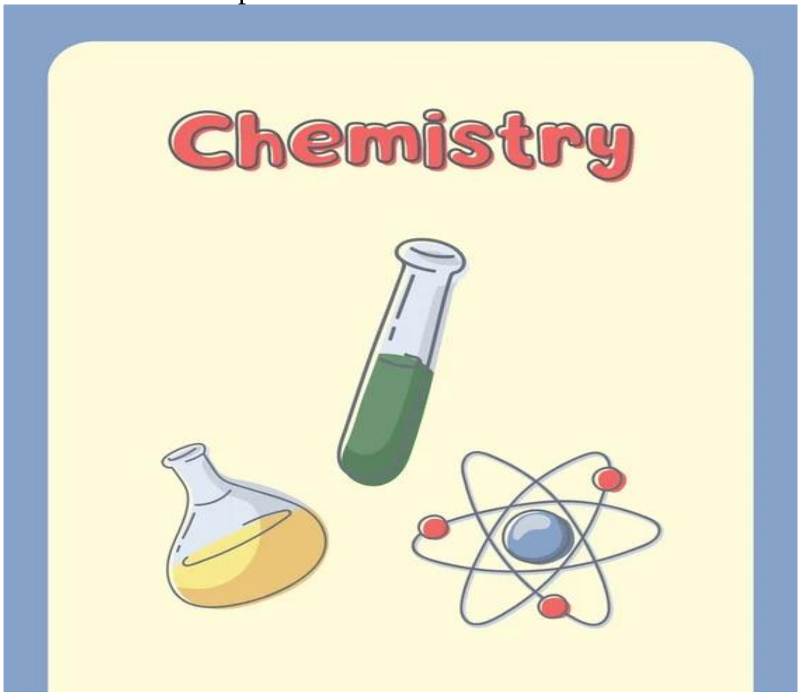
PEOPLE'S DEMOCRATIC REPUBLIC OF ALGERIA
MINISTRY OF HIGHER EDUCATION AND SCIENTIFIC RESEARCH
Ziane Achour University -DJELFA
Faculty of Material and Computer Sciences
Department of Matter Sciences



Structure of Matter Handout Course

Dr. AISSAOUI RAGADIA

2023-2024

The present *Handout Course*
Begins with a Foreword

Chemistry is widely recognized as a fundamental component within the annals of scientific history and the modern global landscape. The field of general chemistry encompasses the study of the reactivity shown by elements and their compounds. Additionally, it offers a comprehensive examination of the fundamental principles that form the basis of the discipline of chemistry. As such, it serves as the foundational component of the basic scientific education provided to aspiring chemists. The foundational education in the field of chemistry for aspiring scientists. This course encompasses the exploration of theoretical advancements and use mathematical methodologies to comprehend specific concepts within the realm of structural chemistry. This course is designed to serve as an excellent educational resource for undergraduate students, particularly those pursuing a first degree in science (L1). Its primary focus is on providing comprehensive instruction in general chemistry within the context of matter sciences and technology, as well as related fields such as medical and biological sciences. The curriculum for Science and Technology students delineates this course into six distinct chapters.

Chapter I: Basic Concepts;
Chapter II: Main Constituents of Matter;
Chapter III: Radioactivity and Nuclear Reactions;
Chapter IV: Electronic Structure of the Atom;
Chapter V: Periodic Classification of Elements;
Chapter VI: The Nature of Chemical Bonds.

Table of contents

CHAPTER I. Basic Concepts

CHAPTER II. Main Constituents of Matter.

CHAPTER III. Radioactivity - Nuclear Reactions.

CHAPTER IV. Electronic Structure of the Atom.

CHAPTER V. Periodic Classification of Elements.

CHAPITRE VI. Chemical Bonds.

CHAPTER I - Basic Concepts.

I. The state of matter

What is Matter in Chemistry? In the field of chemistry, matter refers to any substance that occupies space and possesses mass. According to scientific findings, matter consists of little particles that are imperceptible to the naked sight. It has been empirically noted that matter manifests in several states throughout the natural world. Certain substances exhibit rigidity and maintain a stable shape, such as wood and stone. Conversely, other substances possess the ability to flow and conform to the shape of their container, as exemplified by water. Additionally, there exist forms of matter, such as air, that lack a definitive shape or size. Matter can be categorized into distinct classifications based on their observable physical qualities and the various states in which they manifest. These classifications are commonly referred to as states of matter. There are three states of matter: solid, liquid, and gas.

I.1. Matter Definition Chemistry

Chemistry is an academic discipline that focuses on the investigation of the constituent elements and their respective arrangements within matter, as well as the examination of the many processes by which matter undergoes alteration or conversion. The term "substance" is frequently seen as interchangeable with "matter"; but, within the realm of chemistry, a substance is defined more restrictively. Chemistry encompasses the investigation of the properties and interactions of substances. Chemistry encompasses the study of the composition, structure, and properties of matter, as well as the investigation of the phenomena that arise when various types of matter undergo transformations. The concept of matter theory encompasses the evolving concepts and frameworks employed to elucidate and comprehend the physical realm. A significant portion of matter theory was founded upon a theoretical framework concerning the fundamental constituents known as the elements.

I.2. Solid Definition

- In solids, particles are tightly or closely packed.
- The gaps between the particles are tiny and hence it is tough to compress them.
- Solid has a fixed shape and volume.
- Due to its rigid nature, particles in solid can only vibrate about their mean position and cannot move.
- Force of attraction between particles is adamant.
- The rate of diffusion in solids is very low.
- An example of solids: solid ice, sugar, rock, wood, etc.

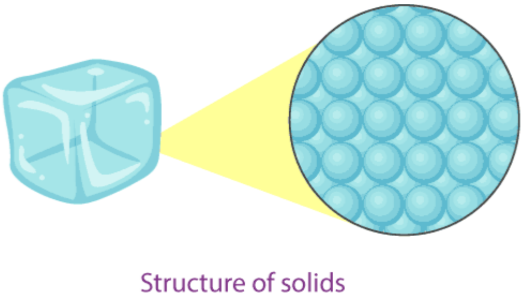


Figure I.1: Structure of solids

I.3. Liquid Definition

- In a liquid state of matter, particles are less tightly packed as compared to solids.
- Liquids take the shape of the container in which they are kept.
- Liquids are difficult to compress as particles have less space between them to move.
- Liquids have fixed volume but no fixed shape.
- The rate of diffusion in liquids is higher than that of solids.
- Force of attraction between the particles is weaker than solids.
- Example of a liquid state of matter: water, milk, blood, coffee, etc.

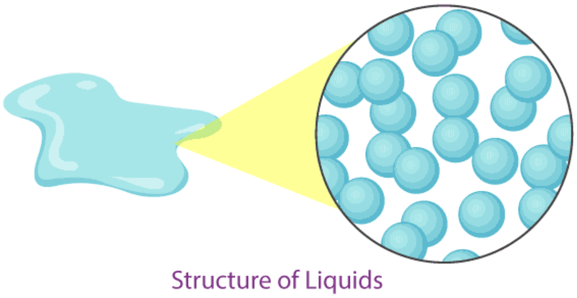


Figure I.2: Structure of liquids

I.4. Gas Definition

- In gases, particles are far apart from each other.
- Force of attraction between the particles is negligible, and they can move freely.
- Gases have neither a fixed volume nor a fixed shape.
- The gaseous state has the highest compressibility as compared to solids and liquids.
- The rate is diffusion is higher than solids and liquids.
- The kinetic energy of particles is higher than in solids and liquids.
- An example of gases: air, helium, nitrogen, oxygen, carbon dioxide, etc.

