

*People's Democratic Republic of Algeria*  
*Ministry of Higher Education and Scientific Research*  
*ZIANE ACHOUR University of Djelfa*



*Faculty of Science and Technology*  
*Department: Common Core Department of state engineer (Process Engineering)*

### ***Learning course***

***Topic: Structure of matter (Chemistry of elements)***

***Level: First year Common Core- state engineer***



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*In the name of Allah, the all-merciful, the all-compassionate*

## **Introduction**

This learning course addresses the fundamental basics of the Structure of Matter (Chemistry of elements) designed for first-year students enrolled in the Common Core Department of state engineer at the Faculty of Science and Technology, and it is also relevant to students specializing in Chemical Process Engineering. The course material provides a comprehensive introduction to the fundamental principles governing the structure of matter. It covers the macroscopic and microscopic aspects of matter, including physical states, phase transitions, and essential quantitative concepts such as the mole, molar quantities, and the law of conservation of mass.

The course explores the main constituents of matter through the development of atomic theory, highlighting atomic structure, isotopes, and methods for determining atomic masses. It introduces the principles of quantum mechanics to explain the electronic structure of atoms, including wave–particle duality and atomic models.

In addition, the course examines the periodic classification of elements and the periodic trends of their physical and chemical properties. It also addresses chemical bonding, focusing on covalent bonds, molecular geometry, and the quantum description of bonding.

Finally, the course presents the fundamentals of radioactivity and nuclear reactions, including types of radiation, radioactive decay kinetics, and their scientific and technological applications.

This course aims to provide students with a solid foundation for understanding the structure and behavior of matter, preparing them for advanced studies in chemistry, physics, and related scientific fields.

The content of this topic is divided into five main chapters according to the CANVAS:

- ✓ **Chapter 1:** Fundamental Concepts
- ✓ **Chapter 2:** Main Constituents of Matter
- ✓ **Chapter 3:** Electronic Structure of the Atom
- ✓ **Chapter 4:** Periodic Classification of Elements
- ✓ **Chapter 5:** Chemical Bonding
- ✓ **Chapter 6:** Radioactivity – Nuclear Reactions

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# Chapter 01: Fundamental Concepts

## Preface

Chemistry is a scientific discipline concerned with the study and understanding of the chemical, physical, and dynamic properties of substances that constitute the matter surrounding us. A fundamental question, however, arises: where should this study begin? Addressing this question requires, as a first step, the acquisition of essential terminology and fundamental concepts that form the basis for a rigorous and systematic understanding of chemical phenomena.

### 1. Definition of matter

Matter is anything that occupies space and has mass. It is composed of atoms, which allow through multiple combinations, the formation of an unlimited number of compounds.

### 2. Matter State

Under normal conditions, there are three distinct states of matter: Solids, liquids, and gases (Figure1).

- **Solids** are relatively rigid and they have fixed shapes and volumes. For example, a rock.
- **Liquids** flow and take the shape of a container, except that it forms a flat or slightly curved upper surface when acted upon by gravity. (In zero gravity, liquids assume a spherical shape).
- **Gases** take both the shape and volume of its container. The volume of gases strongly depends on their temperature and pressure (the amount of force exerted on a given area). Whereas, the volumes of liquids and solids are virtually independent of temperature and pressure.

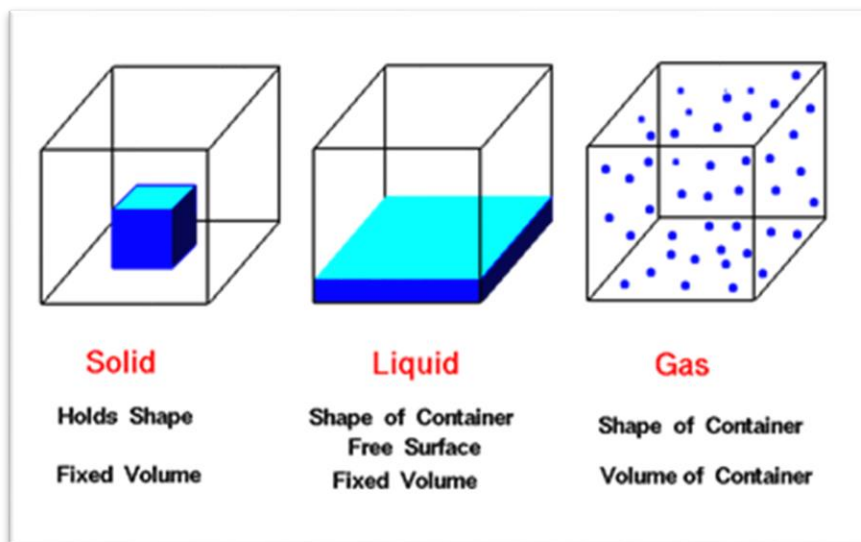


Figure I-1: The Three States of Matter.

## 2.1. Change in matter state

Matter can often change from one physical state to another in a process called a physical change. For example, liquid water heats and forms a gas called steam, and steam can be cooled to form liquid water. However, such changes of state do not affect the chemical composition of the substance.



Figure I- 2: Change in matter states

## 3. Classification of matter

### 3.1. Matter categories

Matter classifies into two broad categories:

#### 3.1.1 Pure substances

The form of pure substances is any matter that has a fixed chemical composition and characteristic properties.

- ✓ Very few samples of matter consist of pure substances; instead, most are mixtures, which are combinations of two or more pure substances in variable proportions in which the individual substances retain their identity.

#### 3.1.2 A mixture

Is a physical combination of two or more pure substances that are not chemically bonded together. Each component in the mixture retains its own chemical properties. Mixtures are generally classified into two main types:

- 1- Homogeneous mixtures:** These have a uniform composition throughout the system. The different components are not visibly distinguishable, even under a microscope. They consist of a single phase. Examples include salt dissolved in water, air, and alloys such as brass.

**2- Heterogeneous mixtures:** These have a non-uniform composition, where the different components can be clearly distinguished. They may consist of two or more phases. Examples include water and oil, sand in water, and granite.

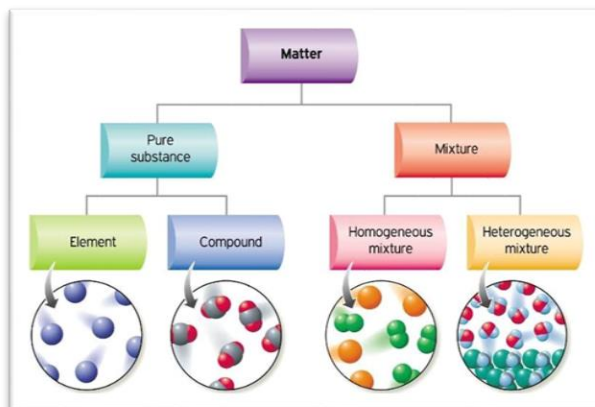


Figure I- 3: Matter categories

### 3.2. Separation of matter

The separation of heterogeneous mixtures by the action of a physical or chemical process gives homogeneous mixtures; the homogeneous can separate again to obtain pure substances.

There are several techniques for separating the constituents of a mixture into pure substances.

- ✓ First, by physical methods, which do not modify the nature of the substances.
- ✓ The second uses chemical methods, which allow the transformation of pure compound substances into simple pure bodies.

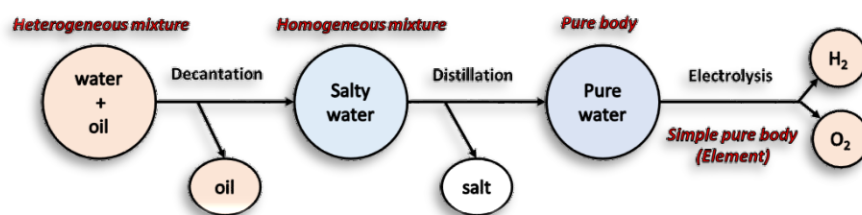


Figure I- 4: Example of mixture separation

Table 1: Separation methods of mixture

Physical separation methods				
Heterogeneous mixtures		Homogeneous mixtures		
Liquid-Liquid	Liquid-Dissolved solid	Liquid-Liquid	Liquid-Solid	Solid –Solid
<ul style="list-style-type: none"> <li>• Distillation</li> <li>• Chromatography</li> </ul>	<ul style="list-style-type: none"> <li>• Evaporation</li> <li>• Crystallization</li> <li>• Chromatography</li> </ul>	<ul style="list-style-type: none"> <li>• Decantation</li> <li>• Centrifugation</li> </ul>	<ul style="list-style-type: none"> <li>• Decantation</li> <li>• Filtration</li> <li>• Centrifugation</li> </ul>	<ul style="list-style-type: none"> <li>• Sieving</li> <li>• Magnetization</li> <li>• Sublimation</li> </ul>
Chemical separation methods				
<ul style="list-style-type: none"> <li>• Thermolysis</li> <li>• Electrolysis</li> </ul>				

## 4. Atoms concepts, Molecules, Ions, Mole and Avogadro number

### 4.1. Atoms concepts

- Matter is composed of exceedingly small particles called atoms. An atom is the smallest unit of an element that can participate in a chemical change. Atoms differ in their masses; each atom is designated by a symbol

*Example: Copper: Cu; Iron: Fe; Oxygen: O;...etc.*

- The atom is unbreakable, so in chemical reactions we do not consider the destruction of atoms. Therefore, it is important to consider the atom as being the unit in each of the elements of the periodic table.
- The atom is an infinitely small quantity of matter, its mass is  $\sim 10^{-26}$ kg, its dimension is of the order of a few Angstroms,

*Exp: the carbon atom C has a diameter d of ( $d=1.8\text{\AA}$ )*

*Note: knowing that  $1\text{\AA} = 10^{-10}\text{m}$*

- A chemical element X is a given species of atoms. It is characterized by an atomic number Z and a mass number A, is designated by an abbreviation called symbol:  $\mathbf{X}_A^Z$

*Exp: Hydrogen ( $Z=1, A=1, \text{symbol H}_1^1$ ); carbon ( $Z=6, A=12, \text{symbol C}_{12}^6$ ); Silicon ( $Z=14, A=28, \text{symbol Si}_{14}^{28}$ )*

### 4.2. Molecules

Molecules are chemical entities composed by two (or more) atoms joined to each other via chemical bond(s).

*Example: H<sub>2</sub>; HCl; H<sub>2</sub>O*

Based on the number of constituents, molecules are divided into two categories:

- **Diatomic molecules:** composed by two identical or different atoms (e.g. O<sub>2</sub>, CO<sub>2</sub>, etc.). as well, a diatomic molecule constituted of:
  - ✓ Two identical atoms is called homonuclear (e.g. H<sub>2</sub>, N<sub>2</sub>, etc.).
  - ✓ Two different atoms is called heteronuclear (e.g. NH<sub>3</sub>, CO<sub>2</sub>, etc.).
- **Polyatomic molecules:** composed by several different atoms (e.g. ICHOHCO<sub>2</sub>H, etc.).

### 4.3. Ions

Ions are electrically charged atoms, or molecules. They come from neutral atoms, or molecules, which have either lost one(s) electron(s) or gained one(s) electron(s).

Example: H<sup>+</sup>; Fe<sup>2+</sup>; O<sup>2-</sup>; NH<sub>2</sub><sup>-</sup>

It should be noted that:

- Cation is ion obtained following a loss of electron(s) (e.g.: Na → Na<sup>+</sup> + 1e<sup>-</sup>)
- Anion ion obtained following a gain of electron(s) (e.g.: Br<sup>-</sup> + 1e<sup>-</sup> → Br<sup>2-</sup>)

#### 4.4. Isotope

Isotope defined as one of two or more species of atoms of a chemical element with the same atomic number and nearly identical chemical behavior but with different atomic masses and physical properties. Every chemical element has one or more isotopes.

For example:



#### 4.5. The mole and Avogadro's number

*a- The mole, or "mol"* is a unit of measurement in chemistry, used to designate a very large number of molecules, atoms, or particles.

##### *b- Avogadro's Constant*

- The number  $6.02214179 \times 10^{23}$  is called Avogadro's number ( $N_A$ ) or Avogadro's constant, defined in the 19th century by scientist *Amedeo Avogadro*.
- The number of units in one mole of any substance is called Avogadro's number or Avogadro's constant. It is equal to  $6.022140857 \times 10^{23}$ . The units may be electrons, ions, atoms, or molecules, depending on the character of the reaction and the nature of the substance.
- Avogadro's number is fundamental to understanding both the makeup of molecules and their interactions and combinations. For example, since one atom of oxygen will combine with two atoms of hydrogen to create one molecule of water ( $H_2O$ ), one mole of oxygen ( $6.022 \times 10^{23}$  of O atoms) will combine with two moles of hydrogen ( $2 \times 6.022 \times 10^{23}$  of H atoms) to make one mole of  $H_2O$ .
- Another property of Avogadro's number is that the mass of one mole of a substance is equal to that substance's molecular weight. For example, the mean molecular weight of water is 18.015 atomic mass units (amu), so 1 mole of water weight 18.015 g. This property simplifies many chemical computations.
- Avogadro's number is typically dimensionless, but when it defines the mole, it can be expressed as  $6.022 \times 10^{23}$  elementary entities/mol. This form shows the role of Avogadro's number as a conversion factor between the number of entities and the number of moles. Therefore, given the relationship  $1 \text{ mol} = 6.022 \times 10^{23} \text{ atoms}$ , converting between moles and atoms of a substance becomes a simple dimensional analysis problem.

## 4.6. Atomic mass and Molecular molar mass

### a- Atomic mass

- Atomic mass is also known as atomic weight. Atomic mass is the weighted average mass of an atom of an element based on the relative natural abundance of that element's isotopes.
- The mass number is a count of the total number of protons and neutrons in an atom's nucleus.
- Atomic mass is the mass of a single atom, calculated by adding the mass of its protons and neutrons. It is measured in atomic mass units (amu), also called daltons (Da). For elements, atomic mass is often used interchangeably with the average atomic weight, which is the weighted average of all the naturally occurring isotopes of that element.
- There is a difference between atomic mass and mass number in Chemistry. The main difference is that the mass number is the sum of the number of protons and neutrons in the nucleus of a given atom, while the atomic mass is the weighted average mass of all the isotopes of an element, measured in atomic mass units (amu). Therefore, the mass number is always an integer, while the atomic mass is often a decimal due to the weight and natural abundance of the different isotopes.

### b- Molar mass

- Is the mass in grams of 1 mole of the substance, it is calculated by summing the atomic masses of all the atoms appearing in chemical formula

$$\text{Molar mass} = \Sigma \text{ atomic mass}$$

For example, the molar mass of NaCl can be calculated for finding the atomic mass of sodium (22.99 g/mol) and the atomic mass of chlorine (35.45 g/mol) and combining them. The molar mass of NaCl is 58.44 g/mol.

$$Mm_{NaCl} = Mm_{Na} + Mm_{Cl} = 22.99 \text{ g/mol} + 35.45 \text{ g/mol} = 58.44 \text{ g/mol}$$

- Although there is no physical way of measuring the number of moles of a compound, we can relate its mass to the number of moles by using the compound's molar mass as a direct conversion factor.
- To convert between mass and number of moles, you can use the molar mass of the substance. Then, you can use Avogadro's number to convert the number of moles to number of atoms.

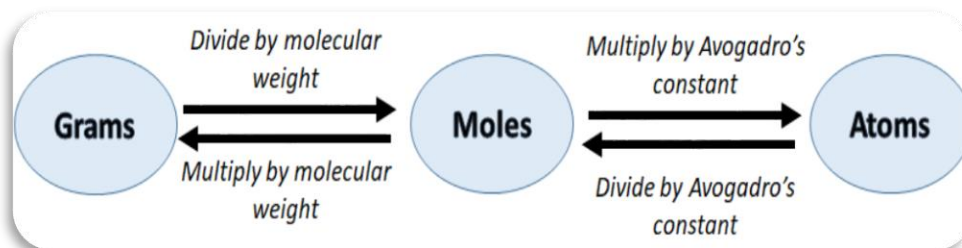


Figure I- 5: Relationship between mass (m) and atomic and molecular molar mass

## 5. The solutions

A solution is a homogeneous mixture of two or more component (called solute) dissolved in a solvent.

- Solvent is any liquid substance that has the power to dissolve other substances.
- Solute is a chemical species (molecular or ionic) dissolved in a solvent.
- This homogeneous mixture (solvent + solute) is called aqueous solution if the solvent is water.
- The solvent is always in much greater quantity than the solute(s).
- This homogeneous mixture (solvent + solute) is called aqueous solution if the solvent is water.

### 5.1. Concentration

Concentrations are quantities with units allowing the proportion of solutes to be determined in relation to that of the solvent. Depending on the nature of the unit chosen, we distinguish molarity, molality and normality.

a. **Molarity** is the number of moles of solute per liter of solution.

$$\text{molarity (mol. L}^{-1}\text{) or (M)} = \frac{\text{moles of solute (mol)}}{\text{volume of solution (litre)}}$$

b. **Molality** is the number of moles of solute per kilogram of solvent.

$$\text{molality (mol. kg}^{-1}\text{) or (M}_L\text{)} = \frac{\text{moles of solute (mol)}}{\text{volume of solution (kg)}}$$

c. **Normality** is the number of equivalents per liter of solution.

$$\text{normality (N)} = \frac{\text{nombre of gram equivalents of solute}}{\text{volume of solution (litre)}}$$

- When substances are present in trace form in a solution, it is common to use the concepts of ppm ppb and ppt.
  - Parts per million = 1 ppm = 1 mg/L
  - Part per million = 1 ppb = 0,001 mg/L
  - Parts per trillion = ppt = 1. 10<sup>-9</sup> mg/L

### 5.2. Density

Density is a substance's mass per unit of volume. The symbol most often used for density is  $\rho$

$$\text{Density } \rho \text{ (g/L)} = \frac{\text{mass of substance (gram)}}{\text{volume of solution (litre)}}$$

### 5.3.Molar fraction

Mass fraction of a constituent i “ $X_i$ ” It is defined as the ratio of the moles number (or mass) of the constituent "i" to the number of total moles (or total mass) "j" of all the constituents present in the solution. The mole fraction has no unit.

$$X_i = \frac{n_i}{\sum n_j} \text{ with } \sum X_i = 1$$

Example: If we have a solution made up of two compounds; the solute (A) and the solvent (B). So, we have:

$$X_A = \frac{n_A}{n_A + n_B} \text{ and } X_B = \frac{n_B}{n_A + n_B} \text{ with } X_A + X_B = 1$$

### 5.4.Dilution

It is often necessary to have a solution with a concentration that is very precisely known. Solutions containing a precise mass of solute in a precise volume of solution are called stock (or mother solution) solutions.

