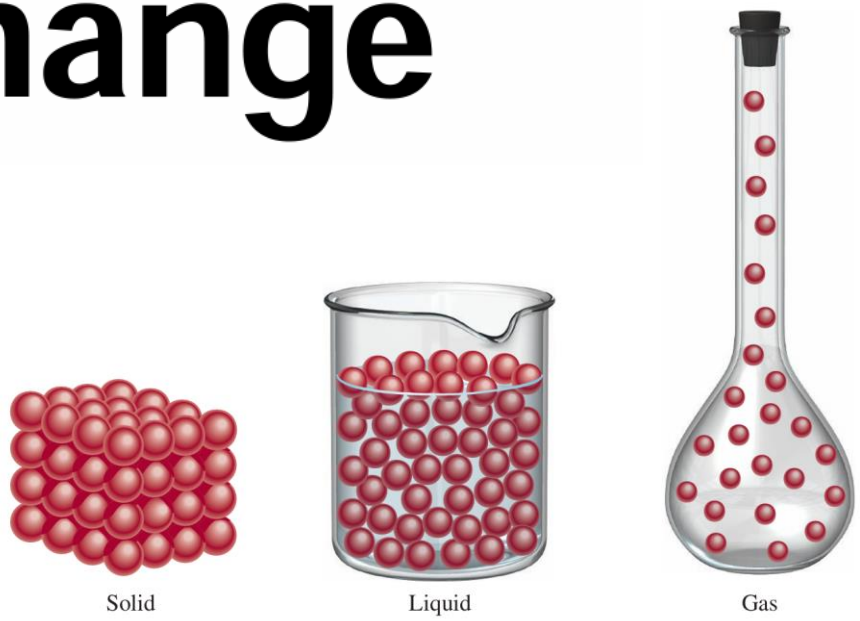
Chapter 1

Chemistry: The Study of Change

Introduction



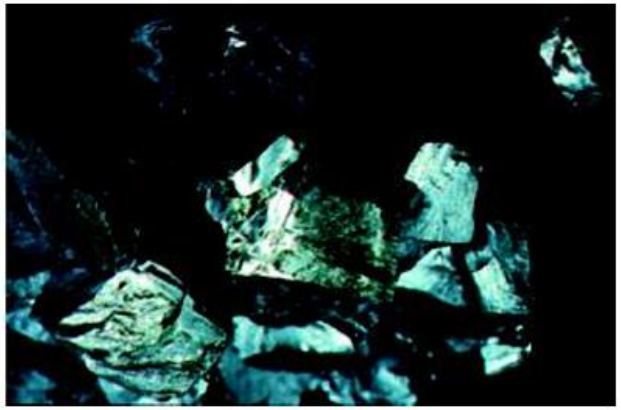
Chemistry is the study of matter and the changes it undergoes.

Matter is anything that occupies space and has mass.

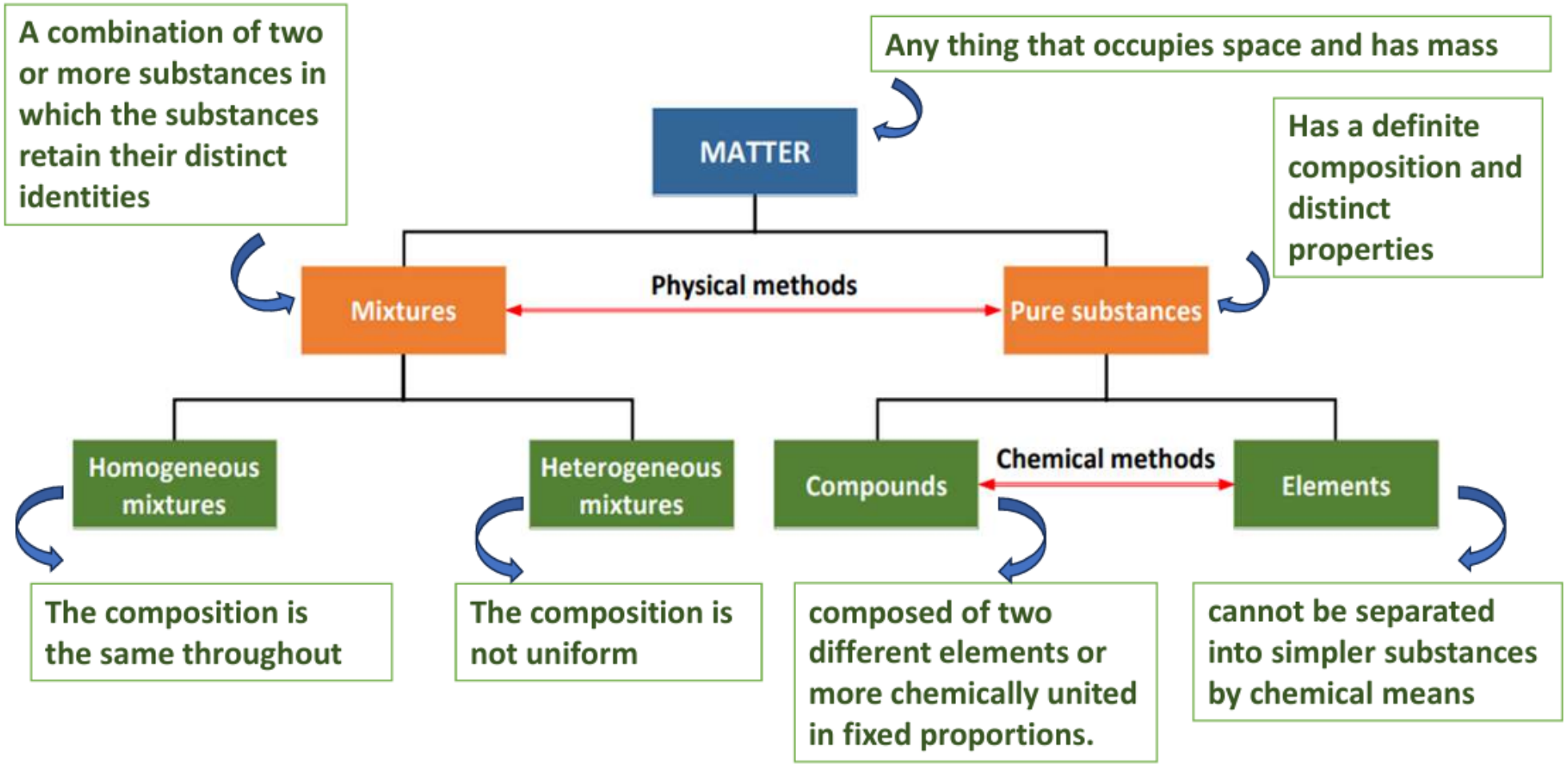
Substance is a form of matter that has a definite composition and distinct properties.

liquid nitrogen

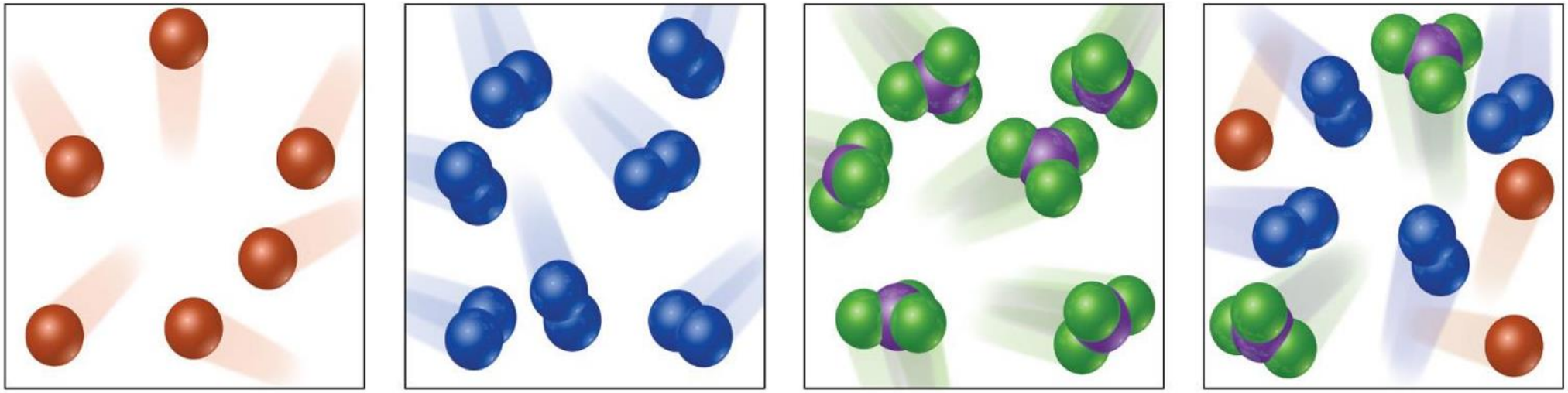
gold ingots



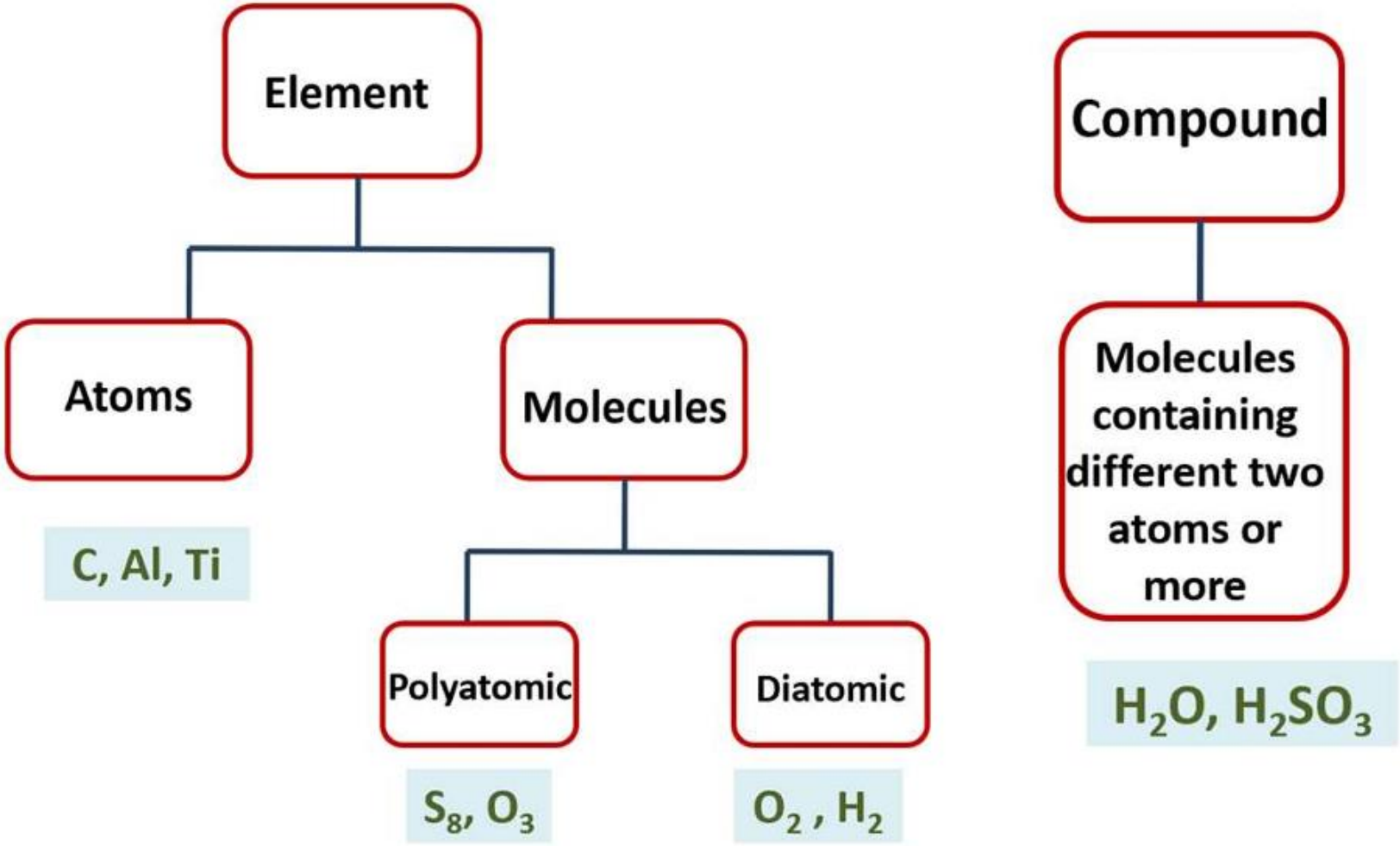
silicon crystals


A combination of two or more substances in which the substances retain their distinct identities
Any thing that occupies space and has mass
MATTER
Has a definite composition and distinct properties
Mixtures
Physical methods
Pure substances
Homogeneous mixtures
Heterogeneous mixtures
Compounds
Chemical methods
Elements
The composition is the same throughout
The composition is not uniform
composed of two different elements or more chemically united in fixed proportions.
cannot be separated into simpler substances by chemical means

Classification of matter according to its composition

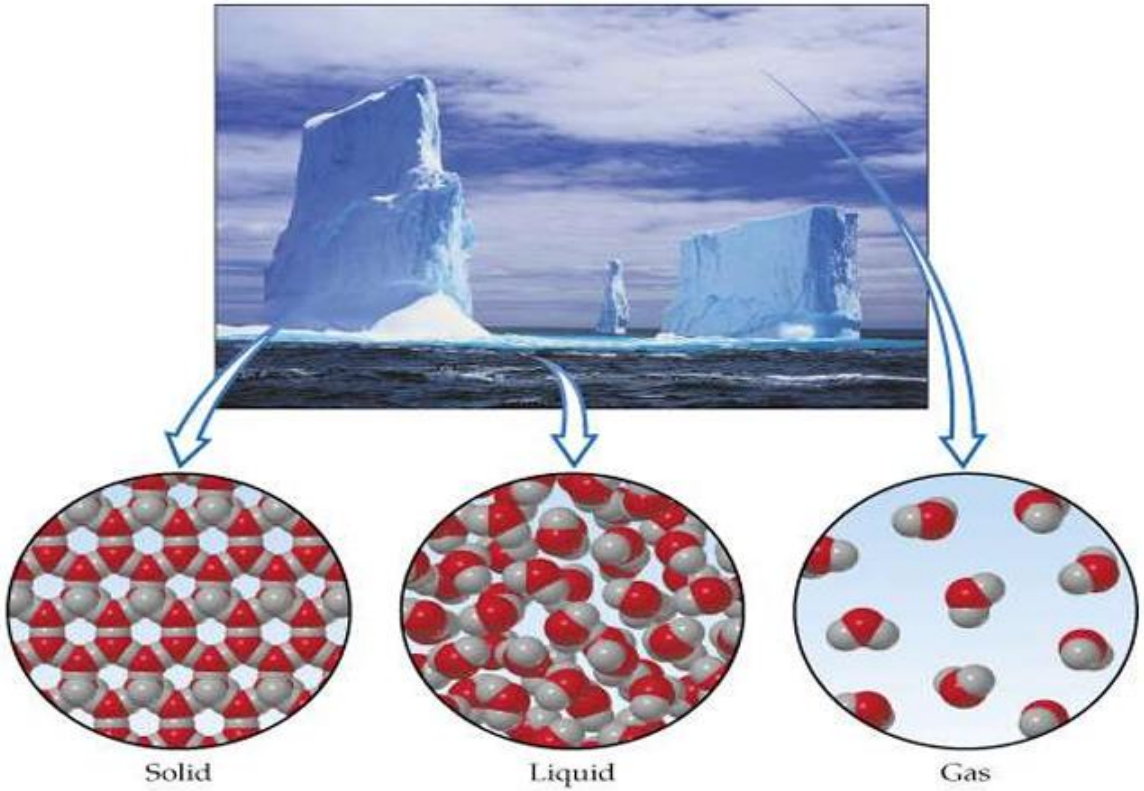


(a) Atoms of an element (b) Molecules of an element (c) Molecules of a compound (d) Mixture of elements and a compound


Element
Atoms
C, Al, Ti
Molecules
Polyatomic
S_8, O_3
Diatomic
O_2 , H_2
Compound
Molecules containing different two atoms or more
H_2O, H_2SO_3

Matter States

The difference between the states is the distance between the molecules.



Physical States of Matter

All matters can exist in three physical states: solid, liquid, and gas.

water is an ideal example: Ice is a solid water-molecules are held together rigidly and are very close to each other. Liquid water-molecules are close together but are free to move around and slide over each other. Steam is a gas water molecules are far apart and move freely and randomly.

1-Solid State

A solid has a definite shape and volume, with particles that cling rigidly to one another. Most commonly occurring solids, such as salt, sugar, quartz, and metals, are crystalline, the material exists in regular, repeating, three dimensional, geometric patterns. Some solids such as plastics, glass, and gels do not have any regular, geometric pattern. Such solids are called amorphous solids.

2-Liquid State

A liquid has a definite volume but not a definite shape, with particles that stick firmly but not rigidly.
Particle mobility gives a liquid fluidity and causes it to take the shape of the container in which it is stored.

3- Gaseous State

A gas has indefinite volume and no fixed shape, with particles that move independently of one another.
The actual volume of the gas is very small compared with the volume of the space occupied by the gas. A gas therefore may be compressed into a very small volume or expanded almost indefinitely.

Physical Changes

are changes in physical properties (such as size, shape, and density) or changes in the state of matter without an accompanying change in composition.

1. **Melting** is the process by which a substance changes from a solid state to a liquid state.

$$ice, snow\ \mathbf{H_2O}_{(s)} \rightarrow \mathbf{H_2O}_{(\ell)}\ liquid\ water$$

2. **Freezing** is the process through which a substance changes from a liquid state to a solid state.

$$liquid\ water\ \mathbf{H_2O}_{(\ell)} \rightarrow \mathbf{H_2O}_{(s)}\ ice$$

3. **Vaporization** or **evaporation** is the process by which a substance changes from a liquid state to a gas state.

$$liquid\ water\ \mathbf{H_2O}_{(\ell)} \rightarrow \mathbf{H_2O}_{(g)}\ water\ vapour$$

4. **Condensation** is the process through which a substance changes from a gas state to a liquid state.

$$water\ vapour\ \mathbf{H_2O}_{(g)} \rightarrow \mathbf{H_2O}_{(\ell)}\ liquid\ water(dew)$$

5. **Deposition** is the process through which a substance changes from a gas state to a solid state, directly.

$$water\ vapour\ \mathbf{H_2O}_{(g)} \rightarrow \mathbf{H_2O}_{(s)}\ frost, snow$$

$$Iodine\ vapour\ \mathbf{I_{2(g)}} \rightarrow \mathbf{I_{2(s)}}\ Iodine\ solid$$

6. **Sublimation** is the process through which a substance changes from a solid state to a gas state, directly.

$$ice, snow\ \mathbf{H_2O}_{(s)} \rightarrow \mathbf{H_2O}_{(g)}\ water\ vapour$$

$$Iodine\ solid\ \mathbf{I_{2(s)}} \rightarrow \mathbf{I_{2(g)}}\ Iodine\ vapour$$

Chemical Changes

new substances are formed that have different properties and compositions from the original material.

$$2Cu_{(s)} + O_{2(g)} \xrightarrow{\Delta} 2CuO_{(s)}$$

$$2H_2O_{(\ell)} \xrightarrow{\text{electric current}} 2H_{2(g)} + O_{2(g)}$$

International System of Units (SI)

An international agreement set up a system of units called the International System of Units, or the SI system. This system is based on the metric system and units derived from the metric system.

Table 1.6. SI Base units

Base quantity	Name of unit	Symbol
Mass	kilogram	kg
Length	meter	m
Time	second	s
Temperature	kelvin	K
Electric current	ampere	A
Amount of substance	mole	mol
Luminous intensity	candela	cd

All other units, called derived units, combine these seven base units.

Table 1.7. Common SI derived units

Derived quantity	Definition of quantity	SI derived unit
Area (A)	Length squared	m^2
Volume (V)	Length cubed	m^3
Density (d)	Mass per unit volume	$kg.m^{-3}(kg/m^3)$
Velocity (v)	Distance travelled per unit time	$m.s^{-1}(m/s)$
Acceleration (a)	Velocity changed per unit time	$m.s^{-2}(m/s^2)$
Force (F)	Mass times acceleration of object	$Newton = N = kg.m.s^{-2}$
Weight (w)	Force of gravity	$Newton = N = kg.m.s^{-2}$
Pressure (P)	Force per unit area	$Pascal = Pa = kg.m^{-1}.s^{-2}$
Work (W)	Force times distance travelled	$Joule = J = kg.m^2.s^{-2}$

Mass and Weight

Mass is the amount of matter in a definite object.
Weight, is the force that gravity (g = 9.8 m. s −2) exerts on an object.

$$\text{Force} = \text{mass} \times \text{acceleration}$$

$$F = m \times a$$

$$\text{Weight} = \text{Force of gravity}$$

$$W = m \times \mathbf{g}$$

The SI base unit of weight is the Newton (N) which equal to:

$$\text{Newton} = N = kg.m.s^{-2}$$

1.14. Example

An African forest elephant has a weight of 25000 N. What is the mass of the African forest elephant? $\mathbf{g} = 9.8\ \mathrm{m.s^{-2}}$

Solution

Weight is another word for the force of gravity. We can solve for the mass using the formula:

$$W = m \times \mathbf{g}$$

$$m = \frac{W}{\mathbf{g}}$$

$$m = \frac{25000\ \mathrm{N}}{\mathbf{g}} = \frac{25000\ \mathrm{kg.m.s^{-2}}}{9.8\ \mathrm{m.s^{-2}}} = 2551.02\ \mathrm{kg}$$

1.15. Example

A man has a mass of 50 kilograms. What is his weight in Newtons? $\mathbf{g} = 9.8\ \mathrm{m.s^{-2}}$

Solution

We can solve it using the formula:

$$W = m \times \mathbf{g}$$

$$W = 50\ \mathrm{kg} \times 9.8\ \mathrm{m.s^{-2}} = 490\ \mathrm{N}$$

1.16. Example

Find the weight of a person on Earth if they have a mass of 65 kg

Solution

We can solve it using the formula:

$$W = m \times \mathbf{g}$$

$$W = 65\ \mathrm{kg} \times 9.8\ \mathrm{m.s^{-2}} = 637\ \mathrm{N}$$

Volume

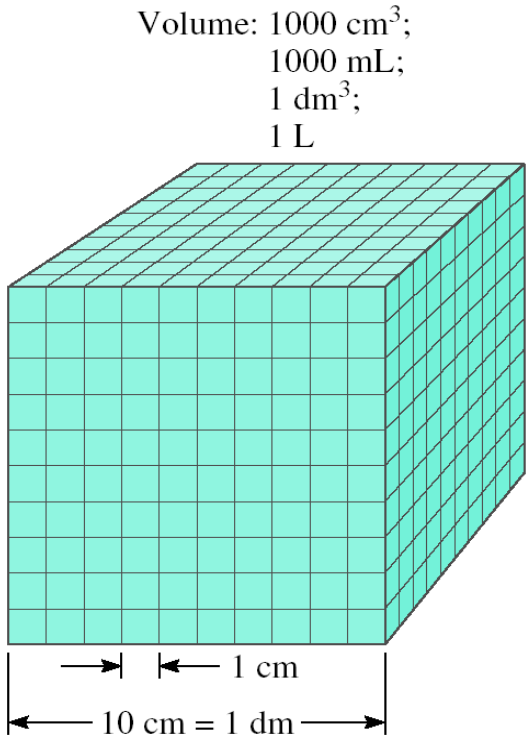
Volume is the space that a substance or an object takes up.
The SI-derived unit for volume is the cubic meter (m^3) and (dm^3).

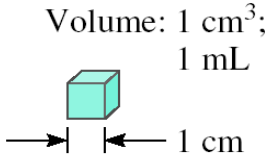
Volumetric flask

$$1\ cm^3 = (1 \times 10^{-2}\ m)^3 = 1 \times 10^{-6}\ m^3$$

$$\boxed{1\ cm^3 = 1\ mL}$$

$$1\ L = 1000\ mL = 1000\ cm^3$$





Another common unit of volume is the liter (L). A liter is the volume occupied by one cubic decimeter of water at 4°C. One liter of volume is equal to 1000 milliliters (mL) or 1000 cm^3 :

1.17. Example

How many millilitres are contained in 3.5 litres?

Solution

We can solve it using the formula:

$$1.0\ \mathrm{L} = 1000\ \mathrm{mL}$$

$$3.5\ \mathrm{L} = x\ \mathrm{mL}$$

$$x = \frac{3.5\mathrm{L} \times 1000\mathrm{mL}}{1.0\mathrm{L}} = 3500\mathrm{mL}$$

1.19. Example

How many cubic centimetres are contained in 3.6 litres?

Solution

We can solve it using the formula:

$$1.0\ \mathrm{L} = 10^3\ \mathrm{cm}^3$$

$$3.6\ \mathrm{L} = 3.6 \times 10^3\ \mathrm{cm}^3$$

Density

The density of an object defined as its mass per unit volume:

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

where d, m, and V denote density, mass, and volume, respectively.

Density usually decreases with temperature.

1.21. Example

The density of mercury, the only metal that is a liquid at room temperature, is $13.6\ \mathrm{g.mL^{-1}}$. Calculate the mass of 5.50 mL of the liquid.

Solution

We are given the density and volume of a liquid and asked to calculate the mass of the liquid. We rearrange Equation of density to give:

$$d = \frac{\mathrm{m}}{\mathrm{V}} \Rightarrow \mathrm{m} = d.\mathrm{V}$$

$$d = \frac{\mathrm{m}}{\mathrm{V}} \Rightarrow \mathrm{m} = 13.6\ \mathrm{g.mL^{-1}} \times 5.50\ \mathrm{mL}$$

$$\mathrm{m} = 74.8\ \mathrm{g}$$

This density corresponds exactly to that of **isopropyl alcohol**, which is therefore the most likely main component of the cleaner.

Scientific Notation

Chemists often deal with numbers that are either extremely large or extremely small.

For example, in 1 g of the element hydrogen there are roughly 602,200,000,000,000,000,000,000 hydrogen atoms. Each hydrogen atom has a mass of only 0.000000000000000000000000166 g.

To avoid mistakes, scientists use power of 10.

Writing a number as the product of a number between 1 and 10 multiplied by 10 raised to some power is called <u>scientific notation.</u>

$$\mathbf{N} \times \mathbf{10}^{\boldsymbol{n}}$$

Where $\mathbf{10} > \mathbf{N} > \mathbf{1}$, and $\boldsymbol{n}$ is power positive or negative

To learn how to write a number in scientific notation, let's consider the number 2468:

1. Move the decimal point in the original number so that it is located after the first nonzero digit.

$$2\ 4\ 6\ 8.0 \Rightarrow 2.468$$ (Decimal moves three places to the left)

2. Multiply this new number by 10 raised to the proper exponent (power). The proper exponent is equal to the number of places that the decimal point was moved.

$$2.468 \times 10^3$$

3. The sign on the exponent indicates the direction the decimal was moved.

moved right : negative exponent $(+n)$, *moved left : positive exponent* $(-n)$

1.3. Example

Write 4500000000 in scientific notation (two significant figures).

Solution

Place the decimal between the **4** and the **5**. Since the decimal was moved nine places to the ***left***, the power of **10** will be **9** and the number **4.5** is multiplied by 10^9

$$4\,5\,0\,0\,0\,0\,0\,0\,0\,0.$$

9 moves

$$4.5 \times 10^9$$

1.4. Example

Write 0.000123 in scientific notation.

Solution

Place the decimal between the 1 and the 2. Since the decimal was moved four places to the ***right***, the power of **10** will be -4 and the number 1.23 is multiplied by 10^{-4}

$$0.0\,0\,0\,1\,2\,3$$

4 moves

$$1.23 \times 10^{-4}$$

Prefixes Used with SI Units

Table 1.3 Prefixes Used with SI Units

Prefix	Symbol	Meaning
peta-	P	1,000,000,000,000,000, or 10^{15}
tera-	T	1,000,000,000,000, or 10^{12}
giga-	G	1,000,000,000, or 10^{9}
mega-	M	1,000,000, or 10^{6}
kilo-	k	1,000, or 10^{3}
deci-	d	1/10, or 10^{-1}
centi-	c	1/100, or 10^{-2}
milli-	m	1/1,000, or 10^{-3}
micro-	μ	1/1,000,000, or 10^{-6}
nano-	n	1/1,000,000,000, or 10^{-9}
pico-	p	1/1,000,000,000,000, or 10^{-12}
femto-	f	1/1,000,000,000,000,000, or 10^{-15}
atto-	a	1/1,000,000,000,000,000,000, or 10^{-18}

1.5. Example

Change scientific notation to normal form of:

(a) 8.86×10^{-8}
(b) 6.57×10^{11}
(c) 4.53×10^{-5}
(d) 4.1×10^{4}
(e) 5.0×10^{-3}
(f) 2.4×10^{22}

Solution

(a) $8.86 \times 10^{-8} = 0.0000000886$
(b) $6.57 \times 10^{11} = 657000000000$
(c) $4.53 \times 10^{-5} = 0.0000453$
(d) $4.1 \times 10^{4} = 41000$
(e) $5.0 \times 10^{-3} = 0.005$
(f) $2.4 \times 10^{22} = 24000000000000000000000$

1.8. Example

Change scientific notation to prefixes notation of:

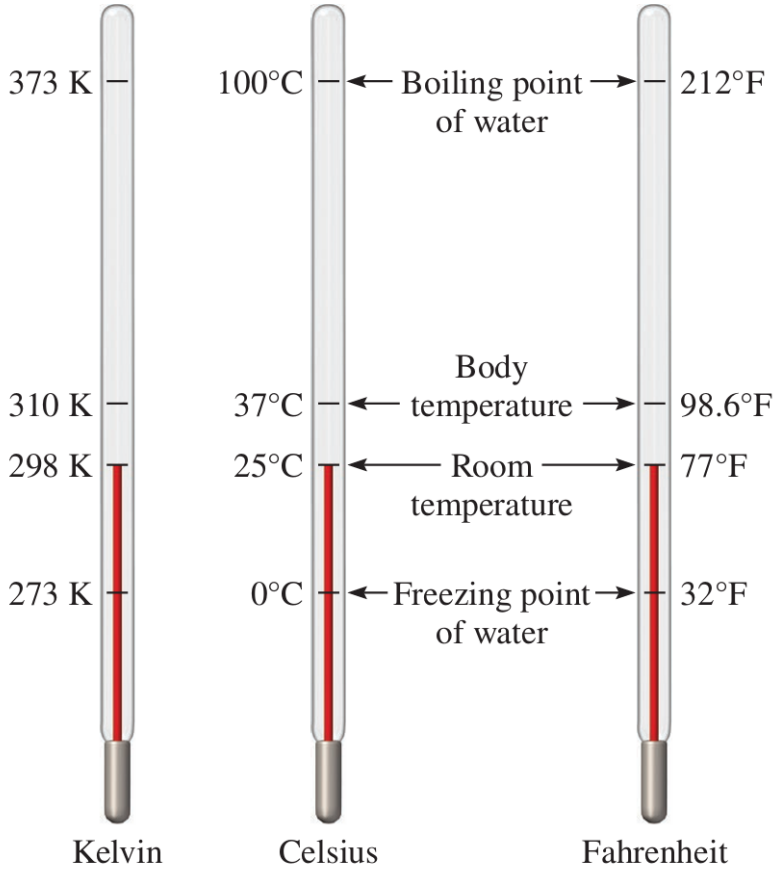
(a) 7.5×10^{10}
(b) 3.2×10^{3}
(c) 1.43×10^{-6}
(d) 3.45×10^{-2}
(e) 1.23×10^{15}
(f) 1.23×10^{-15}

Solution

(a) $7.5 \times 10^{10} = 75G$ (75 Giga)
(b) $3.2 \times 10^{3} = 3.2k$ (3.2 kilo)
(c) $14.3 \times 10^{-6} = 14.3\mu$ (14.3 micro)
(d) $3.45 \times 10^{-2} = 3.45c$ (3.45 centi)
(e) $1.23 \times 10^{15} = 1.23P$ (1.23 Peta)
(f) $1.23 \times 10^{-15} = 1.23f$ (1.23 femto)

Temperature

Three temperature scales are currently in use: The Celsius scale, the Kelvin scale, and the Fahrenheit scale.