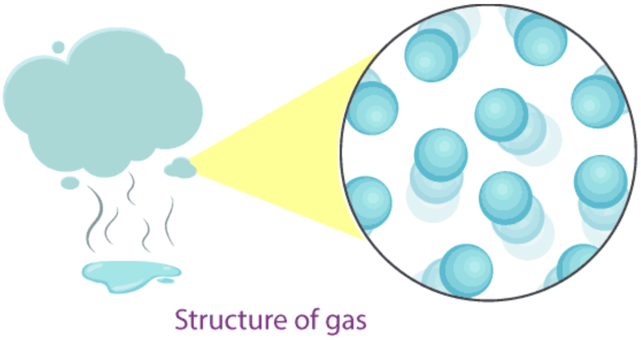


Figure I.2: Structure of gas

II. Change of state of matter

Solid-state, liquid-state, and gaseous-state are three states of matter, and any physical change in their state is called a change of state of matter. These changes are reversible in nature means they can attain any state again and again. This reversible property of the three states depends upon different parameters and conditions which will be discussed below.

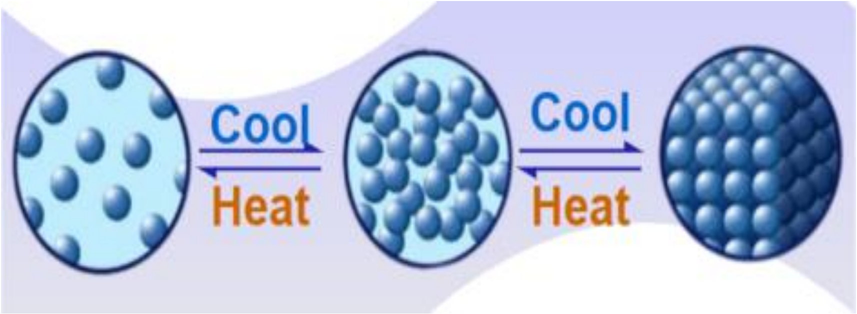


Figure I.3: Change of state of matter

A physical change in a matter is referred to as a change of state of matter. They are reversible modifications that do not require any changes in the matter's chemical composition. Melting, freezing, sublimation, deposition, condensation, and vaporization are examples of common state transitions.

We can understand the meaning of a change of states of matter in one more way i.e. when a solid is heated it changes into liquid, and when a liquid is heated it changes into a gas, and when a gas is cooled it changes to a liquid when a liquid is cooled it changes to solid. And, we can interchange these states by:

- Changing Temperature.
- Changing Pressure.

Why do States of Matter Change?

The change in state occurs due to the following factors:

- Changing the Temperature

- Changing the Pressure
- Changing the Intermolecular Space and Force of Attraction
- Changing the Kinetic Energy of Particle

Let's learn about them Changing the Temperature and Changing the Pressure and the other in detail.

II.1. Changing the Temperature

The temperature effect on heating a matter depends upon the nature of the matter and the conditions required in bringing the change. So, let's discuss all the 6 interchanges between these states now.

II.1.1. Solid to Liquid change

This process is known as **Melting**. The process in which a solid substance changes into a liquid on heating is called melting. On increasing the temperature of the solid the kinetic energy of the particle increase which overcomes the force of attraction between the particles thereby solid melts and is converted into liquid.

II.1.2. Liquid to Gas change

This process is known as **Boiling** or **Vaporization**. The process in which a liquid changes into gas rapidly on heating is called boiling. The temperature at which a liquid boils and changes rapidly into gas at atmospheric pressure is called the boiling point of the liquid.

II.1.3. Gas to Liquid Change

This process is known as **Condensation**. The process of changing gas into liquid by cooling is called condensation. Condensation is the reverse of boiling.

II.1.4. Liquid to Solid Change

This process is known as **Freezing**. The process of transformation of liquid into a solid by cooling is called freezing. Freezing means solidification. It is the reverse of the melting process.

II.1.5. Solid to Gas Change

This process is known as **Sublimation**. The change of solid directly into vapor on heating without passing through the intervening liquid state is called sublimation. The common substances which undergo sublimation are ammonium chloride, iodine, camphor, naphthalene, and anthracene. For example; Solid carbon dioxide (or dry ice) sublimes to form carbon dioxide gas. Naphthalene balls disappear with time without leaving behind any residue.

II.1.6. Gas to Solid Change

This process is known as **Deposition** or **De-sublimation**. It is a thermodynamic process in which gas changes into a solid directly without entering into the liquid phase.

II.2. Changing the Pressure

The physical state of matter can also be changed by changing the pressure. By applying high pressure the particles of a gas can be brought close together means gases can be liquefied easily by applying pressure and reducing temperature. When pressure is applied particles come together thus the force of attraction increases and intermolecular space decreases.

Hence, gas liquefies. When pressure around the solid carbon dioxide is reduced its temperature increases and it directly changes into carbon dioxide gas.

II.3. Inter-conversion of Three States of Matter

The states of matter are inter-convertible. The state of matter can be changed by changing the temperature or pressure. The transition of one state to another is referred to as the inter-conversion of matter. It is a process in which matter transitions from one state to another and then returns to its original state with no change in its chemical makeup. Heating may transform solids into liquids.

III. Homogeneous and heterogeneous systems

What are Mixtures?

Mixtures are formed when two or more substances (elements or compounds) mix together without participating in a chemical change. The substances need not necessarily mix in a definite ratio to form a mixture.

Some examples of mixtures include mixtures of sand and water, mixtures of sugar and salt, and mixtures of lime juice and water. There are two primary types of mixtures, namely homogeneous mixtures and heterogeneous mixtures.

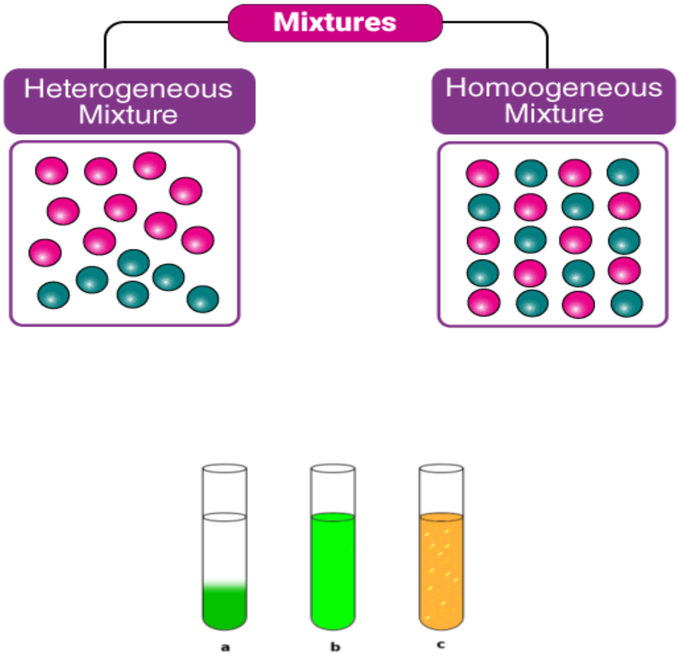


Figure I.4: Homogeneity and heterogeneity; only "b" is homogeneous

III.1. Heterogeneous and Homogeneous Definition

What is a Homogeneous Mixture?