Dilution of an aqueous solution consists of reducing its concentration by adding a solvent (water).

- The initial solution of higher concentration is called the stock solution.
- The final solution of lower concentration is called dilute solution.

During the dilution, the quantity of solute material is conserved such that we can write:

$$n_i = n_f \Rightarrow C_i V_i = C_f V_f$$

Where:

*n*: quantity of material;

*V*: volume

*C*: concentration

*i*: initial, that is to say relative to the mother solution.

*f*: final, that is to say relating to the diluted solution.

- **Dilution factor denoted “F”**. It is defined as the number of times the mother solution is diluted to prepare the daughter solution.

$$F = \frac{C_i}{C_f} = \frac{V_f}{V_i}$$

## 6. The conservation of mass

- In chemical reactions, bonds between atoms are broken and reformed, but the actual atoms present stay the same. Atoms contain the mass in all matter, so the masses on each side of the reaction are always the same.
- The conservation of mass is one of the fundamental principles on which modern chemistry is based. It was discovered by the chemist Antoine Lavoisier in the 1770s. Lavoisier found that mass is conserved in a chemical reaction. The total mass of the products of a chemical reaction is always the same as the total mass of the starting materials consumed in the reaction.

### Example

We consider oxygen and hydrogen molecules combining to form water. Notice how there is no new atoms. They have just re-positioned. Thus, in a chemical reaction, new atoms are not formed, but the original atoms simply rearrange to make different molecules.

The mass of one mole of hydrogen atoms is 1.008 g, and the mass of one mole of oxygen atoms (O) is 15.999 g. Once calculated, the total mass on both sides of the equation is 36.030 g.

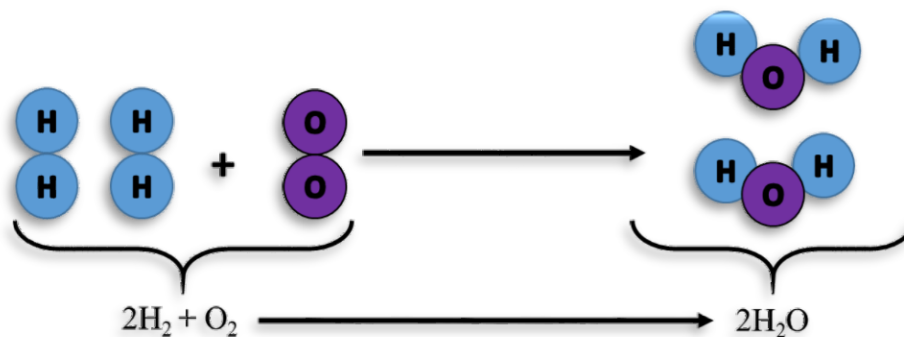


Figure I-7: Example of mass conservation in chemical reaction

## Applied exercises

### Exercise 01

We completely dissolved 1g of NaCl in 90 ml of H<sub>2</sub>O water with a density of 0.998 g/ml. We have obtained 90ml of aqueous solution of Sodium Chloride (NaCl).

1. What does mean aqueous solution?
2. What is the mass percentage of NaCl in this solution?
3. What is the Molar fraction of NaCl in this solution?
4. What is the Molality of NaCl?
5. What is the Molarity of NaCl?

**Given data:**  $M(\text{Na}): 23\text{g/mol}; M(\text{Cl}): 35.5\text{g/mol}$

### Exercise 02

A tablet of vitamin C (500) contains 500 mg of ascorbic acid (C<sub>6</sub>H<sub>8</sub>O<sub>6</sub>).

1. Calculate the molecular mass of vitamin C.
2. How much ascorbic acid material is contained in this tablet ?
3. This effervescent tablet is placed in a 12 ml glass of water .Calculate the molar concentration of the vitamin C solution.
4. How many vitamin c molecules are in this solution?
5. How many molecules of water are in this 12 ml solution?

**Given data:**  $M_C=12\text{g/mol}, M_O=16\text{g/mol}, M_H=1\text{g/mol}$

### Exercise 03

A statue weighs 6175 grams. This statue composed of a mixture based on copper, arsenic and iron, where weigh of the iron is 5 kg and the mass of copper is twice the mass of arsenic.

Calculate for each element:

1. The number of mol;
2. The number of atoms;
3. The mass percentage;
4. The number of neutrons.

**Given data:**  $N_A= 6.02 \times 10^{23} \text{ mol}^{-1}; {}^{56}_{26}\text{Fe}; {}^{63}_{29}\text{Cu}; {}^{75}_{33}\text{As}$

# Chapter 02: The Components of Matter

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## **Preface**

Matter is divisible, but there is a division limit. This limit is called an atom, which comes from the Greek name "atomos", which means indivisible. Around the 15th century, scientists began to advance their knowledge of matter and to question Aristotelian concepts of the world and matter. Robert Boyle (1627-1691), English chemist, matter was made of a few simple substances called elements.

In 1803, the British chemist J. Dalton (1766-1844) studied chemical reactions. He based his theory on the existence of small indivisible particles, atoms. Dalton's atomic theory was not immediately accepted in the scientific community. It did not arise from direct experimental observation like the previous laws; it was rather the result of logical deduction.

In this chapter, we will discuss in more detail the numerous important experiments that contributed to the development of the atomic structural theory and how they helped in the evolution of this theory. Moreover, we will highlight the constituents of matter and, therefore, of the atom, and some physical properties (mass and charge)

## 1. Faraday's Experiment: "Relationship between Matter and Electricity"

Faraday's experiments connect the concepts of electricity and electrons, though they did not directly discover the electron itself, which was later identified by J.J. Thomson. However, Faraday highlighted one of the most significant early indications in discovering the electrical nature of matter, and the relationship between matter and electricity emerged from his experimental research conducted in 1833 in the field of electrochemical analysis. Faraday observes with that the destruction of chemical bonds by electrolysis involves considerable quantities of electricity.

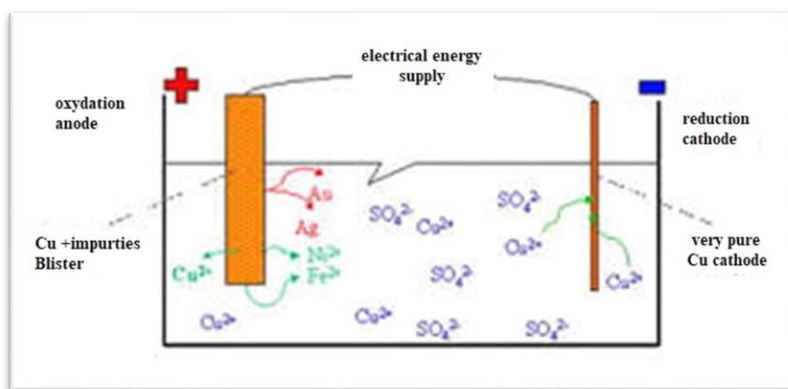


Figure II-1 : Faraday experiment concepts

- Positive Electrode = Anode
- Negative Electrode = Cathode

When passing an electric current through this solution consisting of dissolved copper sulfate in water:

- Positive ions ( $\text{Cu}^{++}$ ) move towards the negative electrode.
- Negative ions ( $\text{SO}_4^{-2}$ ) move towards the positive electrode.
- ✓ Faraday found that the weight of the substance deposited on one of the electrodes is proportional to the amount of electricity passing through the solution. –
- ✓ The product of the weights of the deposited, emitted, or dissolved substances on these electrodes in the quantity of the resulting electricity is proportional to the equivalent weights of the substances. –
- ✓ If we represent  $q$  as the amount of electricity associated with the appearance of a copper atom at the negative electrode. Therefore,  $2q$ ,  $3q$ , ...,  $nq$  represents the amount of electricity resulting from the deposition of 2, 3, ...,  $n$  copper atoms at the cathode. The emergence of these whole number quantities of electricity led scientists to assume that electricity is composed of elementary charges, and that atoms contain such charges.

***Faraday's research challenged the idea that atoms were indivisible and provided a crucial conceptual foundation for Thomson's experiments, which directly led to the identification of the electron as a particle.***

## 2. Atom structure

### 2.1. Electron

#### 2.1.1 Demonstration of Electrons

G. Stoney introduced the concept of the electron, or “atom of electricity”. The experimental demonstration and characterization of this particle came with J.J. Thomson. He proved that matter is made-up of heavy positive particles and electrons, the lighter negative particles, for which he was able to determine the charge and mass.

#### ✚ Experience of J.J. Thomson

Under the effect of very high electrical voltage (40,000 volts) applied between two internal parts of a discharge tube, a beam is emitted from the cathode, called cathode rays and collected by the anode.

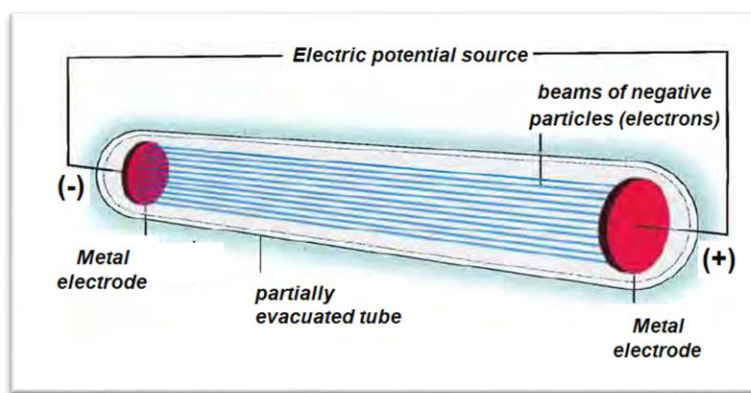


Figure II-2: J.J. Thomson experiment

#### Properties of cathode rays

- Propagate in a rectilinear manner and perpendicular to the cathode.
- They are made up of particles that transport energy.
- They are deflected by an electric field towards the positive pole, which indicates that the particles constituting these rays are negatively charged.

J.J. Thomson thus foresaw the notion of divisible atoms. To respect the classical vision of continuous matter, he proposed the "plum-pudding" model. (Figure II-3 )

He imagined that the electrons, the "plum," moved in a positively charged medium: the "pudding."

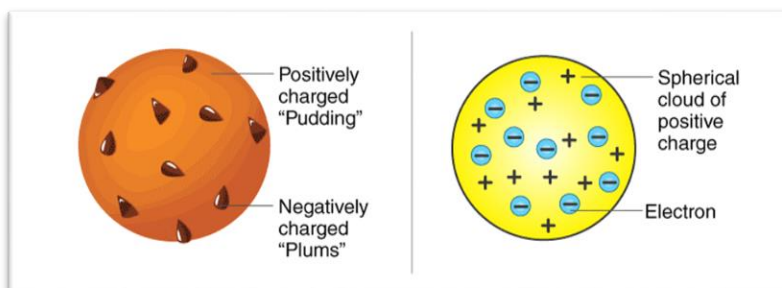


Figure II-3: J.J. Thomson model

### 2.1.2 Experience of Milliken's oil drop

Robert Milliken and Harvey Fletcher constructed the apparatus for the Oil Drop experiment in 1909. It incorporated two metal plates held at a distance by an insulated rod. There were four holes in the plate, out of which three were there to allow light to pass through them, and one was there to allow viewing through the microscope. Ordinary oil was not used for the experiment, as it would evaporate due to the heat of the light and thus could cause an error in the Millikens Oil Drop Experiment. Therefore, the oil typically used in a vacuum apparatus, which has a low vapor pressure, was employed.

#### ✚ Procedures

- Oil passes through the atomizer from where it came in the form of tiny droplets. They pass the droplets through the holes present in the upper plate of the apparatus.
- The downward motions of droplets are observed through a microscope, and the mass of oil droplets is measured, and then their terminal velocity is measured.
- The air inside the chamber is ionized by passing a beam of X-rays through it.
- The electrical charge on these oil droplets acquired by collisions with gaseous ions produced by the ionization of air.
- The electric field is set up between the two plates, and so the motion of charged oil droplets can be affected by the electric field.
- Gravity attracts the oil in a downward direction, and the electric field pushes the charge upward. The strength of the electric field is regulated so that the oil droplet reaches an equilibrium position with gravity.
- The charge over the droplet is calculated at equilibrium, which is dependent on the strength of the electric field and the mass of the droplet.

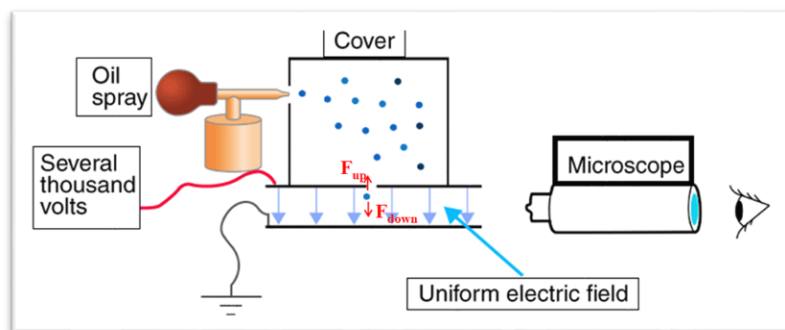


Figure II-4: Milliken's oil drop experiment

$$\left. \begin{array}{l} F_{up} = F_{down} \\ F_{up} = Q \cdot E \\ F_{down} = m \cdot g \end{array} \right\} m \cdot g = Q \cdot E \quad \rightarrow \quad Q = \frac{m \cdot g}{E}$$

Where:  $Q$ : is an electron's charge,  
 $E$ : is the electric field,  
 $m$ : is the droplet's mass,  
 $g$ : is gravity.

- The charge over any oil droplet is always a multiple integral value of  $e$ , which is the smallest electric charge that a charged oil droplet can carry.
- This is the elementary electric charge  $e$ , with  $e = 1,602 \cdot 10^{-19}$  Coulomb
- Knowing the values  $(|e|/m_e)$  and  $(e)$ , we deduce the mass of the electron:  $m_e = 9,108 \cdot 10^{-31}$  kg.

## 2.2.PROTON

### 2.2.1 Goldstein's experiment (Demonstration of the positive charge of the nucleus)

Goldstein's experiment, also known as the canal ray experiment (1886), revealed the existence of positively charged particles, protons, using a cathode ray tube. By modifying the cathode tube to drill holes in it, Goldstein observed a new type of ray passing through the holes from the anode (positively charged) to the cathode (negatively charged), thus proving the existence of a positive charge in the atom.

The principle of the experiment is based on the modification of the cathode tube by drilling holes in the cathode itself.

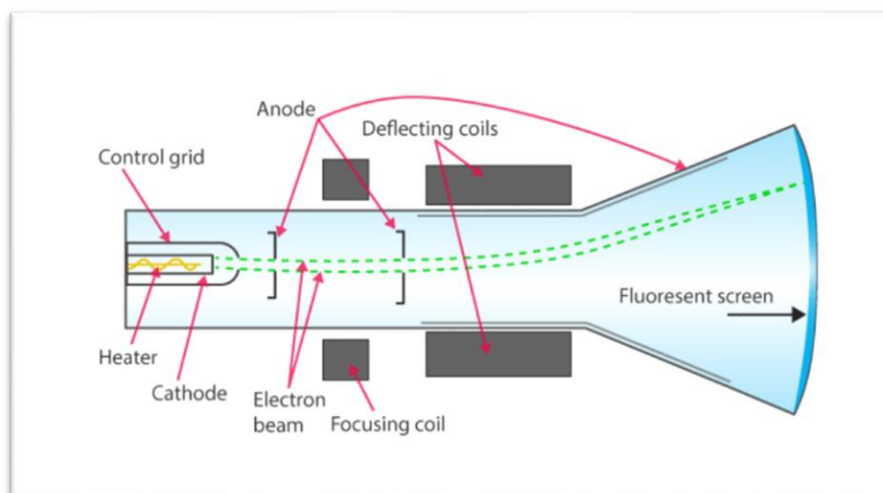


Figure II-5: Canal ray experiment

Goldstein observed the movement of electrons (cathode rays) from the cathode to the anode. Also, He observed a beam of light particles (canal rays) moving in the opposite direction, from the anode to the cathode.

These new canal rays were composed of positively charged particles, later discovered to be the proton. Thus, this experiment reinforced knowledge of atomic structure by showing that the atom contained localized positive charges.