We can convert from the Kelvin scale to the Celsius scale using the equation:

$$T_K = T_C + 273\ K$$

* Mercury, the only metal that exists as a liquid at room temperature, melts at −38.9°C. Convert its melting point to kelvins.

$$T_k = -39.9^oC + 273\ K = 234.1\ K$$

* Convert the boiling point of ethanol at room temperature (351.37 K) in Kelvins to degree Celsius:

$$T_c = 351.37 - 273 = 78.37^oC$$

The following equation is used to convert degrees Celsius to degrees Fahrenheit:

$$T_F = (1.8 \times T_C) + 32°F$$

What temperature on Fahrenheit scale corresponds to −40°C?

Solution

This conversion is carried out by writing:

$$T_F = (1.8 \times T_C) + 32°F$$

$$T_F = (1.8 \times -40) + 32°F = -40°F$$

The temperature at which table salt (sodium chloride) melts is 800 °C. What is this temperature on the Kelvin and Fahrenheit scales?

Solution

We have two conversions, the first one from Celsius to Fahrenheit scale and it is carried out by writing:

$$T_F = (1.8 \times T_C) + 32°F$$

$$T_F = (1.8 \times 800) + 32°F = 1472\ °F$$

the second one from Celsius to Kevin scale and it is carried out by writing:

$$T_K = T_C + 273\ K$$

$$T_K = 800 + 273\ K = 1073\ K$$

The following equation is used to convert degrees Fahrenheit to degrees Celsius:

$$T_C = \frac{(T_F - 32)}{1.8}\,°C$$

Helium has the lowest boiling point of all the elements at −452°F. Convert this temperature to degrees Celsius.

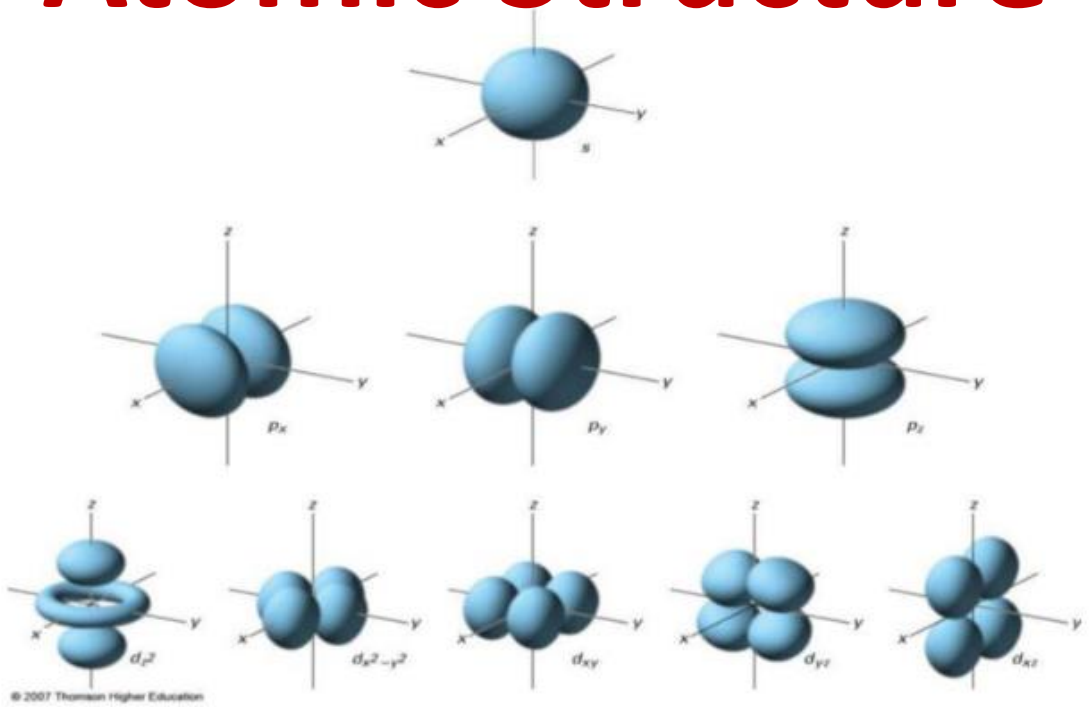
Solution

This conversion is carried out by writing:

$$T_C = \frac{(T_F - 32)}{1.8}\,°C$$

$$T_C = \frac{(-452 - 32)}{1.8}\,°C = -268.89°C$$

Chapter 2
Atomic Structure



Atomic Theory

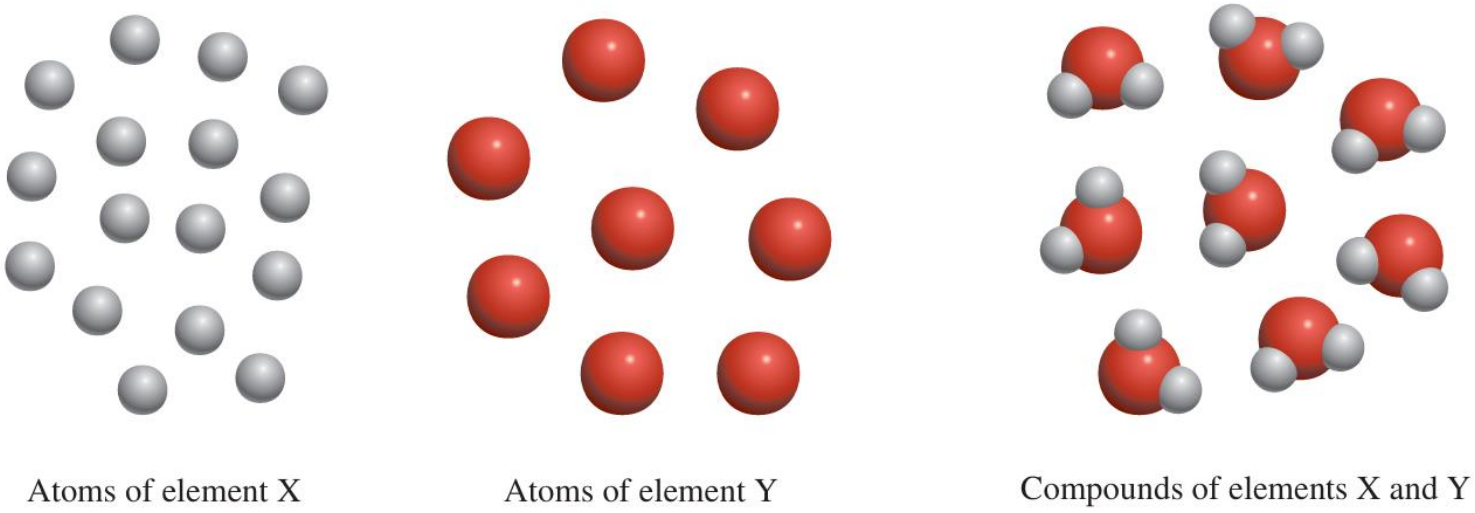
According to Dalton's atomic theory, the hypotheses about the nature of matter can be summarized as follows:

1-Elements are composed of extremely small particles called atoms.

2. All atoms of a given element are identical, having the same size, mass, and chemical properties. The atoms of one element are different from the atoms of all other elements.

3. Compounds are composed of atoms of more than one element. For any given compound, the atoms present are always in the same ratio.

4. A chemical reaction involves only the separation, combination, or rearrangement of atoms; it does not result in the creation or destruction of atoms.



Structure of The Atom

Based on Dalton's model of the atom, we can define an atom as the basic unit of an element that can enter chemical combination. The atom consists of nucleus of protons and neutrons surrounded by a group of electrons.

1- The Neutron (n^0)

The neutron (n^0) is an elementary particle, electrically neutral, located in nucleus.

2. The Proton (p^+)

is an elementary particle with a positive electrical charge, located in nucleus. Its relative charge +1 is equal in magnitude, but opposite in sign, to the charge on the electron.

3-The Electron (e^-)

is an elementary particle with a negative electrical charge, moves around the nucleus. The size of an electron has not been determined exactly, but its diameter is believed to be less than 10^{-12}cm.

Mass Relationships

All atoms can be identified by the number of protons and neutrons they contain. The nucleus of an element contains two types of elementary particles called protons (+) and neutrons (0).

1. Atomic Number (Z)

The atomic number ($\boldsymbol{Z}$) of an element is the number of protons in the nucleus of an atom of that element. In a neutral atom the number of protons is equal to the number of electrons, so the atomic number also indicates the number of electrons present in the atom.

$$\text{Atomic number (Z)} = \text{number of protons in the nucleus}$$

All carbon atoms (Z = 6) have 6 protons, all oxygen atoms (Z = 8) have 8 protons, and all uranium atoms (Z = 92) have 92 protons.

2. Atomic Mass (A) or atomic mass number

The mass number (A) of an element is the sum of the number of protons and the number of neutrons in the nucleus.

$$\text{Mass number (A)} = \text{number of protons} + \text{number of neutrons}$$

$$\text{Mass number (A)} = \text{Atomic number (Z)} + \text{number of neutrons}$$

For example, if the mass number of a particular boron atom is 12 and the atomic number is 5 (indicating 5 protons in the nucleus), then the number of neutrons is:

$$\text{Number of neutrons (N)} = A - Z$$

$$\text{Number of neutrons} = 12 - 5 = 7$$

The subscript (Z) is the atomic number; the superscript (A) is the mass atomic number of an element (E) as follows:

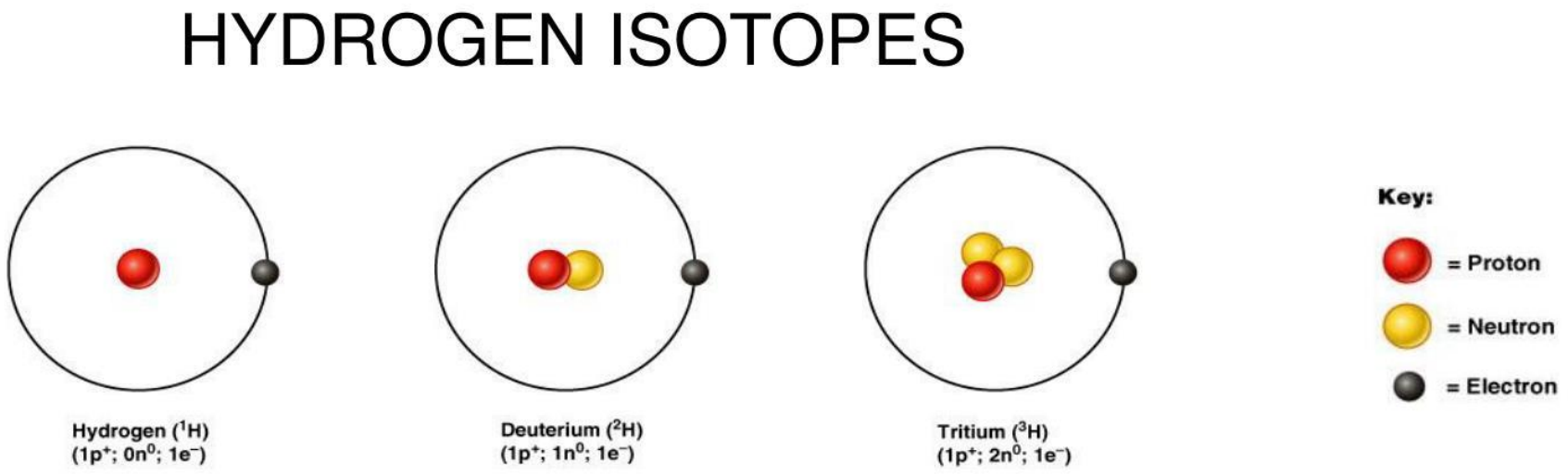
Figure 2.6. The isotopic notation

Homework:

Give the number of protons, neutrons, and electrons in each of the following species: (a) $^{20}_{11}Na$, (b) $^{22}_{11}Na$, (c) ^{17}O, and (d) carbon-14.

Isotopes

Most elements have two or more isotopes. The isotopes are atoms of an element, that have the same atomic number but different mass numbers, or atoms of an element having the same number of protons, but a different number of neutrons.



2.4. Example

How many protons, neutrons, and electrons are in each of the three stable isotopes of oxygen?

$$^{16}_{8}O\ ,\ ^{17}_{8}O\ ,\text{and}\ ^{18}_{8}O$$

Solution

The mass number (A) and the atomic number (Z) of each of the three isotopes are given, so,

$$\text{Atomic number (Z)} = \text{number of protons in the nucleus}$$

$$\text{Mass number (A)} = \text{Atomic number (Z)} + \text{number of neutrons (N)}$$

$$\text{Number of neutrons (N)} = \text{A} - \text{Z}$$

For the first isotope:

(a) The atomic number (Z) is 8, so there are 8 protons.
(b) The mass number (A) is 20, so the number of neutrons (N) is $16 - 8 = 8$.
(c) The number of electrons is the same as the number of protons; that is, 8.

Therefore:

$$^{16}_{8}O \text{ has } 8p^{+}, 8e^{-}, \text{and } 8n^{0}\ (16 - 8)$$

$$^{17}_{8}O \text{ has } 8p^{+}, 8e^{-}, \text{and } 9n^{0}\ (17 - 8)$$

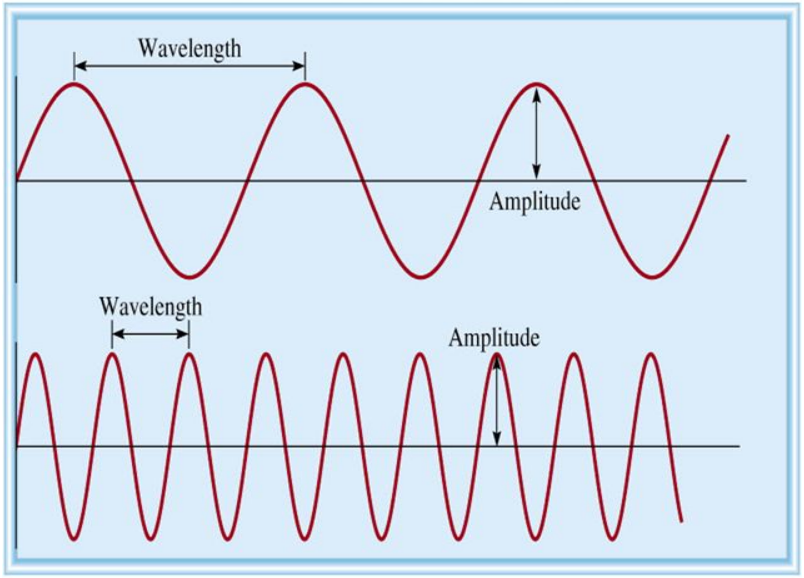
$$^{18}_{8}O \text{ has } 8p^{+}, 8e^{-}, \text{and } 10n^{0}\ (18 - 8)$$

Properties of Waves

Quantum theory enables us to predict and understand the critical role that electrons play in chemistry.

- **Wavelength (λ):** the distance between two consecutive peaks or troughs in a wave.

- **Frequency (ν):** the number of waves that pass through a particular point in 1 second (Hz = 1 cycle/s).
- **Amplitude:** the vertical distance from the midline of a wave to the peak or trough.



Electromagnetic Radiation

- In 1873 James Maxwell proposed that visible light consists of electromagnetic waves or it is an electromagnetic radiation.

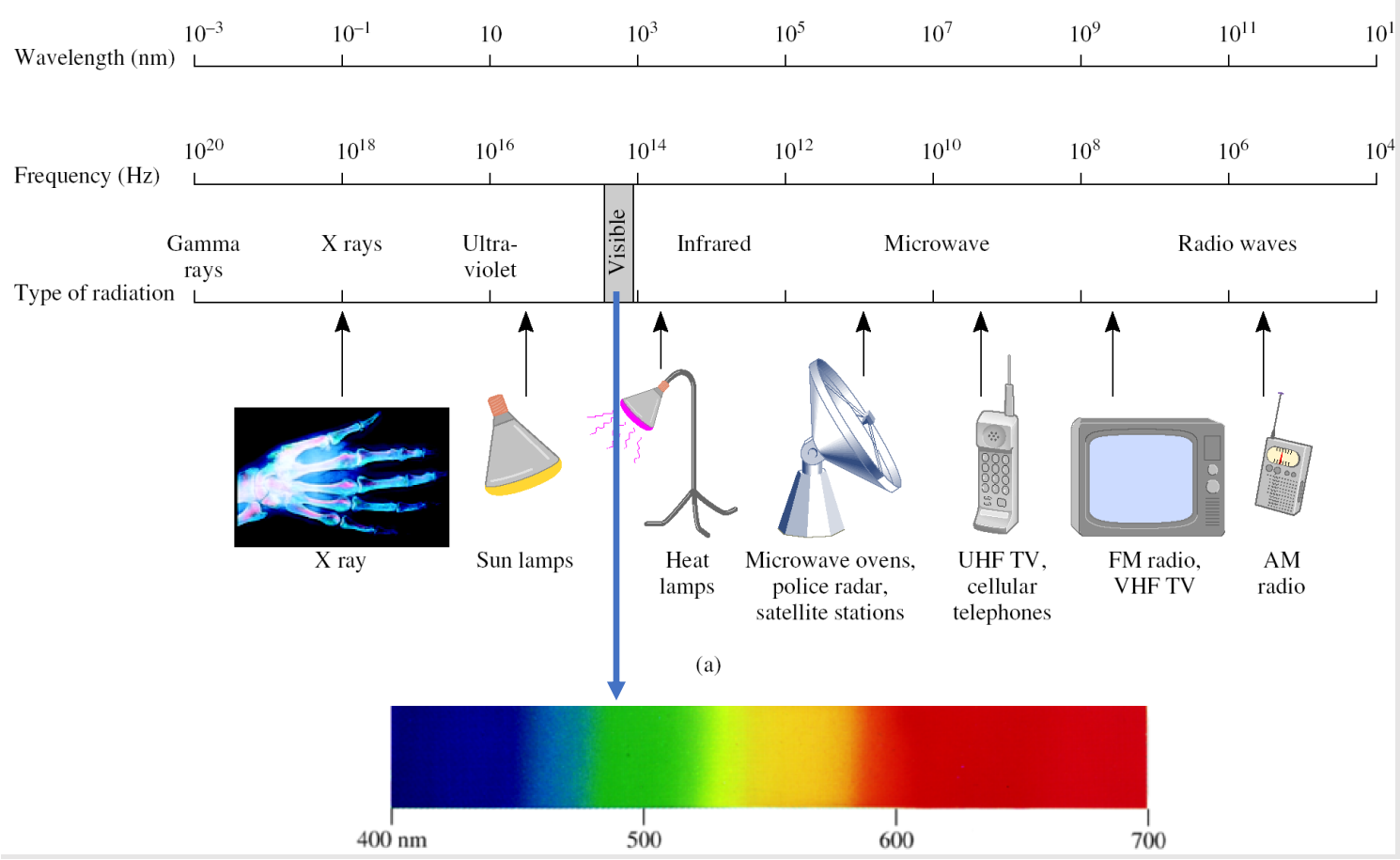
- Electromagnetic radiation: is the emission and transmission of energy in the form of electromagnetic waves.

-All electromagnetic radiation travels at the same velocity in a specific medium (speed of light)

-Speed of light (c) in vacuum = 3×10^8 m/s

$$c = \lambda \times \nu$$

Types of Electromagnetic Radiation



Example 1

The wavelength of the green light from a traffic signal is centered at 522nm . What is the frequency of this radiation?

Given: $\lambda = 522$ nm; c (known)

$$\because\ c = \lambda\ x\ \nu$$

$$\therefore\ \nu = \frac{c}{\lambda} = \frac{3\ x\ 10^{8}\ m/s}{522\ x\ 10^{-9} m} = 5.7 \text{ x } 10^{14}\text{Hz}$$

What is the λ in meter (m) of an electromagnetic wave whose frequency is 3.64 x10^{7} Hz?

Given: ν = 3.64 x107 Hz; c (known)

$$\because\ c = \lambda\ x\ \nu$$

$$\therefore\ \lambda = \frac{c}{\nu} = \frac{3\ x\ 10^{8} m/s}{3.64\ x\ 10^{7}/s} = 8.24 \text{ m}$$

Plank's Quantum Theory

- **Energy (light) is emitted or absorbed in discrete units (quantum).**

  - **Quantum (energy) is given by:**

$$\boldsymbol{E = h\,x\,\nu}$$
$$\boldsymbol{E = h\,x\,\frac{c}{\lambda}}$$

where:
E: is the energy
h: Plank's constant, $h = 6.63\ x\ 10^{-34}$ J.s
ν: frequency of radiation

- **According to quantum theory: energy is always emitted in integrals multiples of $h\nu$ e.g. $h\nu$, $2h\nu$, $3h\nu$, ……**

Example:

Calculate the energy (in J) of a photon with a wavelength of 5.0 x 10^4 nm.

$\lambda = 5.0\ x\ 104\ \text{nm} \rightarrow\ 5.0\ x\ 104\ x\ 10^{-9} = 5.0\ x\ 10^{-5}\text{m}$

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

$$= \frac{6.63\ x\ 10^{-34}\ J.s\ x\ 3.0\ x\ 10^{8} m/s}{5.0 x\ 10^{-5}\ m} = 3.98\ x\ 10^{-21}\text{J}$$

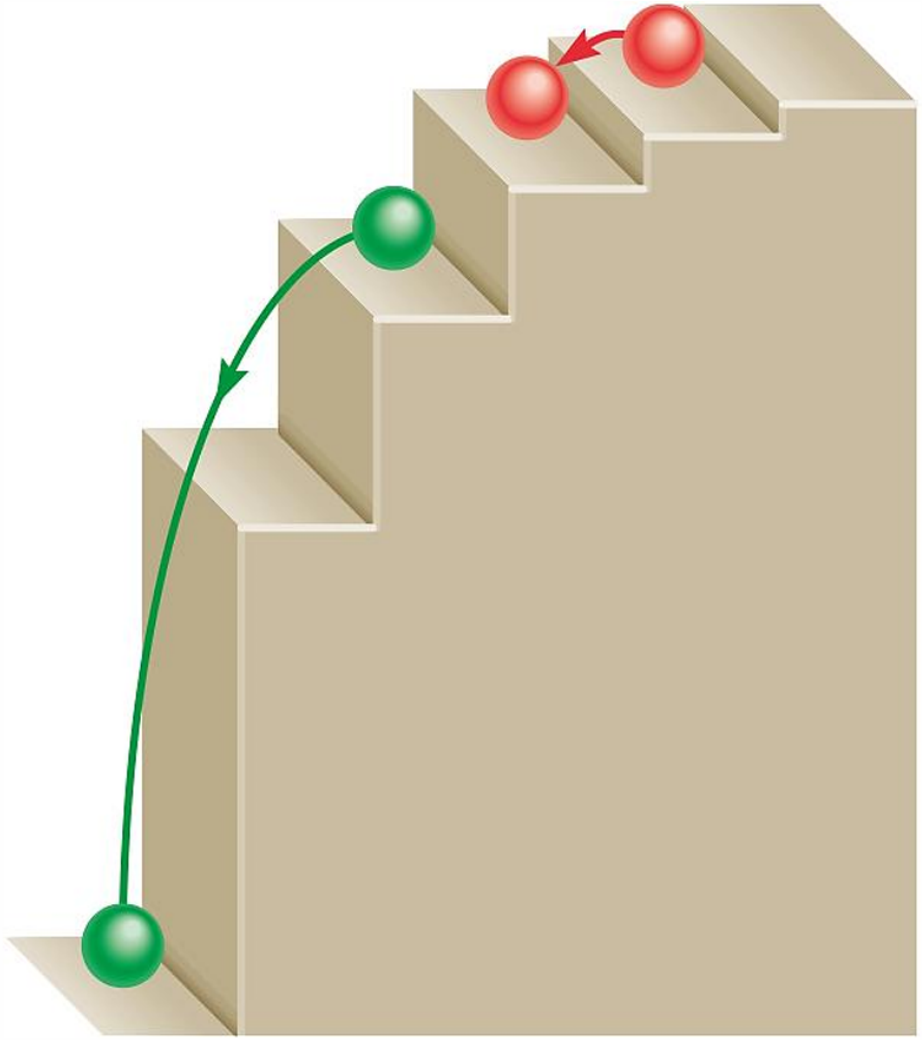
Bohr's Theory of the Hydrogen Atom (1913)

- Neil Bohr: study the emission spectrum of the Hydrogen Atom
- Electron (e^-) can only have specific energy values (quantized)
- light is emitted as e^- moves from one energy level to a lower energy level
- THUS: the emission spectrum of the H atom results from: the excitation of an electron to a higher energy orbit then drops to a lower-energy orbit and emits a quantum of energy (light)

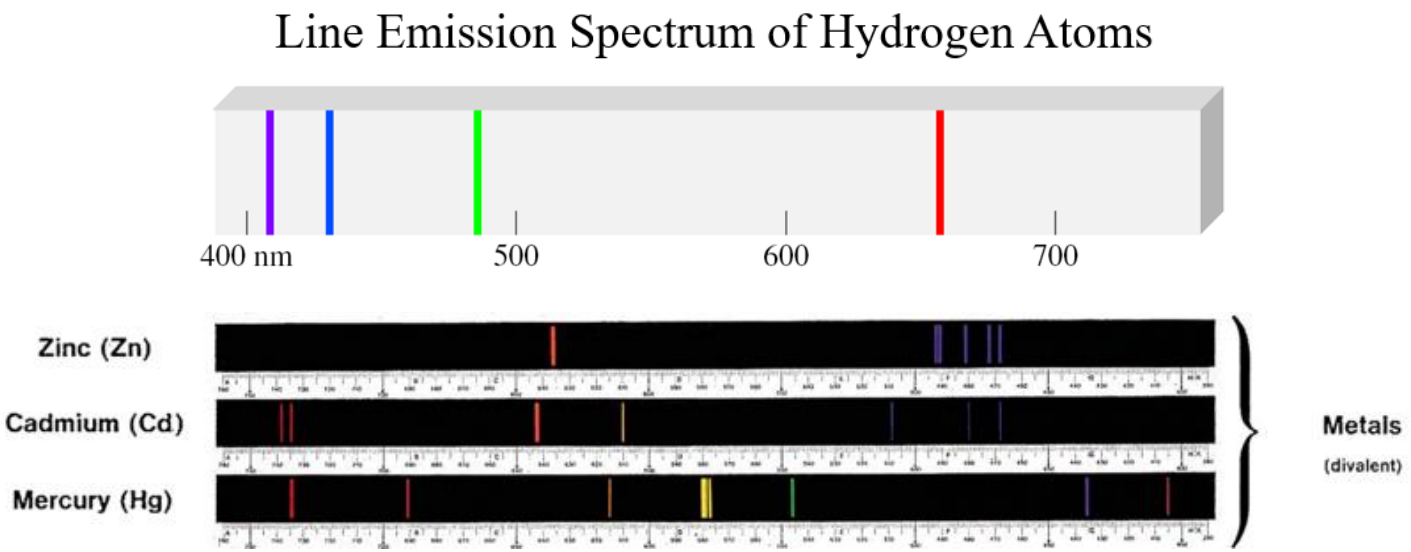
Quantized energy

- When an electron undergoes a transition, it can only exist in an energy level, not between energy levels, because energy levels of the atom are quantized.

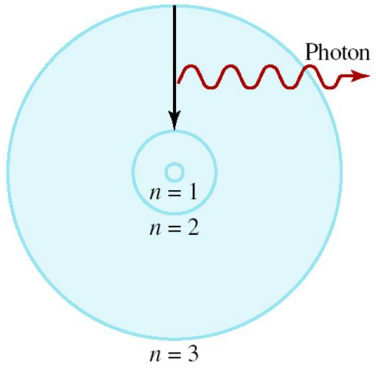
- A way to think about this is a ball on a staircase. The ball can only rest on steps, not between steps, much like how an electron can only exist in an energy level, not between energy levels.



- **Emission Spectra of atoms are bright lines (spectral lines) in the visible spectrum**
- **Emission spectrum of any atom is a fingerprint (lines appeared at specific wavelengths)**



When electron transfers from a higher orbital to a lower emits energy as a wave equals the difference between the two levels



The Uncertainty Principle

- **Werner Heisenberg assumed: It is difficult to determine the position and velocity of the electron at the same time.**

- The best way to explain the motion of the electron is by considering the probability of finding the electron at different positions in the atom **"electron density"** or **"orbitals"**

Quantum Numbers (n, ℓ, mℓ, ms)

- In quantum mechanics, **three quantum numbers** are required to describe the distribution of electrons in hydrogen and other atoms (n, ℓ, m_ℓ) . These numbers are derived from the mathematical solution of the Schrödinger equation for hydrogen atom.