These are the types of mixtures in which the components mixed are uniformly distributed throughout the mixture. In other words, ***"they are uniform throughout"***. We can observe only one phase of matter in a homogeneous mixture. Key points regarding such mixtures are:

- Particles are distributed uniformly
- We can't judge a homogeneous mixture by just seeing it
- Homogeneous mixtures are also called solutions
- Uniform composition
- **Example:** rainwater, vinegar, etc.

What is a Heterogeneous Mixture?

This is a type of mixture in which all the components are completely mixed and all the particles can be seen under a microscope. We can easily identify the components and more than one phase can be seen by naked eyes.

Key points regarding this type of mixture:

- Particles are distributed non-uniformly
- We can judge a heterogeneous mixture by just seeing it
- Non-uniform composition
- **Example:** seawater, pizza, etc.

III.2. Difference between Homogeneous and Heterogeneous Mixture

Homogeneous mixture	Heterogeneous mixture
It has a uniform composition	It has a non-uniform composition
It has only one phase	There are two or more phases
It can't be separated out physically	It can be separated out physically
"Homo" means the same	"hetero" means different
Example: a mixture of alcohol and water	**Example:** a mixture of sodium chloride and sand

Table I: Difference between Homogeneous and Heterogeneous Mixture

IV. Notions of atoms and molecules

IV.1. Structure of the atom

IV.1.1. The nucleus and electrons

Atoms are made up of a very dense, positively charged nucleus surrounded by a cloud of negatively charged electrons. The nucleus is made up of two types of particles (protons and neutrons) called nucleons.

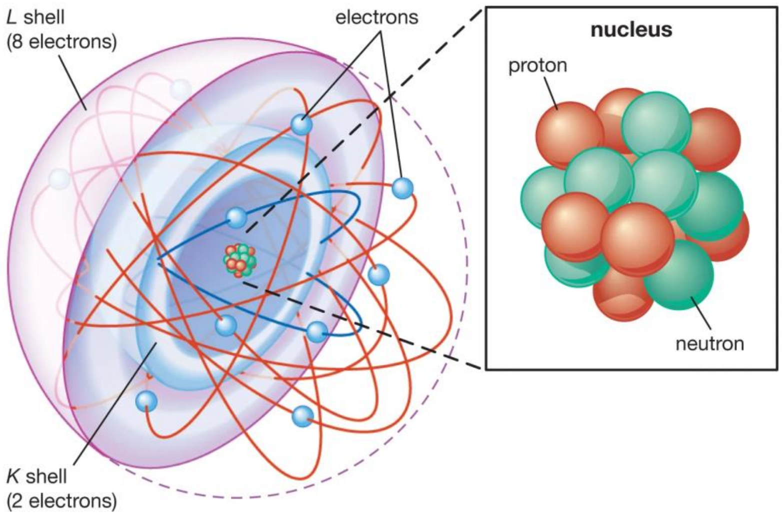


Figure I.5: Structure of the atom

Shell atomic model

In the shell atomic model, electrons occupy different energy levels, or shells. The *K* and *L* shells are shown for a neon atom.

	Electrical load	**Mass**
Nucleus	proton: $q = +\ 1{,}602.10^{-19}$ C	$m_p = 1{,}6726.10^{-27}$ kg $= 1836\ m_e$
	neutron**:** 0	$m_n = 1{,}6747.10^{-27}$ kg $= 1839\ m_e$
	electron: $q = -\ 1{,}602.10^{-19}$ C	$m_e = 9{,}1094.10^{-31}$ kg

IV.1.2. The nuclide

A nuclide is an atomic species symbolized by: **Isotope Symbol**

$$\mathbf{{}^{A}_{Z}X}$$

A: Mass number.

Z: Atomic number.

$$\text{It is defined by} \begin{cases} \text{Z: atomic number} \Rightarrow \text{number of protons} \\ \text{A: mass number} \Rightarrow \text{number of nucleons} \end{cases}$$

Nuclide → ${}^{12}_{6}C$

IV.1.3. Element isotopes

$$\mathbf{A = Z + N}$$

Hence the number of neutrons: **N = A – Z**

Nuclides with the same number of protons (same Z) correspond to the same element.

They have the same name. Example: Magnesium: ${}^{24}_{12}Mg$, ${}^{25}_{12}Mg$, ${}^{26}_{12}Mg$

Isotopes of an element are nuclides with the same atomic number Z, but different mass numbers A.

Example: ${}^{1}_{1}H$ hydrogen and ${}^{2}_{1}H$: deuterium

- Real atomic mass = mass of a real atom: expressed in kg or in u.m.a. (u) (atomic mass unit). The isotope is used as a reference: it is assumed that a real atom weighing $1{,}99625.10^{-26}$ kg corresponds to exactly 12 u ⇒ 1 u = $1{,}66054.10^{-27}$ kg

⇒ $1\ u \approx m_p \approx m_n$

IV.1.4. Avogadro number NA

The number of real atoms contained in 1 mole of the isotope ${}^{12}_{6}C$ of carbon.

Mole = unit of substance and it is assumed that 1 mole of ${}^{12}_{6}\mathrm{C}$ weights exactly 12 g.mol^{-1}

⇒ NA = $12.10^{-3} / 1.99625.10^{-26} = 6.022.10^{23}$ mol^{-1}.

Average atomic mass of an element; mass of this element in a.m.u. considering its isotopes.

$$M = \sum_i \frac{\tau_i M_i}{\sum_i \tau_i}$$

$\tau_1, \tau_2 \dots \tau_n$: % (abundance of the different isotopes of the element) $M_1, M_2, \dots M_n$ their respective atomic masses.

<u>Example:</u>

Natural <u>chlorine</u> contains 75% of the isotope ^{35}Cl and 25% of the isotope ^{37}Cl.

The average atomic mass is: M = (35 x 75) + (37 x 25) / 100 = 35, 5 u.

Molar mass of an element = mass of one mole (symbol: mol) of this element:

mol = set of NA = $6.022.10^{23}$ identical entities (atoms, molecules, particles ...)

<u>Example:</u>

Real atomic mass of 1 atom of the nuclide 14N ≈ 14 u Molar mass of 1 mole of ^{14}N, i.e. the mass of $6.022.10^{23}$ atoms of ^{14}N ≈ 14 g.mol^{-1}

The molar mass (of a mole) of a nuclide expressed in g.mol^{-1} is exactly equal to the atomic mass (of a real atom of this nuclide) expressed in a.m.u.

Molar mass of a molecule = sum of the molar masses of the atoms making up the molecule

Ex: M (H_2O) = (1 x 2) + 16 = 18 g.mol^{-1}.

IV.2. Structure of the molecule

The molecule is the association of two (02) or more atoms such as; H_2O, O_2, CH_3COOH.

IV.2.1. Mole

The mole is the quantity of matter of a system containing N identical entities. It is also defined as the quantity of matter contained in 12 grams of carbon 12 or (^{12}C). Therefore: 1 mole of atoms corresponds to NA = $6.023.\ 10^{23}$

Example:

Determine the number of atoms contained in 12 g of carbon, knowing that the mass of an atom of carbon 12 is 1,9926.10^{-26} Kg. (This mass was determined using a mass spectrometer).