The analysis ( $q/m$  measurement) of these protons allowed the following characteristics to be identified:

- ✓  $q = +e = 1.6022 \cdot 10^{-19} \text{ C}$
- ✓  $m_p = 1.6726 \cdot 10^{-27} \text{ kg} = 1836 \text{ .me}$

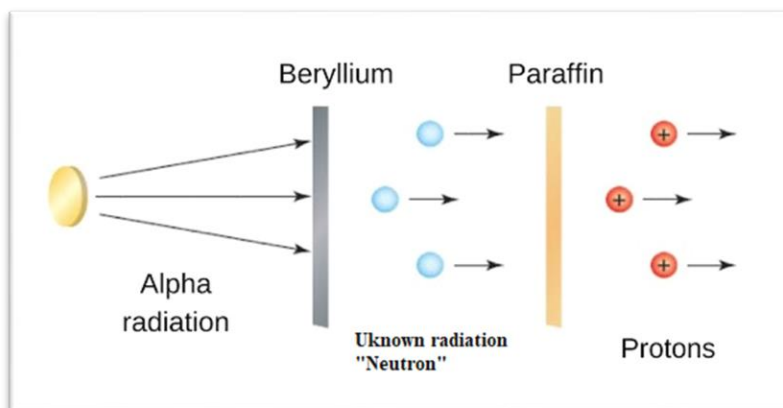
## 2.3.NEUTRON

### 2.3.1 Chadwick's experiment (neutron proof).

The British physicist Sir James Chadwick discovered neutrons in the year 1932. He was awarded the Nobel Prize in Physics in the year 1935 for this discovery.

Chadwick fired alpha radiation at beryllium sheet from a polonium source. This led to the production of an uncharged, penetrating radiation.

- ✓ This radiation was made incident on paraffin wax, a hydrocarbon having a relatively high hydrogen content.
- ✓ The protons ejected from the paraffin wax (when struck by the uncharged radiation) were observed with the help of an ionization chamber.
- ✓ The range of the liberated protons was measured and the interaction between the uncharged radiation and the atoms of several gases was studied by Chadwick.
- ✓ He concluded that the unusually penetrating radiation consisted of uncharged particles having (approximately) the same mass as a proton. These particles were later termed 'neutrons'.



*Figure II-6: Chadwick's experiment concepts*

**NB:** It is important to note that the neutron was first theorized by Ernest Rutherford in the year 1920.

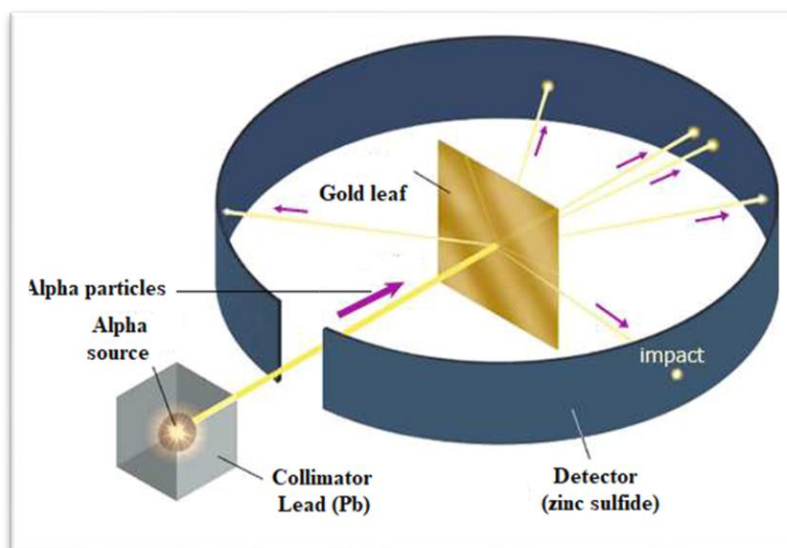
## 2.4.NUCLEUS

### 2.4.1 Rutherford Planetary Model

The Rutherford Planetary Model, proposed in 1911 by Ernest Rutherford, suggests an atom has a small, dense, positively charged nucleus at the centre, with electrons orbiting it in mostly empty space, much like planets orbiting the sun. The Rutherford-Bohr atomic model represents the atom by indicating the number of protons in the nucleus as well as the number of electrons in each of the electron shells. This model follows the Thomson atomic model (or "plum pudding model"), proposed in 1904 by Joseph John Thomson, which was invalidated following the Rutherford experiment or "gold foil experiment" in 1909. Rutherford's model was a major advance in understanding the structure of the atom.

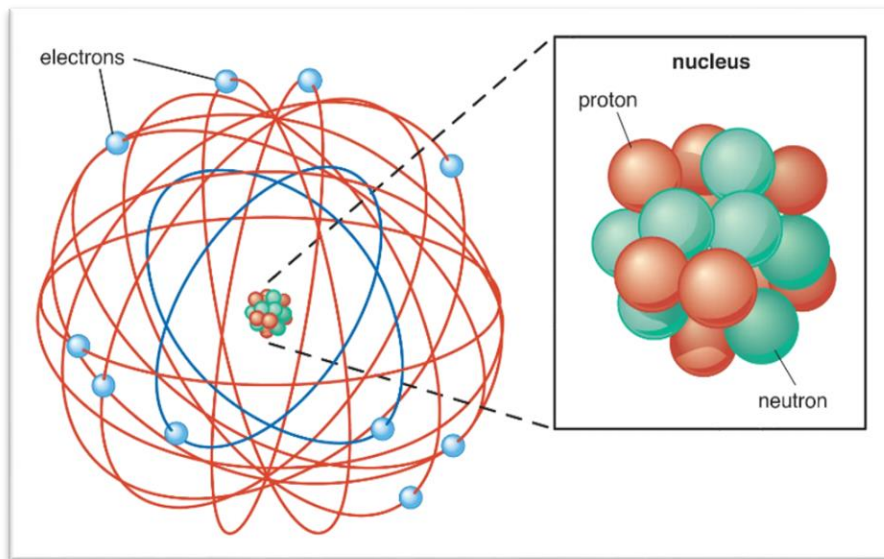
#### Experiment procedures

The experiment consists of bombarding a very thin sheet of metal (Gold) with radiation made up of Helium nuclei ( $\text{He}^{2+}$ ). Bombarding very thin gold sheets with alpha particles, Hans Geiger and Ernest Marsden, the students of Rutherford, observed that a tiny fraction (1 in 8000) of these particles were deflected at a wide angle as if they were bouncing off an obstacle massive. The impacts were observed in the dark under a microscope on a glittering zinc sulphid screen. Rutherford concluded that the atom contained a massive core, with a positive electrical charge, capable of repelling alpha.



*Figure II-7: Rutherford's experiment*

The experiment results led Rutherford to conclude that atoms are not primarily composed of empty space, but rather that the positive charge is concentrated in a small, dense nucleus at the center of the atom, and most of the space in an atom is actually empty. In other words, Rutherford deduced that the atom consists of a positively charged nucleus, around which negatively charged electrons move and remain within a sphere. The nucleus is 10<sup>4</sup> to 10<sup>5</sup> times smaller than the atom and concentrates most of its mass.



*Figure II-8: Rutherford's atom model.*

According to Rutherford, all atoms are composed of a positively charged central nucleus. The core contains two types of ingredient particles:

- Positively charged protons (+):  $q_p = +e = 1.602 \times 10^{-19} \text{ C}$

The mass of the proton:  $m_p = 1.673 \times 10^{-27} \text{ kg} \approx 1836 \text{ me}$

- Neutrons, which are neutral. It's mass:  $m_n = 1,675 \times 10^{-27} \text{ kg}$ .

The atom mass is concentrated in the nucleus.

### 3. Presentation of an atom

#### 3.1 Definition

An atom is the smallest particle of matter that possesses the chemical properties of an element. It consists of a central nucleus containing protons and neutrons, and electrons orbiting the nucleus. In an atom, there are as many positively charged protons as negatively charged electrons: an atom is electrically neutral. The number of protons is the atomic number  $Z$ . The sum of the protons and neutrons is the mass number  $A$ . An atom contains three basic particles namely protons, neutrons and electrons. The nucleus of the atom contains protons and neutrons where protons are positively charged and neutrons are neutral. The electrons are located at the outermost regions called the electron orbits.

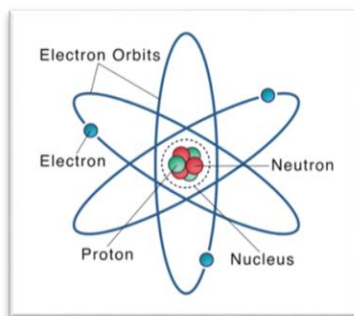


Figure II-9: Structure of atom

In fact, the atom does not often exist in a free state; it combines with others to form molecules.

For example:

- Monatomics (noble gases) He, Ne, Ar
- Diatomic  $H_2$ ,  $O_2$ , NaCl
- Polyatomic  $H_2O$ ,  $H_2SO$

#### 3.2 Nomenclature

An atom is made up of three types of subatomic particles: protons, neutrons, and electrons. The number of protons in an atom's nucleus determines its atomic number, which is used to identify the chemical element to which the atom belongs. We associate a symbol with each chemical element 'X'. It is written in capital letters, for example: hydrogen 'H', oxygen 'O' and carbon 'C'.... or followed by a lower case, for example: chlorine 'Cl', calcium 'Ca', copper 'Cu'...

*The element is represented by:*

**A:** mass number, it designates the number of proton 'P' and neutron 'n'.

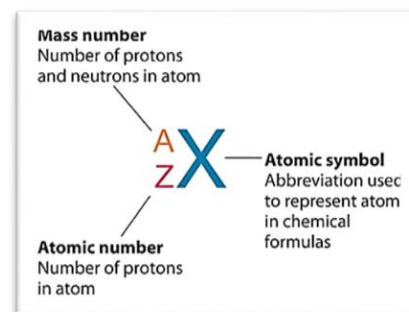
**Z:** atomic number or charge number, it designates the number of protons.

**n:** number of neutrons.

**Example:**

Hydrogen ( $Z=1$ ,  $A=1$ , symbol  $H_1^1$ ); carbon ( $Z=6$ ,  $A=12$ , symbol  $C_{12}^6$ );

Silicon ( $Z=14$ ,  $A=28$ , symbol  $Si_{14}^{28}$ )



### 3.3 Characteristics of atoms

- The proton has a charge of  $+1.60 \times 10^{-19}$  Coulombs, which corresponds to the elementary charge for a mass of  $1.673 \times 10^{-27}$  kg.
- The neutron has a zero charge for a mass of  $1.675 \times 10^{-27}$  kg.
- The nucleus has a positive charge. Neutrons and protons constitute nucleons, which are held together by the strong interaction.
- The electron has a charge of  $-1.60 \times 10^{-19}$  C. Its charge is negative and opposite that of the proton, and it has a mass of  $9.109 \times 10^{-31}$  kg. It is therefore 1,800 times lighter than the proton. The mass of an atom is therefore approximately the same as the mass of its nucleus. An atom has as many electrons as protons; its overall charge is zero.
- The atoms of an element have a characteristic average mass, which is unique to that element.
- Atoms cannot be subdivided, created or destroyed in ordinary chemical reactions. However, these changes can occur in nuclear reactions.
- Atoms of any one element differ in properties from atoms of another element.
- If the element is ionized (charged), the number of electrons is different from the number of protons.
- If the element is an anion (negative charge): we must add the charge number to the proton number.
- If the element is a cation (positive charge): we must subtract the charge number from the proton number.
- There are two types of atoms: non-isotope atoms and isotopes.

### 3.4 Isotopes

Isotopes are atoms of the same element that have the same number of protons in their nucleus, but a different number of neutrons. This means that isotopes have different atomic masses but similar chemical properties. They are therefore groups of atoms that differ only in the number of their neutrons.

**Example:** the Carbon-12 (or  $^{12}\text{C}$ ) contains six protons, six neutrons, and six electrons; therefore, it has a mass number of 12 amu (six protons and six neutrons). Carbon-14 (or  $^{14}\text{C}$ ) contains six protons, eight neutrons, and six electrons; its atomic mass is 14 amu (six protons and eight neutrons).

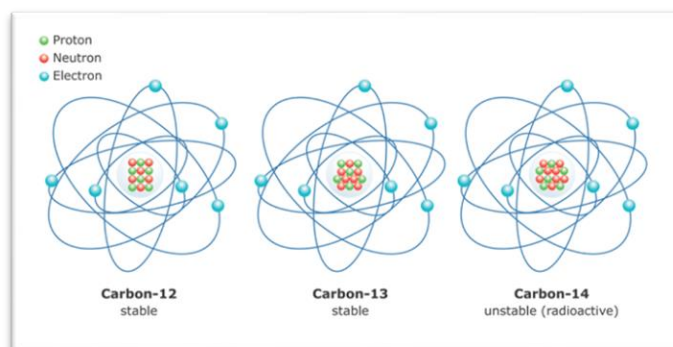


Figure II-10: Isotopes of Carbon

Isotopy is the property of different isotopes of the same element. The relative abundance of isotopes is the proportion of each isotope in a sample of an element. The relative abundance of isotopes varies depending on the element and the sample considered. For example, carbon has three naturally occurring isotopes: carbon-12, carbon-13, and carbon-14. Carbon-12 is the most abundant, representing approximately 98.9% of all carbon atoms in nature. Carbon-13 represents approximately 1.1% of all carbon atoms, and carbon-14 is extremely rare, representing only about one in a trillion carbon atoms.

This abundance is equivalent to the molar fraction of each stable isotope. As an element is made up of a mixture of various isotopes and the proportions of these various isotopes are constant, we can define for each element an average molar mass which will take into account its composition.

### 3.5 Atomic masses

The atomic mass is equal to the sum of the masses of the constituents of the atom:

$$m_a = Z \times m_e + m_N$$

*Z*: atomic number or charge number, it designates the number of protons.

$m_e$ : mass of the electron

$m_N$ : nucleus mass

$$m_N = Z \times m_p + n \times m_n$$

$m_p$ : mass of proton

*n*: number of neutrons

$m_n$ : neutron mass

#### ➤ Mass in amu (Atomic mass unit)

$$\left. \begin{array}{l} 1 \text{uma} \rightarrow 1,67 \times 10^{-27} \text{ kg} \\ x \leftarrow 1 \text{kg} \end{array} \right\} x = 6 \times 10^{+26}$$

$$\rightarrow ma = 26,7768 \times 10^{-27} \times 6 \times 10^{+26}$$

$$\rightarrow ma = 16,06 \text{ uma}$$

In the general case, an element has one or more isotopes; therefore, the atomic mass will be the sum of the proportions relating to each isotope.

$$m = \sum (X_i \times m_i) \text{ uma}$$

Likewise the molar mass will be:

$$M = \sum (X_i \times m_i) \text{ (g/mole)}$$

The atomic mass will take into account its composition; it is given by the following equation:

$$m_a = \frac{\sum (\alpha_i \times m_i)}{\sum (\alpha_i)}$$

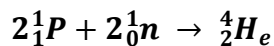
$\alpha_i$ : isotopic abundance or percentage

$m_i$ : atomic mass of isotopes

### 3.6 The cohesion of the nucleus “Stability of nuclei”

#### c. Cohesion energy

We know that in the nucleus, the positively charged protons are concentrated without repelling each other. Therefore, to understand this we need to know the nuclear binding energy.



If we consider the formation of a helium (He) nucleus from nucleons according to the above reaction:

The mass of helium based on the masses of the nuclides is:  $2 \times 1.007278 + 2 \times 1.008665 = 4.031886 \text{ uma}$ .

But the real mass of helium is equal to **4.001503 uma**.

So we have a loss of mass:

$$\Delta m = m_{\text{theoretical}} - m_{\text{real}} \rightarrow \Delta m = 4.031886 - 4.001503 = 0.030383 \text{ uma}$$

The formation of the helium nucleus is accompanied by a significant release of energy; the constituents themselves present this energy in the form of a fraction of its mass according to Einstein's relationship:

$$\Delta E = \Delta m \cdot C^2$$

Where:

C: speed of light

$\Delta E$ : this is the binding energy of the nucleus; it ensures the cohesion of the nucleus.

**NB: A system that evolves by releasing energy sees its mass decrease. Conversely, if it absorbs energy, its mass increases.**

- The equal unit of energy is the Joule (J). However, in nuclear power the most suitable unit is the electron volt (eV). This corresponds to the energy of an electron subjected to a potential difference of 1 volt.  $E = q \cdot U$

$$1 \text{ eV} = 1,602 \cdot 10^{-19} \text{ (Coulomb)} \times 1 \text{ (Volt)} = 1,602 \cdot 10^{-19} \text{ J}$$

$$1 \text{ MeV} = 10^6; \quad \text{eV} = 1,602 \cdot 10^{-13} \text{ J}$$

- We can also find that the energy corresponding to a mass of **1 u** is equal to **931.5 MeV**.

Note that this value is most often given equal to 933 MeV (in the case where rounded values are used; such as  $C = 3.108 \text{ m} \cdot \text{s}^{-1}$ ). The interest of this unit is to make the direct consistency between energy and mass.

#### d. The average energy for nuclear binding

The average energy for nuclear binding  $\Delta E_{\text{moy}}$  is the energy of an atom  $\Delta E$  divided by the number of nucleons. Nuclei that have an average binding energy per nucleon between **6** and **9 Mev** are stable; stability is greater when the average binding energy per nucleon is higher. Isotopes (elements) that have a low average binding energy per nucleon are unstable and are said to be **radioactive**.

For example, for helium nucleus:

$$\Delta E = 28.374 \text{ MeV},$$

So:

$$\Delta E_{\text{moy}} = \frac{28.374}{4} = 7.07 \text{ MeV}$$

**The main rules for identifying stable nuclei are:**

- ✓ For light nuclei ( $Z < 20$ ), stable nuclei have a number of protons equal to the number of neutrons. For heavy nuclei, more neutrons than protons are needed to neutralize the increasing repulsive forces between protons (the density of the nucleus is approximately  $10^{14} \text{ g/cm}^3$ ).
- ✓ 80% of stable nuclei have an even number of protons and 78% have an even number of neutrons.
- ✓ All elements containing more than 83 protons are radioactive, and it is possible to synthesize (artificial) radioisotopes in the laboratory that do not exist in nature.