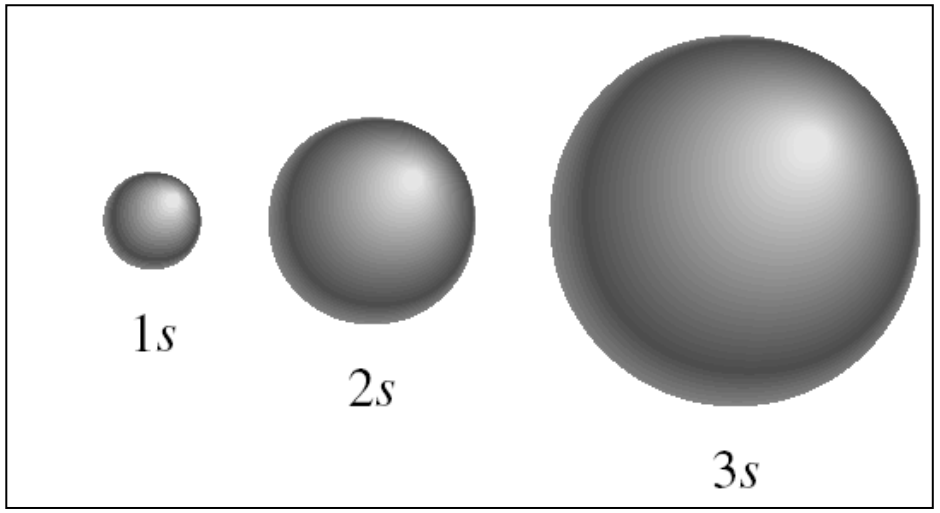
- **The fourth quantum** is the spin quantum number (m_s) describes the behavior of a specific electron and completes the description of the electron in the atoms.

- Electrons in multi-electron atoms can be classified into a series of:

  shells (n) → subshells (ℓ)→ orbitals (m_ℓ)

The Principal Quantum Number (n)

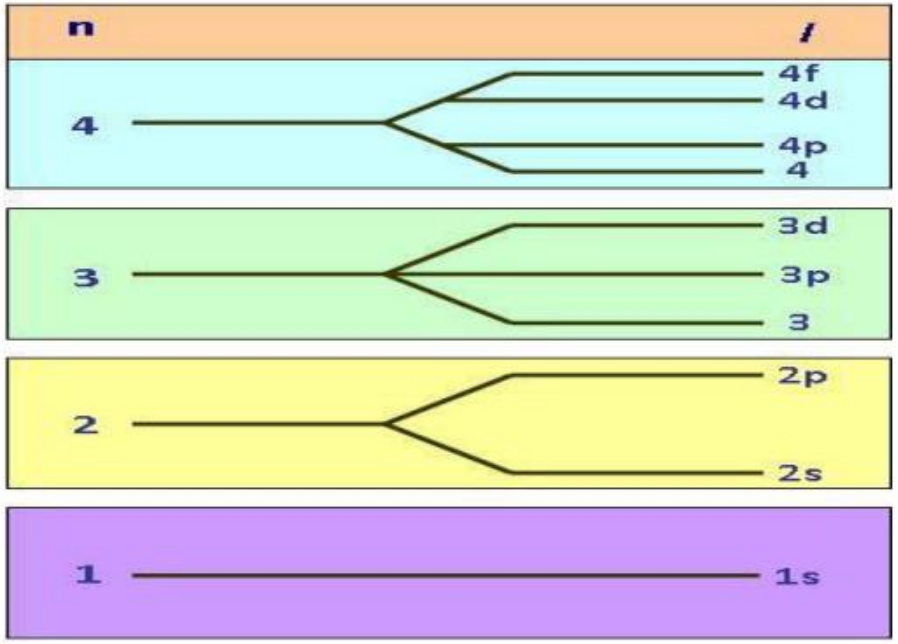
- **determines the energy of an orbital → determines the distance of the electron from the nucleus → Size.**
- **Values:** n = 1, 2 , 3, 4 ……
- Bigger n → larger energy → farther from the nucleus → larger size
- The maximum number of orbitals in $(n) = n^2$
- The maximum number of electrons in $(n) = 2n^2$



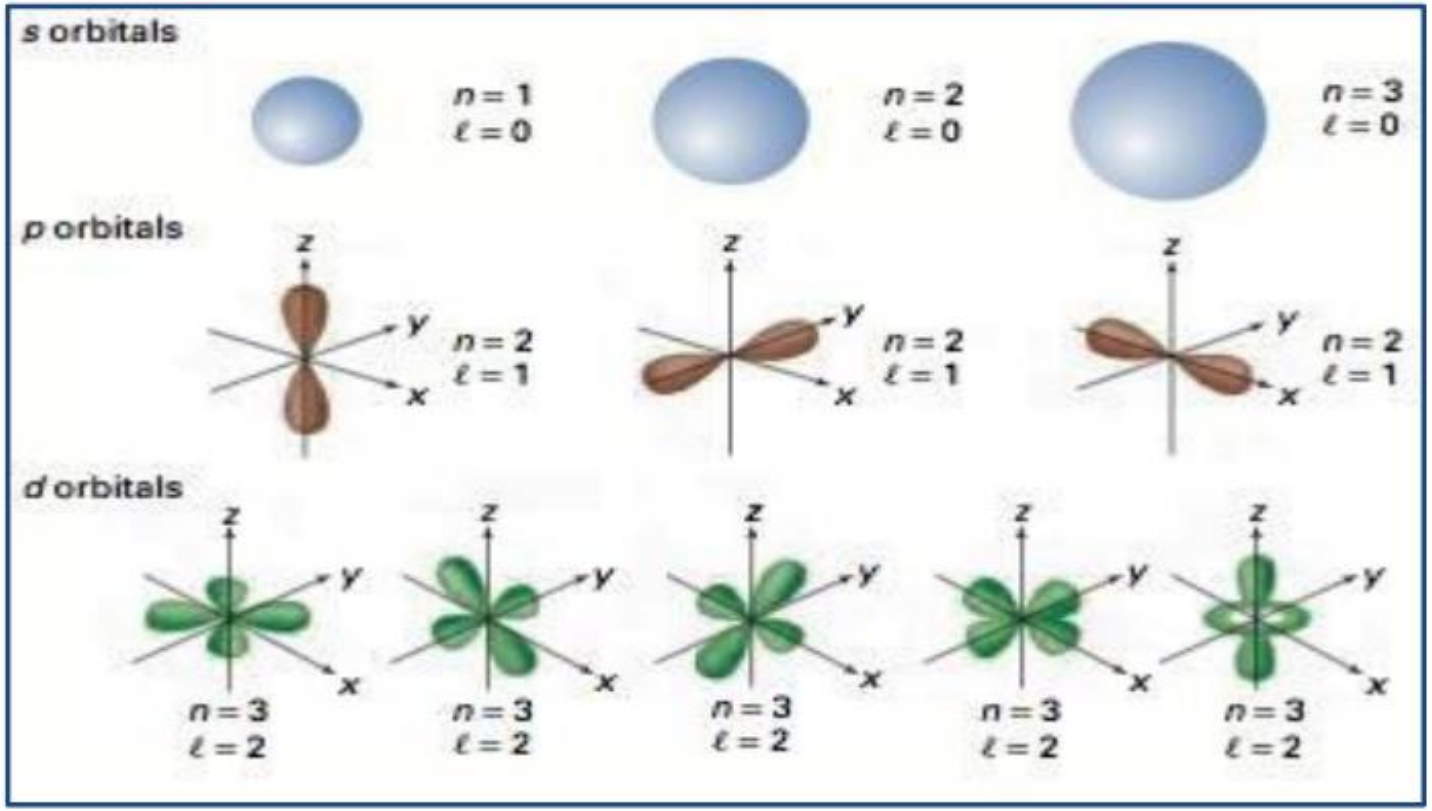
The Angular Momentum Quantum Number (ℓ)

- **determines the shape of the orbital**
- **Values:** ℓ = from 0 to $n-1$
- **The value of ℓ is designated by letters:**

value of ℓ	0	1	2	3	4	5
Name of orbital	*s*	*p*	*d*	*f*	*g*	*h*



Shapes of orbitals



The Magnetic Quantum Number (m_ℓ)

- determines the orientation of the orbital

- depend on the value of ℓ :

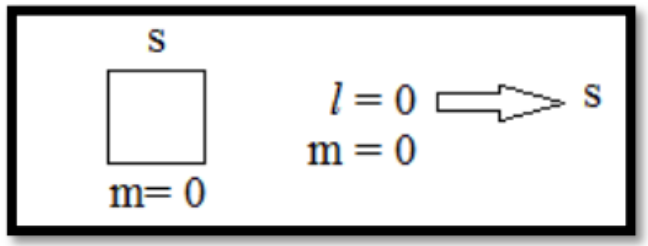
  values of $m_\ell = -\ell$ to $+\ell$

  - The number of orbitals in each subshell ℓ = number of $m_\ell = 2\ell + 1$

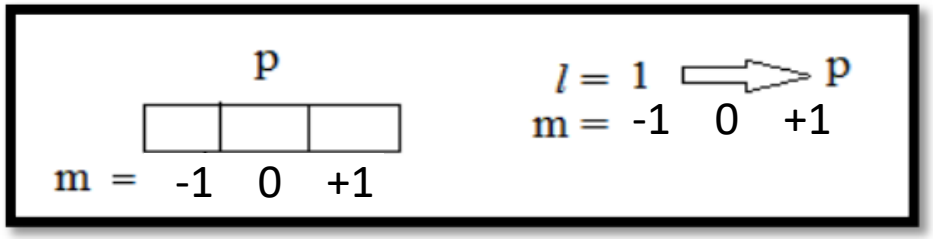
If $\ell = 1$ (p orbital), $m_\ell = -1, 0, +1$

If $\ell = 2$ (d orbital), $m_\ell = -2, -1, 0, +1, +2$

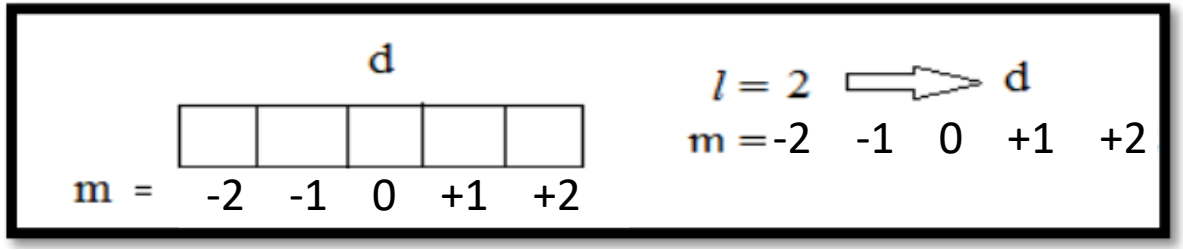
For s orbital there is only one subshell



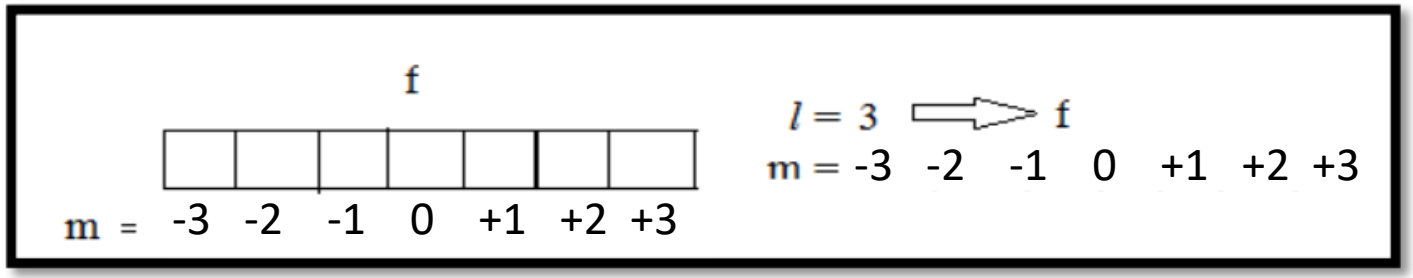
For p orbital there are three subshells



For d orbital there are five subshells



For f orbital there are seven subshells

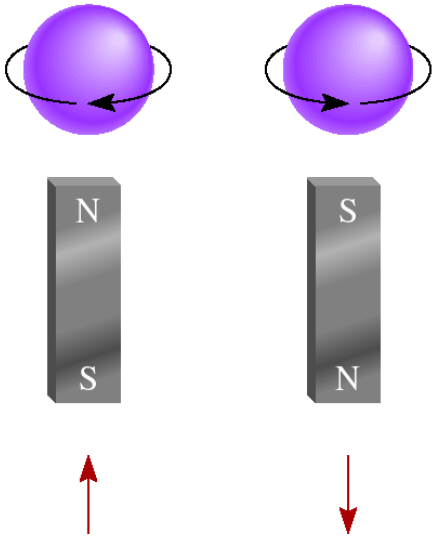


The Electron Spin Quantum Number (m_s)

- **Determines the electron spin**

- **The spin quantum number has only two allowed values:**

$$m_s = +½ \text{ and } -½$$



Which of the following sets of quantum numbers are not allowed?

(a) $n = 3$, $\boxed{\ell = -2}$, $m_\ell = 2$.

(b) $\boxed{n = 0}$, $\ell = 0$, $m_\ell = 0$.

(c) $n = 4$, $\ell = 1$, $m_\ell = 1$, $m_s = +1/2$ OK

(d) $n = 3$, $\ell = 1$, $\boxed{m_\ell = 2}$, $m_s = -1/2$

Exercise:

For $n = 4$, determine the number of allowed subshells and give the designation of each.

$n = 4$

$\ell =$	0,	1,	2	and	3
	$4s$	$4p$	$4d$		$4f$

Number of orbitals per subshell:

1	3	5	7

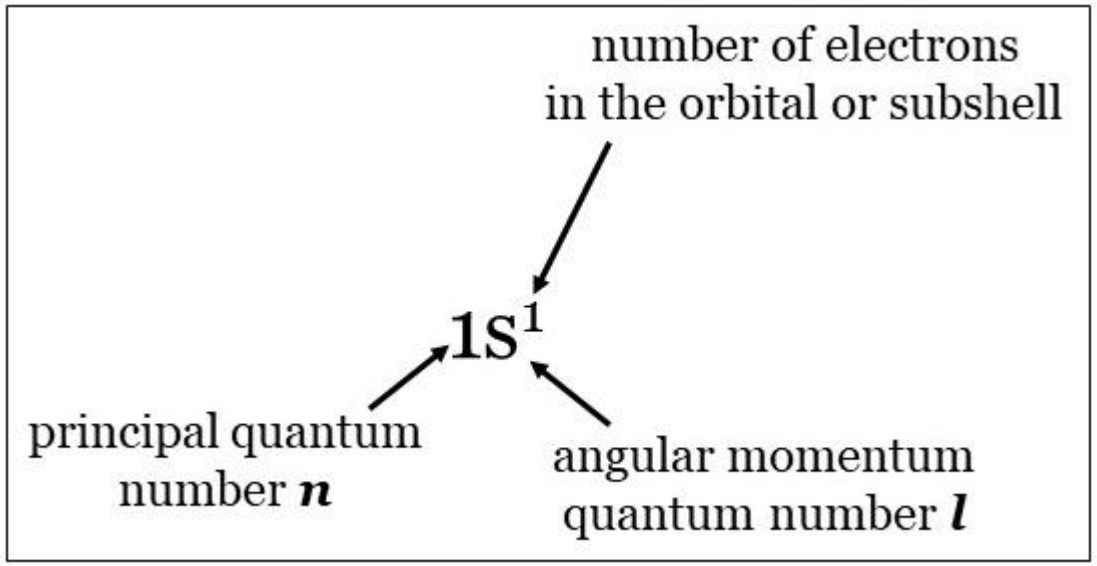
Exercise:

How many orbitals can the subshell $3d$ have?

The electron configuration

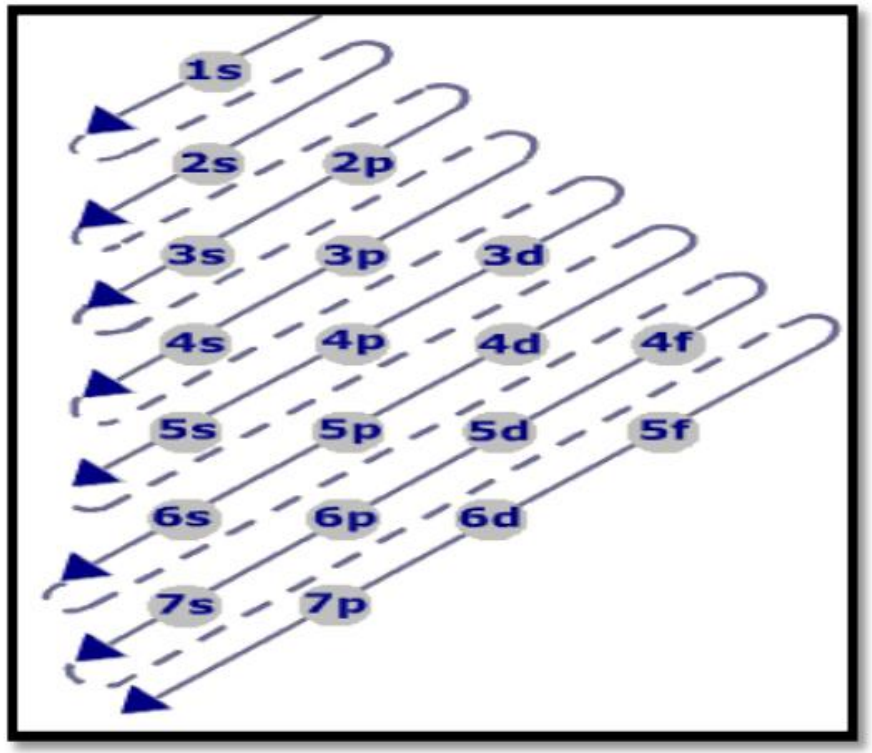
is how the electrons are distributed among the various atomic orbitals in an atom.

- **The four quantum numbers *n*, ℓ, m_{ℓ} and m_s enable us to label completely an electron in any orbital in any atom.**



Aufbau Principle ("Fill up" electrons):
The electron configuration

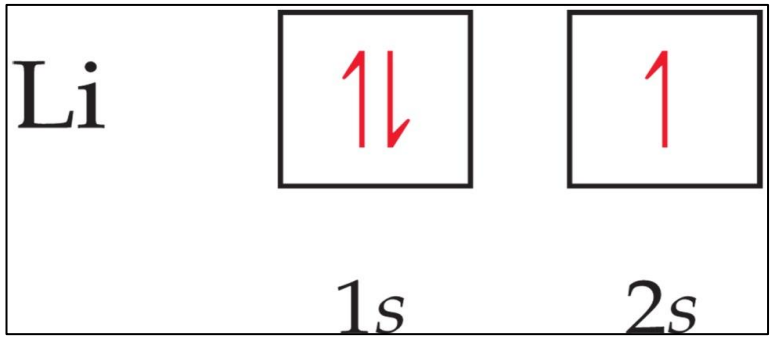
The electrons are added one by one to the atomic orbitals in lowest energy orbitals



Electron configuration

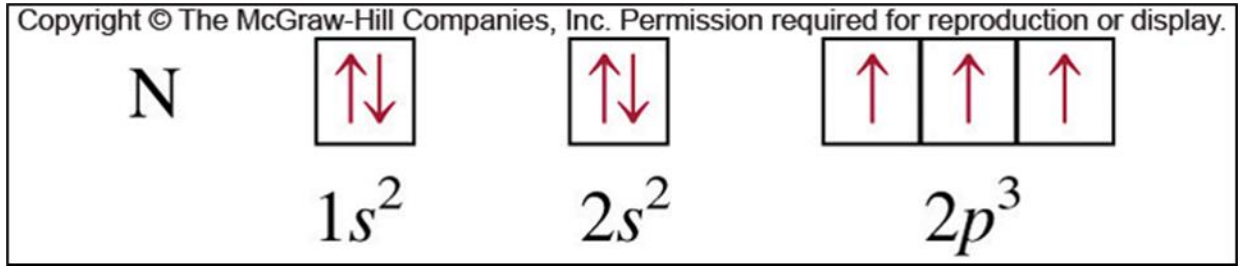
Orbital Diagram

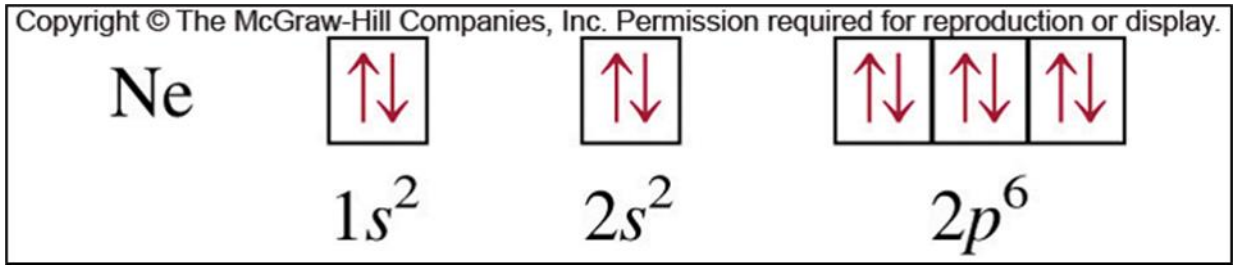
- **Each box represents one orbital.**
- **Half-arrows represent the electrons.**
- **The direction of the arrow represents the spin of the electron.**



Hund's Rule

The most stable arrangement of electrons in subshells is the one with the greatest number of parallel spins





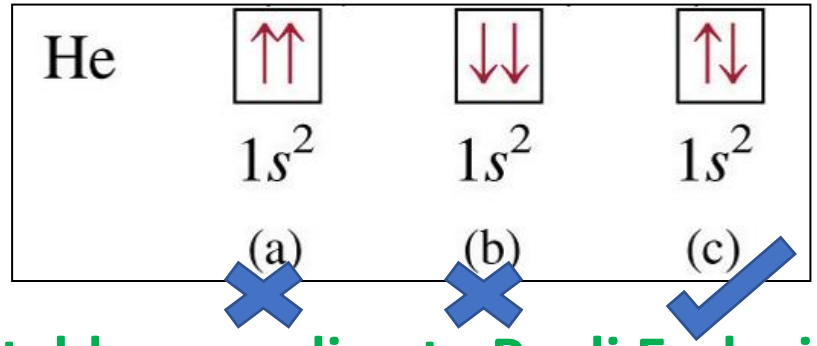
The Pauli Exclusion Principle

<u>NO two</u> electrons in an atom can have the same set of four quantum numbers

<u>Only two</u> electrons may occupy the same atomic orbital (same *n, l, m_l*), and these two electrons must have opposite spins (m_s)

Consider the Helium atom:

$_2$He: $1s^2$



C is acceptable according to Pauli Exclusion Principle

Write the electron configuration for the following elements and ions:

$$Sc, Ni, As, La, Ca^{++}, Fe^{+++}, O^{2-}, Cl^{-}$$

Z= (Sc=21, Ni = 28, As= 33, La=57, Ca =20, Fe =26, O = 8, Cl = 17)

Element	Electron configuration

The Building-Up Principle

- Aufbau Principle ("Fill up" electrons): **the electrons are added one by one to the atomic orbitals in lowest energy orbitals**

- Alkali metals and alkaline earth metals fill the s orbitals last.

- Main group elements fill the p orbitals last.

- Transition metals fill the d orbitals last.

- Lanthanides and actinides fill the (4f) and the (5f) orbitals last, respectively. Elements in same group have same valence shell electron configurations and have similar chemical properties

Short Notation (abbreviation):

In the short notation: the electron configuration of any element except Hydrogen and Helium are represented by a noble gas core, which shows in brackets the noble gas element that most nearly precedes the element being considered, followed by the symbol for the highest filled subshells in the outermost shells.

$_{2}$[He] 2s, $_{10}$[Ne] 3s, $_{18}$[Ar] 4s, 36[Kr] 5s, 54[Xe] 6s

Complete the following table:

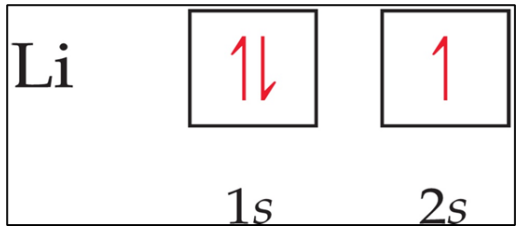
Element	Electron configuration	Short notation (abbreviated)
$_{4}$Be		
$_{11}$Na		
$_{41}$Nb		
$_{25}$Mn		
$_{31}$Ga		

Magnetic properties

Paramagnetic substance: is the substance that contains **net unpaired** electrons in the outermost subshell. Thus it will be attracted by a magnet.

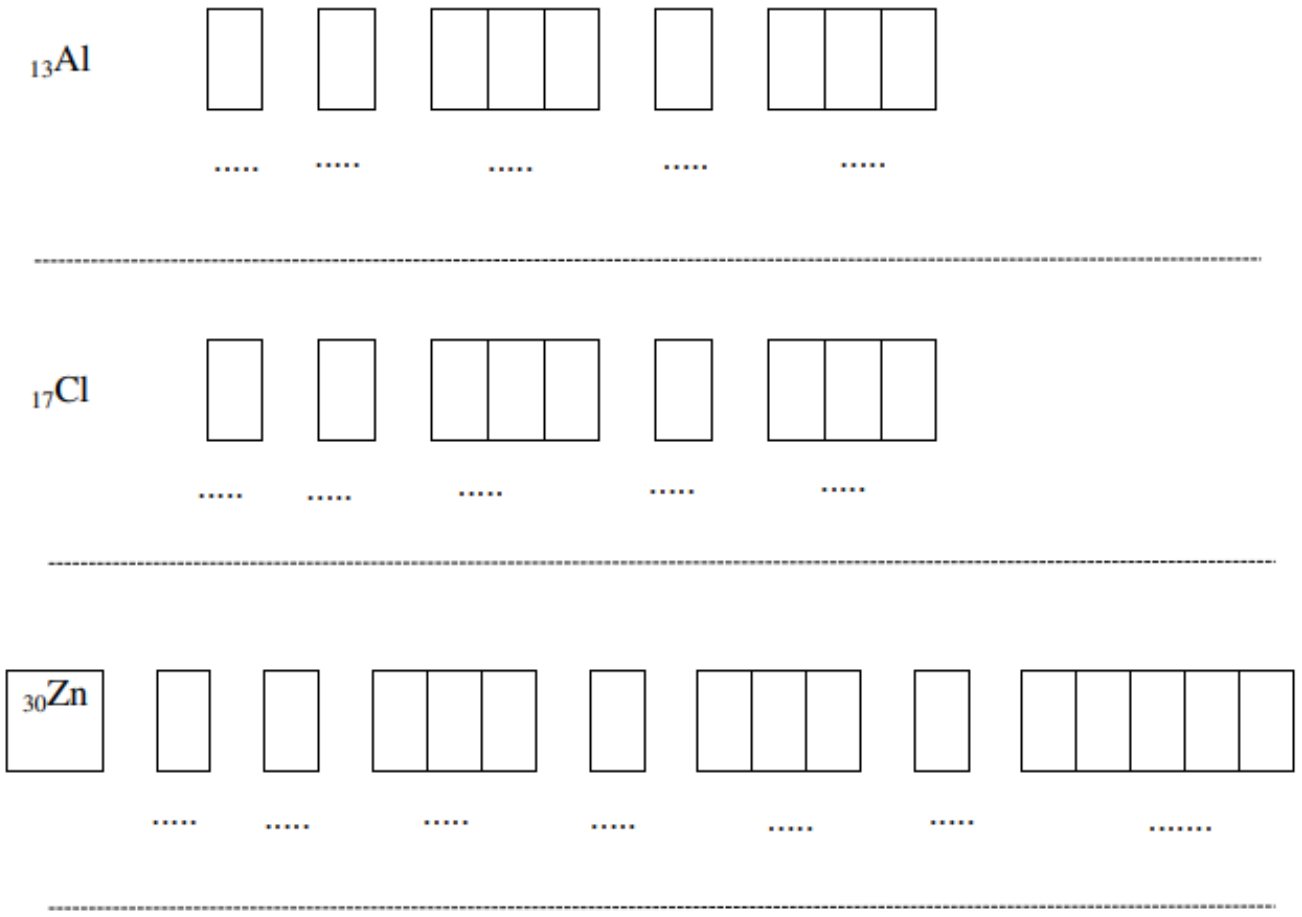
Diamagnetic substance: is the substance that **does not contain net unpaired** electrons (all electrons are paired) in the outermost subshell. Thus it will be slightly repelled by a magnet.

The Li atom contains one unpaired electron and → Li metal is paramagnetic.



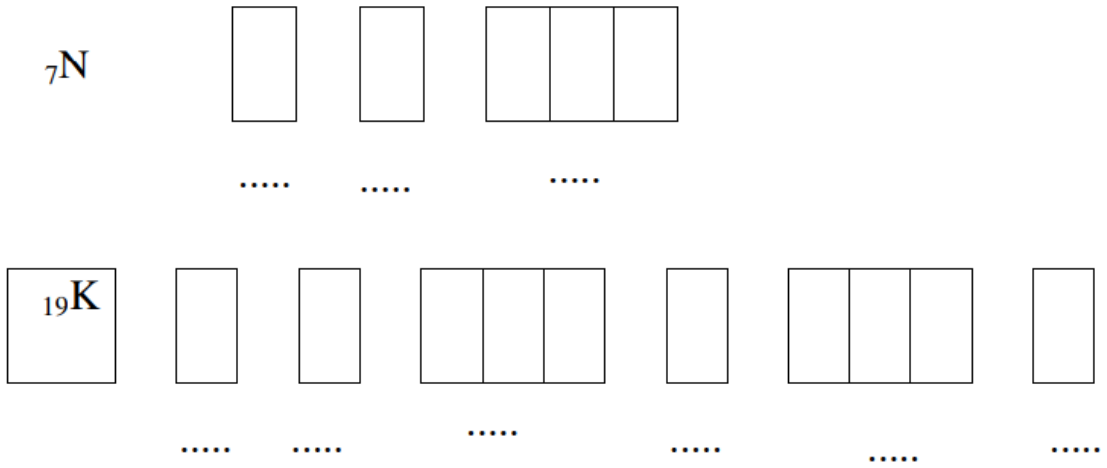
Define the magnetic property for the following elements?

$_{13}Al$, $_{17}Cl$, $_{30}Zn$



Which of the following elements has higher magnetic properties?

$_{7}N$ or $_{19}K$



Example

An atom of a certain element has 15 electrons. Without consulting a periodic table, answer the following questions:

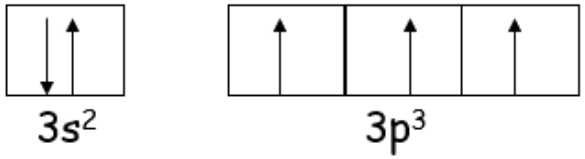
(A)What is the ground-state electron configuration of this element?

Electron configuration: $1s^2\ 2s^2\ 2p^6\ \underline{3s^2\ 3p^3}$

Short notation: [Ne] $3s^2\ 3p^3$

(B) Is the element diamagnetic or paramagnetic?

paramagnetic



Example:

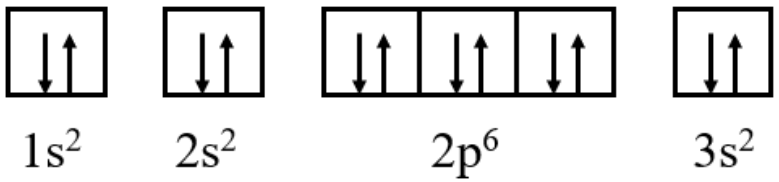
Write the ground-state electron configuration for Mg? is it paramagnetic or diamagnetic?