Solution:

1 mol of (carbon 12) corresponds to ===➔ 12g ====➔ N atoms

1.9926 . 10-26 ====➔1 atom

1 mol = 12 / (1,9926 . 10^{-26}) = 6.023 . 10^{23}

IV.2.2. Atomic molar mass

This is the mass of one mole of atom or of N atoms.

Example:

Determine the mass of a sodium atom (Na) knowing that its atomic molar mass is 23g.

Solution:

1 mole of Na atom ====== 23g ======== 6.023. 10^{23} atoms

1 Na atom ======= m Na g ========= 1 atom

m = 23 / (6,023. 10^{-23}) = (3, 8. 10^{-23}).

IV.2.3. Gram atom

The gram atom of an element is the atomic mass of this element expressed in grams (g).

Example: the gram atom of iron represents 56 g of iron.

The gram atom of oxygen represents 16 g of oxygen.

IV.2.4. Molecular mass

This is the mass of one mole of molecule. It is equal to the sum of the molar masses of the atoms that make up the molecule.

Example:

The $Fe(NO_3)_3$ molecule. The mass of a mole is:

M $Fe(NO_3)_3$ = M Fe + 3* ((MN + (3 * MO)) = 56 + 3 * ((14 + (3 * 16)) = 146 g/mol

The mass of a molecule of $Fe(NO_3)_3$:

1 mol of Fe $(NO_3)_3$ ====== 146 g/mol ======== 6.023. 10^{23} molecules

m Fe(NO3)3 g ========= 1 molecule

m = 146 / (6.023. 10^{-23}) = (8.793. 10^{-23} g)

IV.2.5. Molar volume

This is the volume occupied by one mole of substance. In the case of gases, and under normal conditions of pressure and temperature (n = 1mol; T = 0°C; P = 1 atm): ***V = 22,4 l***

Example:

5.38.10^{19} α particles (He^{2+}) lead to 2 cm^3 of helium gas under normal conditions of temperature and pressure. Determine Avogadro's number.

Solution:

1 mol of (He) ====== 22.4 l ======== N atoms

2 * 10^{-3} l ========= 5.38 * 10^{19} atoms

m = 5,38 * 10^{19} / (2 * 10^{-3}) = (6,025 . 10^{23} g)

IV.2.6. Atomic mass unit (a.m.u.):

The atomic mass unit is defined as the fraction 1 /12 of the mass of a carbon atom 12 (12C).

1uma = 1/12 (mass of a 12C atom).1uma = 1/12* 12/6,023∗10^{23} = 1, 66 * 10^{-24} g

1 uma = 1.666 * 10^{-27} g.

V. Qualitative aspect of matter (Classification of matter)

Matter is made up of atoms which can be identical or different. From this, we can distinguish several types (see the diagram below):

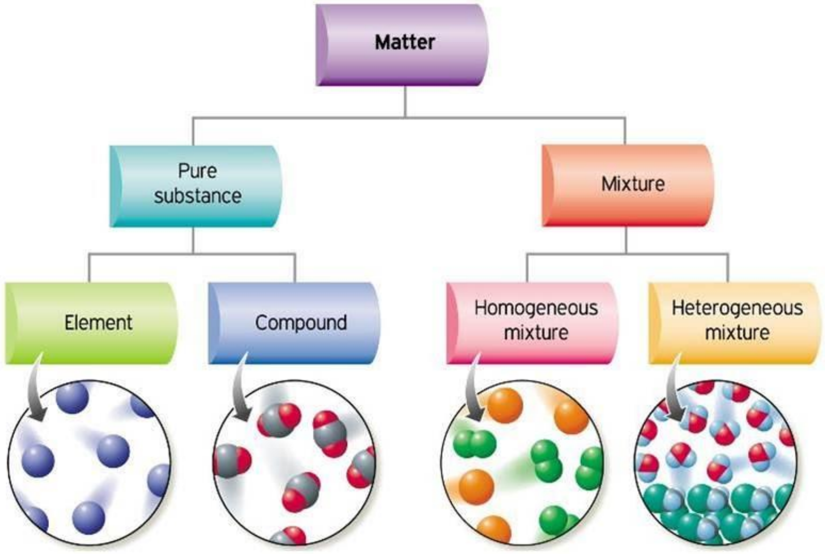


Figure I.6: Classification of matter

1. Simple pure bodies: made up of molecules with identical atoms (Ag, O2, S,...).

2. Compound pure bodies: these are bodies made up of molecules whose atoms are different (NaCl, H_3PO_4, H_2O, etc.).

3. Mixtures: a mixture is a substance made up of different molecules (NaCl + water, Oil + H_2O, ETC.). A distinction is made between

Heterogeneous mixtures: these are mixtures in which we can distinguish, with the naked eye or with the aid of a magnifying instrument, the particles of the bodies that make them up. With the aid of a magnifying instrument. These are mixtures made up of more than one phase.

Homogeneous mixtures: these are mixtures in which we cannot distinguish the particles from the substances that make them up. Particles from their constituent substances. These are mixtures made up of a single phase.

Solution: a homogeneous mixture of pure substances that do not react with each other. The majority (in large proportions) is called the solvent and the dissolved substances are called the solutes.

Water + salt ➔ water (solvent) and salt (solute)

Dilution: diluting an aqueous solution involves reducing its concentration by adding solvent. The initial solution with a higher concentration is called ***the mother solution*** and the solution after dilution is called ***the diluted solution***. After dilution, the quantity of substance is the same. We can write:

$$Cm = n/V$$

$$n = Cm * V$$

Before dilution: $n_1 = C_1 * V_1$

After dilution: $n_2 = C_2 * V_2$

Number of moles is the same: $n_1 = n_2$ (conservation of mass).

Saturation: A solution is said to be saturated if the maximum quantity of solute to be dissolved by the solvent is exceeded. A precipitate appears at the end of the dissolution.

VI. Weight laws

Consider the following chemical reaction:

$$aA + bB \text{ ===}\rightarrow cC + dD$$

The reacting species A and B are called reactants and the resulting species C and D are called products.

The chemical reaction must obey the law of conservation:

Of mass (the mass of the product formed must be equal to the mass of the reactants);

Of charge;

Of matter.

VII. Quantitative aspect of matter

VII.1. The mole number

The mole number is the ratio between the mass of the compound and its molar mass.

$$n\,(mol) = m/M$$

Or: n: mole number,

m: the mass of the compound,

M: the molar mass of the compound.

VII.2. Molar concentration or molarity

The molarity of a solution is the ratio of the number of moles of solute in a volume (expressed in litres) of solution, the unit of which is the mole per litre [mol/l].

It is represented by the symbol M.

VII.3. Molality

The molality of a solution, the unit of which is represented by the symbol m, is the number of moles of solute per kilogram of solvent. ***The molality (m)*** cannot be calculated from ***the molarity (M)*** Or ***normality (N)*** unless the density of the solution is known. This concentration has the advantage of not depending on the volume of the solution and therefore on the temperature and pressure.

VII.4. Weight or mass concentration

Mass concentration is the ratio between the mass of the compound and the volume of the solution.

$$Cm = mi / \textit{solution volume}$$

VII.5. Weight or mass fraction

This is the mass of constituent (i) considered over the total mass of the mixture. It is given by the relationship below:

$$\%mass = mi \ / \ \textit{total mass of the mixture}$$

Example:

A gas mixture consists of 0.2 g of H_2, 0.21 g of N_2 and 0.51 g of NH_3 at a pressure of 1 atmosphere and a temperature of 27°C. Calculate the mole fractions.