## Applied exercises

### Exercise 01

What are the respective numbers of protons, neutrons, and electrons that make up the structure of  ${}_6^{12}\text{C}$ ,  ${}_6^{14}\text{C}$ ,  ${}_8^{16}\text{O}$ ,  ${}_8^{16}\text{O}^-$ ,  ${}_{55}^{25}\text{Mn}$ ,  ${}_{55}^{25}\text{Mn}^{2+}$ .

### Exercise 02

The bombardment of a  ${}_{92}^{235}\text{U}$  nucleus by a neutron releases three neutrons, a lanthanum  ${}_{57}^{146}\text{La}$  nucleus, and a nucleus X.

- Find the atomic number and mass number X.

### Exercise 03

The masses of the proton, neutron, and electron are respectively  $1.6723842 \times 10^{-24}$  g,  $1.6746887 \times 10^{-24}$  g, and  $9.109534 \times 10^{-28}$  g.

- 1) Define the atomic mass unit (amu). Give its value in grams with the same significant figures as the masses of particles of the same order of magnitude.
- 2) Calculate, in amu and to the nearest  $10^{-4}$ , the masses of the proton, neutron, and electron.
- 3) Calculate, using Einstein's relation (mass-energy equivalence), the energy content of one u.m.a expressed in MeV.
- 4) Calculate, using Einstein's relation (mass-energy equivalence), the energy content of one u.m.a expressed in MeV.

### Exercise 04

- 1) Calculate in amu, the theoretical mass of the nitrogen nucleus ( ${}_{7}^{14}\text{N}$ ), compare it with its real value of 14,0075 amu.
- 2) Calculate the cohesion energy of this nucleus in J and MeV.
- 3) The cohesion energy of the oxygen nucleus ( ${}_{8}^{16}\text{O}$ ) is equal to 126 MeV.
  - Calculate the mass of the oxygen core.
  - Which of the nitrogen and oxygen nuclei is the most stable?

**Given Data:**  $1\text{eV} = 1,6 \cdot 10^{-19}$  j;  $N_A = 6,022 \cdot 10^{23}$ ;  $c = 3 \cdot 10^8$  m.s<sup>-1</sup>

# Chapter 03: Electronic Structure of the Atom

## 1. Wave- Corpuscular Duality

In classical physics, we distinguish between two seemingly separate concepts: wave and particle. Particles are small "grains" of matter, localized in space and possessing defined trajectories. Throughout its trajectory, the particle's position and velocity can be known. Waves, on the other hand, are not localized. They have a spatial extent and do not have a trajectory in the strict sense; they do not transport matter but information, momentum, and energy.

Regarding light, numerous experiments demonstrate its wave-like nature: diffraction, interference. Others prove its particle behavior and consider light as a jet of particles (photons): the photoelectric effect (A. Einstein, 1921). The wave and particle aspects must then be considered complementary: light sometimes exhibits wave-like characteristics, sometimes corpuscular ones. This is referred to as Wave- Corpuscular Duality.

### 1.1 Wave nature of light: electromagnetic or light wave and electromagnetic spectrum:

Light is a progressive electromagnetic plane wave (electric field  $E^{\rightarrow}$  and magnetic field  $B^{\rightarrow}$  dependent on space and time). These vectors, themselves orthogonal, are perpendicular to the direction of propagation (Figure III-1).

Light radiation is characterized by:

- Its energy  $E$  (by joules)
- Its wavelength  $\lambda$  (by meters), or spatial period (this is the length, at a given time, after which the wave repeats itself identically).
- We also use the wave number  $\nu$  - defined by:  $\nu = 1/\lambda$  and expressed in  $m^{-1}$
- - Its period  $T$  (by seconds), or temporal period (this is the time, at a given position, after which the wave repeats itself identically). We also use the wave frequency, defined by:  $\nu = c/\lambda$  and expressed in hertz (Hz) or  $s^{-1}$  when  $T$  is expressed in seconds.

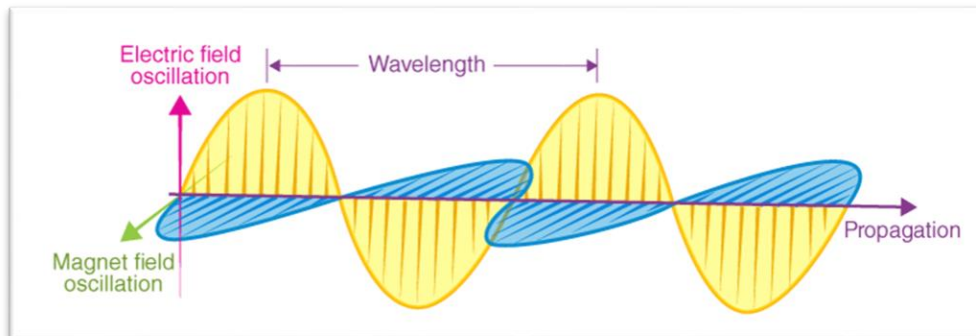


Figure III-1: perpendicular and propagation of waves

Linking the energy of a light radiation, frequency, period and wavelength can be expressed by the following relationships:

$$E = h \nu$$

Where:

$E$  is the energy expressed in joules (in J),

$\nu$  is the frequency in hertz (Hz)

$h$  is Planck's constant,  $h = 6.62 \cdot 10^{-34} \text{ J}\cdot\text{s}$ .

The distance (in meters, m) traveled by light during a period  $T$ , at speed  $c$  (the speed of light in a vacuum,  $c = 3108 \text{ m/s}$ ), is equal to the wavelength. Therefore:

$$\lambda = cT = c/\nu \text{ and consequently } E = hc/\lambda.$$

The very nature of electromagnetic radiation depends on the wavelength and thus on the energy carried. Visible radiation has a wavelength between 400 nm (blue light) and 750 nm (red light).

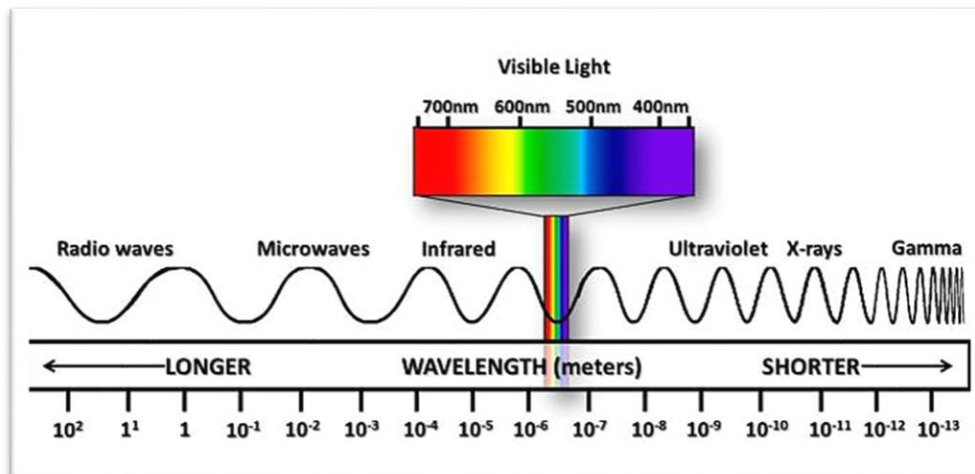
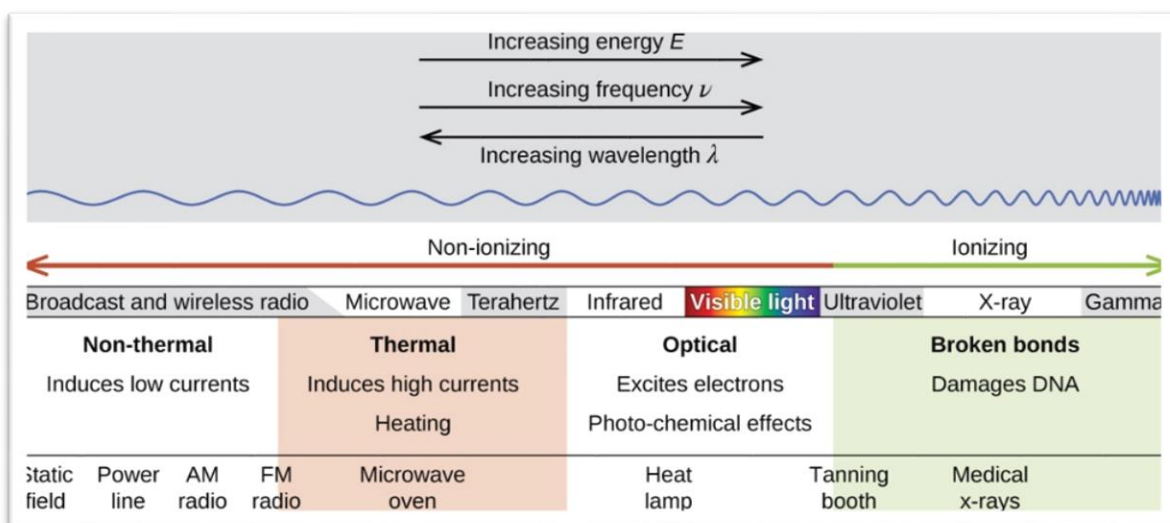


Figure III-2: Electromagnetic spectrum

## 1.2 Properties of Electromagnetic Radiation

- **Photons:** Electromagnetic radiation is emitted as discrete packets of energy called photons. These photons carry light energy and travel at the constant speed of light.
- **Quantized Harmonic Waves:** Electromagnetic radiation can be described as quantized harmonic waves. These waves exhibit specific frequencies and energy levels.
- **Categorization by Wavelength:** Electromagnetic radiation is grouped into different categories based on its wavelength within the electromagnetic spectrum. Each category has distinct properties and applications.

- **Perpendicular Electric and Magnetic Fields:** Electromagnetic waves consist of perpendicular electric and magnetic fields. These fields oscillate in directions that are perpendicular to each other and to the direction of wave propagation.
- **Wavelength, Amplitude, and Frequency:** Electromagnetic radiation exhibits properties such as wavelength, amplitude, and frequency. Wavelength ( $\lambda$ ) represents the distance between two adjacent points in phase, while frequency determines the number of wave cycles per second. Amplitude refers to the maximum displacement of the wave from its equilibrium position.
- **Travel through Empty Space:** Unlike other types of waves, electromagnetic radiation can travel through empty space. It does not require a medium such as a solid, liquid, or gas for propagation.
- **Constant Speed of Light:** The speed of light in a vacuum, denoted as “c,” is a fundamental constant of approximately  $2.99792458 \times 10^8$  m.s<sup>-1</sup>. This speed remains constant for all forms of electromagnetic radiation.
- The different areas of the light (or electromagnetic spectrum) in figure 3, the areas of light that possess short wavelengths are located on the left of the spectrum. All wavelengths from UV (ultraviolet) to  $\gamma$  (gamma) range have the potential to ionize tissues and/or DNA. As a result, individuals who have been exposed to large amounts of these types of radiation in acute time periods could develop cancer. In contrast, visible light (see the rainbow area in the Figure 1) and radiation on the right side of the spectrum has longer wavelengths and does not have the potential to ionize tissues and/or DNA. Visible, infrared (labeled IR), microwave, and radio waves are classified as being nonionizing radiation and have not been linked to cancer.



FigureIII-3: Lower frequency, lower-energy electromagnetic radiation is nonionizing, and higher frequency, higher-energy electromagnetic radiation is ionizing.

### 1.3 Corpuscular Aspect of Light

Each component of white light is a light radiation characterized by a specific color (made up of an infinite number of colors: red, blue, violet, etc.), and each color corresponds to an energy, a frequency, and a wavelength. In its corpuscular aspect, a light radiation can be considered as being composed of very small particles called photons.

Photon, also known as light quantum, is a minute energy packet of electromagnetic radiation. The idea of photon arose in 1905 from Albert Einstein's description of the photoelectric effect, in which he suggested the presence of discrete energy packets during the transmission of light.

Einstein assumed (1905) that radiation behaved in the photoelectric effect like a beam of particles. Each particle is a "grain" (quantum) of light (now called photon) with energy  $E$  proportional to the frequency of the monochromatic radiation that accompanies it.

$$E = h\nu$$

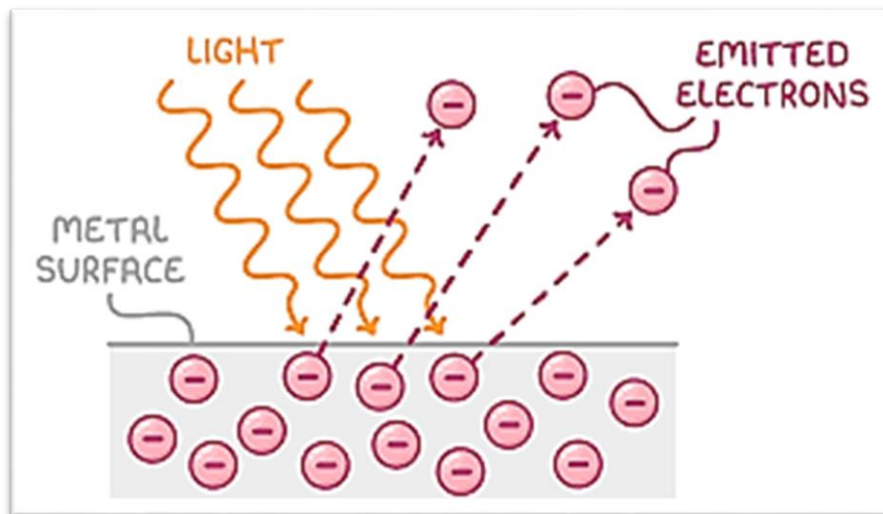
Where:

$h = 6.626 \times 10^{-34} \text{ J}\cdot\text{s}$  (Planck's constant),

$E$ : light energy carried by the radiation in Joules,

### 1.4 Photoelectric effect

When exposed to light (very high-frequency photons), metals release electrons. These electrons interact with the photons, receiving energy. This energy causes the electrons to move at a speed  $v$ , resulting in the flow of an electric current. This is the photoelectric effect (light) (electron movement).  $\nu$ : frequency of the radiation in Hz.



FigureIII-4: Photoelectric effect

## 2. Interaction between Light and Matter

When a light source strikes an object, the object reflects radiation at a specific wavelength and therefore appears a particular color depending on the mechanisms of emission, reflection, absorption, and transmission.

### 2.1 Emission Spectrum of the Hydrogen Atom

The hydrogen spectrum is the set of wavelengths present in the light that the hydrogen atom is capable of emitting. This light spectrum is composed of discrete wavelengths. It is obtained experimentally (Figure III-5) in a discharge tube containing dihydrogen and equipped with two metallic electrodes. The tube contains dihydrogen under low pressure (on the order of millimeters of mercury). A discharge is performed, partially ionizing the dihydrogen ( $H_2$ ). The generated ions are accelerated by the potential difference between the two electrodes and collide at high speed with the dihydrogen molecules, causing dissociation into hydrogen atoms, as well as the excitation of the atoms formed.

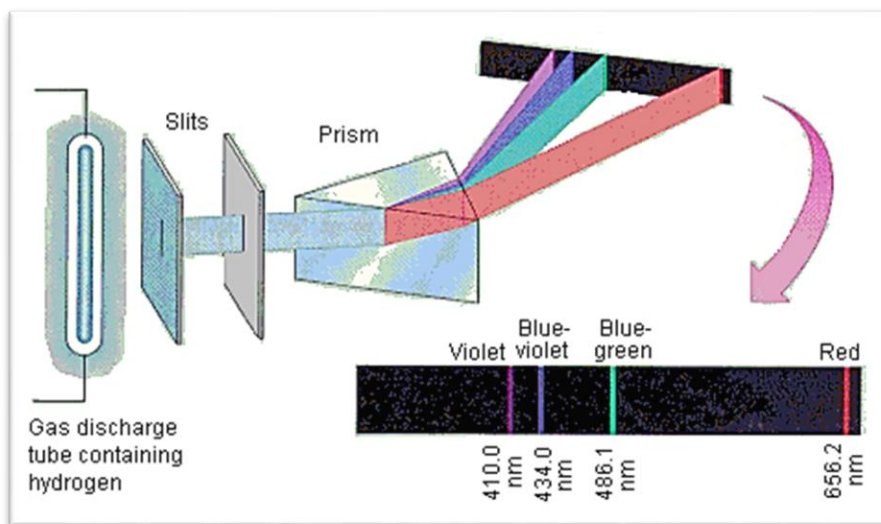


Figure 5: Hydrogen's Atomic Emission Spectrum

Experimentally, the spectrum of the hydrogen atom is obtained by placing a sealed tube containing hydrogen under low pressure in front of the slit of a spectrograph and in which an electric discharge is caused. This discharge excites the hydrogen atoms. When atoms return from the various excited states to lower energy states, electromagnetic radiation is emitted.

The experiments have shown that the emission spectrum of the hydrogen atom exhibits a large number of lines in the ultraviolet, visible, and infrared. The first series was observed by Balmer (a series located in the visible range). Lyman discovered a series in the ultraviolet, and then Paschen located a new series in the infrared range. Subsequently, Brackett and Pfund identified two new lines.

*NB: Within the same series, the lines are not separated by the same wavelength: the lines get closer together when the wavelength decreases and seem to tend towards a limiting line.*

## 2.2 Empirical Balmer-Rydberg relationship

The Balmer relation is given by the following relation:

$$\lambda = B \left( \frac{n^2}{(n^2 - 2^2)} \right)$$

Where:

*B*: Balmer Constant

*n*: Principal quantum number which designates the layer or level. It is a whole number not zero ( $n = 3, 4, 5, \dots \infty$ ).

Several years later, a more general empirical equation for all hydrogen transitions was derived by the physicist Johannes Rydberg. This version of polymer equation is the more generally used equation.