Mg atom has 12 electrons (from: Periodic table (Z = atomic number))

Electron Configuration: $1s^2 2s^2 2p^6\ 3s^2$

Short notation: [Ne] $3s^2$; where: **[Ne] =** $1s^2 2s^2 2p^6$

Orbital Diagram:



So, it is a diamagnetic

Examples:

Which of the following is paramagnetic ? • Mg • Ar • He • **N**	How many unpaired electrons are in Mn ? • 2 • **5** • 4 • 3
Which of the following is diamagnetic ? • **Mg** • Na • N • Li	How many unpaired electrons are in Fe^{2+} ? • 2 • **4** • 5 • 3
How many unpaired electrons are in Mn^{2+} ? • 2 • **5** • 4 • 3	How many unpaired electrons are in Fe^{3+} ? • 2 • **5** • 4 • 3

General Chemistry
Chem101

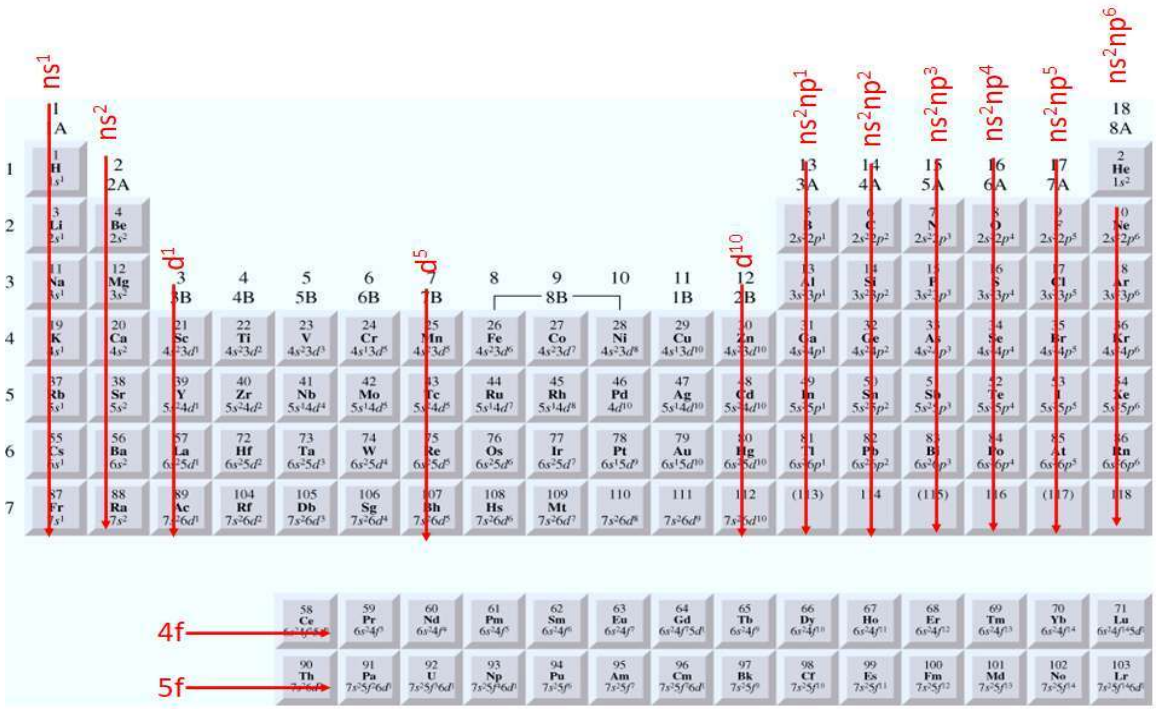
Chapter 3
Periodic Table

❖ Development of the Periodic Table

- Many attempts have been made to arrange the elements.
- When Russian Chemist Dmitri Mendeleev arranged the elements in order of increasing atomic mass, the properties were repeated. Because the properties repeated themselves regularly/periodically on his chart, the system became known as the periodic table.
- Mendeleev's classification was based on the atomic mass, however, this resulted in some inconsistency.
- Later on, after the discovery of the atomic number by Henry Moseley the **elements were arranged by their atomic numbers.**
- Periodic table is divided into four roughly rectangular areas called **blocks**. The rows of the table are called **periods**, and the columns are called **groups**.

Note:

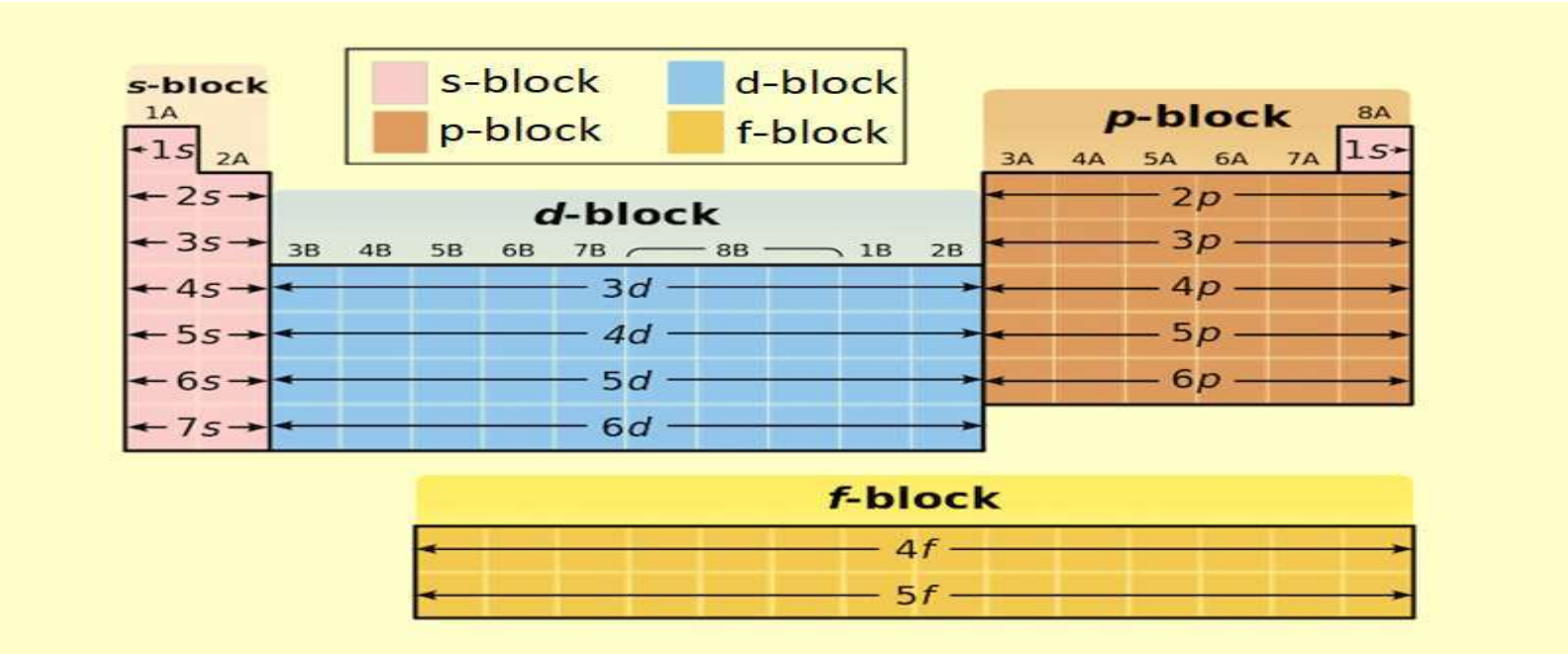
- The number of electrons increases as we go from left to right across the period.
- The value of n increases as we move down the group (from top to bottom).



1. Blocks of the Periodic Table| s-p-d-f Blocks

The periodic table is divided into **<u>four</u>** blocks depending on the type of shells being filled.

- **s-block** is characterized by **alkali metals** and **alkaline earth metals**.
- **p-block** is characterized by **metals, non-metals, and metalloids** of groups 3 to 8.
- **d-block** is characterized **by metals with variable (transition**) oxidation states.
- **f-block** is characterized by **Lanthanide and Actinide metals**.



How to find the block for an element in the periodic table ?

1. write the electronic configuration of the element
2. The orbital which receives the last electron represents the block of the element

Examples:

$_{3}$**Li: $1s^2\ 2\underline{s}^1$** ⟹ **s-block**

$_{6}$**C :$1s^2\ 2s^2\ 2\underline{p}^2$** ⟹ **p-block**

$_{21}$**Sc: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3\underline{d}^1$** ⟹ **d-block**

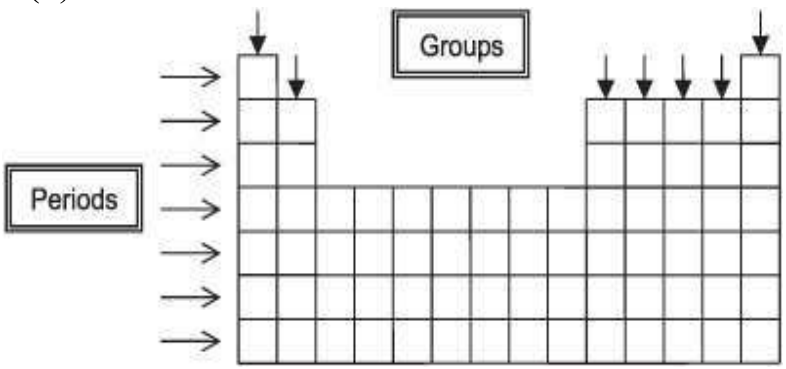
$_{58}$**Ce: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 5s^2\ 4d^{10}5p^6\ 6s^2\ 4\underline{f}^2$** ⟹ **f-block**

2. Periods of the Periodic Table

- A **period** in the periodic table is a row of chemical elements
- There are currently **seven complete periods** in the periodic table

How to find the period for an element in the periodic table ?

1. write the electronic configuration of the element
2. the number of the period is equal to the highest principal quantum number (n) of the elements



➢ Period 1 (K)

- Highest principal quantum number **n=1**
- contains only two elements hydrogen and helium

Examples: $_{1}H:\underline{1}s^{1}$ $_{2}He:\underline{1}s^{2}$

➢ Period 2 (L)

- Highest principal quantum number **n=2**
- contains the elements lithium, beryllium, boron, carbon, nitrogen, oxygen, fluorine, and neon.

Examples: $_{3}Li : 1s^{2}\ \underline{2}s^{1}$ $_{6}C : 1s^{2}\ 2s^{2}\ \underline{2}p^{2}$

➢ Period 3 (M)

- Highest principal quantum number **n=3**
- contains 8 elements beginning with sodium and ending with argon.

Example: $_{11}Na : 1s^{2}\ 2s^{2}\ 2p^{6}\ \underline{3}s^{1}$

➢ Period 4 (N)

- Highest principal quantum number **n=4**
- contains 18 elements beginning with potassium and ending with krypton

Example: $_{21}Sc$: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ \underline{4}s^2\ 3d^1$

➢ Period 5 (O)

- Highest principal quantum number **n=5**
- contains 18 elements, beginning with rubidium and ending with xenon

Example: $_{38}Sr$: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ \underline{5}s^2$

➢ Period 6 (P)

- Highest principal quantum number **n=6**
- contains 32 elements beginning with caesium and ending with radon

Example: $_{58}Ce$: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 5s^2\ 4d^{10}\ 5p^6\ \underline{6}s^2\ 4f^2$

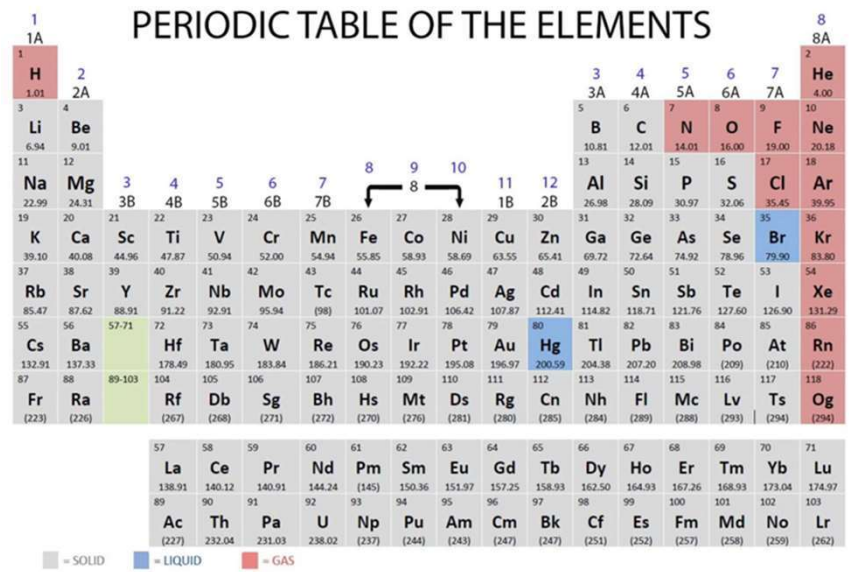
➢ Period 7 (Q)

- Highest principal quantum number **n=7**
- ontains 32 elements beginning with francium

Example: $_{87}Fr$:[Rn] $\underline{7}s^1$

3. Groups of the Periodic Table

- **The elements are arranged in 18 vertical columns called groups. Groups are labeled at the top of each column.**
- **The elements can also be classified into the main-group elements (or representative elements) in the columns labeled 1, 2 and 13–18 Group A and transition metals located in columns 3-12 Group B**



3.1. Group A elements

How to find the group for an element in the periodic table ?

1. write the electronic configuration of the element
2. Get the **total number** of electrons (e) in the outer **subshells/incomplete subshells (ns,np):** This gives the 'Group number'

➢ Group 1A

Elements of group 1A (**alkali metals**) have only one valence electron in their highest-energy orbitals (ns^1).

Example: $_3Li : 1s^2\ \mathbf{2s^1}$ group 1A

➢ Group 2A

Elements of group 2A (**alkaline earth metals**) have only one valence electron in their highest-energy orbitals (ns^2).

Example: $_4Be : 1s^2\ \mathbf{2s^2}$ group 2A

- **Group 3A**

Elements of group 3A have **three** valence electron in their highest-energy orbitals **(ns^2p^1).**

Example: $_5B$: $1s^2$ **$2s^2$ $2p^1$** **group 3A**

- **Group 4A**

Elements of group 4A have **four** valence electron in their highest-energy orbitals **(ns^2p^2).**

Example: $_6C$: $1s^2$ **$2s^2$ $2p^2$** **group 4A**

- **Group 5A**

Elements of group 5A have **five** valence electron in their highest-energy orbitals **(ns^2p^3).**

Example: $_7N$: $1s^2$ **$2s^2$ $2p^3$** **group 5A**

- **Group 6A**

Elements of group 6A have **six** valence electron in their highest-energy orbitals **(ns^2p^4).**

Example: $_8O$: $1s^2$ **$2s^2$ $2p^4$** **group 6A**

- **Group 7A**

Elements of group 7A (**halogens**) have **seven** valence electron in their highest-energy orbitals **(ns^2p^5).**

Example: $_9F$: $1s^2$ **$2s^2$ $2p^5$** **group 7A**

- **Group 8A**

Elements of group 8A (**noble gases** or **inert gases**) have **six** valence electron in their highest-energy orbitals **(ns^2p^6).**

Example: $_{10}Ne$: $1s^2$ **$2s^2$ $2p^6$** **group 8A**

3.2. Group B elements

- The **transition elements** or **transition metals** occupy the short columns in the center of the periodic table, between Group 2A and Group 3A. They are sometimes called the ***d*-block elements**,
- the transition metals in general have electron configurations of **ns^2 (n-1)d**

How to find the group for Transition elements?

1. write the electronic configuration of the element

➢ **If the number of electrons (e) in *d*-orbitals is less than five**

Get the **total number** of electrons (e) in the outer **subshells ns, (n-1)d :** This gives the 'Group number'

Examples:

$_{21}Sc$: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ \mathbf{4s^2\ 3d^1}$	**Group 3B**
$_{22}Ti$: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ \mathbf{4s^2\ 3d^2}$	**Group 4B**
$_{23}V$: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ \mathbf{4s^2\ 3d^3}$	**Group 5B**
$_{24}Cr$: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ \mathbf{4s^1\ 3d^5}$	**Group 6B**
$_{25}Mn$: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ \mathbf{4s^2\ 3d^5}$	**Group 7B**

- **If the number of electrons (e) in *d*-orbitals is more than five and less than ten**

The group is 8B

Examples:

$_{26}Fe$: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ \mathbf{4s^2\ 3d^6}$	**Group 8B**
$_{27}Co$: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ \mathbf{4s^2\ 3d^7}$	**Group 8B**
$_{28}Ni$: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ \mathbf{4s^2\ 3d^8}$	**Group 8B**

- **If the number of electrons (e) in *d*-orbitals equals ten**

Get the **total number** of electrons (e) in the outer **subshells s:** This gives the 'Group number'

Examples:

$_{29}Cu$: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ \mathbf{4s^1\ 3d^{10}}$	**Group 1B**
$_{27}Zn$: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ \mathbf{4s^2\ 3d^{10}}$	**Group 2B**

Examples:

1- The element with the valance electron configuration of $3s^2\ 3p^3$ is:

a) Carbon

b) Nitrogen

c) Phosphorus

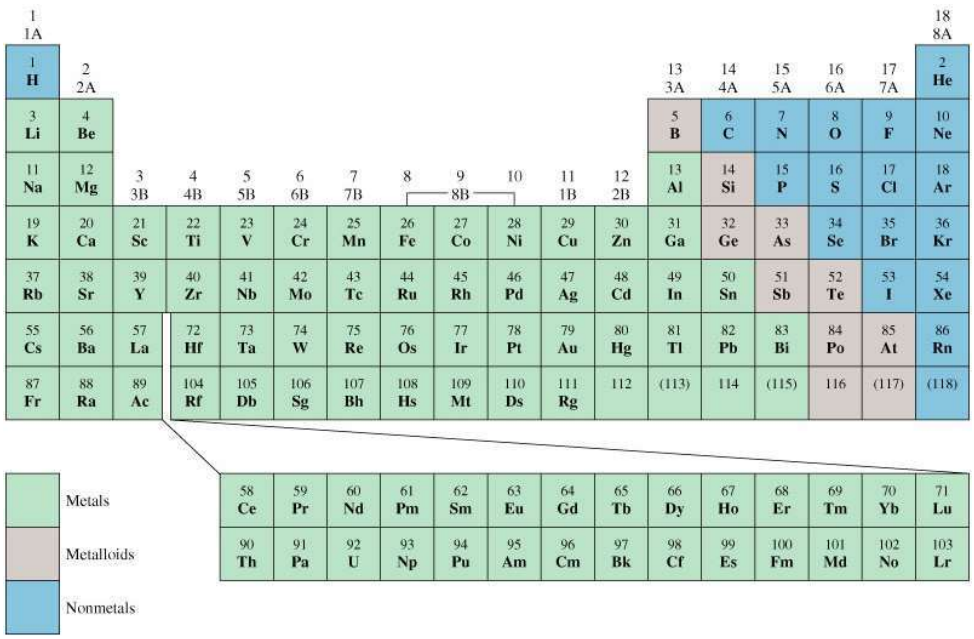
d) Neon

2- Which of the following sets of elements are expected to have similar chemical properties?

a) Sulfur and phosphorous

b) Sulfur and oxygen

c) Sulfur and argon



3-Titanium (Ti) element is found in the periodic table in:

a) s-block
b) P-block
c) d-block
d) f-block

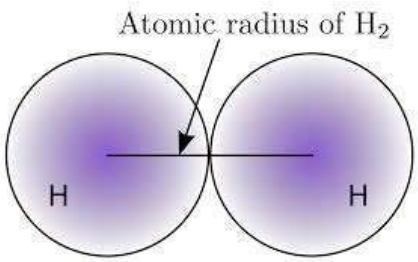
4- The general formula of an element in group 8A is

a) S^2
b) S^1
c) s^2p^6
d) s^1p^1

5- Iron is located in group --------- and period ----------

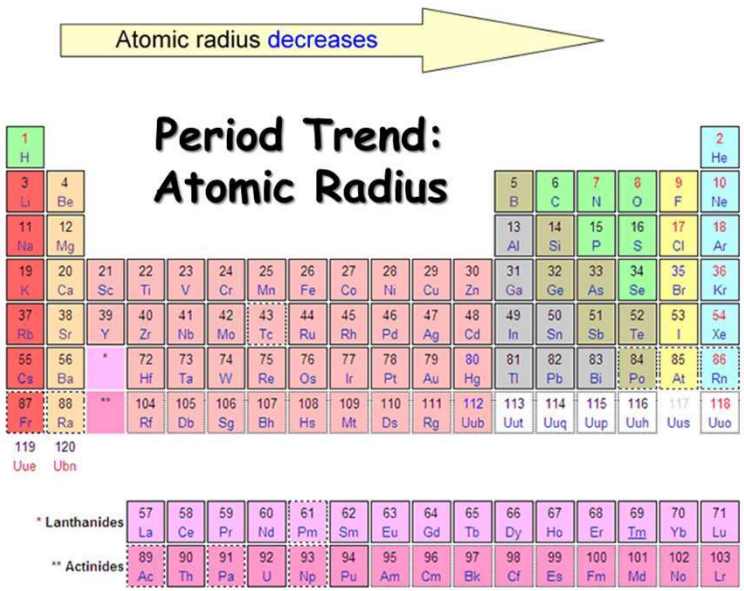
4. Periodic Variation in Physical Properties

4.1. Atomic Radius



- The size of the atom is defined by the ATOMIC RADIUS.
- **Atomic Radius (AR) :** is one-half the distance between the two nuclei in two adjacent metal atoms or in a diatomic molecule.

- **In the same period:** n is the same → the added valence electron is more strongly attracted by the nucleus → As a result, the atomic radius decreases from left to right across the period.



Examples:

Element	period	group
$_4$Be: **1s^{2}2s^2**	2	**2A**
$_5$B: **1s^{2}2s^2**2p^1	2	**3A**
$_6$C: **1s^{2}2s^2**2p^2	2	**4A**

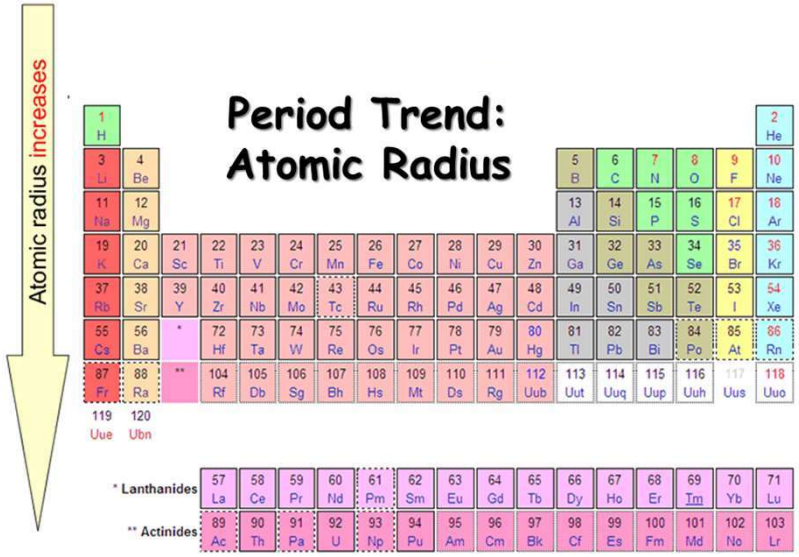
the atomic radius decreases from Beryllium (Be) to Carbon (C) (same period)

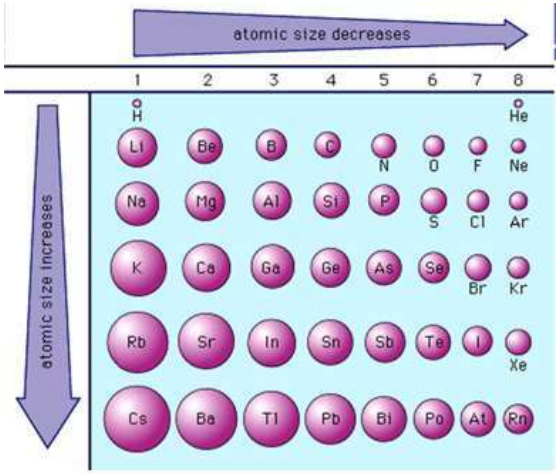
In the same group: The atomic radius increases from top to bottom as the electrons are added to new energy shells (n increases).

Examples:

Element	period	group
$_{1}H$: **1**s^1	1	**1A**
$_{3}Li$: **1**s^2**2**s^1	2	**1A**
$_{11}Na$:1s^2 2s^2 2p^6 **3**s^1	3	**1A**

the atomic radius increases from Hydrogen (H) to Sodium (Na) (same group)





Referring to a periodic table, arrange the following atoms in order of increasing atomic radius: P, Si, N.

Increasing means from small to large

(Small) N < P < Si (Large)

Arrange the following atoms in order of decreasing radius: C , Li, Be .

Decreasing means from large to small

(Large) Li > Be > C (Small)

Which choice below correctly lists the elements in order of increasing atomic radii?

a- Na < Mg < K < Rb

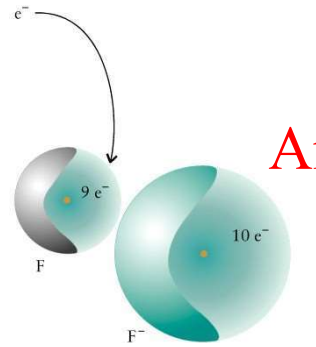
b- Mg < Na < K < Rb

c- Rb < K < Na < Mg

d- Rb < K < Mg < Na

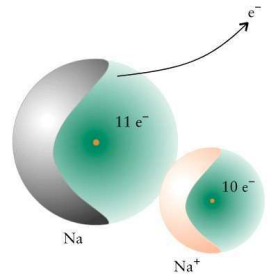
4.2. Ionic Radius

- **Ionic Radius:** is the radius of cations or anions.
- **Anions:** gain electrons → The **ionic radius increases** because the nuclear charge remains the same but the repulsion resulting from the additional electrons increases the size.



Anion

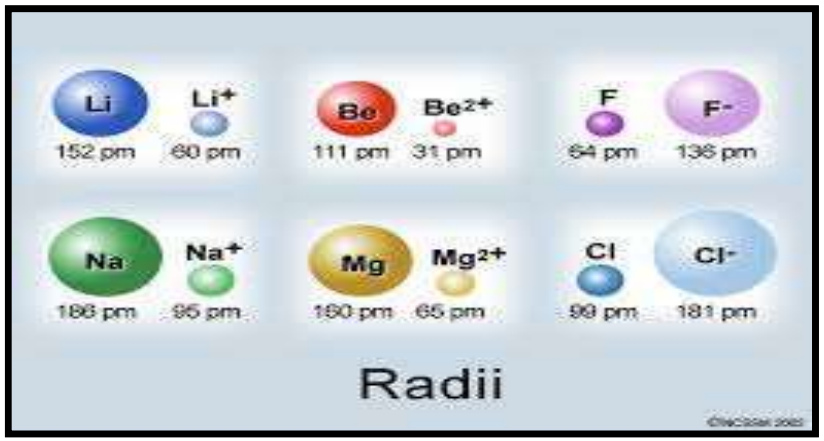
- **Cations:** lose electrons → The **ionic radius decreases** because the removal of one or more electrons from an atom reduces electron-electron repulsion while the nuclear charge remains the same. This leads to shrink the electron clouds.



Cation

Na> Na⁺

$_{11}Na$:$1s^2$ $2s^2$ $2p^6$ $3s^1$
$_{11}Na^+$:$1s^2$ $2s^2$ $2p^6$



F <F⁻

$_9F$: $1s^2$ $2s^2$ $2p^5$
F^- : $1s^2$ $2s^2$ $2p^6$

Order the following according to the increase in the atomic/ionic radius.

N^{3-} Li^{+} C O^{2-}

a) $C < Li^{+} < O^{2-} < N^{3-}$

b) $N^{3-} < O^{2-} < C < Li^{+}$

c) $Li^{+} < C < N^{3-} < O^{2-}$

d) $Li^{+} < C < O^{2-} < N^{3-}$

4.3. Ionization Energy

- **Ionization Energy (IE) :** is the minimum energy in (kJ/mol) required to remove an electron from a gaseous atom in its ground state.
- For a many-electron atom, the amount of energy required to remove the first electron from the atom in its ground state is called the first ionization energy (I_1). The amounts of energy required to remove the second and third electrons are called the second and third ionization energies (I_2 and I_3), respectively.

- When an electron is removed from the atom, the repulsion among the remaining electrons decreases because the nuclear charge remains constant. However, more energy is needed to remove another electron from the positively charged ion.

$$I_1 < I_2 < I_3$$

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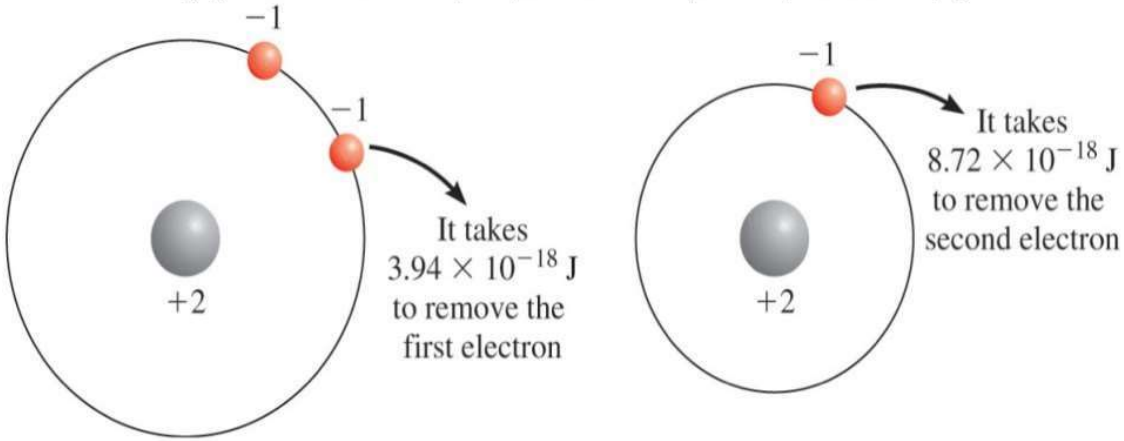
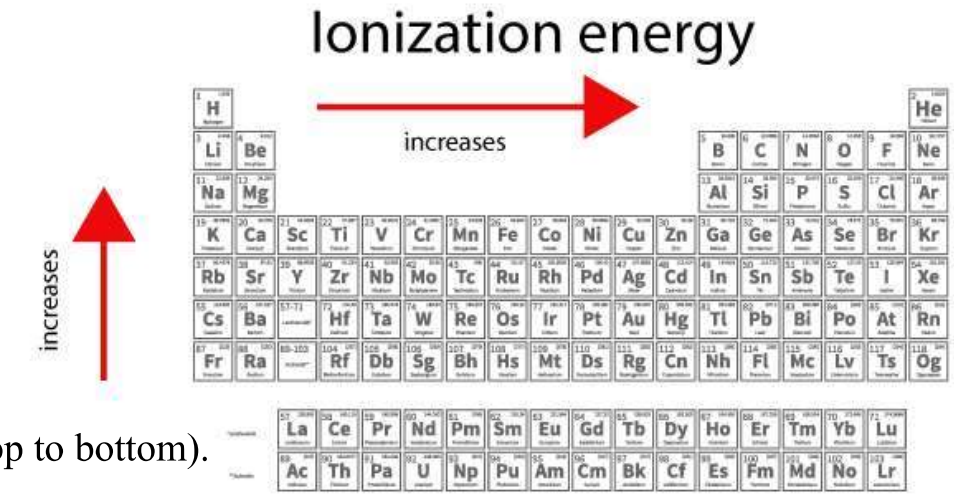


❖ **In the same period:** n is the same → the added valence electron is more strongly attracted by the nucleus → As a result, the ionization energy increases from left to right across the period.