Solution:

We have: $\%mass = mi \ / \ \textit{total mass of the mixture}$

M tot = $mH_2 + mN_2 + mNH_3 = 0.2 + 0.21 + 0.51 = 0.92$ g

$XH_2 = mH_2 / mtot$ = 0.2/ 0.92 = 0.2174 or 21.74% in mass

$XN_2 = mN_2 / mtot$ = 0.21/0.92 = 0.2282 or 22.82% in mass

$XNH_3 = mNH_3/ mtot$ = 0.51/0.92 = 0.5543 or 55.43% in mass

VII.6. Title

The title of a solution is the mass, in g, of solution in 1 ml of solvent. It is given by the following relationship: $\boldsymbol{TA/B = mA/VA}$

VII.7. Mole fraction

The mole fraction XA of a constituent A of a solution is the ratio of the number of moles of this constituent to the total number of moles of all the constituents of the solution. The sum of the mole fractions of all the constituents of a solution is 1.

$$\boldsymbol{XA = XA/ ntot}$$

Or: n tot = the sum of the number of mol of all the constituents of the solute.

VII.8. Normal concentration or normality

The normality of a solution is the number of gram equivalents of solute contained in one liter of solution. This measure of concentration is inseparable from a particular chemical reaction (acid-base or oxidation-reduction reaction) which is implicitly considered.

The unit of normality is the gram equivalent per litre, represented by the symbol N:

1 N = 1 eg/l.

Given the definition of equivalent mass, the normality of a solution will always be an integer multiple (1, 2, 3, ...) of its molarity, i.e. : N = Z *M

Gram equivalent (g.e.): this is the ratio of the mass of the solute in the pure state to its molar mass or atomic mass. Equivalent molar or atomic mass (m_{eq}): this is the molar or atomic mass of the element in question, divided by the number of electrons. Element to the number of electron, proton or hydroxyl exchanged during a reaction.

$$CN = N = neq \text{ of solute}/V = m \text{ of solute } /meq /V = m \text{ of solute}/M /Z/V$$

With: M: Molar mass of solute; Z: Number of proton, electron or hydroxyl exchanged.

VII.9. Volumic mass and density

VII.9.1. Volumic mass

Density is a physical quantity which characterises the mass of a material per unit of volume. It is determined by the ratio:

$$\rho = m/V \ Kg /m^3 \text{ or } g /cm^3$$

Where m is the mass of the homogeneous substance occupying a volume V.

VII.9.2. Density:

a. Solid-liquid density

The density of a solid or liquid in relation to water is the ratio of the mass of a certain volume of this body to the same mass of a volume of water. To the same mass of volume of water. It is given by the following relationship

$$d = \rho \text{ pure compounds } (\text{s ou l}) /\rho eau = m/V/m'/ V = m/m'$$

b. Density of gases

In the case of gases or vapors, the gaseous reference body is air at the same temperature and pressure, under the same pressure.

VIII. Raoult's laws

At a given temperature, any pure liquid is in equilibrium with its vapour phase.molecular level by: Condensation rate = Vaporisation rate. For Raoult, who was the first to study the phenomenon: "The vapor pressure of the solvent (A) of a mixture (A, B) is proportional to its molar fraction in the mixture".

$$P_A = X_A * P_A^{Sat}$$

CHAPTER II: Main constituents of matter.

I. Introduction: FARADAY's experiment

Around the 10th century, FRANKLIN by rubbing bars of glass or wax with a silk cloth, observed phenomena of attraction and repulsion between the bars. Observed phenomena of attraction and repulsion between the bars, which implies the existence of an electric fluid. After this experiment, FARADAY, by carrying out the electrolysis of water, was able to establish a relationship between the quantity of matter and the quantity of electricity.

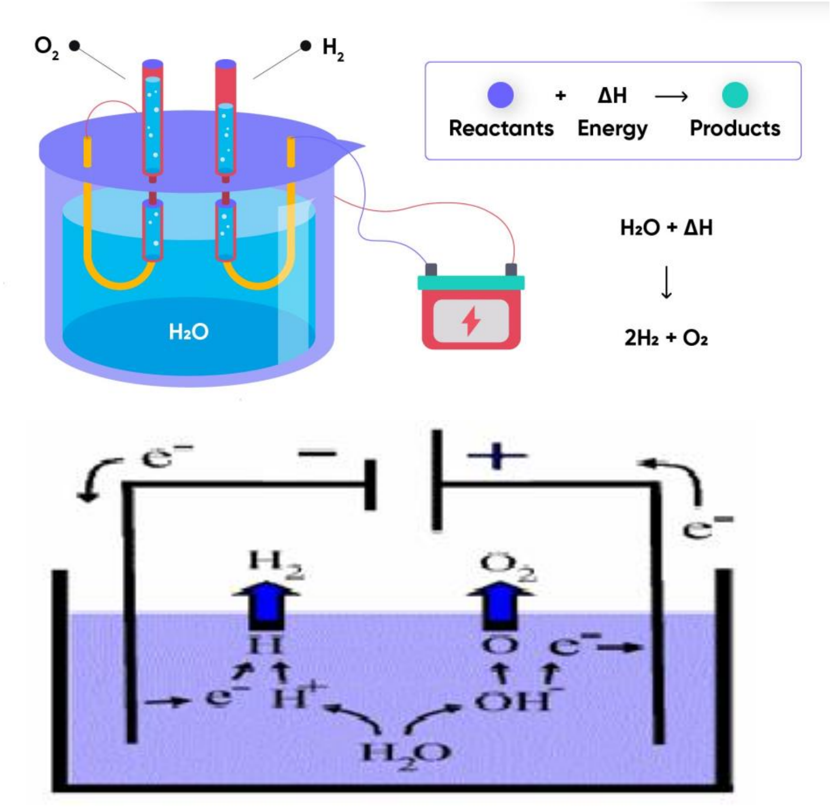


Figure II.1: Diagram of water electrolysis

Now that we have hydrogen gas floating to the surface, lets take a look at the hydroxide ion. The negatively charged hydroxide ions travel to the position anode where an electron is removed and completes the circuit. The hydroxide ion then recombines with three other hydroxide molecules to from 1 molecule of oxygen and 2 molecules of water:

$$4OH^- \rightarrow O_2 + 2H_2O + 4e^-$$

N * e- = 1 Faraday = 96500 Colomb

$$m = \frac{A * I * t}{n * F} \quad \text{with} \quad Q = I * t \quad \text{we have } m = \frac{A * Q}{n * F}$$

Q = I * t: quantity of electricity

A = atomic mass of the element:

n = number of electrons exchanged during the reaction in question

F = Faraday number

t = time

Several experiments have been carried out to identify the different elementary particles of matter. Have been carried out. These particles were discovered between 1875 and 1910: the proton, the neutron and the electron.

* CROOKES: Discovery of the electron

* GOLDSTEIN: Discovery of the proton

* CHADWIK: Discovery of the neutron.

II. Highlighting the constituents of matter

II.1. The electron

The characteristics of the electron were obtained from the work of **CROOKES, J. PERRIN, MILLIKAN and J.J. THOMSON.**

a- CROOKES experiment and characteristics of cathode radiation:

The CROOKES experiment consists of applying a ddp of 50 KV to a gas in a glass tube between two electrodes. Various phenomena are observed:

*At atmospheric pressure, the current does not flow. So the gas does not conduct of electricity.