Rydberg relationship which is given by the following:

$$\frac{1}{\lambda} = R_H \left( \frac{1}{(n')^2} - \frac{1}{(n^2)} \right)$$

Where:

$R_H$ : Constant =  $10973731.57m^{-1}$

*n*: Principal quantum number

The Rydberg equation is applicable to any spectral series of hydrogen (see the following table)

$n'$	$n$	name	Spectral region
1	$2 \rightarrow \infty$	Lyman series	UV
<b>2</b>	<b><math>3 \rightarrow \infty</math></b>	<b>Balmer series</b>	<b>Visible</b>
3	$4 \rightarrow \infty$	Pashen series	IR
4	$5 \rightarrow \infty$	Brackette series	Far IR
5	$6 \rightarrow \infty$	Pfund series	Far IR
6	$7 \rightarrow \infty$	Humphrey series	Far IR

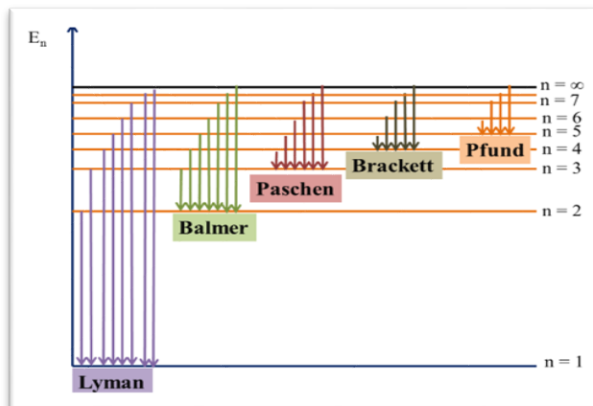


Figure III-6: spectral series of hydrogen

### 3. Classical Model of the Atom

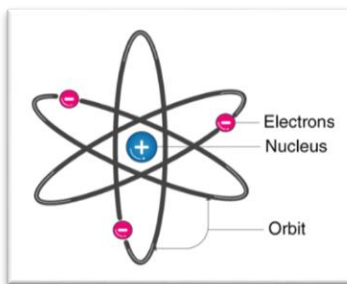
The atomic model, the discovery of what an atom looks like, is the result of reflection and experiments that took place over several centuries. The atomic model has evolved, been modified, and been questioned throughout history.

#### 3.1 Rutherford's Model

Rutherford hypothesized that the atom consists of a dense, positively charged nucleus containing the majority of the atom's mass, around which electrons orbit like planets around the sun under the influence of gravitational forces. This model is also called the planetary model.

Rutherford used classical mechanics as the physical law to study the motion of the electron, considering that: The electron is subject to two equal and opposite forces: the Coulombic force of attraction of the nucleus and the centrifugal (repulsive) force.

**The total energy of the system = kinetic energy + potential energy**

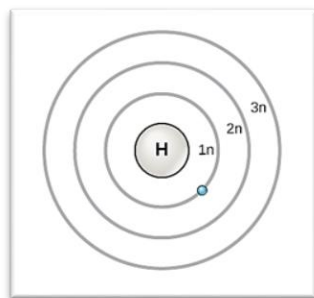


*Figure III-7: Rutherford's planetary model of the atom*

#### 3.2 Bohr model

##### 3.2.1 Description (case of the hydrogen atom)

In 1913, Danish scientist Niels Bohr (1885–1962) developed an early model of the atom where, The Bohr model shows the atom as a central nucleus containing protons and neutrons with the electrons in circular orbitals at specific distances from the nucleus (Figure III-8). These orbits form electron shells or energy levels, which are a way of visualizing the number of electrons in the various shells. These energy levels are designated by a number and the symbol "n." For example, the 1n shell represents the first energy level located closest to the nucleus.



*Figure III-8. The Bohr model postulated that electron orbited the nucleus in shells of fixed distance.*

An electron normally exists in the lowest energy shell available, which is the one closest to the nucleus. Energy from a photon of light can bump it up to a higher energy shell, but this situation is unstable and the electron quickly decays back to the ground state.

**Bohr proposes four hypotheses:**

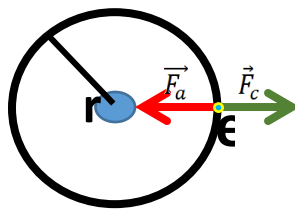
- In the atom, the nucleus is stationary while the electron of mass  $m$  moves around the nucleus in a circular orbit of radius  $r$ .
- The electron can only be found in privileged orbits without emitting energy; they are called "stationary orbits".
- When an electron passes from one level to another it emits or absorbs energy:  $\Delta E = h \cdot \nu$
- The angular momentum of the electron can only take integer values (quantification of angular momentum):

$$mvr = \frac{n \cdot h}{2\pi}$$

Where,  
 $n$  = number of corresponding energy shell; 1, 2, 3 .....  
 $m$  = mass of the electron  
 $v$  = velocity  
 $r$  = radius  
 $h$  = Plank's constant

**3.2.2 Quantitative aspect of the Bohr atom**

The system is stable by two forces: the attractive force  $\vec{F}_a$  and the centrifugal force  $\vec{F}_c$ .



Attractive force given by Columbus' law:

$$\vec{F}_a = \frac{Z \times k \times e^2}{r_n^2}$$

Centrifugal force given by the following relation:

$$\vec{F}_c = \frac{m \times v^2}{r_n}$$

At equilibrium

$$|\vec{F}_a| = |\vec{F}_c| \text{ so, } \frac{Z \times k \times e^2}{r_n^2} = \frac{m \times v^2}{r_n}$$

The angular momentum of the electron

$$m \times v \times r_n = \frac{n \times h}{2\pi} \leftrightarrow (m \times v \times r_n)^2 = \left(\frac{n \times h}{2\pi}\right)^2$$

$$m \times v^2 = \frac{n^2 \times h^2}{4 \times m \times \pi^2 \times r_n^2}$$

From the above equations:

$$\frac{Z \times k \times e^2}{r_n} = \frac{n^2 \times h^2}{4 \times m \times \pi^2 \times r_n^2} \rightarrow r_n = \frac{n^2 \times h^2}{4 \times m \times Z \times k \times \pi^2 \times e^2}$$

Where,  $r_n$  is the radius of the orbit where the electron circulates and it is quantified.

### 3.2.3 Energy of the electron in a stationary orbit

- ✓ The total energy of the system:  $E_T = E_C + E_P$
- ✓ Kinetic energy:  $E_C = 1/2 m \times v^2$
- ✓ The potential energy is due to the attraction of the nucleus:

$$E_P = \frac{Z \times k \times e^2}{r_n}; \frac{Z \times k \times e^2}{r_n} = m \times v^2$$

$$\frac{Z \times k \times e^2}{2 \times r_n} = \frac{1}{2} m \times v^2$$

$$E_T = \frac{Z \times k \times e^2}{2 \times r_n} - \frac{Z \times k \times e^2}{r_n} \rightarrow E_T = -\frac{Z \times k \times e^2}{2 \times r_n} \rightarrow E_T = -\frac{2 \times m \times Z^2 \times k^2 \times \pi^2 \times e^4}{n^2 \times h^2}$$

- ✓ The energy of the electron is quantized (it is a function of 'n').

$$k = 9109; e = 1.602 \times 10^{-19} \text{ C}; m = 9.1 \times 10^{-31} \text{ kg and } 1\text{eV} = 1.602 \times 10^{-19} \text{ J}$$

$$r_n = \frac{h^2}{4 \times m \times k \times \pi^2 \times e^2} \times \frac{n^2}{Z} = 5,30 \times 10^{-11} \times \frac{n^2}{Z} \text{ (m)} = 0,53 \times \frac{n^2}{Z} \text{ (A}^0\text{)}$$

$$E_T = \frac{2 \times m \times k^2 \times \pi^2 \times e^4}{h^2} \times \frac{Z^2}{n^2} = 21,78 \times 10^{-19} \times \frac{Z^2}{n^2} \text{ (J)} = 13,61 \times \frac{Z^2}{n^2} \text{ (eV)}$$

### 3.2.4 Relationship between wave number and energy levels

$$\Delta E = h\nu$$

$$\Delta E = E_{n_2} - E_{n_1}$$



$$\Delta E = \left( \frac{2 \times m \times Z^2 \times k^2 \times \pi^2 \times e^4}{n_2^2 \times h^2} - \frac{2 \times m \times Z^2 \times k^2 \times \pi^2 \times e^4}{n_1^2 \times h^2} \right)$$

$$\Delta E = \left( \frac{2 \times m \times Z^2 \times k^2 \times \pi^2 \times e^4}{h^2} \times \left( \frac{1}{n_2^2} - \frac{1}{n_1^2} \right) \right) \rightarrow h \times \nu$$

$$= \left( \frac{2 \times m \times Z^2 \times k^2 \times \pi^2 \times e^4}{h^2} \times \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \right)$$

$$\nu = \left( \frac{2 \times m \times Z^2 \times k^2 \times \pi^2 \times e^4}{h^3} \times \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \right)$$

$$\nu = \frac{C}{\lambda}$$

Where:

$C$  is speed of light =  $3 \times 10^8$  m/s

$\lambda$  is wavelength

$$\frac{C}{\lambda} = \left( \frac{2 \times m \times Z^2 \times k^2 \times \pi^2 \times e^4}{h^3} \times \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \right)$$

$$\frac{1}{\lambda} = \left( \frac{2 \times m \times Z^2 \times k^2 \times \pi^2 \times e^4}{C \times h^3} \times \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \right)$$

$$\bar{\nu} = \frac{1}{\lambda}; \text{ where } \bar{\nu} \text{ is wave number (cm}^{-1}\text{)}$$

$$\bar{\nu} = \left( \frac{2 \times m \times Z^2 \times k^2 \times \pi^2 \times e^4}{C \times h^3} \times \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \right)$$

$$\bar{\nu} = R_H \times \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right), \quad \text{where } R_H \text{ Rydberg constant}$$

### 3.2.5 Atomic Absorption Spectra

An electron cannot absorb or release energy, that is to say radiated, only by passing from one level (orbit) to another. The quantity of energy absorbed or emitted is equal to the energy difference between the two levels (Planck relation).

$$E_T = E_i - E_f$$

#### a) Absorption

When an electron passes from a level of orbit  $n$  of radius  $r_n$  to an orbit  $n+1$  of radius  $r_{n+1}$ , it absorbs radiation of frequency  $\nu_{n+1 \rightarrow n}$

#### b) Emission

When an electron goes from a level of  $n+1$  to a level  $n$ , it emits radiation of frequency  $\nu_{n+1 \rightarrow n}$

➤ *Continuous Spectrum*



➤ *Emission lines*



➤ *Absorption lines*



Figure III-9: Spectral lines

### 3.2.6 Limitations of Bohr Atomic Model Theory

- It violates the Heisenberg Uncertainty Principle. The Bohr atomic model theory considers electrons to have both a known radius and orbit i.e. known position and momentum at the same time, which is impossible according to Heisenberg.
- The Bohr atomic model theory made correct predictions for smaller sized atoms like hydrogen, but poor spectral predictions are obtained when larger atoms are considered.
- It failed to explain the Zeeman effect when the spectral line is split into several components in the presence of a magnetic field.
- It failed to explain the Stark effect when the spectral line gets split up into fine lines in the presence of an electric field.

#### 4. Electronic configuration

The electron configuration of an element describes how electrons are distributed in its atomic orbitals. Electron configurations of atoms follow a standard notation in which all electron-containing atomic subshells (with the number of electrons they hold written in superscript) are placed in a sequence.

Electrons in an atom are grouped around the nucleus into **shells**.

**a) Shell (electron):** A grouping of electrons in an atom according to energy.

The farther a shell is from the nucleus, the larger it is, the more electrons it can hold, and the higher the energies of those electrons.

The first shell (closest to the nucleus) can hold two electrons. The second shell can hold 8 electrons. The third shell can hold 18 electrons.

Within the shells, electrons are further grouped into **subshells** of four different types, identified as s, p, d, and f in order of increasing energy.

- The 1<sup>st</sup> shell has only an s subshell;
- The 2<sup>nd</sup> shell has an s and a p subshell;
- The 3<sup>rd</sup> shell has s, p, and d subshells,
- The 4<sup>th</sup> has s, p, d and f subshells.

The number of subshells is equal to the shell number.

A specific subshell is symbolized by writing the number of the shell, followed by the letter for the subshell.

**b) Subshell (electron):** A grouping of electrons in a shell according to the shape of the region of space they occupy.

**c) Orbital:** A region of space within an atom where an electron in a given subshell can be found.

Within each subshell, electrons are grouped into **orbitals**, regions of space within an atom where the specific electrons are most likely to be found. Each orbital holds two electrons which differ in a property known as spin.

Shell number:	1	2	3	4
Subshell designation:	s	s, p	s, p, d	s, p, d, f
Number of orbitals:	1	1, 3	1, 3, 5	1, 3, 5, 7

Any orbital can hold a maximum of 2 electrons with opposite spin.

- 1<sup>st</sup> shell has one 1s orbital and holds 2 electrons.
- 2<sup>nd</sup> shell holds 8 electrons; 2 in a 2s orbital and 6 in three 2p orbitals.
- 3<sup>rd</sup> shell holds 18 electrons; 2 in a 3s orbital; 6 in three 3p orbitals; and 10 in five 3d orbitals.
- 4<sup>th</sup> shell holds 32 electrons; 2 in a 4s orbital; 6 in three 4p orbitals; 10 in five 4d orbitals; and 14 in seven 4f orbitals.

Table III-1: Electron distribution in atom

Shell number	1	2	3	4
Subshell designation	s	s , p	s , p , d	s , p , d , f
Number of orbitals	1	1 , 3	1 , 3 , 5	1 , 3 , 5 , 7
Number of electron	2	2 , 6	2 , 6 , 10	2 , 6 , 10 , 14
Total electron capacity	2	8	18	32

The exact arrangement of electrons in an atom's shells and subshells is the atom's electron configuration. We construct the configuration by following different empirical rules:

#### 4.1 Construction (or filling) rule

The number of electrons is distributed so that the atom has the lowest possible energy in the ground state. We therefore "fill" the orbitals respecting the Pauli principle, starting with the lowest energies, step by step (Klechkowski rule), until the electrons are exhausted.

The energy of the atom is the sum of the hydrogen energies of the individual electrons.

#### 4.2 Klechkowski rule

Empirically, we see that the filling of the orbitals takes place in order as in the following figure:

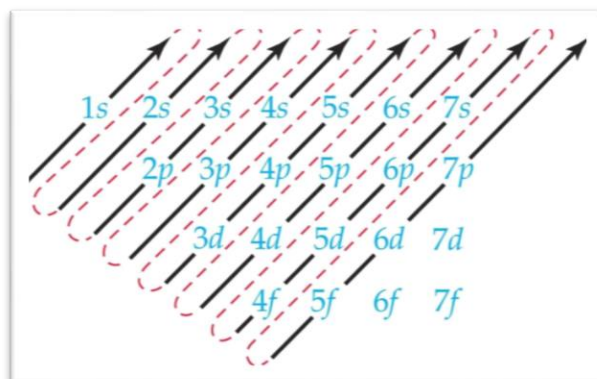


Figure III-11: Simple scheme to help remember the order in which the orbitals are filled

*NB: there are many atoms that are exceptions to this rule; in order of increasing Z: Cr, Cu, Nb, Mo, Ru, Rh, Pd, Ag, La, Gd, Pt, Au, Ac, Th, Pa, U.*

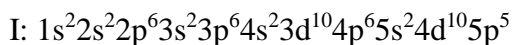
### 4.3 Hund's rule:

When electrons can occupy orbitals of the same energy in different distinct ways, the lowest energy state is the one where the greatest numbers of spins are parallel. When a subshell is not complete, the electrons occupy the maximum number of orbitals with spins in the same direction.

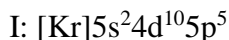
Hund's rule is essential when we are interested in a detailed electronic configuration, such as the one where the orbitals are represented by boxes. Thus, each atomic orbital is filled with at most two electrons, and then their spins are necessarily opposite (antiparallel).

### 4.4 Notation

To help describe the appropriate notation for electron configuration, it is best to do so through example. For this example, we will use the iodine atom. There are two ways in which electron configuration can be written:



or



In both of these types of notations, the order of the energy levels must be written by increased energy, showing the number of electrons in each subshell as an exponent. In the short notation, you place brackets around the *preceding* noble gas element followed by the valence shell electron configuration. The periodic table shows that krypton (Kr) is the previous noble gas listed before iodine. The noble gas configuration encompasses the energy states lower than the valence shell electrons. Therefore, in this case  $[\text{Kr}] = 1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6$ .

### 4.5 Slater's Rules

The general principle behind Slater's Rule is that the actual charge felt by an electron is equal to what you'd expect the charge to be from a certain number of protons, but minus a certain amount of charge from other electrons. Slater's rules allow you to estimate the effective nuclear charge  $Z_{\text{eff}}$  from the real number of protons in the nucleus and the effective shielding of electrons in each orbital "shell" (e.g., to compare the effective nuclear charge and shielding 3d and 4s in transition metals). Slater's rules are fairly simple and produce fairly accurate predictions of things like the electron configurations and ionization energies.

$$Z_{\text{eff}} = Z - \sigma_{ij}$$

Where  $\sigma_{ij}$  is screen constant

**The screening constant** is the summation of contribution of each electron in screening from the force of the nucleus according to Slater's Rule. The contribution of electrons of each orbital is different and its values are provided by Slater's Rule. Also effective nuclear charge can be defined as the net attraction or net positive charge experienced by an electron in a multi-electron atom.