Examples:

Element	period	group
$_5B$: $1s^2 2s^2 2p^1$	2	**3A**
$_6C$: $1s^2 2s^2 2p^2$	2	**4A**
$_7N$: $1s^2 2s^2 2p^3$	2	**5A**

IE: $_7N > {}_6C > {}_5B$



❖ **In the same group:** The IE decreases down the groups (from top to bottom).

Examples:

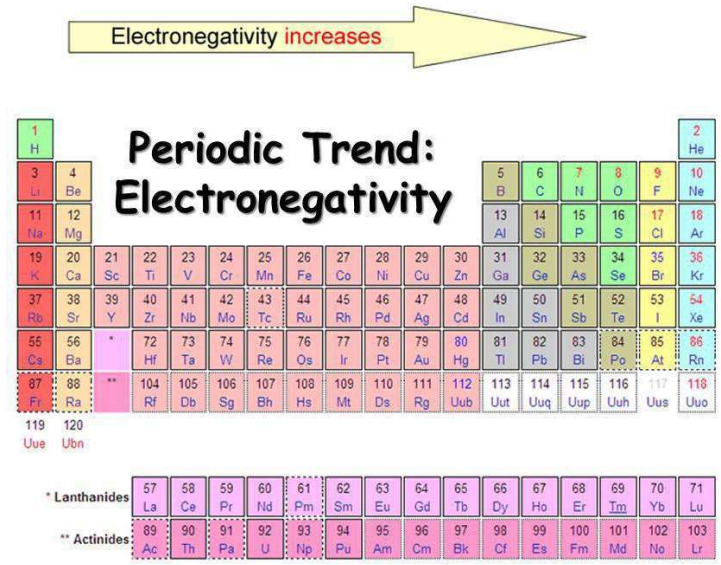
Element	period	group
$_3Li$: $1s^2 2s^1$	2	**1A**
$_{11}Na$:$1s^2\ 2s^2\ 2p^6\ 3s^1$	3	**1A**
$_{19}K$:$1s^2\ 2s^2\ 2p^6\ 3s^2 3p^6\ 4s^1$	4	**1A**

IE: $_3Li > {}_{11}Na > {}_{19}K$

4.4. Electronegativity

- **Electronegativity:** is the ability of an atom to attract toward itself the electrons in a chemical bond.
- High electronegativity → able to pick up electrons easily
- Nonmetals have high electronegativity, On the other hand, metals have lower electronegativity.

❖ **In the same period:** n is the same → the added valence electron is more strongly attracted by the nucleus → As a result, the Electronegativity increases from left to right across the period.



Examples:

Element	period	group
$_5B$: $1s^2 2s^2 2p^1$	2	**3A**
$_6C$: $1s^2 2s^2 2p^2$	2	**4A**
$_7N$: $1s^2 2s^2 2p^3$	2	**5A**

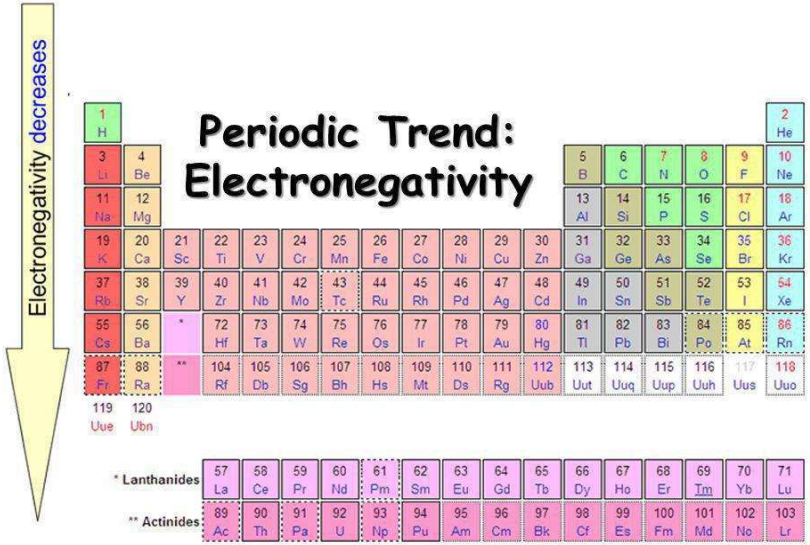
Electronegativity: $_7N > {}_6C > {}_5B$

- **In the same group:** The electronegativity decreases down the groups (from top to bottom).

Examples:

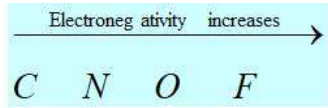
Element	period	group
$_{3}Li$: **1**s^2**2**s^1	2	**1A**
$_{11}Na$:$1s^2$ $2s^2$ $2p^6$ **3**s^1	3	**1A**
$_{19}K$:$1s^2$ $2s^2$ $2p^6$ **3**$s^2 3p^6$ **4**s^1	4	**1A**

Electronegativity: $_{3}Li$ > $_{11}Na$ > $_{19}K$



Example:

Which choice below correctly lists the elements in order of increasing electronegativity?

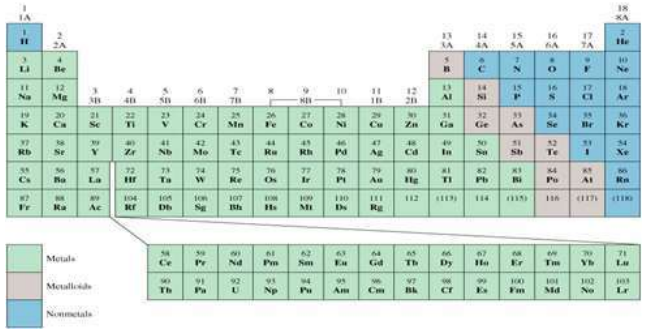


a) **C < N < O < F**

b) N < C < O < F

c) N < C < F < O

d) C < N < F < O



Which atom should have a smaller first ionization energy: oxygen or sulphur?

Both oxygen and sulphur atoms are in group 6 but different period, the valence electrons in sulphur are farther from the nucleus → removing of them is easier

THUS: I_1 (S) < I_1 (O)

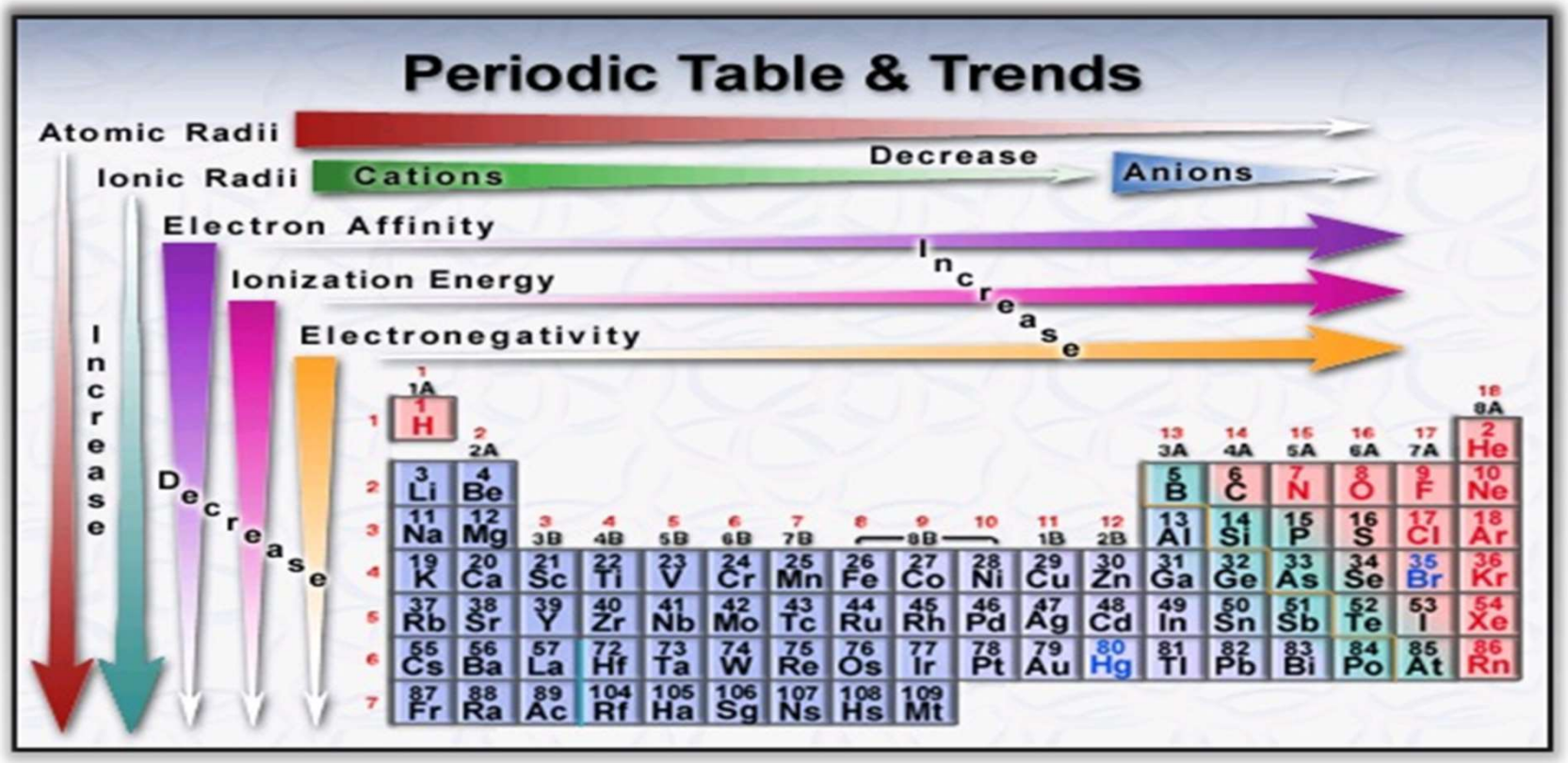
Which atom should have a higher second ionization energy (Li or Be)?

Li ($2s^1$) < Be ($2s^2$) … first ionization energy

Li^+ ($1s^2$) > Be^+ ($2s^1$) … second ionization energy

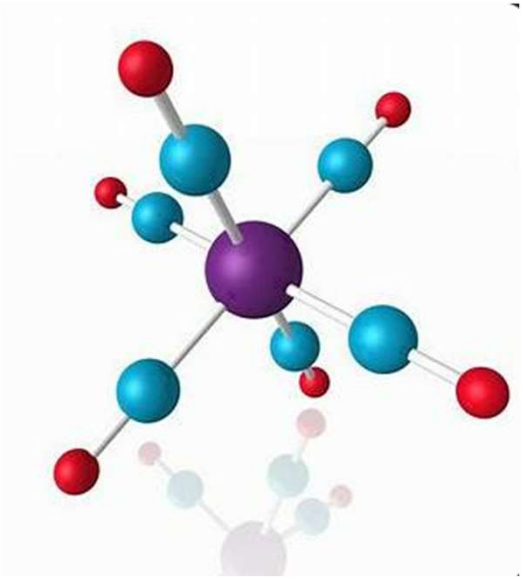
Because 1s electrons shield 2s electrons much more effectively than they shield each other , we predict that it should be easier to remove a 2s electron from Be^+ than to remove a 1s electron from Li^+

Summary

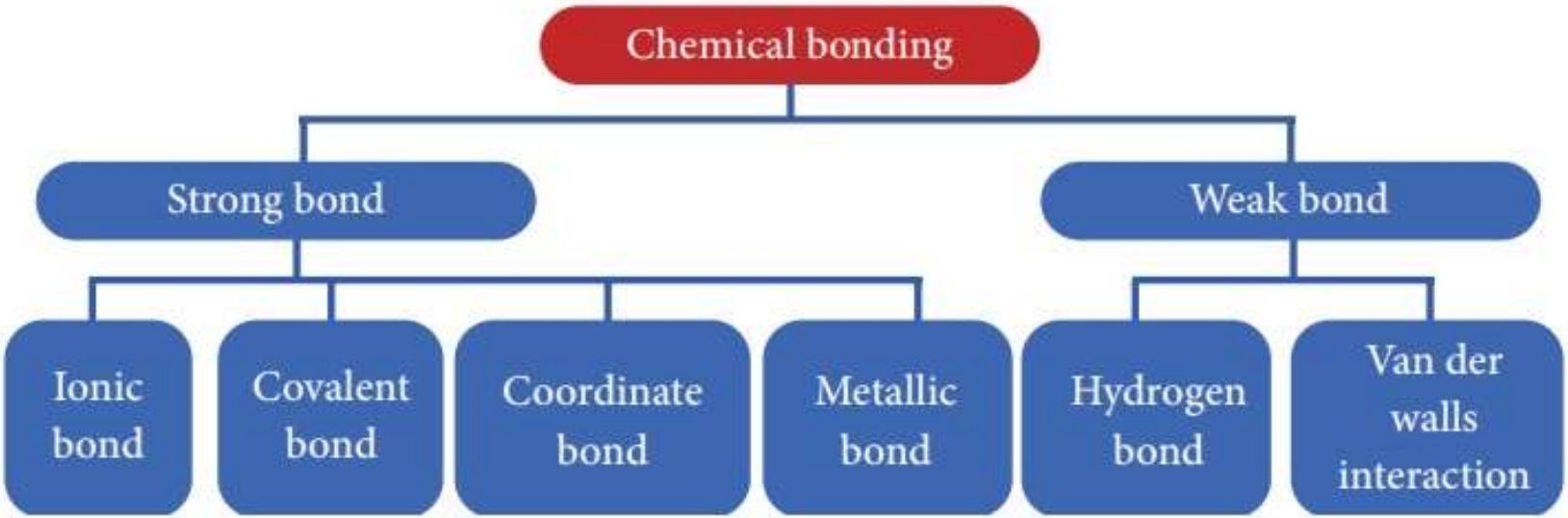

Periodic Table & Trends
Atomic Radii
Decrease
Ionic Radii
Cations
Anions
Electron Affinity
Ionization Energy
Increase
Electronegativity
Increase
Decrease

Chapter 4

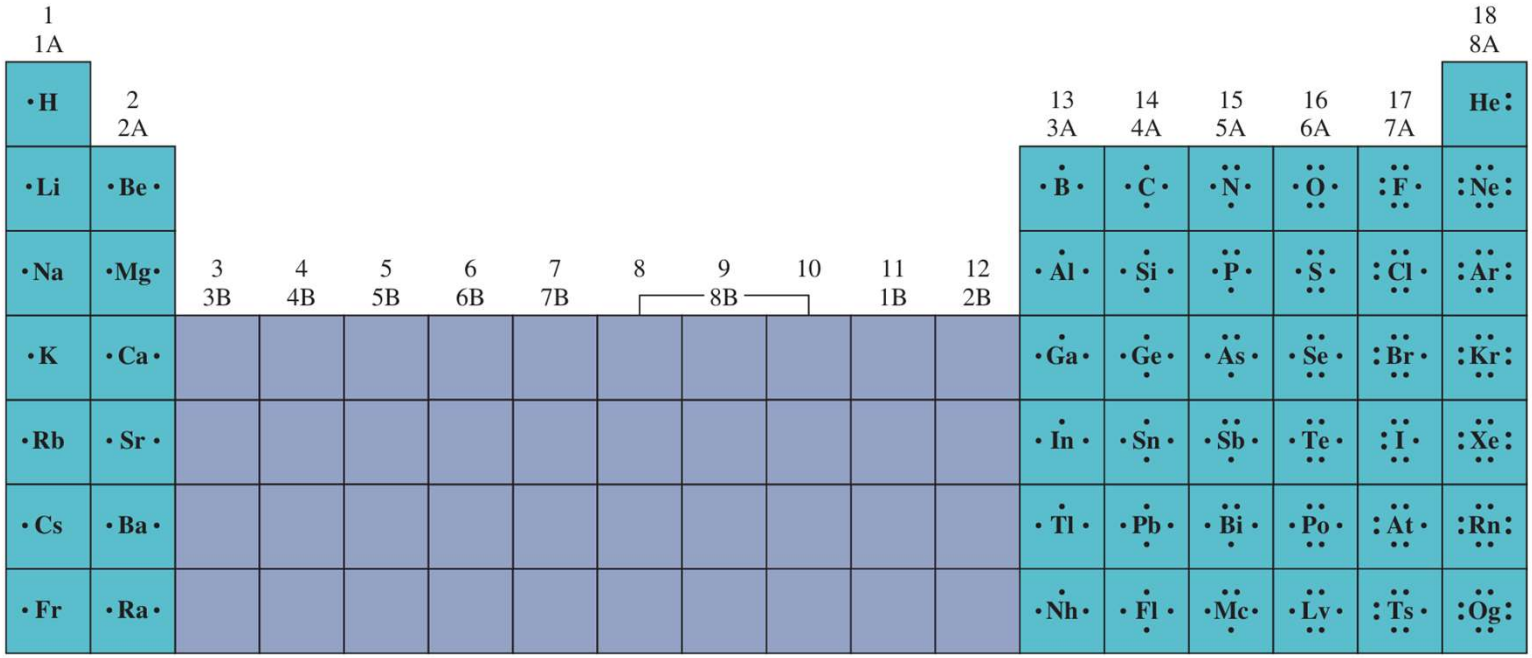
Introduction of Chemical Bonding



When atoms interact to form a chemical bond, only their outer regions are in contact. For this reason, when we study chemical bonding, we are concerned primarily with the valence electrons of the atoms.



A Lewis dot symbol consists of the symbol of an element and one dot for each valence electron in an atom of the element.



Lewis dot symbols for the representative elements and the noble gases.

- **The ability of an atom in a molecule to attract shared electrons is called electronegativity. When two atoms combine, the difference between their electronegativities is an indication of the type of bond that will form.**

The ionic bond

- **An ionic bond is the electrostatic force that holds ions together in an ionic compound.**

$$\cdot\,\mathrm{Li} \quad + \quad :\ddot{\underset{\cdot\cdot}{\mathrm{F}}}\cdot \quad \longrightarrow \quad \mathrm{Li}^{+} \quad :\ddot{\underset{\cdot\cdot}{\mathrm{F}}}:^{-} \quad (\text{or LiF})$$

$$1s^2 2s^1 \qquad 1s^2 2s^2 2p^5 \qquad\qquad 1s^2 \quad 1s^2 2s^2 2p^6$$

For convenience, imagine that this reaction occurs in separate steps—first the ionization of Li:

$$\cdot\mathrm{Li} \longrightarrow \mathrm{Li}^{+} + e^{-}$$

and then the acceptance of an electron by F:

$$:\ddot{\underset{\cdot\cdot}{\mathrm{F}}}\cdot + e^{-} \longrightarrow :\ddot{\underset{\cdot\cdot}{\mathrm{F}}}:^{-}$$

Next, imagine the two separate ions joining to form a LiF unit:

$$\mathrm{Li}^{+} + :\ddot{\underset{\cdot\cdot}{\mathrm{F}}}:^{-} \longrightarrow \mathrm{Li}^{+} : \ddot{\underset{\cdot\cdot}{\mathrm{F}}}:^{-}$$

Many other common reactions lead to the formation of ionic bonds. For instance, sodium chloride NaCl:

More examples of ionic bonds:

Ca^{2+} $:\ddot{\underset{\cdot\cdot}{O}}:^{2-}$ **(or** CaO **)** Calcium Oxide

$2Li^{+}$ $:\ddot{\underset{\cdot\cdot}{O}}:^{2-}$ (or Li_2O) Lithium Oxide

Mg^{2+} $2F^{-}$ (or MgF_2) Magnesium Fluoride

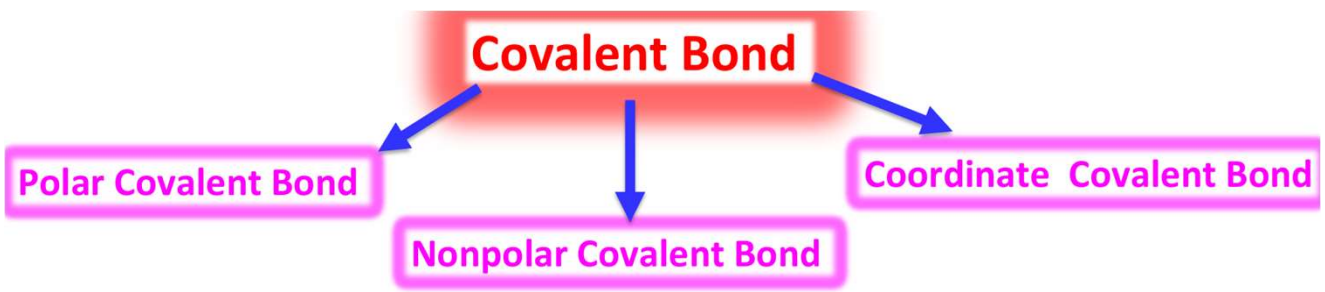
$2Na^{+}$ O^{2-} (Na_2O) Sodium Oxide

The Covalent Bond

The covalent bond is the attraction force that results from the sharing of an electron pair between two atoms forming a molecule. Covalent compounds are compounds that contain only covalent bonds.

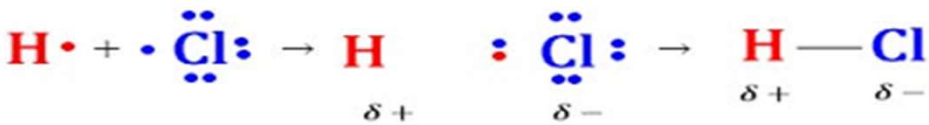
$$\mathrm{H} \cdot + \cdot \mathrm{H} \longrightarrow \mathrm{H} : \mathrm{H}$$

When two atoms have a small difference in electronegativity, we observe electron sharing and covalent bonding. This type of bonding most commonly occurs between nonmetal atoms.



Polar Covalent Bond (polar bond)

It is bond in which the bonding electrons spend more time near one atom (has high electronegativity) than the other (has low electronegativity).



When electron pair spend more time near the atom with high electronegativity, it give a partial negative charge δ^- and becomes a negative pole. The other atom had a partial positive charge δ^+ and becomes a positive pole.

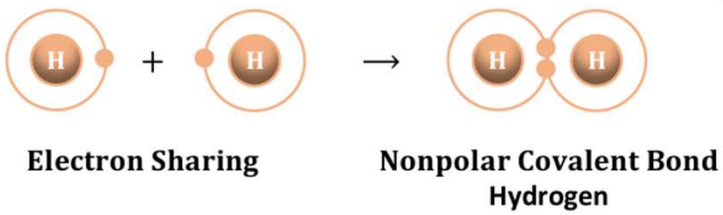
Examples:

H_2O, CO, CO_2, HF

Nonpolar Covalent Bond

It is a covalent bond in which the bonding electrons shared equally between two atoms. So, No electronegativity difference between the tow atoms.

Example; H_2



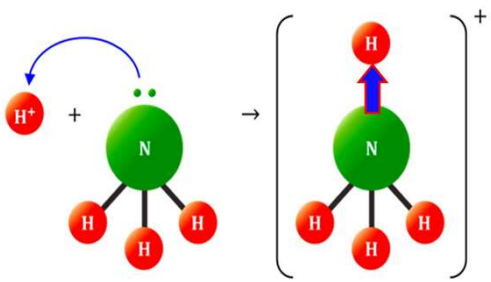
More examples:

O_2, F_2, Cl_2, N_2, Br_2

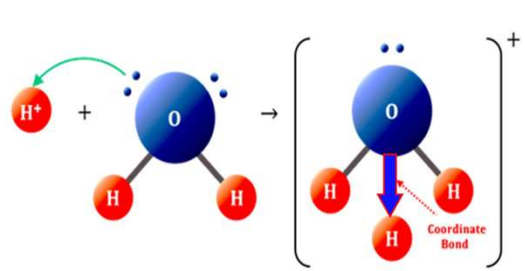
Coordinate Covalent Bond (Dative Covalent Bond)

is a covalent bond (a shared pair of electrons) in which both electrons come from the same atom. We represent the coordinate bond by an arrow directed from the donor atom to the acceptor atom

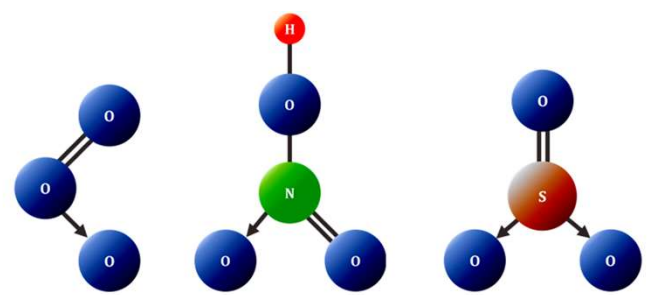
Examples;



Ammonium Ion
NH_4^+



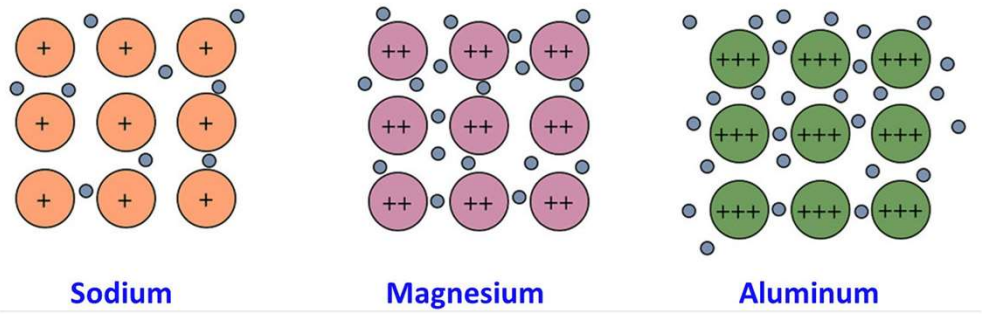
Hydronium Ion
H_3O^+



O_3 **HNO_3** **SO_3**

Metallic Bond

It is the force of attraction between positive metallic atomic cores (ions) and surrounded delocalized valence electrons. Unlike the localized electrons in covalent bonding, electrons in metallic bonding are delocalized, moving freely throughout the piece of metal.



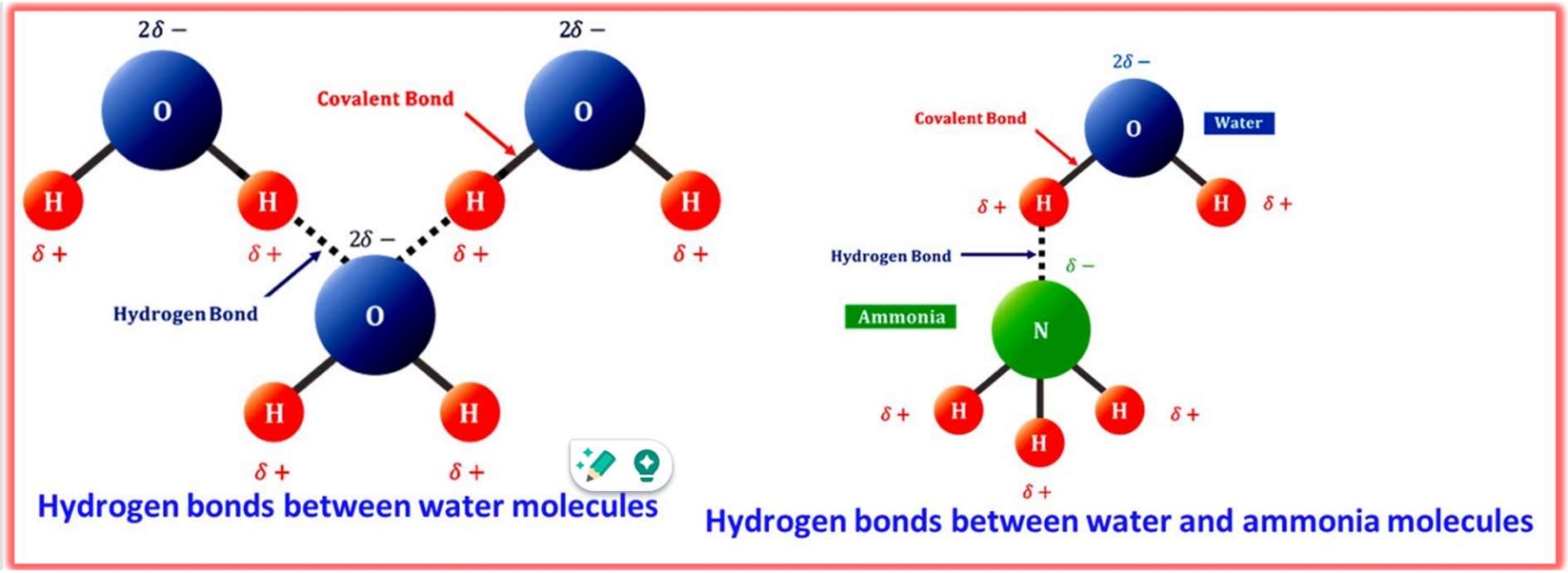
The softness and low melting point of sodium can be explained by the relatively low number of electrons in the electron sea and the relatively small charge on the sodium cation compared to magnesium and aluminum.

Hydrogen Bond

-It is a special type of intermolecular force of dipole-dipole attraction arises between molecules that have H atom covalently bonded to a small, highly electronegative atom with lone electron pairs such as a N, O, S or F atom.

-As a result, the partially positive H of one molecule is attracted to the partially negative lone pair on the N, O, S or F of another molecule.