* At pressures of between 0.01 and 0.1 atmospheres, the gas becomes luminescent.

This radiation from the cathode, responsible for a faint greenish glow, is called the cathode ray; For CROOKES, the radiation consists of negative particles in motion. An initial anions resulting from the impact of molecules on the cathode.

SCHUSTER then put forward the hypothesis of a negative particle resulting from the ionization of the gas and common to all bodies. (1st approach to the electron).

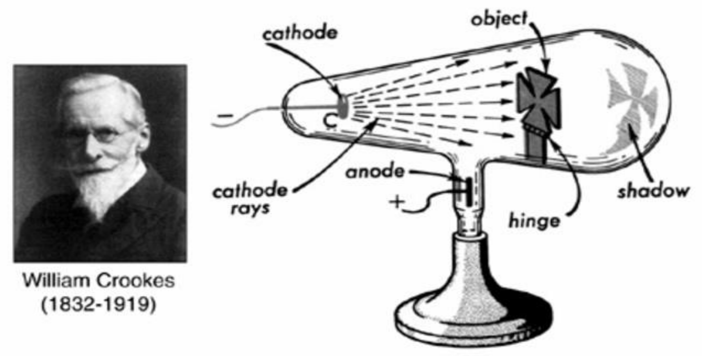


Figure II.2: Illustration of the Crookes X-ray tube.

The concept of negative electricity:

This is the work of JEAN PERRIN, who collected cathode radiation in a Faraday cylinder connected to an electroscope: he noticed that the leaves diverged as a result of the appearance of a negative charge. When subjected to an electric or magnetic field, cathode rays undergo a deviation that prevents them from being charged which prevents it from charging the electroscope .Since all these experiments are independent of the nature of the electrodes and the gas in the tube, the particles making up the cathode rays must be present in all bodies. This is the concept of the electron.

a. J.J. THOMSON experiment (1912): Determination of the e/m ratio

Using the laws of electromagnetism, **J.J. THOMSON** was able to determine the ratio between the charge and mass of the electron. Measurement of the e/m ratio is based on the deflection of an electrified particle by an electric and magnetic field.

b.1. Description of the device

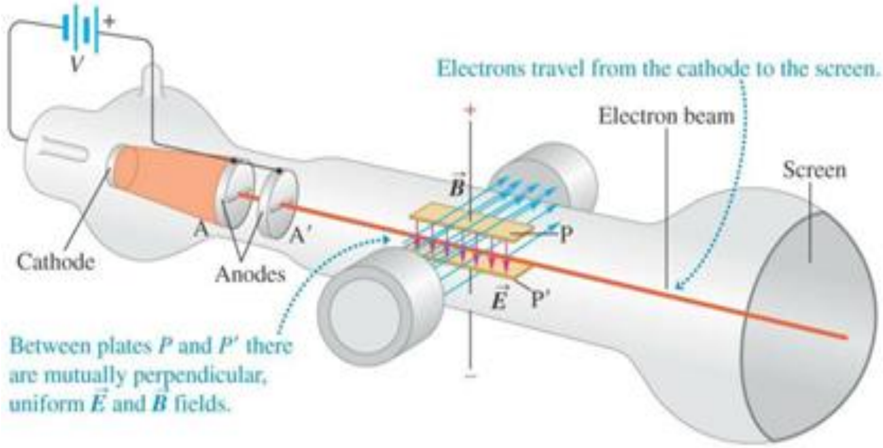


Figure II.3: Diagram of e/m ratio measurement.

Left: Place where the gas is introduced at very high pressure. The ions formed are accelerated by a ddp and pass through the hollow cathode C. From the moment the ions arrive at the hollow cathode, they are no longer subject to any force, and the velocity acquired in the electric field remains constant. Velocity acquired in the electric field remains constant.

Ampoule: Accelerated charged particles pass through an ampoule in a vacuum to avoid any obstacle to their propagation. The propagation of these particles. The accelerated particles pass through a vacuum bulb that flares (widens) towards the receiver so as not to disturb the trajectories of the particles. The bottom of the ampoule has a large surface. It is covered with a thin layer of a solid luminescent material (platinum barium cyanide barium platinocyanide; zinc superlide; ....), which has the property of emitting visible light radiation at any point where an ion strikes it.

The electromagnetic analyzer: this is placed outside the bulb near the cathode. It is made up of an electromagnet and a capacitor whose armatures have exactly the same shape, so that the electromagnetic signals are visible. Exactly the same shape, so that the electric and magnetic fields are rigorously superimposed. This operation produces linear ion trajectories.

b.2. Study of the deviations of the channel rays

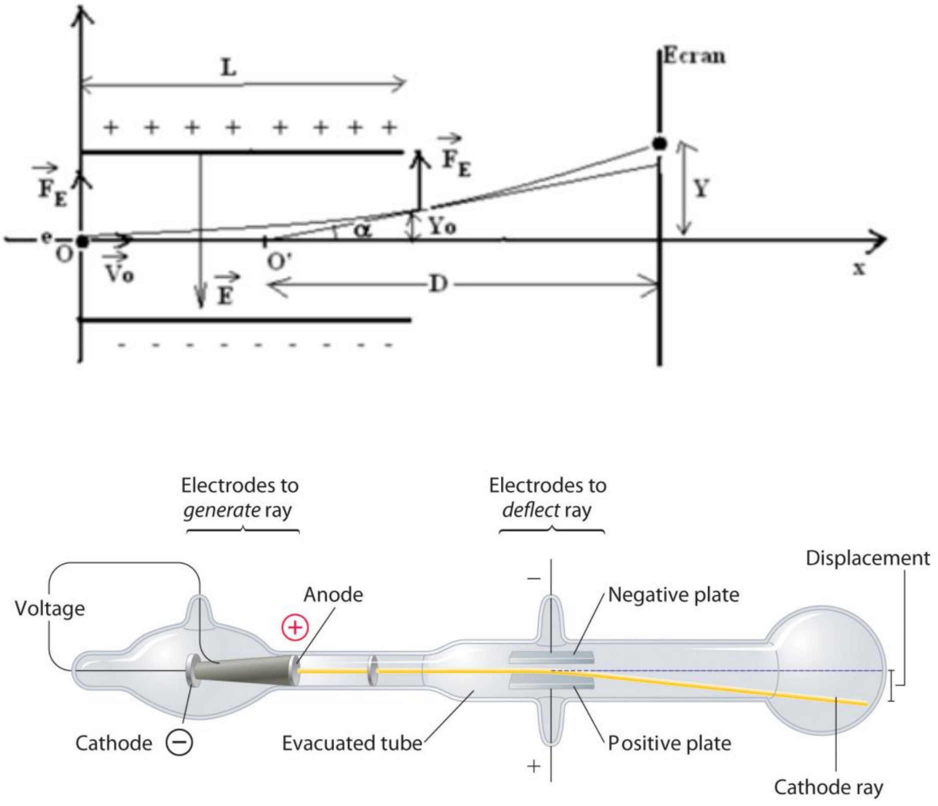


Figure II.4: Deflection of cathode rays.

Action of an electric field:

Consider a particle m with charge q = - e, travelling at speed V_0.

- If the capacitor is not charged, the particle moves along OX.