Table III-2:  $\sigma_{ij}$  values ("screening" of  $e_i$  by  $e_j$ )

		$e_j$							
		1s	2s, 2p	3s, 3p	3d	4s, 4p	4d	4f	5s, 5p
$e_i$	1s	0,31	0	0	0	0	0	0	0
	2s, 2p	0,85	0,35	0	0	0	0	0	0
	3s, 3p	1	0,85	0,35	0	0	0	0	0
	3d	1	1	1	0,35	0	0	0	0
	4s, 4p	1	1	0,85	0,85	0,35	0	0	0
	4d	1	1	1	1	1	0,35	0	0
	4f	1	1	1	1	1	1	0,35	0
	5s, 5p	1	1	1	1	0,85	0,85	0,85	0,35

## Applied exercises

### Exercise 01

1. What energy must the ion of  $\text{Li}^{2+}$  absorb to move the electron from the fundamental level to the second level excited?
2. What is the wavelength of radiation that is capable of causing this transition?
3. Calculate in eV and in joules, the ionization energy of the  $\text{Li}^{2+}$  ion, from the second state excited.

**Given data:** Li ( $Z=3$ );  $1\text{eV} = 1.6 \times 10^{-19}$  Joules;  $h = 6.62 \times 10^{-34}$  J.s;  $c = 3.108 \text{ m.s}^{-1}$ ,

### Exercise 02

The emission spectrum of hydrogenic ion  ${}_Z\text{X}^{n+}$  consists of series of lines whose wavelength  $\lambda$  (in meters)

verify the relationship :  $\frac{1}{\lambda} = 0.176 \cdot 10^9 \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$

- a) Determine the atomic number ( $Z$ ) of this hydrogen ion and its charge
- b) What is the variation of the energy of this hydrogenic ion during its transition from ground to excited state ( $n=3$ )
- c) Calculate the ionization energy of this hydrogenic ion from the excited state

# Chapter 04: Periodic Classification of Elements

## Preface

The Periodic Classification of Elements is a central concept in chemistry that has evolved progressively over time. The earliest classification, known as the classical periodic table, was established by Dmitri Ivanovich Mendeleev, who organized elements according to their atomic masses and observed the periodic recurrence of their properties.

With the advancement of atomic theory, this classification was refined by Henry Moseley, who demonstrated that atomic number, rather than atomic mass, is the fundamental basis of periodicity. This led to the modern periodic table, which is directly based on electronic structure.

The classical and modern periodic tables are therefore closely related, as the modern form is an improved version of Mendeleev's original system. The modern classification corrects previous inconsistencies and provides a more accurate and scientific organization of elements.

This chapter introduces the evolution of the periodic table, the transition from the classical to the modern approach, and the fundamental principles that govern the classification of elements.

### 1. Mendeleev's Periodic Table

*Russian chemist Dmitri Ivanovich Mendeleev* put forth his periodic table in 1869. He observed that the properties of elements, both physical and chemical, were periodically related to the atomic mass of the elements. The **Periodic Law** (also referred to as Mendeleev's Law), states that the chemical properties of elements are a periodic function of their atomic weights.

#### 1.1. The advantages of Mendeleev's Periodic table

- The inclusion of these newly discovered elements did not disturb the periodic table. Examples include germanium, gallium, and scandium.
- It was used to correct the wrong atomic weights in use at that time.
- A variance from the atomic weight order was provided by Mendeleev's table.

#### 1.2. The limitations of Mendeleev's Periodic table

- Hydrogen's position was in the group of alkali metals but hydrogen also exhibited halogen like qualities.
- Isotopes were positioned differently since this type of classification of elements was done by considering the atomic weight of the element. Therefore – protium, deuterium, and tritium would occupy varying positions in Mendeleev's table.
- An anomalous positioning of a few elements showed that the atomic masses did not increase regularly from one element to the next. An example of this would be the placement of cobalt (atomic mass of 58.9) before nickel (atomic mass of 58.7).

These methods were the foundation on which the modern periodic table was built. However, the greatest contributor to the modern periodic table was Dmitri Mendeleev. Mendeleev is also known as the Father of the Modern Periodic Table. The modern periodic law is also called Mendeleev's Law to honour him.

Mendeleev Table															
H 1.01															
Li 6.94	Be 9.01	B 10.8	C 12.0	N 14.0	O 16.0	F 19.0									
Na 23.0	Mg 24.3	Al 27.0	Si 28.1	P 31.0	S 32.1	Cl 35.5									
K 39.1	Ca 40.01		Ti 47.9	V 50.9	Cr 52.0	Mn 54.9	Fe 55.9	Co 58.9	Ni 58.7						
Cu 63.5	Zn 65.4			As 74.9	Se 79.0	Br 79.9									
Rb 85.5	Sr 87.6	Y 88.9	Zr 91.2	Nb 92.9	Mo 95.9		Ru 101	Rh 103	Pd 106						
Ag 108	Cd 112	In 115	Sn 119	Sb 122	Te 128	I 127									
Ce 133	Ba 137	La 139		Ta 181	W 184		Os 194	Ir 192	Pt 195						
Au 197	Hg 201	Tl 204	Pb 207	Bi 209											
			Th 232		U 238										

Figure VI-1: The classical Mendeleev table

## 2. Modern periodic table

In the year 1913, English physicist **Henry Moseley** studied the wavelength of the characteristic x-rays by using different metals as anti cathode and showed that the square root of the frequency of the line is related to the atomic number. On the basis of the above observations Moseley gave the **modern periodic law** which states that:

“Physical and chemical properties of the elements are the periodic function of their atomic numbers”.

The atomic mass of an element is due to the mass of protons and neutrons present in the nucleus of its atom. Since the nucleus is located inside an atom, It is not very much linked with the properties of the element, particularly the chemical properties. These are related to the number of electrons and also the distributions of the electrons in the different energy shells. The elements with different electronic arrangements of atoms possess different chemical properties. As the number of electrons in an atom is given by the atomic number and not by the mass number, therefore atomic number should form the basis of the classification of the elements in the periodic table and not atomic mass as predicted by Mendeleev.

Repetitions of the similar properties of the elements placed in a group and separated by certain definite gap of atomic number are known as Periodicity.

### 3. Classification of elements in periodic table

The periodic table is a consequence of electronic configurations. The periodic table is based on the formation of groups consisting of elements (with atomic number  $Z$ ) having similar properties.

- The periodic table is made up of 4 blocks: s, p, d and f.
- The elements of the same horizontal row of the periodic table constitute a period. There are 7 of them.
- The elements of the same column having the same electronic configuration of the outer layer constitute a family or group.



Figure VI-2: Periodic table

The periodic table is made up of 18 columns divided into 9 groups. The first 7 each have two subgroups A and B depending on the state of the external electrons.

- **Subgroup A:** contains elements whose outer layer is  $ns\ np$ .
- **Subgroup B:** contains atoms which have a state  $d$ .

The indices **I, II, III,...** indicate the number of electrons in the outer shell, called valence electrons.

- ✚ **Block s:** The s block consists of the elements present in columns 1 (alkali metals) and 2 (alkaline earth metals) of the periodic table of the elements, as well as hydrogen and helium. They are so called because their highest occupied orbital (in energy) is of type s.
- ✚ **Block p:** The P block consists of the elements present in columns 13 to 18 of the periodic table of elements. They are so called because their highest occupied orbital (in energy) is p-type. This block

includes icosagens (column 13), crystallogens (column 14), pnictogens (column 15), chalcogens (column 16), halogens (column 17), and rare gases (column 18), exception of Helium.

✚ **Block d:** Block d consists of the elements present in columns 3 to 12 of the periodic table. They are called so because the highest (in energy) orbital occupied is of type d.

✚ **Block f:** Block f is made up of the internal transition elements of the periodic table: lanthanides and actinides. They are so called because the highest orbital (in energy) occupied by these atoms is of type f

### 3.1. Chemical families

The element families considered as the most important, by their use or their abundance, are:

#### a) Alkalis:

Located on the far left of the periodic table, alkalis have only one electron on their lowest energy level. They will tend to easily give up this electron to saturate the previous energy level and become stable like a rare gas. During a chemical reaction, they are ready to donate this valence electron to non-metals; they therefore form ionic bonds. The elements of the group (IA) have a centered cubic crystal structure. They are light, silvery-white metals that oxidize easily and melt at low temperatures.

#### b) Alkaline earths:

Group (IIA), the alkaline earth metals, contains 6 elements: (Be, Mg, Ca, Sr, Ba and Ra) which is radioactive. These elements are very electropositive, they are light, soft and very reactive metals. In water, the elements of group (IIA) give soluble bases of formula they react easily with many non-metals.

#### c) Halogens:

They are non-metals that share certain characteristics: they do not conduct electric current, they have a dull appearance, they are not malleable and they cannot be rolled. It is the only family in the periodic table where we find elements in liquid, gaseous and solid states.

These elements have seven valence electrons, and they will have strong tendencies to react with other elements, either through an ionic bond or through a covalent bond, in order to acquire the electronic structure of rare gases.

#### d) Transition metals

These are the elements whose last shell is saturated with two electrons while the subshell (d) is incompletely filled. This family is in fact grouped over the same period and includes elements with atomic numbers between 21 and 30 (from Scandium to Zinc). It has the characteristics of metals but its chemical behavior is quite particular.

#### e) Noble gases:

The elements of these families are distinguished by the almost total absence of their chemical activity, hence their great stability. Helium is a monatomic gas. The forces of attraction between the atoms of this gas are very weak. It is the only known substance that cannot be solidified at a certain temperature without increasing the pressure. The other rare gases have very close similarities with helium. Apart from radon, which is a product of the decay of uranium or radium, the others are found in small quantities in the air. Helium is the second most abundant element in the universe.

*The byte rule: Noble gases have great chemical inertia, they give practically no reaction. They are sometimes called noble gases because they refuse to mix with other elements in chemical compounds. These are mono-atomic gases. This great stability is due to their electronic configuration which reveals a saturated valence shell with 8 electrons.*

### 4. Periodicity of properties

The basic law governing modern periodic table states that the properties of elements are periodic functions of their atomic number. These properties reappear at regular intervals or follow a particular trend at regular intervals. This phenomenon is known as the periodicity of elements.

The periodic properties of elements occur due to the recurrence of similar electronic configuration that is having the same number of electrons in the outermost orbit. In a particular group, the number of valence electrons remains the same. On the other hand, the number of valence electrons increases, as we move from left to right across a period. The chemical property of an element depends on the number of electrons in the valence shell.

#### 4.1. Atomic radius $r_a$

We can define the atomic radius as being half the distance between the centers of the two atoms linked by a single bond.

- Over a period: if  $Z$  increases then  $r_a$  decreases
- On a column: if  $Z$  increases then  $r_a$  increases

#### 4.2. Ionic radius $r_i$

In a general way:

- ✓ Cations are smaller than their parent atoms:  $r_i$  (cation)  $<$   $r_a$
- ✓ Anions are larger than their parent atoms:  $r_i$  (anion)  $>$   $r_a$
- ✓ For ions with the same electronic configuration ( $S^{2-}$ ,  $Cl^-$ ,  $K^+$ ,  $Ca^{2+}$ ,  $Ti^{4+}$ , ...). if  $Z$  increases;  $r_i$  decreases
- ✓ At equal charges, the ionic radius varies in the same direction as the atomic radius: if  $Z$  increases then  $r_i$  decreases.

## Applied exercises

### Exercise 01

Consider the following elements:  ${}^4\text{Be}$ ,  ${}^8\text{O}$ ,  ${}^9\text{F}$ ,  ${}^{10}\text{Ne}$ ,  ${}^{17}\text{Cl}$ ,  ${}^{24}\text{Cr}$ ,  ${}^{28}\text{Ni}$ ,  ${}^{30}\text{Zn}$ ,  ${}^{37}\text{Rb}$ ,  ${}^{42}\text{Mo}$ ,  ${}^{46}\text{Pb}$ ,  ${}^{54}\text{Xe}$ ;  ${}^{56}\text{Ba}$

- 1) Give the electronic structure of these elements and represent the outer layer electrons with quantum boxes
- 2) Situate these elements in the periodic table.
- 3) Classify these elements by ionization energy in ascending order.

### Exercise 02

1. Give the position of the following elements in the periodic table:  ${}^7\text{N}$ ,  ${}^{17}\text{Cl}$ ,  ${}^{21}\text{Sc}$ ,  ${}^{24}\text{Cr}$ ,  ${}^{26}\text{Fe}$ ,  ${}^{29}\text{Cu}$ ,  ${}^{30}\text{Zn}$ ,  ${}^{47}\text{Ag}$ .
2. Cesium (Sb) belongs to the same family as nitrogen ( ${}^7\text{N}$ ) and to the same period as silver ( ${}^{47}\text{Ag}$ ). Give its electronic configuration and its atomic number  $Z$ .
3. Determine the energy of the first ionization of nitrogen ( ${}^7\text{N}$ ).

# Chapter 05: Chemical Bonding

## Preface

Chemical bonds arise from the intrinsic properties of atoms. In general, atoms rarely exist in an isolated state, with the exception of noble gases (and, under certain conditions, hydrogen). Instead, they tend to combine to form molecules or extended structures that are more stable than individual atoms.

The interactions between atoms lead to the formation of **strong chemical bonds**, such as covalent and ionic bonds. In contrast, interactions between molecules are generally weaker and include forces such as hydrogen bonding. These interactions play a key role in determining the physical and chemical properties of substances.

### 1. Formation of Chemical Bonds

The formation of a chemical bond between atoms is accompanied by a release of energy, which corresponds to the stabilization of the system. Conversely, breaking a bond requires an input of energy equal in magnitude to the bond dissociation energy.

As a result, the molecule formed possesses a lower total energy than the separated atoms from which it originates, making it thermodynamically more stable.

### 2. Types of chemical bonds

There are four types of bonds hold the atoms together in a molecule, depending on the ways by which the atoms arrange their outermost shell electrons to get an eight electron outermost shell configuration.

- Covalent bond
- Ionic bond
- Co-ordinate bond
- Metallic bond

These bonds are strong; however, attractive forces between the atoms are comparatively weaker; and are called **weaker bonds**. In these bonds, the bonding atoms retain their identity and are of the following types:

- Hydrogen bond: involves bonding of hydrogen atom with two strongly electronegative atoms ( e.g., N, O and F)
- Van der Waals interaction: involves interaction between atoms or molecules with inert gas configuration.

## 2.1. Covalent bond

These are the bonds that form between atoms with similar electronegativities  $\phi$ . This bond is formed by a pair of electrons (this is then a single bond, denoted  $\phi$ ) or several pairs (multiple bonds: one  $\phi$  bond and one or two  $\pi$  bonds).

There are two ways to form a covalent bond:

- Each atom contributes one unpaired electron; the bond is called a normal covalent bond:



- One atom provides a lone pair and the other receives it in an empty space; the bond is called dative covalent or coordination:



*Note: In reality, these two types of bonds are completely identical and indistinguishable.*

### 2.1.1 Properties

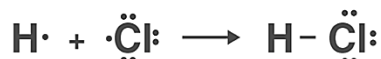
- Covalent bonding does not result in the formation of new electrons. The bond only pairs them.
- They are very powerful chemical bonds that exist between atoms.
- A covalent bond normally contains an energy of about ~80 kilocalories per mole (kcal/mol).
- Covalent bonds rarely break spontaneously after it is formed.
- Covalent bonds are directional, where the atoms that are bonded showcase specific orientations relative to one another.
- Most compounds having covalent bonds exhibit relatively low melting points and boiling points.
- Compounds with covalent bonds usually have lower enthalpies of vaporisation and fusion.
- Compounds formed by covalent bonding don't conduct electricity due to the lack of free electrons.
- Covalent compounds are not soluble in water.

### 2.1.2 Types of Covalent Bonds

Depending upon the number of shared electron pairs, the covalent bond can be classified into:

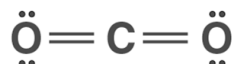
- Single Bonds:** is formed when only one pair of electrons is shared between the two participating atoms. It is represented by one dash (-). Although this form of covalent bond has a smaller density and is weaker than a double and triple bond, it is the most stable.

*For example, the HCL molecule has one hydrogen atom with one valence electron and one chlorine atom with seven valence electrons. In this case, a single bond is formed between hydrogen and chlorine by sharing one electron.*



- b) Double Bonds:** is formed when two pairs of electrons are shared between the two participating atoms. It is represented by two dashes (=). Double covalent bonds are much stronger than single bonds, but they are less stable.

*For example, a carbon dioxide molecule has one carbon atom with six valence electrons and two oxygen atoms with four valence electrons. To complete its octet, carbon shares two of its valence electrons with one oxygen atom and two with another oxygen atom. Each oxygen atom shares its two electrons with carbon, and therefore there are two double bonds in CO<sub>2</sub>.*



*Oxygen Molecule: In the formation of the oxygen molecule, each oxygen atom has six electrons in its valence shell. Each atom requires two more electrons to complete its octet. Therefore, the atoms share two electrons each to form the oxygen molecule. Since two electron pairs are shared, there is a double bond between the two oxygen atoms.*



- c) Triple Bond:** is formed when three pairs of electrons are shared between the two participating atoms. Triple covalent bonds are represented by three dashes ( $\equiv$ ) and are the least stable type of covalent bonds.

*For example, in the formation of a nitrogen molecule, each nitrogen atom having five valence electrons provides three electrons to form three electron pairs for sharing. Thus, a triple bond is formed between the two nitrogen atoms.*



- d) Polar Covalent Bond:** exists where the unequal sharing of electrons occurs due to the difference in the electronegativity of combining atoms. More electronegative atoms will have a stronger pull for electrons. The electronegative difference between the atoms is greater than zero and less than 2.0. As a result, the shared pair of electrons will be closer to that atom.

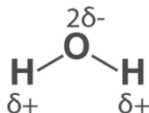
*For example, molecules form hydrogen bonding as a result of an unbalanced electrostatic potential. In this case, the hydrogen atom interacts with electronegative fluorine, hydrogen, or oxygen.*

- e) Nonpolar Covalent Bond:** is formed whenever there is an equal share of electrons between atoms. The electronegativity difference between two atoms is zero. It occurs wherever the combining atoms have similar electron affinity (diatomic elements).