-and a hydrogen bond (H bond) form –H···O–, –H···N–, –H···S–and –H···F–.
-We represent hydrogen bond by dotted line.
- hydrogen bonding is a weaker form of chemical bonding.


2δ −
O
H
δ +
Covalent Bond
Hydrogen Bond
Water
Ammonia
N
Hydrogen bonds between water molecules
Hydrogen bonds between water and ammonia molecules

Predicting Bond Types

A property that helps us distinguish between bonds is electronegativity.
By using electronegativity values of the elements (Pauling scale) we can determine the type of bond.

increase

H 2.20	He																
Li 0.98	Be 1.57											B 2.04	C 2.55	N 3.04	O 3.44	F 3.98	Ne
Na 0.93	Mg 1.31											Al 1.61	Si 1.9	P 2.19	S 2.58	Cl 3.16	Ar
K 0.82	Ca 1.0	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 1.9	Zn 1.65	Ga 1.81	Ge 2.01	As 2.18	Se 2.55	Br 2.96	Kr 3.0
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 2.2	Ag 1.93	Cd 1.69	In 1.78	Sn 1.96	Sb 2.05	Te 2.1	I 2.66	Xe 2.6
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 2.2	Pt 2.2	Au 2.4	Hg 1.9	Tl 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2	Rn
Fr 0.7	Ra 0.9	Ac 1.1															

- **Ionic bonds typically form when the difference in electronegativity ΔE is between two atoms is greater than 1.6 ($\Delta E > 1.6$).**
- **Nonpolar Covalent Bonds: These occur when the electronegativity difference is zero ($\Delta E = 0$)**
- **Polar Covalent Bonds: These occur when the electronegativity difference is between 0 and 1.6.($0 < \Delta E < 1.6$).**

Example:

Predict the type of bonds using Pauling scale of electronegativity

Na-Cl	3.16 - 0.93 = 2.23	Ionic bond
C-H	2.55 - 2.2= 0.35	polar covalent bond
O-O	3.44 - 3.44 = 0	Nonpolar covalent bond
N-H	3.04 -2.2 = 0.84	polar covalent bond

Chapter 5

Chemical Calculations

Atomic mass

Atomic mass is the mass of an atom in atomic mass units (amu)

amu definition: the mass exactly equal to 1/12 the mass of one ^{12}C atom

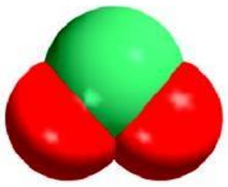
^{12}C = 6p, 6n = 12.00 amu

Experiment shows one atom ^{1}H = 8.400% of ^{12}C atom thus; mass of one atom ^{1}H = 1.008 amu
(12.00 x 0.08400)

^{16}O = 16.00 amu, ^{26}Fe = 55.85 amu, …

Molecular Mass

Molecular mass (or molecular weight) is the sum of the atomic masses (in amu) in a molecule.



SO_2

1S	32.07 amu
2O	+ (2 x 16.00 amu)
SO_2	64.07 amu

Example

1- Calculate the molecular mass of $Ba(NO_3)_2$

Molecular mass of $Ba(NO_3)_2$ =

= (1 × atomic mass of Ba) + (2 × atomic mass of N) + (6 × atomic mass of O)

= 137.3 amu + (2 × 14.01 amu) + (6 × 16.00 amu) = 261.3 amu

2- Calculate the Molecular mass of NH_4NO_3

Molecular mass of NH_4NO_3 =

= (2 × atomic mass of N) + (4 × atomic mass of H) + (3 × atomic mass of O)

= (2 × 14.01 amu) + (4 × 1.008 amu) + (3 × 16.00 amu) = 80.05 amu

The Mole

The Mole (mol): A unit to count numbers of particles

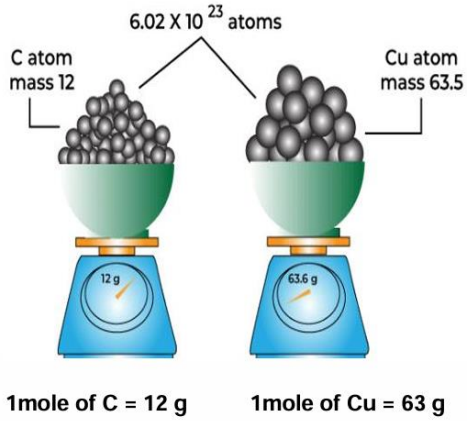
Dozen = 12

Pair = 2

The ***mole (mol)*** is the amount of a substance that contains as many elementary entities as there are atoms in exactly 12.00 grams of ^{12}C

1 mol = N_A = 6.0221367 x 10^{23}

Avogadro's number (N_A)



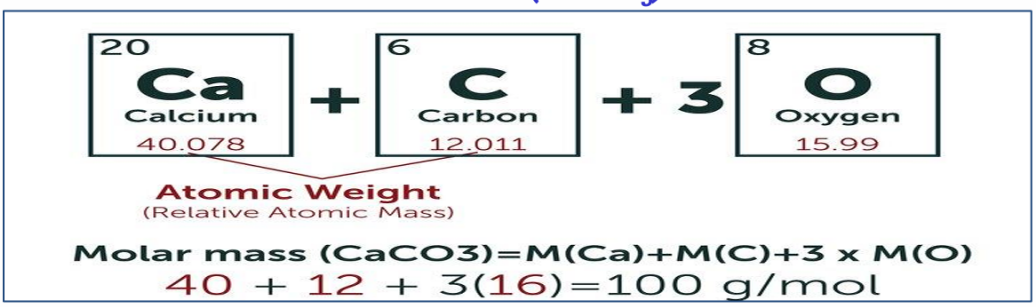
Molar mass (M_m)

M_m is defined as the total mass of one mole of the substance. It is frequently expressed in terms of 'grams per mole' (g/mol).

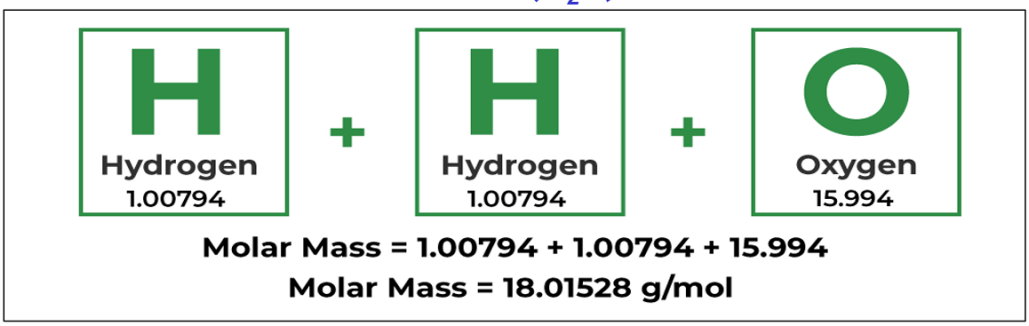
Molar mass = Atomic mass or Molecular mass but in(g/mol) unit.

Molar mass (Mm)

1- Calculate the Molar mass of ($CaCO_3$)



2- Calculate the Molar mass of (H_2O)



Important!

The number of moles formula is as follows:

$$n\ (mol) = \frac{m\ (g)}{Mw\ (g/mol)}$$

Determine how many moles are in 95 g of MnO_2.

Mw(MnO_2)= (1x 54.94) + (2 x 16)= 86.94 g/mol

$$n = \frac{m}{Mw} = \frac{95}{86.94} = 1.092 \text{ mol}$$

We can also determine the number of (atoms, molecules, or particles) using the following formula:

$$N = n\,(mol) \times N_A$$

Where:
N = number of atoms or molecules
n= number of moles
N_A= Avogadro's Number= 6.022 x 10^{23}

Examples

1) How many grams of Ag are in 0.0342 mol of Ag?

Solution

Mass (g) of Ag $= n \times M_m$

m_{Ag} = 0.0342 mol ×107.9 (g/mol) = 3.69 g of Ag

2) How many iron (Fe) atoms are in 95.8 g of Fe?

Solution

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

$$n\,(mol) \text{ of Fe} = \frac{95.8\,(g) \text{ of Fe}}{55.85\,(g/mol) \text{ of Fe}} = 1.72 \text{ mol of Fe}$$

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

$$N_{Fe}(\text{atoms}) = 1.72 \text{ mol} \times 6.022 \times 10^{23} \text{ atoms/mol}$$

$$= 1.04 \times 10^{24} \text{ atoms } Fe$$

3) How many formula units are in 41.6 g of ammonium carbonate $(NH_4)_2CO_3$?

Solution

$$\text{n (mol) of } (NH_4)_2CO_3 = \frac{\text{M (g) of } (NH_4)_2CO_3}{\text{M}_m\text{(g/mol) of } (NH_4)_2CO_3}$$

$$\text{n (mol) of } (NH_4)_2CO_3 = \frac{41.6 \text{ (g) of } (NH_4)_2CO_3}{96.09 \text{ (g/mol) of } (NH_4)_2CO_3} = 0.433 \text{ mol}$$

$$\text{N (no. of formula units)} = \text{n (mol) of } (NH_4)_2CO_3 \times 6.022 \times 10^{23}$$

$$\text{N (no. of formula units)} = 0.433 \text{ mol of } (NH_4)_2CO_3 \times 6.02 \times 10^{23} \text{formula units/mol}$$

$$= 2.61 \times 10^{23} \text{ formula units } (NH_4)_2CO_3$$

Chemical Reaction

A process in which one or more substances is changed into one or more new substances is a ***chemical reaction***

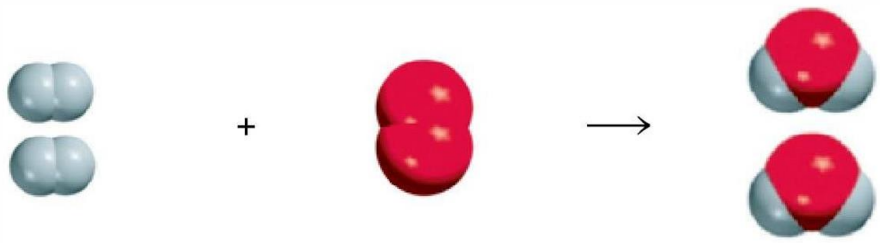
A ***chemical equation*** uses chemical symbols to show what happens during a chemical reaction

reactants $\longrightarrow$ products

3 ways of representing the reaction of H_2 with O_2 to form H_2O

Two hydrogen molecules + One oxygen molecule $\longrightarrow$ Two water molecules

$2H_2 + O_2 \longrightarrow 2H_2O$



How to Balance a Chemical Equation

- When balancing a chemical reaction you may add coefficients in front of the compounds to balance the reaction, but you may **not** change the …
  - subscripts.
  - Changing the subscripts changes the compound.

Reactants | Product

$N_2 + H_2 \longrightarrow NH_3$

Atom Counts	Atom Counts
Nitrogen: 2	Nitrogen: 1
↑ From the Subscript	
Hydrogen: 2	Hydrogen: 3

When balancing a chemical equation, there should be equal numbers of every atom on both sides of the equation

$$N_2 + 3H_2 \longrightarrow 2NH_3$$

Balance the following equations:

- $Al + O_2 \rightarrow Al_2O_3$
- $CO_2 + H_2 \rightarrow CH_4 + H_2O$

Chemical calculations

Calculate the mass of magnesium oxide (MgO) produced from the burning of 20 g of magnesium? Mg= 24

Answer:

1-balance the equation:

$$2Mg + O_2 \longrightarrow 2MgO$$

From the equation:

$$2 \text{ mol Mg} \longrightarrow 2 \text{ mol MgO}$$

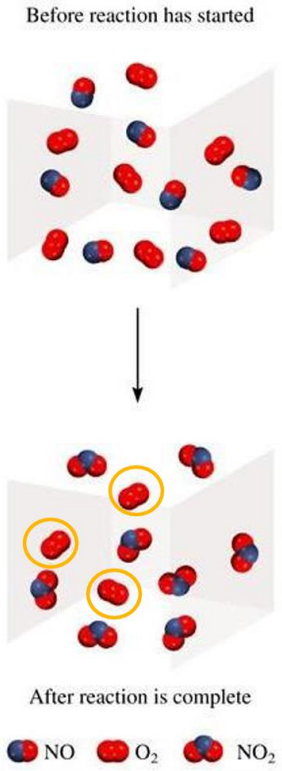
2-Calculate the Mm, then find the mass.

For Mg	for MgO
$n=\frac{m}{Mm}$	$n=\frac{m}{Mm}$
$2=\frac{m}{24}$	$2=\frac{m}{40}$
m= 2x24= 48 g	m= 2x40= 80 g

3-from the calculation.

48g Mg → 80g MgO
20 g Mg → ? MgO

$$m_{(MgO)} = \frac{20x80}{48} = 33.3 \text{ g of MgO}$$



Limiting Reagent

Reactant **used up first** in the reaction

$$2NO + O_2 \longrightarrow 2NO_2$$

NO is the **limiting** reagent

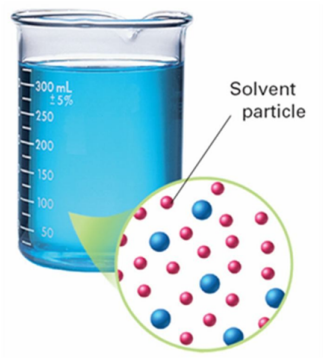
O_2 is the **excess** reagent

Chapter 6

Solutions

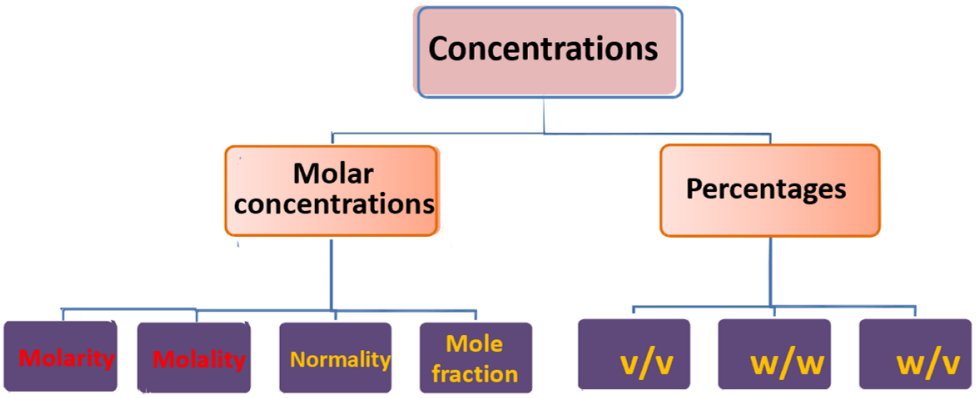
Solutions

Solution: a homogeneous mixture of two or more substances
Solute: a substance that is being dissolved (smaller amount)
Solvent: a substance which dissolves a solute (larger amount)



Concentrations

The ***concentration*** of a solution is the amount of solute present in a given quantity of a solvent or solution.



Molarity

The number of moles of solute dissolved in one liter of solution.

$$\text{Molarity } (M) = \frac{\text{moles of solute}}{\text{liters of solution}}$$

***What is the molarity of a solution containing 1.4 mol of acetic acid in 250.0 mL of solution?**

$$\text{Molarity} = \frac{\text{number of moles of solute mol}}{\text{Volume of solution (L)}}$$

$$\text{Molarity} = \text{C} = \frac{n_{\text{acetic acid}}\ \text{mol}}{\text{Volume of solution (L)}} = \frac{1.4\ \text{mol}}{0.25\ \text{L}} = 5.6\ \text{mol/L}\ \ (5.6\text{M})$$

***What is the molarity of a solution made by dissolving 2.00 g of potassium chlorate in enough water to make 150.0 mL of solution?**
(molar mass $KClO_3$ = 122.6 g/ mol).

1) $$n_{KClO_3}\ (\text{mol}) = \frac{2.00\ (\text{g})}{122.6\ (\text{g/mol})} = 0.0163\ \text{mol}\ KClO_3$$

2) $$\text{volume of solution (L)} = \frac{150.0\ \text{mL}}{1000} = 0.15\ \text{L}$$

3) Finding molarity:

$$\text{Molarity} = \text{C} = \frac{n_{KClO_3}\ \text{mol}}{\text{Volume of solution L}} = \frac{0.0163\ \text{mol}}{0.15\ \text{L}} = 0.1087\ \text{mol/L}\ \ (0.1087\text{M})$$

Molality

The number of moles of solute dissolved in one kilogram of solvent

$$m = \frac{\text{moles of solute}}{\text{mass of solvent (kg)}}$$

The units of molality are moles per kilogram (mol/kg), or molal (m)

***What is the molality of a solution prepared by dissolving 32.0 g of CaCl2 in 271 g of water?**

1) $$\text{Moles of } CaCl_2 (\text{mol}) = \frac{\text{mass of } CaCl_2 \text{ (g)}}{\text{Molar mass of } CaCl_2 (\text{g/mol})}$$

$$n_{CaCl_2} = \frac{m_{CaCl_2}}{M_{CaCl_2}}$$

$$n_{CaCl_2} = \frac{32.0 \text{ g}}{110.98 \text{ g/mol}} = 0.288 \text{ mol of } CaCl_2$$

2) Determine the mass of solvent (water) in kilograms:

$$W_2 = W_{water}(\text{kg}) = \frac{m_{water}(\text{g})}{1000} = \frac{271}{1000} = 0.271\text{kg}$$

3) Finding molality:

$$\text{Molality} = \boldsymbol{m} = \frac{n_{CaCl_2}(\text{mol})}{\text{kilogram of solvent (kg)}} = 1.06(\text{mol/kg}) = 1.06\, m$$

***Calculate the molality of a sulfuric acid solution containing 24.4 g of sulfuric acid in 198 g of water. The molar mass of sulfuric acid is 98.09 g**

1) $$n_{H_2SO_4} = \frac{m_{H_2SO_4}}{M_{H_2SO_4}}$$

$$n_{H_2SO_4} = \frac{24.4 \text{ g}}{95.09 \text{ g/mol}} = 0.249 \text{ mol } H_2SO_4$$

---

2) Determine the mass of solvent (water) in kilograms:

$$W_2 = W_{water}(\text{kg}) = \frac{m_{water}(\text{g})}{1000} = \frac{198}{1000} = 0.198\text{kg}$$

---

3) Finding molality:

$$\text{Molality} = \boldsymbol{m} = \frac{0.249 \text{ mol}}{0.198\text{kg}} = 1.26(\text{mol/kg}) = 1.06\, m$$

Mole fraction (x_i)

$$\text{Mole fraction} = \frac{\text{number of moles of substance (mol)}}{\text{total number of moles of solution (mol)}}$$

If we have n_A mole of solute A and n_B mole of solute B dissolved in n_C mole of solvent C so, the mole fraction for all these components can be express as follow:

$$\frac{n_A}{n_A + n_B + n_C} = x_A = A$$

$$\frac{n_B}{n_A + n_B + n_C} = x_B = B$$

$$\frac{n_C}{n_A + n_B + n_C} = x_C = C$$

Note that:

$X_i = X_A + X_B + X_C = 1$

What are the mole fractions of glucose and water in a solution containing 5.67 g of glucose $C_6H_{12}O_6$, dissolved in 25.2 g of water?

1)

$$\text{The moles of glucose (mol)} = \frac{\text{mass of glucose (g)}}{\text{molar mass of glucose (g/mol)}}$$

$$n_{\text{glucose}}\ \text{(mol)} = \frac{5.67\ \text{(g)}}{180.2\ \text{(g/mol)}} = 0.0315\ \text{mol glucose}$$

2)

$$\text{The moles of water (mol)} = \frac{\text{mass of water (g)}}{\text{molar mass of water (g/mol)}}$$

$$n_{\text{water}}\ \text{(mol)} = \frac{25.2\ \text{(g)}}{18.0\ \text{(g/mol)}} = 1.40\ \text{mol water}$$

3)

$$\text{moles of solution} = \text{moles of water} + \text{moles of glucose}$$

$$\text{moles of solution (mol)} = 1.40\ \text{(mol)} + 0.0315\ \text{(mol)} = 1.4315\ \text{(mol)}$$

4)

$$x_{\text{glucose}} = x_2 = \frac{0.0315\ \text{(mol)}}{1.4315\ \text{(mol)}} = 0.0220$$

5)

$$x_{\text{water}} = x_1 = \frac{1.40\ \text{(mol)}}{1.4315\ \text{(mol)}} = 0.978$$

w% weight percentage

W% of solute is the mass of solute m_{solute} (in gram) dissolved in 100 g of solution.

$$W\% = \frac{m_{solute}}{m_{solution}} \times 100$$

Remember !!

$$m_{solution} = m_{solute} + m_{solvent}$$

***What is the mass percent of sodium hydroxide in a solution that is made by dissolving 8.00 g NaOH in 50.0 g H_2O?**

1)

$$W\% = \frac{m_{NaOH}\ (g)}{m_{solution}\ (g)} \times 100$$

2)

$$m_{solution}\ (g) = m_{water}\ (g) + m_{NaOH}\ (g)$$
$$m_{solution}\ (g) = 50.0\ (g) + 8.00\ (g) = 58.00\ g$$

3) Finding mass percentage of NaOH:

$$W\% = \frac{8.00\ (g)}{58.00\ (g)} \times 100 = 13.79\ \%$$

Chapter 7
Thermochemistry

Energy Changes in Chemical Reactions

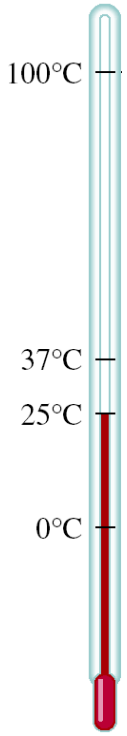
All Chemical reactions absorb or produce (release) energy in the form of heat.

- **Heat is the thermal energy transfer between two bodies at different temperatures.**

- **Temperature is a measure of the thermal energy.**

Temperature ≠ Thermal Energy

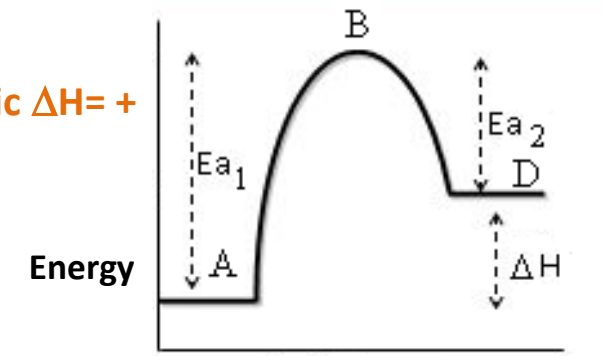
- **Thermal Energy is always transferred from a warmer to a cooler object!!**



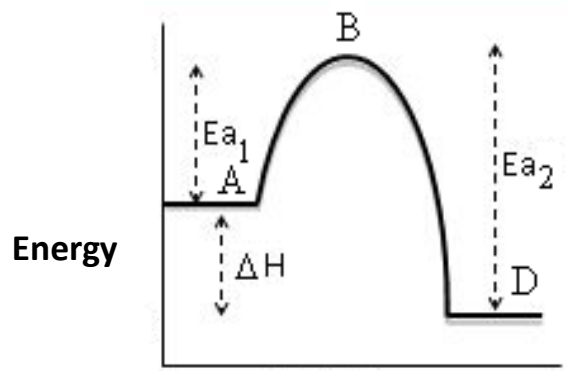
Thermochemistry studies the changes in Heat Energy within a Chemical Reaction

- Energy can be gained or lost in the form of heat during a chemical reaction
- When heat energy is gained (or absorbed), a reaction is called endothermic
- When heat energy is lost (or released), a reaction is called exothermic
- The change in heat is represented by the symbol ΔH

Endothermic ΔH= +

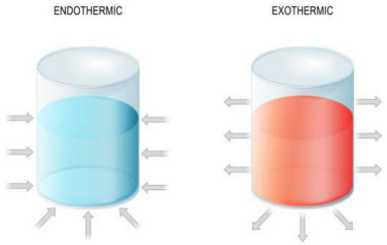


Exothermic ΔH= -



$$\text{energy} + 2HgO_{(s)} \longrightarrow 2Hg_{(L)} + O_{2(g)}$$

$$2H_{2\,(g)} + O_{2\,(g)} \longrightarrow 2H_2O_{\,(L)} + \text{energy}$$



Heat energy

Heat energy is a form of energy transferred between two (or more) systems or a system and its surroundings by the effect of temperature difference.

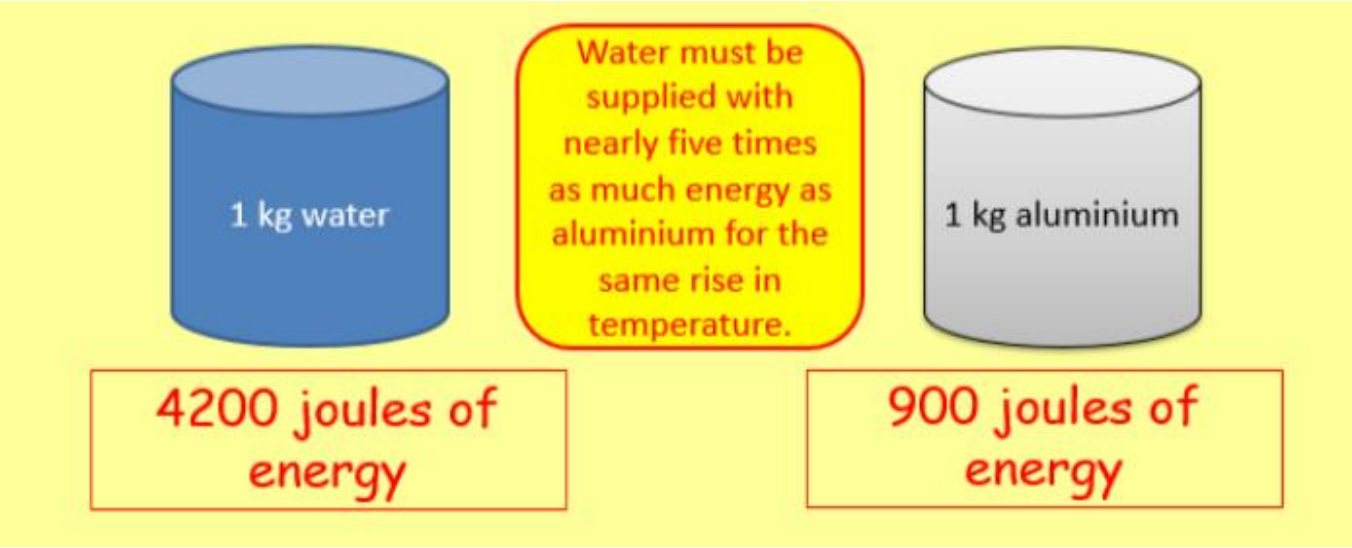
The SI unit of the heat energy transferred is expressed in joule (J), another used unit is calorie

$$1 \text{ cal} = 4.186 \text{ J}$$

Calorie: is the energy needed to raise the temperature of 1 g of water through 1 °C (now usually defined as 4.1868 joules).

Specific Heat (s)

- The specific heat of a substance is the amount of heat required to raise the temperature of 1 g of substance by 1°C.
- It is measured in J/ g °C.
- Specific heat of water = 4.2 J/g °C
- Specific heat of aluminum = 0.9 J/g °C



Heat Capacity (C)

- **The amount of heat required to raise the temperature of a given quantity of the substance by one degree Celsius or kelvin.** (J/ ^{o}C or J/K)

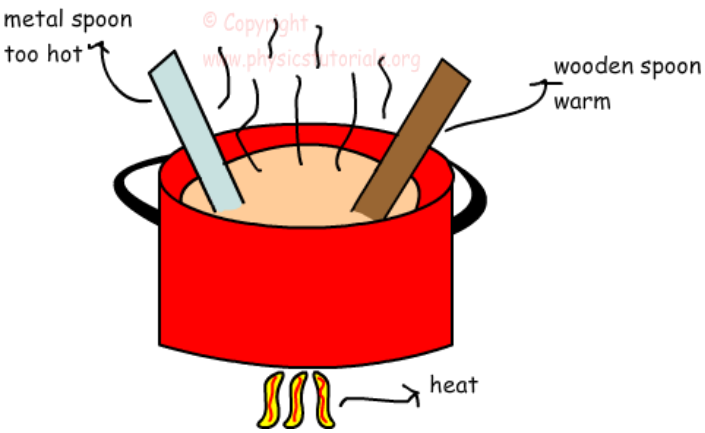
- **This value changes as the mass changes (the greater mass, the greater its heat capacity)**
- **The heat capacity (C) of a pure substance can be expressed as**

$$C = S \times m$$

C= heat capacity

S= specific heat

m= mass of an object



Specific heats of some common substances

Substance	Specific Heat (J/g.°C)
Al	0.900
Au	0.129
C (graphite)	0.720
C (diamond)	0.502
Cu	0.385
Fe	0.444
Hg	0.139
H_2O	4.184
C_2H_5OH	2.46

Heat of reaction (q)

Is the amount of heat absorbed or released by a system at a certain temperature. The relationship between q, and temperature change, Δt, is:

$$q = C \cdot \Delta t$$

- q = magnitude of heat
- C = heat capacity (J/°C)
- Δt = change in temp

For a pure substance of mass m, the expression of q can be written as

$$q = S \times m \times \Delta t$$

- q = magnitude of heat
- m = mass
- S= specific heat of substance (J/g·°C)
- Δt = change in temp

Examples

The specific heat of copper is 0.382 J/g•°C. How much heat is absorbed by a copper plate with a mass of 135.5 g to raise its temperature from 25.0°C to an oven temperature of 215°C?

q= S x m x Δt

q = (135.5 g)(0.382 J/g·°C)(215°C – 25.0 °C)

q = 9835 J

How much heat is given off by a 50.0 g sample of copper when it cools from 80.0 to 50.0°C?

q= S x m x Δt

q = (50.0 g)(0.382 J/g·°C)(50.0 °C - 80.0 °C)

q = (50.0 g)(0.382 J/g·°C)(-30.0 °C)

q = -573 J (neg. sign because heat is given off)

The temperature of a piece of copper with a mass of 95.4 g increases from 25.0 °C to 48.0 °C when the metal absorbs 849 J of heat. What is the specific heat of copper, C_{Cu}?

q= S x m x Δt

849 J = (95.4 g)(C_{Cu})(48.0 °C - 25.0 °C)

C_{Cu}= (849 J) / (95.4 g)(23.0°C)

C_{Cu} = 0.387 J/g•°C

Enthalpy of Chemical Reactions

For any reaction of the type

Reactants ⟶ products

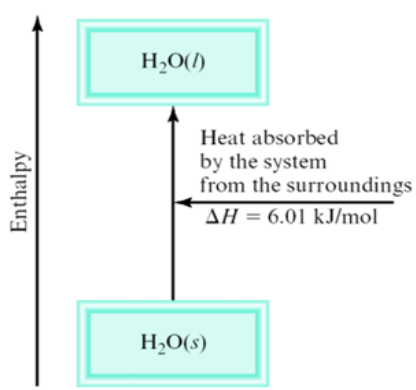
Enthalpy of reaction, ΔH, is the difference between the enthalpies of the products and the enthalpies of the reactants:

$$\Delta H = H(\text{products}) - H(\text{reactants})$$

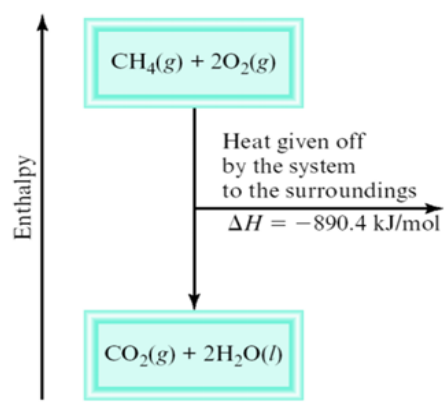
ΔH = heat released or absorbed during a reaction **at constant pressure**

- **For an endothermic process**
  ΔH is positive (that is, ΔH > 0).