- If the capacitor is charged, the electron is subjected to a force towards the positive plate along OY of magnitude:

$$Fe = e * E = m_e * \gamma \qquad (1)$$

Following OX: uniform rectilinear motion γn = 0

$$X = V_0 * t \qquad (2)$$

Following OY: uniformly accelerated motion

$$\gamma = \frac{e*E}{m} \qquad (3)$$

Along OY, the motion is uniformly accelerated, so we can write:

$$m * \frac{d^2*y}{dt^2} = e * E \qquad (4)$$

By integrating this equation assuming: at t = 0, y = 0 we find:

$$y_0 = \frac{1}{2}\gamma t^2 = \frac{1}{2}\frac{e}{m}E * t^2 \qquad (5)$$

Following OX: x = V_0 * t → $t = x/V_0$

$$y_0 = \frac{1}{2}\frac{e}{m}\frac{x^2}{V0^2} \qquad (6)$$

At the capacitor output: x = L

$$y_0 = \frac{1}{2}\frac{e}{m}\frac{E * L^2}{V0^2} \qquad (7)$$

Deflection of the electron in a uniform magnetic field:

The electron driven by a velocity $\overrightarrow{Vo}$ perpendicular to the magnetic field $\vec{B}$, is subjected to a force magnetic force $\overrightarrow{Fm}$ opposite to the electric force $\overrightarrow{Fe}$ of intensity:

$$F_m = e * V_0 * B \sin\alpha = e * V_0 * B \qquad (8)$$

$\overrightarrow{Vo}$ is perpendicular to$\vec{B}$: sin α = 1.

The direction of this force is given by the rule of the three fingers of the right hand: the thumb, index finger indicating the direction of the magnetic field, the speed and the magnetic force respectively. The electron's trajectory within the magnetic field is circular with a radius (r) equal to:

$$r = \frac{me * Vo}{e * B} \qquad (9)$$

Deducted from: the magnetic force is equal to the centrifugal force hence:

$$\overrightarrow{|Fc|} = me\,\frac{V0^2}{r} = e * V_0 * B => \frac{me * Vo}{e * B} \qquad (10)$$

Simultaneous action of the two fields:

By applying simultaneously and acting appropriately on the intensities of E and B, we can avoid This means:

$$|\overrightarrow{Fe}| = |\overrightarrow{Fm}| => e * E = e * V_0 * B => V_0 = \frac{E}{B} \qquad (11)$$

Replacing the expression for V0 in the expression for y_0:

$$y_0 = \frac{1}{2}\frac{e}{mo}\frac{E * L^2}{E^2}\,B^2 = \frac{1}{2}\frac{e}{me}\frac{B^2 * L^2}{E}$$

$$\frac{e}{me} = \frac{2*E*ys}{B^2*L^2} \qquad (12)$$

From the measurement of y_0, the experimental parameters E and B and knowing L, it is possible to calculate e/m:

$$\frac{\mathrm{e}}{\mathrm{me}} = 1{,}759 * 10^{11}\ \mathrm{C/Kg}$$

c. MILLIKAN experiment: Determination of the charge |e| and deduction of its mass

c.1. Description of the apparatus:

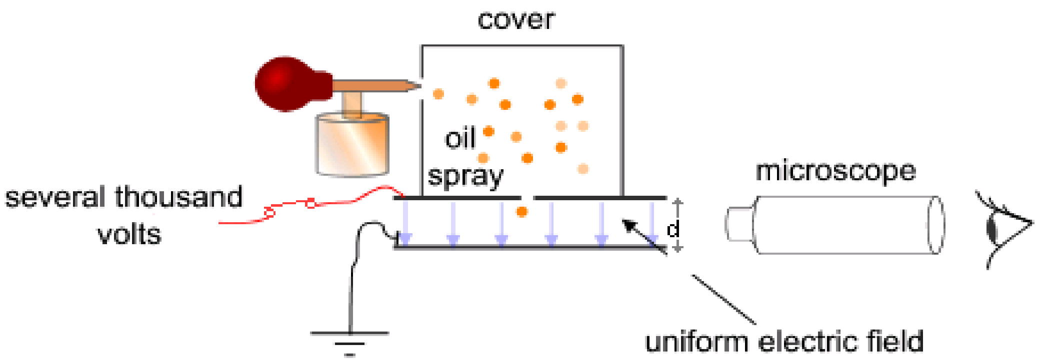
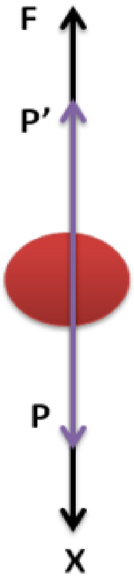


Figure II.5: The MILIKAN experiment.

The experiment involves spraying droplets of oil into the air between the plates of a condenser. Under the effect of X-rays (R-X), the gas becomes ionized and the oil droplets become electrically charged with electricity. The movement of these droplets between the plates of the condenser is followed using a microscope (**Figure II.5**). The radius of the droplets is assumed to be constant.

In the absence of an electric field: the droplet falls freely, subject to the three forces:



Gravity:

$$P = m * g = \rho * V * g = \frac{4}{3}\pi r^3 g \qquad (13)$$

Where: ρ: the density of the oil.

Archimedean thrust due to air of density ρ_a:

$$P' = \pi_A = \frac{4}{3}\pi r^3 \rho_a\, g \qquad (14)$$

Viscous friction force given by Stockes law:

$$F = + 6\pi\eta\, r\, V_0 \qquad (15)$$

Where; V_0: Droplet velocity; r: Droplet radius

It can be seen that the droplets quickly reach a limiting velocity, at which point the acceleration is zero:

$$\sum\overrightarrow{Fex} = \overrightarrow{m * \gamma} = 0 \Rightarrow P - P' - F = 0$$

Let:

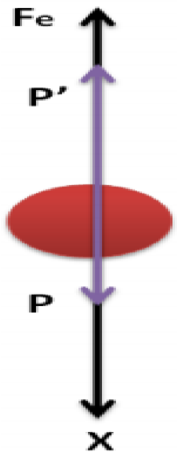
$$\frac{4}{3}\pi r^3 \rho\, g - \frac{4}{3}\pi r^3 \rho_a\, g - 6\pi\eta\, r\, V_0 = 0$$

$$\frac{4}{3} r^2 (\rho - \rho_a)\, g - 6\,\eta V_0 = 0 \Rightarrow r^2 = \frac{9}{2}\,\frac{\eta V0}{2\,(\rho - \rho a\,)g} \qquad (16)$$

By measuring the free-fall velocity V0 of the droplets, we can determine the average radius of the droplets. (The velocity is calculated by measuring the time (t) taken by a droplet to travel a distance d a distance d marked by the microscope ($V0 = d/t$).

c.2. In the presence of an electric field

When the electric field is activated, the droplets move upwards or downwards of the droplets.



Consider a positively charged droplet ($q>0$). The charged droplets are subjected, in the field, to an electric force (F_e):

$$F_e = q * E \qquad (17)$$

An electric field E can be applied so that a droplet is stationary (force of friction are zero) then $F = 0$:

$$\sum \overrightarrow{Fex} = 0 \Rightarrow P - P' - F = 0$$

$$P - q * E - P' - F_e = 0$$

$$q * E = P - P' = \frac{4}{3} \pi r^3 * (\rho - \rho_a) * g \qquad (18)$$

The charge q can then be determined.