*For example, Nonpolar Covalent Bond is found in gas molecules like hydrogen gas, nitrogen gas, etc.*

### 2.1.3. Polarization of Covalent Bonds

It is observed that in the sigma bonds between two different atoms, the electron cloud is always closer to the more electronegative of the two atoms participating in the sigma bond. Due to this, there is a permanent dipole that arises in the bond, and the covalent bond is said to be polarized.



An illustration describing the polarity of the covalent bonds in a water molecule is provided above. The more electronegative atom is said to have a partial negative charge, and the less electronegative atom has a partial positive charge in the polar covalent bond.

### 2.1.4 Lewis structure

G.N. Lewis introduced electron dots symbols (Lewis symbols, or Lewis structures) to denote valence electrons in an atom. According to this method:

- 1) Symbol of an element represents the nucleus and the inner electrons which do not participate in bond formation.
- 2) Number of dot on the symbol represents Valence electron.

For example :

- Hydrogen atom contains 1 electron in its valence shell; thus, its Lewis symbol is :  $\dot{H}$   
Here, H represents the hydrogen nucleus and the dot (.) represents 1 valence electron in hydrogen atom
- Electronic configuration of chlorine is 2,8,7; thus, number of valence electrons is 7 and Lewis symbol of chlorine atom is



Here, Cl represents the chlorine nucleus and 10 (2,8) inner electrons; and the 7 dots represent valence electron in chlorine atom.

#### c) Rules of Lewis structure

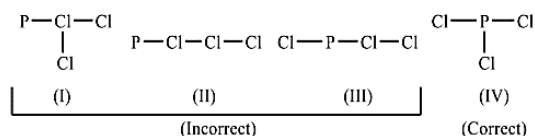
##### Step 1: Choice of central atom

The correct structure of a molecule is obtained by properly arranging the atoms of the combining elements. Generally, the atom with the largest number of bonds is placed as the **central atom** of the structure.

Example:  $PCl_3$  (Phosphorus trichloride)

Among the proposed skeleton structures for  $PCl_3$ , only structure IV is correct because:

- Chlorine (Cl) atoms cannot form more than one covalent bond
- Phosphorus (P) can form multiple covalent bonds



### **Step 2: Valence electron distribution**

The total number of available valence electrons in a molecule is calculated and distributed so that:

- Each atom (except hydrogen) is surrounded by **8 electrons (octet rule)**
- Hydrogen follows the **duet rule (2 electrons only)**
- Shared electrons are counted for both bonded atoms

**Step 3:** valence electrons on the two combining atoms are shown differently. Dots are placed on one atom, and crosses are placed on the other atom.

#### **d) Limitation of Lewis structure**

Lewis theory explains **how atoms connect**, but it does not fully describe:

- Bond geometry
- Bond energy
- Electron distribution in space

For that, more advanced models like **Valence Bond Theory** or **Molecular Orbital Theory** are used.

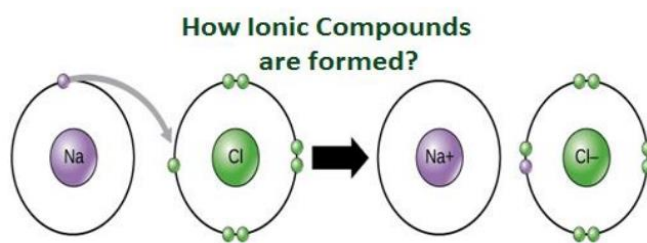
## **2.2. Ionic bond**

Ionic bonds are formed by the complete transfer of electrons from one atom to another, resulting in the formation of charged particles called ions. These ions are held together by strong electrostatic forces of attraction.

- ✓ An ionic bond forms when one atom donates electrons to achieve a stable noble gas electron configuration, while another atom accepts these electrons to achieve the same stability. In other words, an ionic bond is the chemical bond formed through the transfer of electrons between atoms.
- ✓ Ionic bonding is also known as electrovalent bonding, and compounds formed through this type of bonding are called ionic compounds. Therefore, ionic compounds consist of positively and negatively charged ions.
- ✓ Ionic bonds typically form between a metal and a non-metal. In this reaction, electrons are transferred from the metal to the non-metal, and the resulting ions are held together by electrostatic attraction.

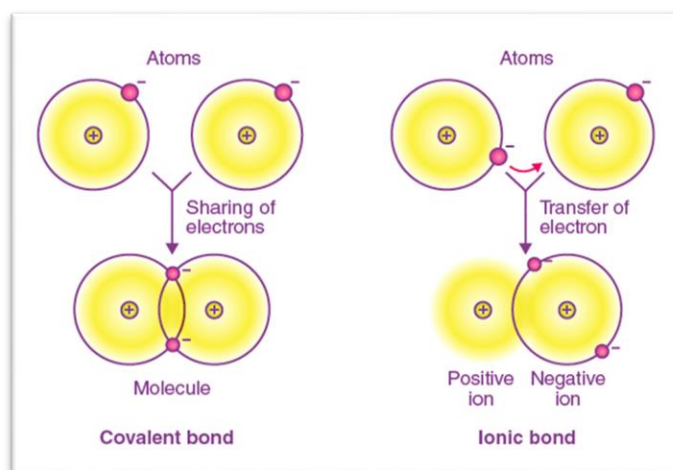
*For an example: **Formation of Sodium Chloride:*** Sodium is a metal whereas chlorine is a non-metal. Sodium metal reacts with chlorine to form an ionic compound, sodium chloride. Now we will see how sodium chloride is formed and what changes take place in the electronic arrangements of sodium and chlorine atoms in the formation of this compound. The atomic number of sodium is 11, so its electronic configuration is  $1s^2, 2s^2, 2p^6, 3s^1$ . Sodium has only one electron in its outermost shell. So, sodium atom will donate one electron to chlorine atom and forms a sodium ion i.e.  $\text{Na}^+$ . On the other side chlorine atomic number is 17, its electronic configuration is  $1s^2, 2s^2, 2p^6, 3s^2, 3p^5$ . Therefore, chlorine atom has 7 electrons

in the outermost shell and needs one more electron to achieve stable electronic configuration or inert gas configuration. So, a chlorine atom takes one electron from sodium atom and forms a negatively charged chloride ion i.e.  $\text{Cl}^-$ .



### 2.3 Difference between Covalent and Ionic Bonds

Covalent bonds and ionic bonds are types of atomic bonds. These bonds are different in their properties and structure. Covalent bonds include pairs of electrons by two atoms binding them in a fixed orientation, while a bond between two ions is called an ionic bond.



*Figure V-1: Covalent vs Ionic Bonds*

Covalent bonding occurs between two non-metallic atoms, characterised by the sharing of electron pairs between the atoms and other covalent bonds with an electronegativity difference greater than 2.0 ( $<2.0$ ). In the case of covalent bond formation, polyatomic ions are formed, whereas the ionic bond is formed as a result of electrostatic attraction between the oppositely charged ions.

### 3. Repulsion Model or VSEPR or Gillespie Model

- ✓ The Lewis model does not account for the geometric shape of molecules. However, experience shows that molecules have a well-defined shape. Several authors (Sidgwick, Powell, Nyholm, and later Gillespie) proposed the valence shell electron pair repulsion (VSEPR) model.
- ✓ In the VSEPR model, it is assumed that the arrangement, within a molecule, of atoms bonded to a given atom A, considered central, is achieved by distributing the valence electron pairs of this atom in such a way that the electrostatic repulsions between these pairs balance each other. The rules obtained from these models are often called Gillespie's rules.
- ✓ Two atoms can join together through several bonds simultaneously; these are called multiple bonds. There are three types of bonds: single, double, and triple, which are symbolized by lines



Where:

A: The central atom under consideration.

X<sub>n</sub>: The bonds (due to valence pairs), n being their number (X, a multiple bond, counts as a single bond).

E<sub>m</sub>: The non-bonding electron pairs, in number m.

Depending on the value of n + m, the molecule will have a linear form (n + m = 2), an equilateral triangle (n + m = 3), a tetrahedron (n + m = 4), .....

Bonding electron pairs	Lone pairs	Electron domains (Steric #)	Shape	Ideal bond angle (example's bond angle)	Example	Image
2	0	2	linear	180°	CO <sub>2</sub>	
3	0	3	trigonal planar	120°	BF <sub>3</sub>	
2	1	3	bent	120° (119°)	SO <sub>2</sub>	
4	0	4	tetrahedral	109.5°	CH <sub>4</sub>	
3	1	4	trigonal pyramidal	107°	NH <sub>3</sub>	
2	2	4	angular	109.5° (104.5°)	H <sub>2</sub> O	
5	0	5	trigonal bipyramidal	90°, 120°, 180°	PCl <sub>5</sub>	
4	1	5	seesaw	180°, 120°, 90° (173.1°, 101.6°)	SF <sub>4</sub>	
3	2	5	T-shaped	90°, 180° (87.5°, < 180°)	ClF <sub>3</sub>	
2	3	5	linear	180°	XeF <sub>2</sub>	
6	0	6	octahedral	90°, 180°	SF <sub>6</sub>	
5	1	6	square pyramidal	90° (84.8°), 180°	BrF <sub>5</sub>	
4	2	6	square planar	90°, 180°	XeF <sub>4</sub>	
7	0	7	pentagonal bipyramidal	90°, 72°, 180°	IF <sub>7</sub>	

Figure V-2: VSEPR table of molecular geometries:

## 4. The Covalent Bond in the Quantum Model

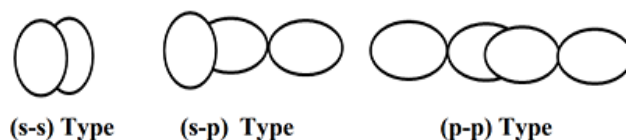
### *Physical Aspect of the Covalent Bond*

As in the case of the atom, a molecular Schrödinger equation can be written, whose solution provides wave functions describing the behavior of electrons in a molecule.

An exact solution of this equation is only possible in the simplest case, namely the dihydrogen molecule ( $H_2$ ). For other molecules, only approximate methods can be used.

The chemical bond is formed through the overlap of atomic orbitals, leading to the formation of molecular orbitals. This overlap can occur in two different ways, corresponding to two different types of bonds.

#### *c) Axial overlap leading to $\sigma$ -type bonds*



#### *d) Lateral overlap leading to $\pi$ -type bonds*



Lateral overlap of the p-p type

$\sigma$  and  $\pi$  bonds are two different types of bonds. In general,  $\sigma$ -type bonds are stronger than  $\pi$ -type bonds because they correspond to a greater overlap.

## 5. Hybridization of Atomic Orbitals

- ✓ The case of molecules with more than two atoms is more complex than that of diatomic molecules. The main additional difficulty lies in incorporating molecular geometry.
- ✓ The use of normal atomic orbitals cannot explain the different geometric shapes of molecules involving identical atomic orbitals. For this, we resort to the concept of atomic orbital hybridization.
- ✓ It can be shown mathematically that any linear combination of two or more wave functions that are solutions to the Schrödinger equation is itself a solution to that Schrödinger equation. This mathematical property is the basis of the atomic orbital hybridization technique.

We begin by identifying the atomic orbitals involved in the bonds under consideration. Each atomic orbital is associated with a mathematical function and a specific geometric shape. We determine the actual geometric shape of the molecule by applying the VSEPR method.

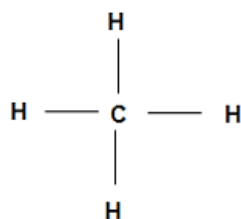
We then mathematically determine the linear combination of the initial atomic orbitals that will lead to new orbitals called hybrid orbitals, whose geometric shape will correspond to the actual shape of the molecule being studied.

The linear combination of atomic orbitals to form hybrid orbitals then allows us to explain the formation of molecular orbitals through the overlap of these hybrid atomic orbitals.

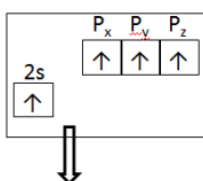
### e) Linear combination of 4 atomic orbitals

#### Example: methane

This molecule is a tetrahedral molecule of type AX<sub>4</sub>. Its Lewis structure is as follows:

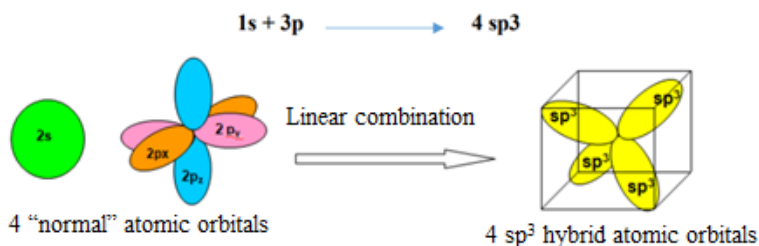


The methane molecule has a regular tetrahedral shape (as predicted by VSEPR theory), and it satisfies the octet rule. However, the bond angle of 109.5° and the equal C–H bond lengths are not consistent with the original atomic orbitals of carbon. To explain this, four equivalent hybrid orbitals are formed through the linear combination of atomic orbitals. This process is called sp<sup>3</sup> hybridization of carbon. These four sp<sup>3</sup> hybrid orbitals correspond to lower-energy, more stable states for the valence electrons. They form four identical covalent bonds arranged symmetrically with bond angles of 109.5°.

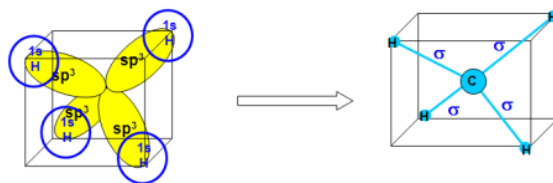


4 hybrid orbitals sp<sup>3</sup>

Since the orbitals are spherical and the p orbitals point along the three Cartesian axes, the formation of a tetrahedral molecule cannot be explained simply. The atomic orbitals involved in its formation are the 2s and 2p orbitals of the carbon atom, which will overlap with the 1s orbitals of hydrogen.



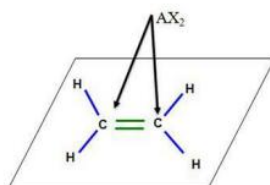
Once the hybrid atomic orbitals are obtained, the molecular orbitals are constructed by overlapping them with the four **1s** atomic orbitals of the four hydrogen atoms. The overlap can only be axial, resulting in four  $\sigma$  bonds. These four bonds will obviously point in the directions of a tetrahedron centered on the carbon atom.



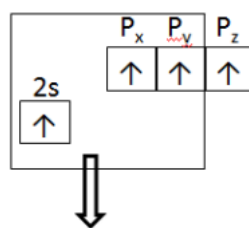
### f) Linear combination of 3 atomic orbitals

#### Example: ethane

$C_2H_4$  this molecule is planar with HCH and HCC angles of  $120^\circ$ , as illustrated in the following diagram:

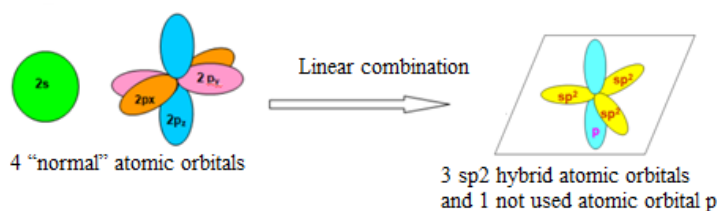


The VSEPR method allows us to predict the value of the  $120^\circ$  angles using the  $AX_3$  geometry around the two carbon atoms, but it doesn't explain why the molecule is planar. Indeed, there's no inherent requirement that the two triangles be coplanar. To describe this molecule,  $sp^3$  hybridization is unsuitable; we will use  $sp^2$  hybridization. The superscript 2 here indicates that only two p orbitals will combine with the s orbital to obtain this type of hybrid orbital. Therefore, one p orbital will remain on each carbon atom.

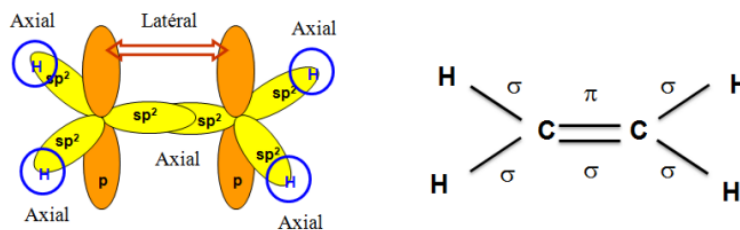


3 hybrid orbital  $sp^2$

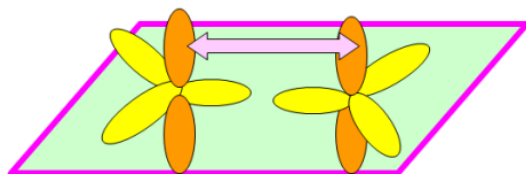
These  $sp^2$  hybrid orbitals will point in the directions of an equilateral triangle centered on the carbon atom.



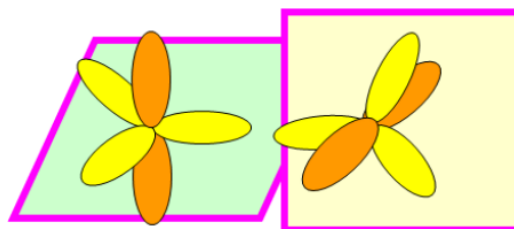
Once the  $sp^2$  hybrid orbitals are obtained, the molecule is formed by the overlap of atomic orbitals (AOs), which will give rise to molecular orbitals (MOs). Due to the unused p orbital, a  $\pi$  bond will be created in addition to the  $\sigma$  bonds.



It is the presence of this bond that explains the planarity of the molecule. Indeed, for lateral overlap to occur, the two p orbitals must be parallel to each other.