- **For an *exothermic process***
  ΔH is negative (that is, $\Delta H < 0$).

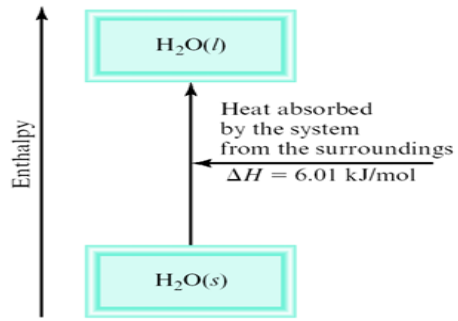


$H_{\text{products}} > H_{\text{reactants}}$



$H_{\text{products}} < H_{\text{reactants}}$

Thermochemical equations show the enthalpy changes as well as the mass relationships.



Is ΔH negative or positive?

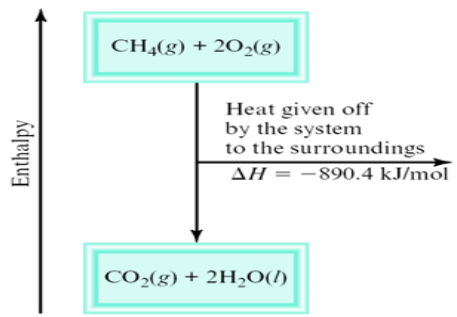
System absorbs heat

So, it is Endothermic

$\Delta H > 0$

6.01 kJ are absorbed for every 1 mole of ice melts at 0^{0}C and 1 atm.

$$H_2O\ (s) \longrightarrow H_2O\ (l) \qquad \Delta H = 6.01\ \text{kJ/mol}$$



Is ΔH negative or positive?

System gives off heat

So, it is Exothermic

$\Delta H < 0$

890.4 kJ are released for every 1 mole of methane that is combusted at 25^{0}C and 1 atm.

$$CH_{4(g)} + 2O_{2(g)} \longrightarrow CO_{2\ (g)} + 2H_2O_{(l)} \qquad \Delta H = -890.4\ \text{kJ/mol}$$

- **The stoichiometric coefficients always refer to the number of moles of a substance**

$$H_2O\ (s) \longrightarrow H_2O\ (l) \qquad \Delta H = 6.01\ \text{kJ/mol}$$

- **If you reverse a reaction, the sign of ΔH changes**

$$H_2O\ (l) \longrightarrow H_2O\ (s) \qquad \Delta H = -6.01\ \text{kJ/mol}$$

- **If you multiply both sides of the equation by a factor *n*, then ΔH must change by the same factor *n*.**

$$2H_2O\ (s) \longrightarrow 2H_2O\ (l) \qquad \Delta H = 2 \times 6.01 = 12.0\ \text{kJ}$$

Standard enthalpy of formation (ΔH_f^0) is the heat change that results when one mole of a compound is formed from its elements at STP. (1 atm, and 25°C)

The standard enthalpy of formation of any **element in its most stable form is zero.**

$\Delta H_f^0\ (O_2) = 0$

$\Delta H_f^0\ (C, \text{graphite}) = 0$

$\Delta H_f^0\ (O_3) = 142\text{kJ/mol}$

$\Delta H_f^0\ (C, \text{diamond}) = 1.90\ \text{kJ/mol}$

TABLE 6.4 Standard Enthalpies of Formation of Some Inorganic Substances at 25°C

Substance	ΔH_f°(kJ/mol)	Substance	ΔH_f°(kJ/mol)
$Ag(s)$	0	$H_2O_2(l)$	−187.6
$AgCl(s)$	−127.0	$Hg(l)$	0
$Al(s)$	0	$I_2(s)$	0
$Al_2O_3(s)$	−1669.8	$HI(g)$	25.9
$Br_2(l)$	0	$Mg(s)$	0
$HBr(g)$	−36.2	$MgO(s)$	−601.8
C(graphite)	0	$MgCO_3(s)$	−1112.9
C(diamond)	1.90	$N_2(g)$	0
$CO(g)$	−110.5	$NH_3(g)$	−46.3
$CO_2(g)$	−393.5	$NO(g)$	90.4
$Ca(s)$	0	$NO_2(g)$	33.85
$CaO(s)$	−635.6	$N_2O(g)$	81.56
$CaCO_3(s)$	−1206.9	$N_2O_4(g)$	9.66
$Cl_2(g)$	0	$O(g)$	249.4
$HCl(g)$	−92.3	$O_2(g)$	0
$Cu(s)$	0	$O_3(g)$	142.2
$CuO(s)$	−155.2	S(rhombic)	0
$F_2(g)$	0	S(monoclinic)	0.30
$HF(g)$	−271.6	$SO_2(g)$	−296.1
$H(g)$	218.2	$SO_3(g)$	−395.2
$H_2(g)$	0	$H_2S(g)$	−20.15
$H_2O(g)$	−241.8	$Zn(s)$	0
$H_2O(l)$	−285.8	$ZnO(s)$	−348.0

Problem:

Calculate the heat of combustion of methanol, ΔH^o_{rxn} for

$$CH_3OH(g) + 3/2\ O_2(g) \rightarrow CO_2(g) + 2\ H_2O(g)$$

$\Delta H_f^o CH_3OH$ = -238.6 KJ/mol

$\Delta H_f^o CO_2$ = -393.5

$\Delta H_f^o O_2$ = 0 KJ/mol

$\Delta H_f^o H_2O$ = -285.8

$$\Delta H^o_{rxn} = H^o_{f(products)} - H^o_{f(reactants)}$$

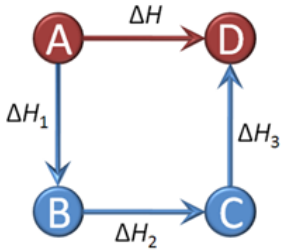
$$= [-393.5 + 2(-285.8)] - [-238.6 + 0]$$

$$= -726.5 \text{ KJ/mol}$$

(Hess's Law)

- **Many compounds cannot be directly synthesized from their elements.**
- **The reaction proceeds too slowly, or side reactions produce substances other than the desired compound.**

Hess's Law: **When reactants are converted to products, the change in enthalpy is the same whether the reaction takes place in one step or in a series of steps.**



$$\Delta H_4 = \Delta H_1 + \Delta H_2 + \Delta H_3$$

Calculate the enthalpy for this reaction

$2C(s) + H_2(g) \text{ ---> } C_2H_2(g)$	$\Delta H° = ???$ kJ

Given the following thermochemical equations:

$C_2H_2(g) + (5/2)O_2(g) \text{ ---> } 2CO_2(g) + H_2O(\ell)$	$\Delta H° = -1299.5$ kJ
$C(s) + O_2(g) \text{ ---> } CO_2(g)$	$\Delta H° = -393.5$ kJ
$H_2(g) + (1/2)O_2(g) \text{ ---> } H_2O(\ell)$	$\Delta H° = -285.8$ kJ

Solution:

1) Determine what must be done to the given equations to get the target equation:

a) first eq: flip it to have C_2H_2 on the product side

b) second eq: multiply it by two to get 2C

c) third eq: do nothing. We need one H_2 on the reactant side and that's what we have.

$2CO_2(g) + H_2O(\ell) \text{ ---> } C_2H_2(g) + (5/2)O_2(g)$ $\Delta H° = +1299.5$ kJ

$2C(s) + 2O_2(g) \text{ ---> } 2CO_2(g)$ $\Delta H° = -787.0$ kJ

$H_2(g) + (1/2)O_2(g) \text{ ---> } H_2O(\ell)$ $\Delta H° = -285.8$ kJ

Notice that the **ΔH values changed as well**

Add up ΔH values for our answer:

+1299.5 kJ + (-787 kJ) + (-285.8 kJ) = **+226.7 kJ**

The formation of CO_2 takes place in one step and produces the following energy

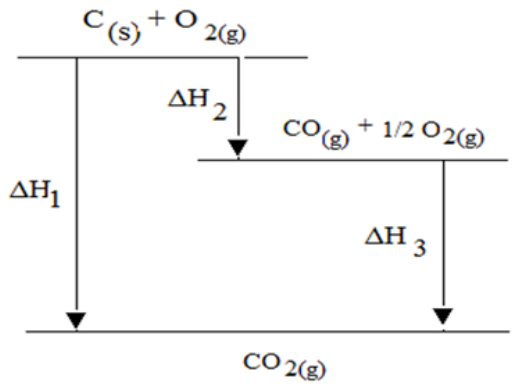
$$C_{(s)} + O_{2(g)} \rightarrow CO_{2(g)} \qquad \Delta H_1 = -393 \text{ kJ}$$

It can also be done in two steps and produce the same energy:

$$C_{(s)} + \frac{1}{2} O_{2(g)} \rightarrow CO_{(g)} \qquad \Delta H_2 = -110 \text{ kJ}$$

$$CO_{(g)} + \frac{1}{2} O_{2(g)} \rightarrow CO_{2(g)} \qquad \Delta H_3 = -283 \text{ kJ}$$

We note that ΔH1 = ΔH2 + ΔH3



An example of the importance of Hess's law

Graphite (C graphite) and diamond (C diamond) are the allotropes of carbon, and it has been found that graphite is the most stable form under normal atmospheric pressure.

$$\text{C(diamond)} \xrightarrow{\text{millions of years}} \text{C(graphite)}$$

Practically, it is very difficult to measure the change in enthalpy of the previous reaction, because of the time it takes. But it can be calculated by Hess's law.

We know that the change in enthalpy of each of the following two reactions can be measured separately:

1) $C(diamond) + O_{2\,(g)} \longrightarrow CO_{2\,(g)}$ $\Delta H = -395.4$ kJ

2) $C(graphite) + O_{2\,(g)} \longrightarrow CO_{2\,(g)}$ $\Delta H = -393.5$ kJ

If we <u>reverse</u> equation (2) we get

3) $CO_{2\,(g)} \longrightarrow C(graphite) + O_{2\,(g)}$ $\Delta H = +393.5$ kJ

Adding equations 1 and 3, we get the required equation

$$C(diamond) + \cancel{O_{2\,(g)}} \longrightarrow \cancel{CO_{2\,(g)}} \qquad \Delta H = -395.4 \text{ kJ}$$

$$\cancel{CO_{2\,(g)}} \longrightarrow C(graphite) + \cancel{O_{2\,(g)}} \qquad \Delta H = +393.5 \text{ kJ}$$

$$C(diamond) \longrightarrow C(graphite) \qquad \Delta H = -1.9 \text{ kJ}$$

So, the transformation of diamond into graphite occurs in an <u>exothermic</u> process

Example 2 :

$$2CO_{(g)} + O_{2(g)} \rightarrow 2CO_{2(g)} \qquad \Delta H_1 = -566\ kJ$$

$$4CO_{(g)} + 2O_{2(g)} \rightarrow 4CO_{2(g)} \qquad \Delta H_2 = -1132 kJ$$

Note that the second reaction is the same as the first multiplied by 2 so:

$$\Delta H_2 = 2x\ \Delta H_1$$

$$\Delta H_2 = 2 \text{ x } -566 = -1132 \text{ kJ}$$

Example 3 :

Calculate the energy of the following reaction:

$$2S_{(S)} + 3O_{2\,(g)} \longrightarrow 2SO_{3\,(g)} \qquad \Delta H = ?$$

Knowing that:

1) $S(s) + O_2\,(g) \longrightarrow SO_2\,(g) \qquad \Delta H = -297$ kJ

2) $2SO_3\,(g) \longrightarrow 2SO_2\,(g) + O_2\,(g) \qquad \Delta H = -198$ kJ

Solution:

To get the first reaction, we must combine the previous two reactions after making the following changes:

a) We multiply the first reaction by 2
b) Reverse the second reaction

$$2S(s) + 2O_2\,(g) \longrightarrow 2\cancel{SO_2}\,(g) \qquad \Delta H = 2\,(-297)\ kJ$$

$$2\cancel{SO_2}\,(g) + O_2\,(g) \longrightarrow 2SO_3\,(g) \qquad \Delta H = +198\ kJ$$

$$2S\,(s) + 3O_2\,(g) \longrightarrow 2SO_3\,(g) \qquad \Delta H = -396\ kJ$$

Chapter 8
Gaseous state

NEOM GREEN HYDROGEN COMPANY

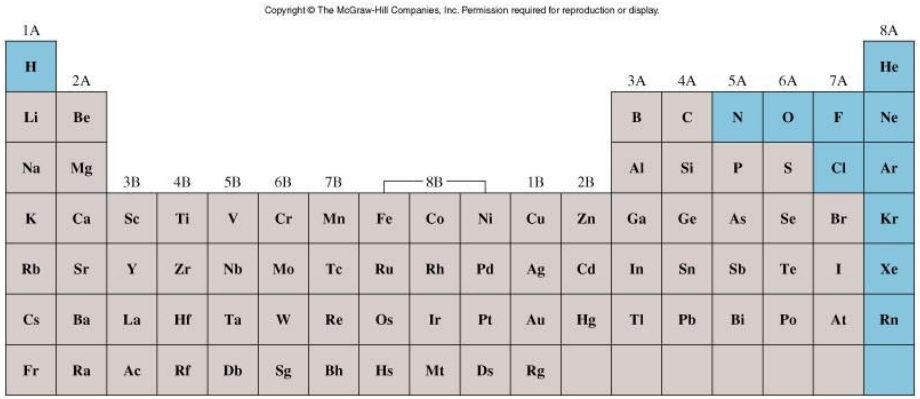
شركة نيوم للهيدروجين الأخضر

Gases

Gases :have indefinite volume and no fixed shape

1-Substances that exist as Gases in the periodic table at 25 °C and 1 atm. (blue boxes) are:

- **Noble gases are monoatomic, e.g., He, Ne, Ar.**
- **Other gases are diatomic, e.g., H_2, N_2, O_2**



Physical Characteristics of Gases

- **Gases assume the volume and shape of their containers.**
- **Gases are the most compressible state of matter.**
- **Gases have much lower densities than liquids and solids.**

2- Pressure of the Gas

- **Gas is in constant motion → gas exert a pressure on the wall of the container.**
- **Pascal (Pa) is the SI unit of pressure.**
- **Other units for pressure are: atmosphere (atm), millimetre of mercury (mmHg), Torr (torr) etc.**

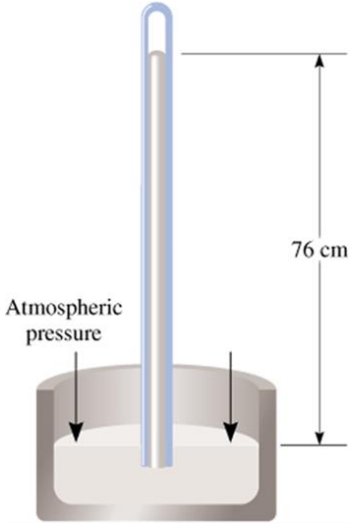
Atmospheric pressure

The pressure that supports a column of mercury exactly 760 mm high at 0 °C at sea level.

Standard atmospheric pressure (1 atm)

A Barometer:

A device that can weigh the atmosphere above us!



Barometer

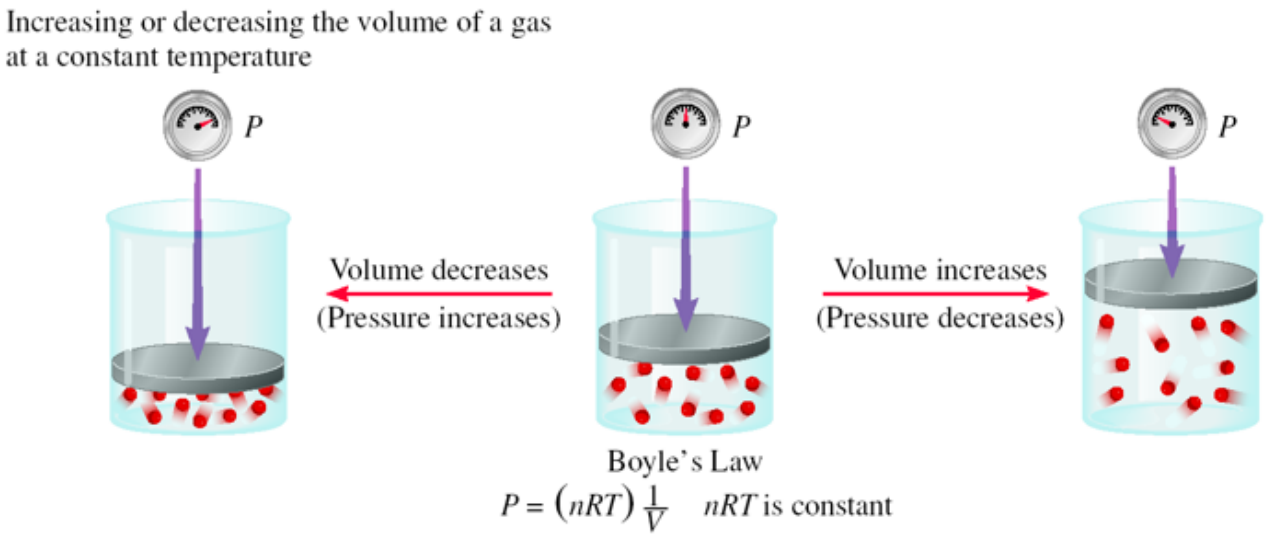
- **1 torr= 1mmHg**
- **1 atm= 760 mmHg**
- **1 atm= 1.01×10^2 kPa**
- **1 atm= 1.01×10^5 Pa**

3- The Gas Laws :

- **Any gas has a pressure P, Volume V, temperature T, and amount (number of moles) n.**
- **Scientists study the relationship between these factors by using several gas laws**

Pressure-Volume Relationship: Boyle's Law

Boyle's Law states that: the pressure of a fixed amount of gas (n is constant) at a constant temperature is inversely proportional to the volume of the gas.



Boyle's Law:

At constant T & n : $P_1V_1 = P_2V_2$

Example

A sample of chlorine gas occupies a volume of 946 mL at a pressure of 726 mmHg. What is the pressure of the gas (in mmHg) if the volume is reduced at constant temperature to 154 mL?

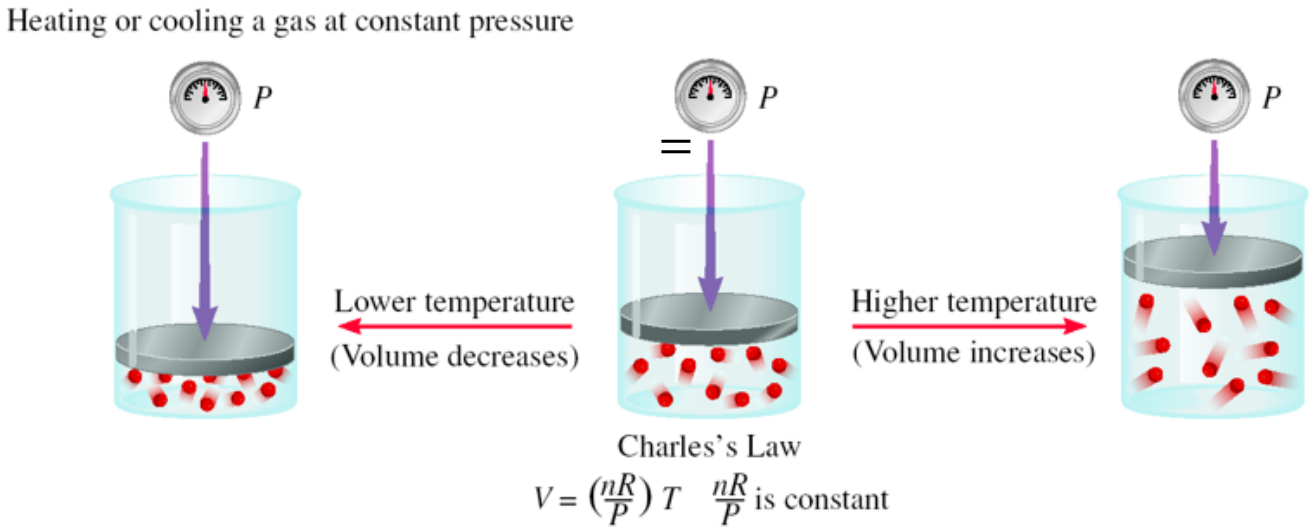
P_1 = 726 mmHg; V_1 = 946 mL P_2 = ? ; V_2 = 154 mL

Boyle's Law: $P_1 V_1 = P_2 V_2$

$$P_2 = \frac{P_1V_1}{V_2} = \frac{726 \text{ mmHg x } 946 \text{ mL}}{154 \text{ mL}} = 4460 \text{ mmHg}$$

Temperature-Volume Relationship: Charles's and Gay-Lussac's Law

- **Charles's and Gay-Lussac's Law states that:** the volume of a fixed amount of gas (n is constant) at a constant pressure is directly proportional to the *absolute temperature* of the gas.



Charles's Law:

At constant P & n : $\frac{V_1}{T_1} = \frac{V_2}{T_2}$

Example

A sample of carbon monoxide gas occupies 3.20 L at 125 °C. At what temperature will the gas occupy a volume of 1.54 L if the pressure remains constant?

$V_1 = 3.20$ L; $T_1 = 125\ ^\circ C \rightarrow K$; $T_1 = 125 + 273.15 = 398.15$ K

$V_2 = 1.54$ L ; $T_2 = ?$

Charles's Law: $V_1T_2 = V_2T_1$

$$T_2 = \frac{V_2T_1}{V_1} = \frac{1.54\ \text{L} \times 398.15\ \text{K}}{3.2\ \text{L}} = 192\ \text{K}$$

Example

Gas occupies 6 L at 37 °C. What will be its volume when its temperature is decreased to half if the pressure remains constant?

V_1=6L , T_1=37 °C

V_2=??? , T_2=½ T_1

$$V_1T_2=V_2T_1$$

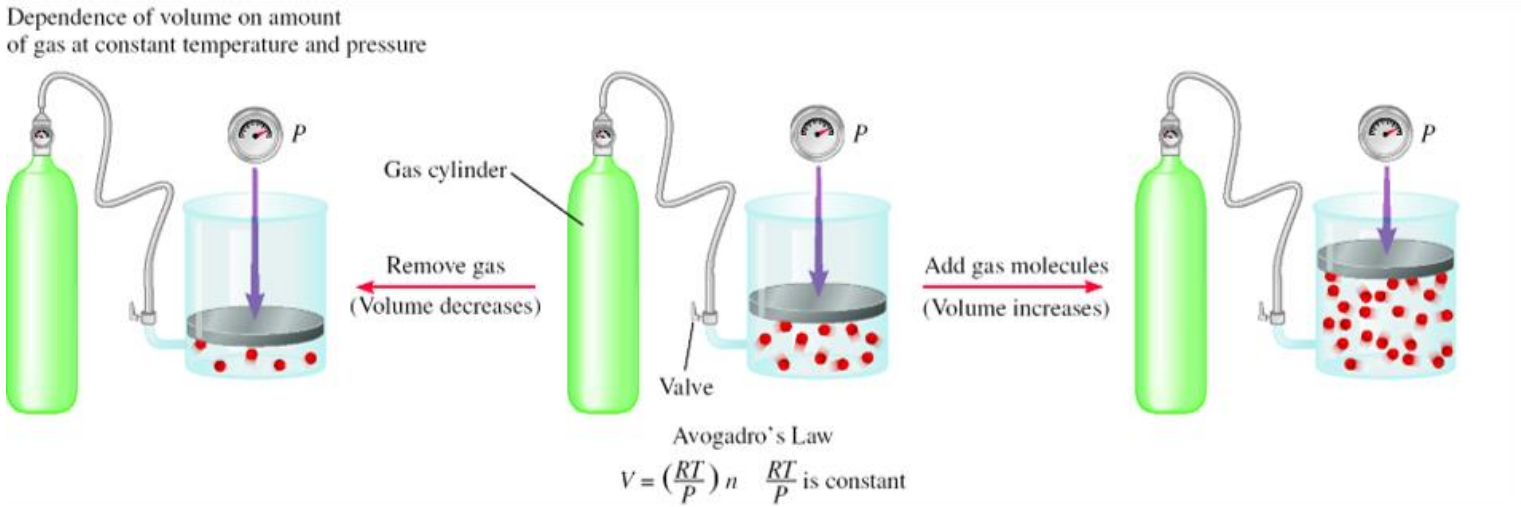
$$V_1\tfrac{1}{2}T_1=V_2T_1$$

$$V_2 = \tfrac{1}{2}V_1$$

$$V_2 = \tfrac{1}{2}(6) = 3L$$

Amount-Volume relationship: Avogadro's Law

- **Avogadro's Law states that:** at constant pressure and temperature, the volume is directly proportional to the number of moles of the gas.



Avogadro's Law:

At constant T & P : $\frac{V_1}{n1} = \frac{V_2}{n_2}$

Example

2 moles of gas occupy 6 L. what will be the volume of 7 moles at constant temperature and at constant pressure ?

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

$$\frac{6}{2} = \frac{V_2}{7}$$

$$V_2 = \frac{6x7}{2} = 21\ L$$

The Ideal Gas Equation

Ideal Gas Equation $PV = nRT$

P = pressure atm , V = volume in Liters n = moles T = temperature in Kelvin R = gas constant

- **The value of *R* that you use is based on your units of pressure:**

R=0.08206 $\frac{L.atm}{mol.K}$ **or R= 62.4** $\frac{L.mmHg}{mol.K}$ **or R=8.314** $\frac{L.KPa}{mol.K}$

- **STP: Standard pressure and temperature condition**

  Standard temperature 0 °C = 273.15 K Standard pressure 1 atm

- **FACT:** One mole of any gas at the STP condition will occupy a volume equal to 22.41 L.

Examples

Calculate the pressure (in atm) exerted by 1.82 moles of the sulphur hexafluoride in a steel vessel of volume 5.43 L at 69.5 °C.

Given: n = 1.82 mol; V = 5.43 L; T =69.5 + 273.15 = 342.65 K ;

R = 0.0821 L.atm/mol.K

Find: P ? → PV = nRT (ideal gas equation)

$$P = \frac{nRT}{V} = \frac{1.82\ \text{mol} \times 0.0821\ \frac{\text{L.atm}}{\text{mol.K}} \times 342.65\ \text{K}}{5.43\ \text{L}} = 9.42\ \text{atm}$$

What is the volume of 2 mol O_2 gas at STP?

$$PV = nRT$$

$$V = nRT/P$$

$$V = 2 \times 0.0821 \times 273 / 1$$

$$V = 44.85\ \text{L}$$

What is the volume of 2 g O_2 gas at 4 atm and 35 °C?

$$PV = nRT$$

$$V = nRT/P$$

$$T = 35 + 273 = 308\ \text{K}$$

$$V = 2 \times 0.0821 \times 308 / 32 \times 4$$

$$V = 0.395\ \text{L}$$

Calculate the volume (in liters) occupied by 7.40 g of NH_3 at STP .

Given: m = 7.40 g → n; P = 1 atm; T = 273.15 K;

R = 0.0821 L.atm/mol.K

Find: V ?

Method (1): PV = nRT

$$n = \frac{m}{Mw} = \frac{7.4\ g}{17\ g/mol} = 0.435\ mol$$

$$V = \frac{nRT}{P} = \frac{0.435\ mol \times 0.0821\ \frac{L.atm}{mol.K} \times 273.15\ K}{1\ atm} = 9.74\ L$$

Method (2):

$$n = \frac{m}{MM} = \frac{7.4\ g}{17\ g/mol} = 0.435\ mol$$

1 mol NH_3 → 22.4 L

0.435 mol NH_3 → ? L

$$V = \frac{0.435\ mol \times 22.4\ L}{1\ mol} = 9.74\ L$$

Combined Gas Law

- **The ideal gas equation is useful if we have only one condition, i.e., only one P, one V, one T, and one n. Thus, knowing three of them → calculate the fourth**
- **The modified ideal gas equation (combined gas law) combines Boyle's law, Charles's law, and Gay-Lussac's law.**

$$\frac{P_1V_1}{n_1T_1} = \frac{P_2V_2}{n_2T_2}$$

Constant n & T →

$$P_1V_1 = P_2V_2$$

Boyle's law

Constant n & P →

$$\frac{V_1}{T_1} = \frac{V_2}{T_2} \Rightarrow V_1T_2 = V_2T_1$$

Charles's law

Constant P & T →

$$\frac{V_1}{n_1} = \frac{V_2}{n_2} \Rightarrow V_1n_2 = V_2n_1$$

Avogadro's law

Example

A small bubble rises from the bottom of a lake, where the temperature and pressure are 8 °C and 6.4 atm, to the water surface, where the temperature and pressure are 25 °C and 1 atm. Calculate the final volume (in mL) of the bubble if its initial volume was 2.1 mL.