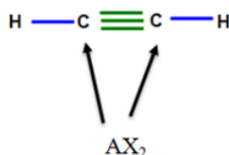


As shown in the diagram above, the  $sp^2$  hybrid orbitals are in the same plane and the pure p orbitals are parallel, therefore  $\pi$  bonding is possible. In the case of the diagram below, the  $sp^2$  orbitals are in two different planes and the p orbitals are non-parallel, therefore  $\pi$  bonding is impossible.

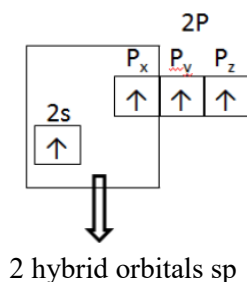


### g) Linear combination of 2 atomic orbitals

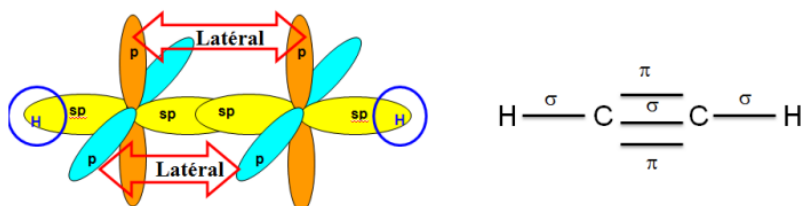
Example: Acetylene:  $C_2H_2$ : linear molecule



To describe this molecule, we will use hybrid atomic orbitals obtained by linear combination of the 2s atomic orbital and a single 2p atomic orbital. This results in 2 hybrid sp atomic orbitals and 2 atomic orbitals that remain pure 2p.



These hybrid orbitals are denoted sp and point 180° apart. As before, the molecule will be formed by the overlap of the hybrid atomic orbitals with each other and with the 1s orbitals of hydrogen. Here, two lateral overlaps will lead to the formation of two π bonds.



### h) Other Types of Hybridization

To obtain the other types of molecular geometry AX5 and AX6, we will use hybrid orbitals involving d-type atomic orbitals:  $sp^3d$  for AX5 and  $sp^3d^2$  or  $d^2sp^3$  for AX6. The most frequent cases of atomic orbital hybridization correspond to the geometric forms already described in the VSEPR method.

## 6. The LCAO Method

### c) Mathematical Aspect of the Covalent Bond

This method consists of considering the molecular wave function as a Linear Combination of Atomic Orbitals (LCAO).

*Example: Dihydrogen molecule  $H_2$*

The electron of the hydrogen atom HA occupies the 1sA atomic orbital. It is therefore described by the wave function  $\Psi_A$ .

The electron of the hydrogen atom HB occupies the 1sB atomic orbital. It is therefore described by the wave function  $\Psi_B$ .

In the HA-HB molecule, the two bonding electrons occupy a molecular orbital.

They are described by the function  $\Psi_{AB}$ , which is a linear combination of the functions  $\Psi_A$  and  $\Psi_B$ , calculated using this formula:

$$\Psi_{AB} = a\Psi_A + b\Psi_B$$

#### d) Energy aspect of the covalent bond

Ultimately, by overlapping, the two atomic orbitals of the same energy give rise to two molecular orbitals of different energies: one stabilized bonding orbital and the other destabilized antibonding orbital.

It can be shown, and we will accept, that the destabilization of the antibonding orbital is greater than the stabilization of the bonding orbital.

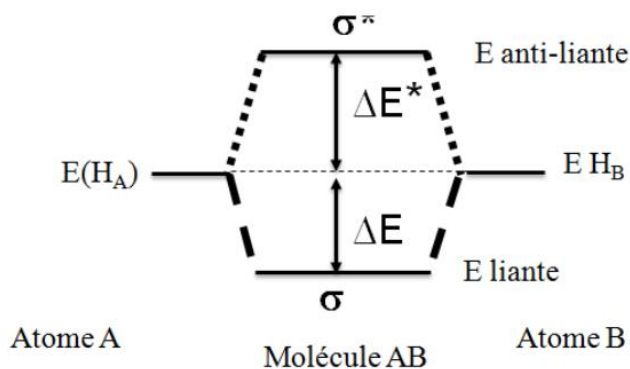


Figure V-3: Energy levels of the bonding and antibonding orbitals of the AB molecule.

The energy differences between molecular levels correspond to the emission (or absorption) of photons in the UV and visible ranges.

The various filling rules used for atoms will also be valid for molecules. They can be summarized as follows:

- A given molecular orbital contains a maximum of 2 electrons.
- An electron is placed in each molecular orbital of the same energy before pairing two electrons in the same level.

The order in which molecular levels are filled by electrons is shown in the diagram below:

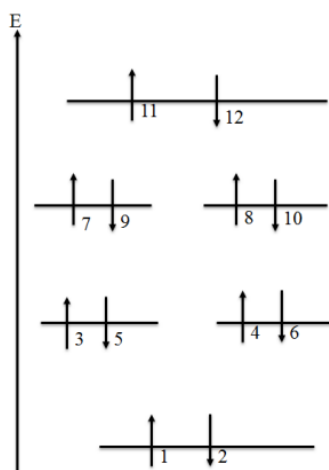


Figure V-4: Order of filling of molecular levels by electrons.

## Applied exercises

### Exercise 01

1. Give the Lewis dot notation for the following molecules and ions:  $\text{H}_2$ ;  $\text{Cl}_2$ ;  $\text{H}_2\text{O}$ ;  $\text{H}_3\text{O}^+$ ;  $\text{NH}_3$ ;  $\text{NH}_4^+$ ;  $\text{CH}_4$ ;  $\text{C}_2\text{H}_6$ ;  $\text{SF}_4$ ;  $\text{SF}_6$ ;  $\text{PCl}_3$ ;  $\text{PCl}_5$ ;  $\text{NCl}_3$
2. Which of these compounds do not obey the octet rule?
3. Based on the electronic structures of sulfur and phosphorus atoms, explain the formation of the molecules  $\text{SF}_6$  and  $\text{PCl}_5$ .
4. Predict the different possible valences of phosphorus. Both chlorides  $\text{PCl}_3$  and  $\text{PCl}_5$  exist. Explain why only the compound  $\text{NCl}_3$  is known, while the compound  $\text{NCl}_5$  does not exist.

### Exercise 02

1. Summarize the main results obtained during the study of H-H bond formation.
2. What molecular orbitals can form during the overlap of the s-s, s-p, and p-p orbitals?
3. Represent the spatial arrangement of these molecular orbitals.

**Chapter 06:**  
**Radioactivity**  
**Nuclear reactions**

## Preface

Radioactivity is the natural property of certain atomic nuclei to spontaneously emit radiation. This corresponds to a spontaneous search for nuclear stability.

This emission of radiation accompanies the phenomenon of radioactive disintegration, which transforms the nucleus of the “father” element (X) into a daughter nucleus (Y). Thus, the nucleus of a radioactive isotope will spontaneously transform into a nucleus of a more stable isotope of the same element, or even into a nucleus of an isotope of another chemical element.

### 1. Definition

Radioactivity is defined as the emission of particles and radiation from nuclear reactions. These nuclear reactions include radioactive decay by unstable atomic nuclei, fission, and fusion.

The spontaneous emission of radiation from the nucleus of certain elements constitutes radioactivity. It was discovered by Becquerel in 1896 who showed that Uranium salts impress a photographic plate.

**a) Natural radioactivity** is all the elements present on earth that exist in nature.

Examples:

- *Uranium-238 & Thorium-232*: Found in rocks and soil, decaying into radon gas, a major source of natural radiation.
- *Potassium-40 (K-40)*: Present in foods like bananas, beans, and meat, essential for life but radioactive.
- *Carbon-14 (C-14)*: Naturally occurring isotope found in all living things, used for dating.
- *Cosmic Rays*: High-energy particles from space interacting with Earth's atmosphere.

**b) Artificial radioactivity** is that obtained by bombardment of atomic nuclei by particles (neutrons, protons, particles ( $\alpha$ ), electrons, positrons, etc.).

Examples:

- *Technetium-99m (Tc-99m)*: Used extensively in medical scans (SPECT) for imaging bones, heart, and brain.
- *Iodine-131 (I-131)*: Used to treat thyroid cancer and hyperthyroidism.
- *Cobalt-60 (Co-60)*: Used in radiation therapy for cancer treatment and industrial sterilization.
- *Plutonium & Americium*: Produced in nuclear reactors, used in smoke detectors (Americium-241).
- *Tritium (H-3)*: Used in self-powered lighting (betalights) and as a tracer.

## 2. Types

Typically, the breakup occurs with the emission of one or more particles, called  $\alpha$  particles,  $\beta$  particles, and  $\gamma$  rays.

- $\beta$  particles we have already seen: they are negatively charged (or sometimes positively charged) electrons.
- $\alpha$  particles are helium nuclei (two protons plus two neutrons).
- $\gamma$  rays are particles of light. They are very energetic particles of light, but they are electromagnetic waves, or rays, nevertheless.

These three types of emitted particles ( $\alpha$ ,  $\beta$ , and  $\gamma$ ) have obvious differences, but can easily be distinguished by the way they are (or are not) deflected by a magnetic field.

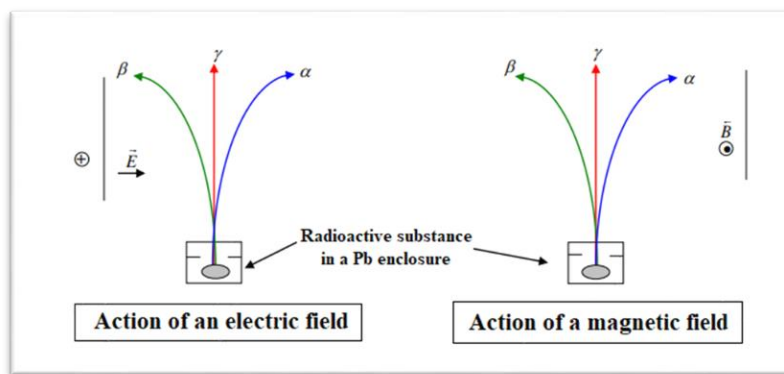
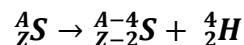


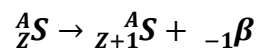
Figure VI-1: The forms of radioactivity

- ✚ **The  $\alpha$  rays** deflected to the right (in both cases) are made up of heavy positive particles. These are helium  $\text{He}^{2+}$  nuclei. When an  $A$  particle ( ${}^4_2\text{He}^{27}$ ) is emitted, the atomic number of the radioactive action decreases by 2 units and its mass by  $u$ .

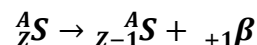


- ✚ **The  $\beta$  rays** deviate to the left (in both cases) by measurements it has been shown that they are electrons. The  $\beta$  rays are more penetrating than  $\alpha$ . There are two kinds of  $\beta$ :

- Certain nuclei emit negative electrons (negatons)  $\beta^-$ , in this case the atomic mass remains constant, but the atomic number increases by one unit:



- Certain nuclei emit positive electrons (positron)  $\beta^+$ , in this case the atomic number decreases by one unit:



- ✚ **The  $\gamma$  rays** are not deflected. These are electromagnetic radiations of very short wavelengths (1 to  $10^{-9}$  A) equivalent to the X-ray; these rays have very high energy and they are very penetrating, but less

ionizing. The  $\gamma$  emission causes integrations, changes neither A nor Z. However, the mass balance shows that the mass of the elements at the start is greater than the mass of the elements we end up with. This difference is transformed into energy.

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

Where:

$E$  is energy

$h$  is Planck constant

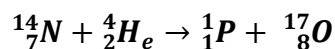
$v$  is frequency

$c$  is speed of light

$\lambda$  is wavelength

### 3. Artificial radioactivity and nuclear reactions

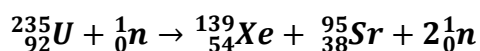
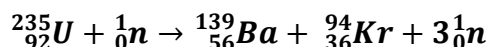
This is the radioactivity caused on certain nuclei following human intervention. The first artificial radioactive nuclei were obtained by Rutherford in 1919, by bombarding nitrogen atoms with  $\alpha$  particles which led to the formation of new nuclei (isotope of oxygen and proton).



### 4. Types of nuclear reactions

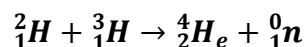
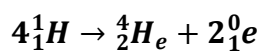
#### a. Nuclear fission

When the atoms with very high mass number A bombarded by neutrons can undergo breakage leading to lighter atoms and regeneration of neutrons.



#### b. Nuclear fusion

During this type of reaction, two light nuclei will fuse to give a heavier and diverse atom.



#### c. Transmutation

These reactions produce nuclides with a mass number equal to or very close to that of the nuclide which served as the target. The nuclides formed are stable or radioactive.

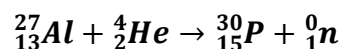


Figure VI-2: Types of Nuclear reactions

## 5. Kinetics of radioactive decay

### a. Radioactive decay law

The decomposition of a radioactive element can be very rapid, a few milliseconds, or extremely long, several or thousands of years. This decomposition is defined by the rate law of a first order reaction. According to the radioactive decay law, when a radioactive material undergoes either  $\alpha$  or  $\beta$  or  $\gamma$  decay, the number of nuclei undergoing the decay per unit time is proportional to the total number of nuclei in the given sample material.

The radioactive decay law states that “*The probability per unit time that a nucleus will decay is a constant, independent of time*”.

$$\frac{d[N]}{dt} = -\lambda N = \frac{d[N]}{N} = -\lambda t$$

Where:

$[N]$  represents the concentration of the radioactive species at time  $t$ .

$\lambda$  is the constant of proportionality ( or radioactive decay constant or disintegration constant).. its units:  $s^{-1}$ ,  $min^{-1}$ ,  $h^{-1}$ ,  $day^{-1}$ , ....

- The total decay rate  $R$  of a radioactive sample is called the activity of that sample which is represented with the unit Becquerel, in honour of its scientist.

$$1 \text{ becquerel (Bq)} = 1 \text{ decay per second (d.p.s).}$$

- Another unit is the curie:

$$1 \text{ curie ( Ci)} = 3.7 \times 10^{10} \text{ Bq.}$$

$$\int_{N_0}^{N_t} \frac{dN}{N} = -\lambda \int_0^t dt \rightarrow (LnN)_{N_0}^{N_t} = -\lambda(t)_0^t$$

$$LnN_t - LnN_0 = -\lambda t \rightarrow Ln \frac{N_t}{N_0} = -\lambda t$$

$$\frac{N_t}{N_0} = e^{-\lambda t}$$

Where:

$[N_0]$  represents the initial concentration of the radioactive species at time  $t = 0$ .

### b. Activity of a radioactive nucleus

The activity of a radioactivity is represented by the number of decays that occur per second.

$$A = \lambda N_t \rightarrow A = N_0 \times e^{-\lambda t} \rightarrow A = A_0 \times e^{-\lambda t}$$

$$A_0 = \lambda \times N_0$$

**c. Radioactive half-life or half-life time**

Half-life is the length of time it takes for half of the radioactive atoms of a specific radionuclide to decay. A good rule of thumb is that, after seven half-lives, you will have less than one percent of the original amount of radiation.

It is obtained by replacing  $t = T$  and  $N_t = N_0 / 2$

$$\int_{N_0}^{\frac{N_0}{2}} \frac{dN}{N} = -\lambda \int_0^T dt \rightarrow (\ln N)_{\frac{N_0}{2}}^{N_0} = -\lambda(t)_0^T$$

$$\ln N_0 - \ln \frac{N_0}{2} = -\lambda T \rightarrow \ln \frac{N_0}{\frac{N_0}{2}} = -\lambda T$$

$$\ln N_0 - \ln 2 - \ln N_0 = -\lambda T \rightarrow \ln 2 = \lambda T$$

$$t_{1/2} = T = \ln 2 / \lambda$$

**6. Applications of radioactivity**

The use of radiation can be positive and negative

Positive	Negative
<ul style="list-style-type: none"> <li>✓ Medicine: imaging, radio, scanner, scintigraphy, radiotherapy, sterilization of materials and instruments, example: Detection of cancerous tumors, Study of brain functioning.</li> <li>✓ Science: Dating, example: the age of rocks (Half-life (T1/2))</li> <li>✓ Food: sterilization and conservation</li> <li>✓ Agriculture: tracers</li> <li>✓ Environment: marking</li> <li>✓ Energy: electricity production</li> </ul>	<ul style="list-style-type: none"> <li>✓ Nuclear tests and bombs</li> <li>✓ Waste</li> <li>✓ Accidents</li> </ul>

## Applied exercises

### Exercise 01

The Rubidium ( ${}^{84}_{37}\text{Rb}$ ) nucleus disintegrates spontaneously by emitting  $\beta$  particle

- 1- Write the decay reaction.
- 2- At time  $t_0$ , a sample of Rb contains  $3.2 \times 10^{20}$  nuclei. After 5 minutes, a quantity of  $3.1 \times 10^{20}$  nuclei disintegrates. Calculate:
  - a) The radioactive constant and the half-life  $T$ .
  - b) The time required for only  $1.6 \times 10^{10}$  nuclei of Rb to remain.
  - c) What is the mass of Rb that will have an activity of 1 Curie? Data:  $1\text{Ci} = 3,7 \cdot 10^{10}$  dps

### Exercise 02

1. Through natural radioactivity, radium transforms into an inert gas and radon. A 35.38% decay of radium occurs every 1000 years.
  - a) Determine the radioactive decay constant of this transformation and the half-life  $T$ .
  - b) What is the mass of radium with an activity of 1 Ci?
2. What is the activity, expressed in curies, of a radioactive source consisting of 500 mg of strontium ( ${}^{90}\text{Sr}$ ) if its half-life is 28 years?
  - a) What happens to this activity one year later?
  - b) After how much time is this activity reduced by 10%?

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