Given: T_1 = 8 °C = 281 K; P_1 = 6.4 atm; V_1 = 2.1 mL; P_2 = 1 atm; T_2 = 25 °C = 298K; Assume $n_1 = n_2$

Find: V_2 (in mL)?

$$\frac{P_1V_1}{n_1T_1} = \frac{P_2V_2}{n_2T_2} \quad , \quad \because n_1 = n_2 \quad \therefore \quad \frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2}$$

$$V_2 = \frac{P_1V_1T_2}{P_2T_1} = \frac{6.4 \text{ atm x } 2.1 \text{ mL x } 298 \text{ K}}{1 \text{ atm x } 281\ K} = 14 \text{ mL}$$

Density of gas Calculations

If we rearrange the ideal gas equation → we can calculate the density of the gas

- $PV = nRT$
- $P = \frac{n}{V} RT$
- $\frac{n}{V} = \frac{P}{RT}$

$$\because n = \frac{m}{Mw}$$

$$\therefore \frac{m}{V \times Mw} = \frac{P}{RT}$$

$$\frac{m}{V} = \frac{P \times Mw}{RT} \quad , \quad \because d = \frac{m}{V}$$

$$\therefore d = \frac{P \times Mw}{RT}$$

Example

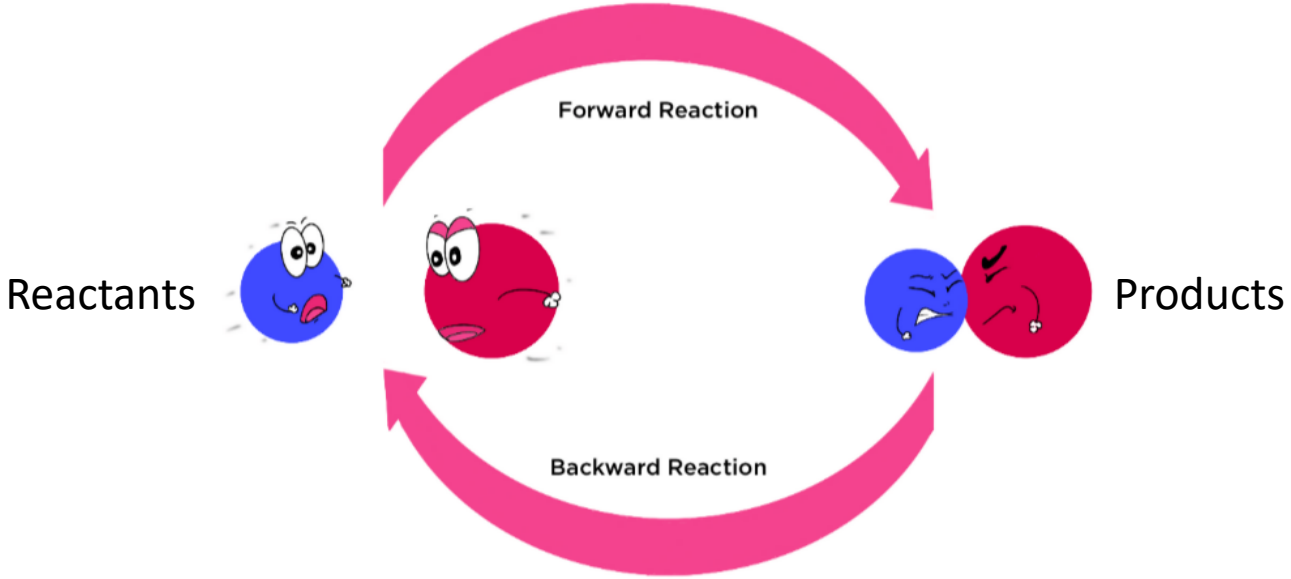
Calculate the density of CO_2 in g/L at 0.990 atm and 55 ˚C.

Given: P = 0.990 atm; T = 55 ˚C + 273 = 328 K

Find: d (in g/L) ??

$$d = \frac{P\ xMw}{R\ T} = \frac{0.99\ atm\ x\ 44.01\ g/mol}{0.0821\ \frac{L.atm}{mol.K}\ x\ 328\ K} = 1.62\ g/L$$

Chapter 9
Chemical Equilibrium



Types of chemical reactions:

Chemical reactions may be completed (irreversible), and all reactants are converted to the product.

and some are not; these reactions are called reversible reactions (the reactants are not completely converted to products, the products may react with each other and produce reactants again).

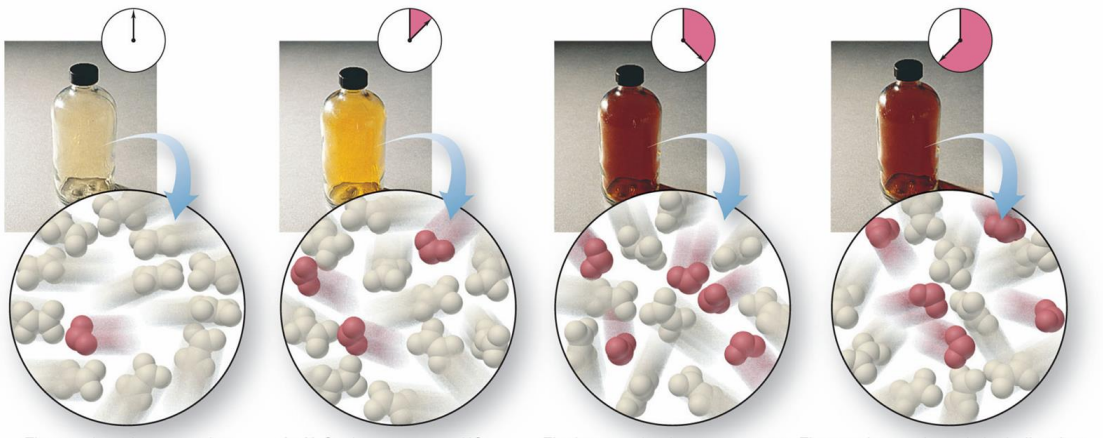
Reactions are reversible and, under suitable conditions, will reach a state of equilibrium.

At equilibrium, the concentrations of products and reactants no longer change because the rates of the forward and reverse reactions are equal.

At equilibrium: $rate_{forward} = rate_{reverse}$

Reaching equilibrium on the macroscopic and molecular levels.

$$N_2O_4(g) \rightleftharpoons 2NO_2(g)$$



The reaction mixture consists mostly of colorless N_2O_4.

As N_2O_4 decomposes to NO_2, the mixture becomes pale brown.

The brown color deepens as more N_2O_4 decomposes and NO_2 is produced, until the color reaches a maximum at equilibrium.

The reaction continues in both directions at equal rates, so the concentrations of NO_2 and N_2O_4, and therefore the color, no longer change.

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The Equilibrium Constant

Consider the reaction $N_2O_4(g) \rightleftharpoons 2NO_2(g)$

At equilibrium $rate_{fwd} = rate_{rev}$

The reaction rate is equal to the product of the concentrations (raised to the appropriate exponents) multiplied by the reaction rate constant:

so $k_{fwd}[N_2O_4]_{eq} = k_{rev}[NO_2]^2_{eq}$

then $\frac{k_{fwd}}{k_{rev}} = \frac{[NO_2]^2_{eq}}{[N_2O_4]_{eq}}$

The ratio of constants gives a new constant, the equilibrium constant:

$$\boxed{K = \frac{k_{fwd}}{k_{rev}} = \frac{[NO_2]^2_{eq}}{[N_2O_4]_{eq}}}$$

From the equation:

[ ] is the molarity concentration

A ***small*** value for *K* indicates that the reaction yields little product before reaching equilibrium. The reaction favors the ***reactants***.

A ***large*** value for *K* indicates that the reaction reaches equilibrium with very little reactant remaining. The reaction favors the ***products***.

Write the equilibrium constant for the following reactions:

(a) $2\,O_3(g) \rightleftharpoons 3\,O_2(g)$

(b) $2\,NO(g) + Cl_2(g) \rightleftharpoons 2\,NOCl(g)$

The answers:

(a)Kc = $\frac{[O_2]^3}{[O_2]^2}$ (b)Kc = $\frac{[NOCl]^2}{[NO]^2 . [Cl_2]}$

K for heterogeneous equilibrium

A heterogeneous equilibrium involves reactants and/or products in different phases.

$$CaCO_3(s) \rightleftharpoons CaO(s) + CO_2(g)$$

A pure solid or liquid always has the same concentration (the same number of moles) per liter of solid or liquid. Pure solids and liquids are omitted from the expression for K.

So, the equilibrium constant can be written as:

$$K_c = [CO_2]$$

Write the equilibrium constant for the following reaction:

$$Na(s) + H_2O(l) \rightleftharpoons NaOH(aq) + H_2(g)$$

The answer:

$$K_c = [NaOH]^2[H_2]$$

Expressing Equilibria with Pressure Terms K_c and K_p

K for a reaction may be expressed using partial pressures of gaseous reactants instead of molarity.
The partial pressure of each gas is directly proportional to its molarity.

$$2NO(g) + O_2(g) \rightleftharpoons 2NO_2(g)$$

If we have an ideal gas, then
PV= nRT $\longrightarrow$ P = [gas]RT

C = n/V = P/RT

$$K_p = \frac{P^2_{NO_2}}{P^2_{NO} \times P_{O_2}} \qquad K_C = \frac{[NO_2]^2}{[NO]^2\,[O_2]}$$

$$K_p = K_c\,(RT)^{\Delta n(gas)}$$

If the amount (mol) of gas does not change in the reaction, $\Delta n_{gas} = 0$ and Kp = Kc.

Example 1:

In the following reactions, the concentrations of [CO]=0.012M, $[Cl_2]$=0.054 and $[COCl_2]$=0.14M. Find the Kc and Kp for this reaction. If you know R=0.0821, T= 74 °C

$$CO\ (g) + Cl_2\ (g) \rightleftharpoons COCl_2\ (g)$$

The answer:

$$CO\ (g) + Cl_2\ (g) \rightleftharpoons COCl_2\ (g)$$

$$K_c = \frac{[COCl_2]}{[CO][Cl_2]} = \frac{0.14}{0.012 \times 0.054} = 220$$

$$\boxed{K_p = K_c(RT)^{\Delta n}}$$

$\Delta n = 1 - 2 = -1$ $\quad R = 0.0821$ $\quad T = 273 + 74 = 347$ K

$$K_p = 220 \times (0.0821 \times 347)^{-1} = 7.7$$

Example 2:

Consider the following reaction:

$$SO_2(g) + NO_2(g) \rightleftharpoons NO(g) + SO_3(g)$$

If the K_c of this equilibrium reaction is 85.0 at 733 K, what is the K_p of this reaction?

$$Kp = Kc\,(RT)^{\Delta n}$$

$$\Delta n = 2-2=0$$

$$Kp = 85.0\,(0.0821 \times 733)^0$$

$$Kp = 85.0$$

Le Châtelier's Principle

When a chemical system at equilibrium is disturbed, it reattains equilibrium by undergoing a ***net reaction*** that ***reduces*** the effect of the disturbance.

A system is disturbed when a change in conditions forces it temporarily out of equilibrium.

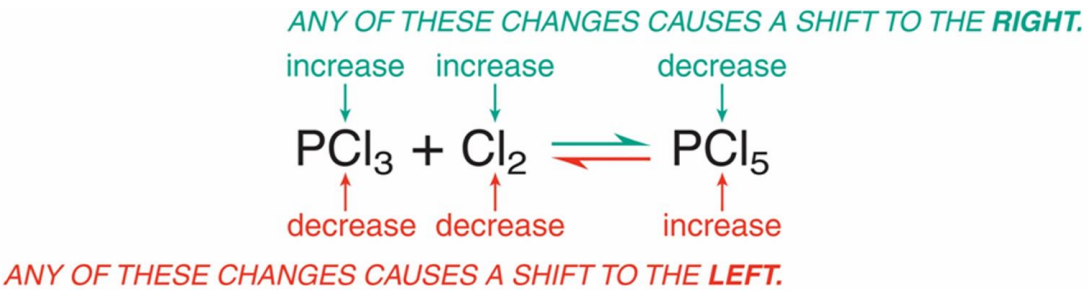
The system responds to a disturbance by a ***shift*** in the equilibrium ***position***.

A shift ***to the left*** is a net reaction from product to reactant.

A shift ***to the right*** is a net reaction from reactant to product.

The Effect of a Change in Concentration

- system will shift away from the added component or towards a removed component
- a change in conc. of a pure solid or liquid does not cause an equil. shift
- Ex: $N_2 + 3H_2 \rightarrow 2NH_3$
  - if more N_2 is added, then equilibrium position shifts to the right
  - if some NH_3 is removed, then equilibrium position shifts to the right



PROBLEM: To improve air quality and obtain a useful product, chemists often remove sulfur from coal and natural gas by treating the contaminant hydrogen sulfide with O_2:

$$2H_2S(g) + O_2(g) \rightleftharpoons 2S(s) + 2H_2O(g)$$

What happens

(a) if O_2 is added? **(b)** if sulfur is added?

SOLUTION:

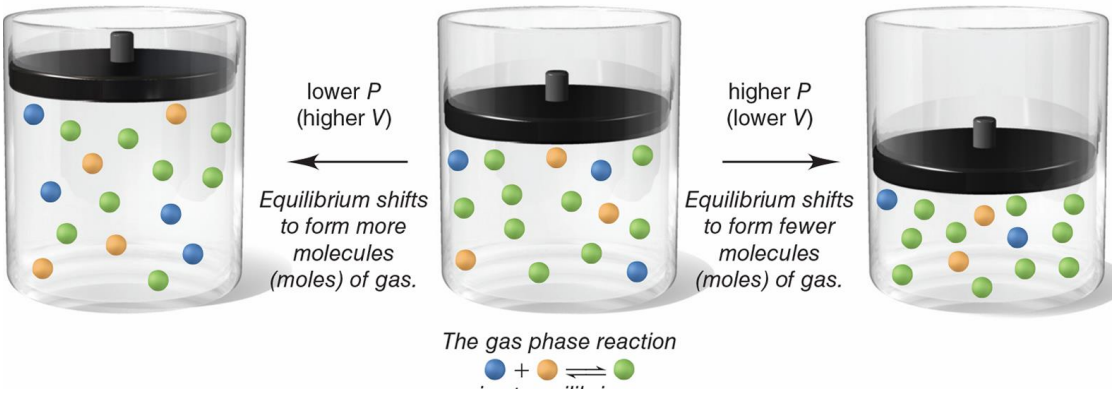
(a) When O_2 is added, the reaction proceeds to the right

(b) When Sulfur is added, the reaction proceeds to the left

The Effect of a Change in Pressure (Volume)

Changes in pressure affect equilibrium systems containing gaseous components.

- **Increase in total pressure :** shift of the equilibrium in the direction of a reduction in the number of moles of gaseous compounds.
- **Decrease in total pressure :** shift of the equilibrium in the direction of an increase in the number of moles of gaseous compounds.



PROBLEM: How would you change the volume of each of the following reactions to *increase* the yield of the products?

(a) $CaCO_3(s) \rightleftharpoons CaO(s) + CO_2(g)$

(b) $S(s) + 3F_2(g) \rightleftharpoons SF_6(g)$

(c) $Cl_2(g) + I_2(g) \rightleftharpoons 2ICl(g)$

SOLUTION:

(a) CO_2 is the only gas present. To increase its yield, we should **increase the volume** (decrease the pressure).

(b) There are more moles of gaseous reactants than products ($\Delta n_{gas} > 0$), so we should **decrease the volume** (increase the pressure) to shift the equilibrium to the right.

(c) The number of moles of gas is the same in both the reactants and the products ($\Delta n_{gas} = 0$); therefore **a change in volume will have no effect**.

The Effect of a Change in Temperature

To determine the effect of a change in temperature on equilibrium, heat is considered a component of the system.

Heat is a ***product*** in an ***exothermic*** reaction ($\Delta H < 0$).
Heat is a ***reactant*** in an ***endothermic*** reaction ($\Delta H > 0$).

An ***increase*** in temperature ***adds*** heat, which favors the ***endothermic*** reaction.

A ***decrease*** in temperature ***removes*** heat, which favors the ***exothermic*** reaction.

PROBLEM: How does an *increase* in temperature affect the equilibrium concentration of the underlined substance and *K* for each of the following reactions?

(a) $CaO(s) + H_2O(l) \rightleftharpoons \underline{Ca(OH)_2}(aq)$ $\Delta H^\circ = -82$ kJ

(b) $CaCO_3(s) \rightleftharpoons CaO(s) + \underline{CO_2}(g)$ $\Delta H^\circ = 178$ kJ

(c) $\underline{SO_2}(g) \rightleftharpoons S(s) + O_2(g)$ $\Delta H^\circ = 297$ kJ

SOLUTION:

(a) $CaO(s) + H_2O(l) \rightleftharpoons \underline{Ca(OH)_2}(aq)$ + heat

Because the reaction is Exothermic, the increase in temperature will shift the reaction to the left, so **$[Ca(OH)_2]$ and *K* will decrease.**

(b) $CaCO_3(s)$ + heat $\rightleftharpoons CaO(s) + \underline{CO_2}(g)$

Because the reaction is Endothermic, the increase in temperature will shift the reaction to the right, so **$[CO_2]$ and *K* will increase.**

(c) $\underline{SO_2}(g)$ + heat $\rightleftharpoons S(s) + O_2(g)$

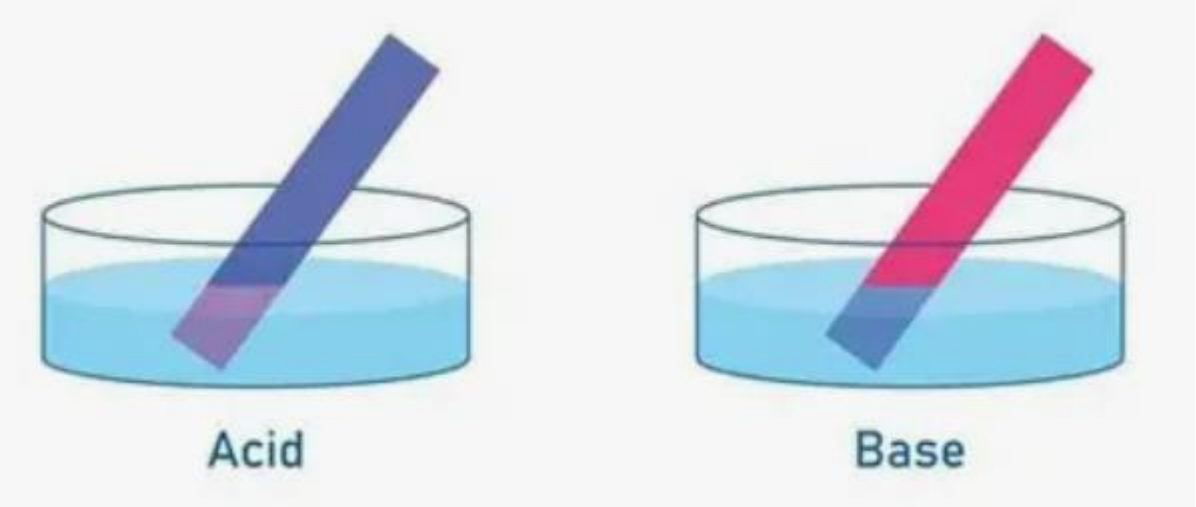
Because the reaction is Endothermic, the increase in temperature will shift the reaction to the right, so **$[SO_2]$ will decrease and *K* will increase**.

Catalysts and Equilibrium

A catalyst speeds up a reaction by lowering its activation energy. A catalyst therefore speeds up the forward and reverse reactions to the same extent.

A catalyst causes a reaction to reach equilibrium more quickly, but has ***no effect*** on the equilibrium position.

Chapter 10
Ionic Equilibrium



Ionic Equilibrium

Ionic equilibria: The equilibrium between ions and unionized molecules in the solutions is called as ionic Equilibria.

Unionized molecule $\rightleftharpoons$ Ions

Ionic equilibria

$$CH_3COOH\ (aq) \leftrightharpoons H^+\ (aq) + CH_3COO^-\ (aq)$$

Dissociation is a chemical reaction in which a molecule or compound breaks into smaller pieces, such as ions, atoms, or radicals.

Electrolyte and Nonelectrolyte Solutions

Electrolytes are chemical compounds that can break down into ions when dissolved in water. These ions can conduct electricity through this aqueous solution.

$NaCl(s) \rightarrow Na^+(aq) + Cl^-(aq)$

Nonelectrolytes are chemical compounds whose aqueous solutions cannot conduct electricity through the solution.

C_2H_5OH - ethyl alcohol
$C_6H_{12}O_6$ - glucose

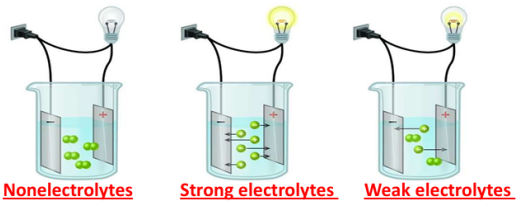
Electrolytes

Strong electrolytes are compounds that can completely dissociate into its ions when dissolved in water.

Ex: strong acids, strong bases, ionic salts
- HCl (hydrochloric acid)
- NaOH (sodium hydroxide)
- NaCl, $MgCl_2$

Weak electrolytes are compounds that partially dissociate into its ions when dissolved in water.

Ex: weak acids, weak bases
- CH_3COOH - acetic acid
- NH_3 - ammonia
- H_2O - water



Acids & Bases

Acids	Molecular formula
hydrochloric acid	HCl
Nitric Acid	HNO_3
sulfuric acid	H_2SO_4
Sulfurous Acid	H_2SO_3
Carbonic Acid	H_2CO_3
Phosphoric Acid	H_3PO_4

Bases	Molecular formula
Sodium Hydroxide	$NaOH$
Potassium Hydroxide	KOH
Ammonium Hydroxide	NH_4OH
Aluminum Hydroxide	$Al(OH)_3$
ammonia	NH_3
Lithium Hydroxide	$LiOH$

ACIDS	BASES
Acids are sour in taste.	They are bitter in taste.
Acids change the color of litmus from blue to red.	Bases change the color of litmus from red to blue.
They produce H^+ ions when mixed with water. $HCl + H_2O \longrightarrow H^+ + Cl^-$	These substances release hydroxide ions (OH^- ions) when dissolved in water. $NaOH \longrightarrow Na^+ + OH^-$
Acids and bases react to form salt and water. $HCl + NaOH \longrightarrow NaCl + H_2O$	Acids and bases react to form salt and water. $HCl + NaOH \longrightarrow NaCl + H_2O$
Acids react with carbonates and hydrogen carbonates to form a salt, water, and carbon dioxide gas. $HCl + Na_2CO_3 \longrightarrow 2NaCl + H_2O + CO_2$	Bases don't react with metal carbonates because metal carbonates have basic nature.
Acids tend to evolve hydrogen gas whilst reacting with an active metal such as Zn, Mg, etc. $H_2SO_4 + Zn \longrightarrow ZnSO_4 + H_2$	Alkalis (bases that are soluble in water) react with metals to produce salt and hydrogen gas. $2\,NaOH + Zn \longrightarrow Na_2ZnO_2 + H_2$

Various theory for Acids and Bases

- **Arrhenius theory**
- **Bronsted Lowry Theory**
- **Lewis theory**

Three theories used to explain acids and bases

Arrhenius theory

Acid

Substance which gives **H^+** ions in aqueous solution and combined with H_2O to forms ion(**H_3O^+**).

Ex:-

$HCl \xrightarrow{H_2O} \mathbf{H_3O^+} + Cl^-$

$HNO_3 \xrightarrow{H_2O} \mathbf{H_3O^+} + NO_3^-$

$CH_3COOH \xrightarrow{H_2O} \mathbf{H_3O^+} + CH_3COO^-$

Base

Substance which gives **OH^-** ions in aqueous solution.

Ex:-

$NaOH \xrightarrow{H_2O} Na^+ + \mathbf{OH^-}$

$Ca(OH)_2 \xrightarrow{H_2O} Ca^{2+} + 2\mathbf{OH^-}$

$NH_3 + H_2O \longrightarrow NH^{+4} + \mathbf{OH^-}$

Bronsted- Lowry theory

Acid

Substance which donate H^+ ion to other substance.

Base

Substance which accept H^+ ion from other substance

$$HCl + NH_3 \longrightarrow Cl^- + NH_4^+$$

donates H^+ ion — accepts H^+ ion — conjugate Base — conjugate Acid

Conjugate Base The base which is produced, when acid donates H^+ ion is called as Conjugated base.

Conjugate Acid The acid which is produced, when base accept H^+ ion is called as Conjugated Acid.

Acid	$-H^+$ →	Conjugated Base
Base	$+H^+$ →	Conjugated Acid

Lewis theory

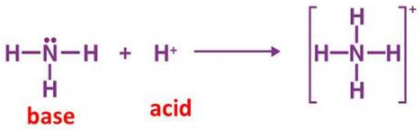
Acid

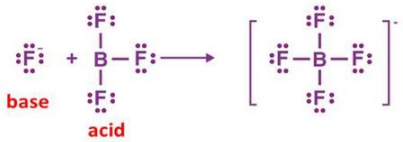
The species which accept shared electron pair.

Base

The species which donate shared electron pair.

Ex,





Dissociation of strong acid	Dissociation of strong base
Strong acids, like HCl, almost 100% dissociate into ions when they dissolve in water. For exampleHCl,HNO_3, H_2SO_4	Strong bases almost %100 dissociate into ions when dissolved in water. For example, NaOH,KOH.
$HCl + H_2O \rightleftharpoons H^+(aq) + Cl^-(aq)$ 0% 100%	$NaOH + H_2O \rightleftharpoons Na^+(aq) + OH^-(aq)$ 0% 100%
Dissociation of weak acid	**Dissociation of weak base**
Weak acids dissolve in water but partially dissociate into ions. For example, CH_3COOH, HF, HCOOH.	Weak bases partially dissociate into ions when dissolved in water. For example , $Fe(OH)_3$, $Cu(OH)_2$
$CH_3COOH + H_2O \rightleftharpoons H^+(aq) + CH_3COO^-(aq)$ approx 99% approx 1% Ka = Dissociation constant of acid	$NH_3 + H_2O \rightleftharpoons NH_4^+(aq) + OH^-(aq)$ > 99% < 1% Kb = Dissociation Constant of Base

Dissociation of Water

Water partially dissociates into ions according to the equation: $H_2O \rightleftharpoons H^+ + OH^-$

This dissociation can be expressed according to the equilibrium law:

$$K = \frac{[H^+][OH^-]}{[H_2O]}$$

$$K[H_2O] = [H^+][OH^-]$$

However, the concentration of water is in huge excess and effectively remains constant (to a very close approximation), as only a tiny fraction of the molecules break apart. The $[H_2O]$ term can be removed and a new constant, Kw, defined.

$$K_W = [H^+][OH^-]$$

The constant Kw, sometimes called the ionic product of water remains unchanged at constant temperature

$$K_W = [H^+][OH^-] = 1x\ 10^{-14}$$

$$[H^+] = 1 \times 10^{-7}\ M$$

$$[OH^-] = 1 \times 10^{-7}\ M$$

Types of solution

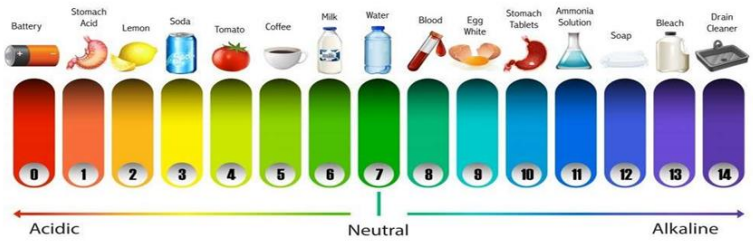
Acidic Solution	Neutral solution	Basic Solution
pH<7	pH=7	pH>7
$[H^+]>10^{-7}$	$[H^+]=[OH^-]=10^{-7}$	$[H^+]<10^{-7}$

Acidic solutions have a higher H^+ concentration than water (greater than 1×10^{-7}M), while basic (alkaline) solutions have a lower H^+ concentration (less than 1×10^{-7}M).

Typically, the hydrogen ion concentration of a solution is expressed in terms of pH.

pH scale

pH is a measure of how acidic/basic water is



acidic	neutral	basic
$[H^+] > [OH^-]$	$[H^+] = [OH^-]$	$[H^+] < [OH^-]$
$[H^+] > 1 \times 10^{-7}$	$[H^+] = 1 \times 10^{-7}$	$[H^+] < 1 \times 10^{-7}$
pH < 7	pH = 7	pH > 7

pH is really a measure of the relative amount of free hydrogen and hydroxyl ions in the water.
Water that has more free hydrogen ions is acidic, whereas water that has more free hydroxyl ions is basic.

pH is calculated as the negative log of a solution's hydrogen ion concentration:

$$pH = -\log [H^+]$$

The pOH is then calculated using the expression

$$pOH = -\log [OH^-]$$

Relationship Between pH and pOH

The pH and pOH of a water solution at 25°C are related by the following equation

$$pOH + pH = 14$$

pH can be measured using pH meter

★ What is the pH of HCl solution whose hydrogen ion concentration is 0.3 *M*?

$[H^+] = 0.3\ M$

$pH = -\log [H^+] = -\log 0.3 = 0.52$

The $[H^+]$ or $[H_3O^+]$ represent the hydrogen ion concentration

★ If the concentration of $[H_3O^+]$ in ammonia solution is 7.41×10^{-12} What is the pH?

$pH = -\log [H_3O^+]$

$pH = -\log 7.41 \times 10^{-12} = 11.13$

★ What is the pH of a 2×10^{-3} *M* HNO_3 solution?

$$HNO_3\ (aq) + H_2O\ (l) \longrightarrow H_3O^+\ (aq) + NO_3^-\ (aq)$$

$pH = -\log [H^+] = -\log [H_3O^+] = -\log(0.002) = 2.7$

★ What is the pH of a 1.8×10^{-2} *M* OH^- solution?

$pOH = -\log [OH^-] = -\log (1.8 \times 10^{-2}) = 1.74$

$pH + pOH = 14$

$pH = 14.00 - pOH = 14.00 - 1{,}74 = 12.26$

★ H^+ ion concentration of the rainwater collected in a certain day was 1.5×10^{-5} M . What is the pH of rainwater ?

$$pH = -\log [H^+]$$

$$pH = -\log 1.5 \times 10^{-5} = 4.82$$

★ The OH^- ion concentration of a blood sample is 2.5×10^{-7} *M*. What is the pH of the blood?

$$pH + pOH = 14.00$$

$$pOH = -\log [OH^-] = -\log (2.5 \times 10^{-7}) = 6.60$$

$$pH = 14.00 - pOH = 14.00 - 6.60 = 7.40$$

BUFFER SOLUTIONS

The solution which do not change its PH, when small amount of strong acid or strong base is added to it, is called as buffer solution.

Buffer solutions are used in a wide variety of chemical applications. One example of a buffer solution found in nature is blood. The normal pH of human blood is 7.4. Some people suffer from alkalosis when experiencing severe anxiety. Alkalosis is a condition in which the pH of the blood is too high. The opposite condition - a blood pH lower than 7.4 is called acidosis .

Types of Buffer solution

Acidic buffer solution is a solution which contains Weak acid + salt of weak acid

Basic buffer solution is a solution which contains Weak base + salt of weak base

Properties of Buffer

pH do not change

- By addition of strong acid or strong base
- By addition of H_2O(dilution)
- By keeping it for long time

Application of buffer

- In biochemical system
- Agriculture
- Industry
- Medicine

Buffer Solution Examples

- Acetic acid (weak acid CH_3COOH) and a salt containing its conjugate base, the acetate anion (CH_3COO-), such as sodium acetate (CH_3COONa)

CH_3COOH/ CH_3COONa

- Ammonia (weak base NH_3) and a salt containing its conjugate acid, the ammonium cation, such as Ammonium Hydroxide (NH_4OH)

NH_3 / NH_4OH