MILLIKAN showed that the charges captured by the droplets were all multiples of the elementary charge (e):

$$e = 1{,}6 * 10^{-19} \text{ Colomb}$$

Knowing the ratio e/m, we can deduce the mass of the electron at rest:

$$m_e = 9{,}109 * 10^{-31} \text{ Kg}$$

II.2. The proton: GOLDSTEIN experiment (Demonstration of the positive charge of the nucleus)

The proton was discovered by ***GOLDSTEIN*** in the channel rays. ***GOLDSTEIN*** took up ***CROOKES***' experiment by provoking an electric discharge in a gas, hydrogen. This is decomposed into H^+ by the cathode rays (the ddp ionizes the H_2 molecules to form H^+). The proton beam is observed behind the cathode.

Analysis (q/m measurement) of these protons revealed the following characteristics:

$$q = +e = 1{,}6*10^{-19}\ Colomb$$

$$m_p = 1{,}6726*10^{-27}\ Kg = 1836 * m_e$$

II.3. The neutron: *CHADWICK* experiment (demonstration of the neutron)

Bombardment of a beryllium target by α particulates emits radiation which, by acting on paraffin, causes protons to be expelled. The radiation emitted by beryllium is not deflected by an electric or magnetic field. It can only be electromagnetic radiation electromagnetic radiation or a beam of neutral particles. ***CHADWICK*** demonstrated that it was a beam of neutrons formed during the collision according to the reaction below:

$${}^{9}_{4}\mathrm{Be} + {}^{4}_{2}He \rightarrow {}^{12}_{6}\mathrm{C} + {}^{0}_{1}\eta$$

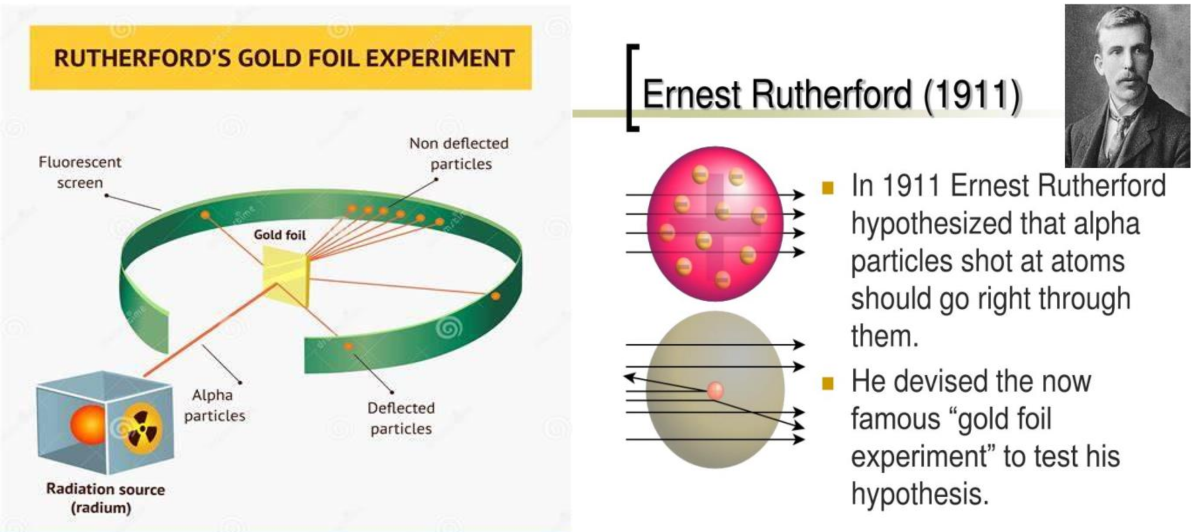
Whose characteristics are as follows?

$$q = 0\ Colomb$$

$$m_n = 1{,}6749*10^{-27}\ Kg\ \ ;\ m_p \approx m_n$$

III. RUTHERFORD's model

The ***RUTHERFORD*** experiment involves bombarding a very thin sheet of gold with helium nuclei of helium (He^{+2}). By studying the trajectories of the particles, he found that most of them passed through the gold foil. Particulates passed through the gold sheet without being deflected, and that a small number of them were either strongly deflected as they passed through it, or sent backwards: these were the particles that passed close to the positive charges. These were the ones that passed close to the positive charges. This shows that the material of the gold leaf is concentrated in particles (very small in volume) that are far apart in size and positively charged positively charged particles that were called the atom's nuclei.



- In 1911 Ernest Rutherford hypothesized that alpha particles shot at atoms should go right through them.
- He devised the now famous "gold foil experiment" to test his hypothesis.

Figure II.6: The Rutherford experiment

Rutherford deduced that the positive charge of each atom is collected in a very small volume compared to that of the atom.

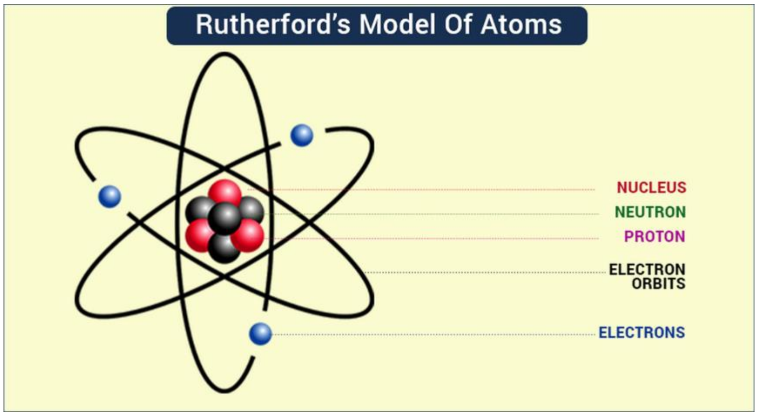


Figure II.7: RUTHERFORD model

Model:

An atom can be model led by a structure with a central compact body called the nucleus, which is positively charged nucleus. The atom is eclectically neutral and is described as a dense, positively-charged nucleus around which electrons gravitate, like the planets around the sun around which electrons gravitate like planets around the sun. The nucleus is made up of nucleons: Protons and neutrons.

IV. Presentation and characteristics of the atom

The atom is characterised by the following values: Z: Number of protons or electrons, N: Number of neutrons. By convention, an element is represented by the symbol:

$$ {}_{Z}^{A}X $$

Z: is the atomic number or charge number;

A: is called the number or mass number and represents the number of nucleons:

$$A = Z + N$$

For any given element, the number of protons is fixed, but the number of neutrons cans vary. Atomic mass unit (u m a). In the international system, the unit of mass is the Kg. It is totally unsuitable at the elementary level for the atom scale for the atom. Hence the need for another unit, the atomic mass unit (u m a) with:

$$1\ uma = 1{,}66 * 10^{-27}\ Kg$$

$$1\ uma = \frac{1}{12}\frac{12}{N_A}\ \frac{10^{-3}}{6.023 * 10^{23}}$$

$$m_e = 9{,}109 * 10^{-31} Kg = \frac{9{,}109 * 10^{-31}}{1.66 * 10^{-27}} = 5{,}5 * 10^{-4} uma$$

$$m_p = 1{,}673 * 10^{-27}\ Kg = 1{,}0074\ uma$$

$$m_n = 1{,}675 * 10^{-27}\ Kg = 1{,}0087\ uma$$

Note:

The average mass of an atom in (amu) and the mass of a mole of atom in gram (g) are numerically equal.

As each nucleon has a mass close to the atomic mass unit (1uma), the mass of the nucleus is approximately equal to : A = Z + N

Since the mass of the electrons is negligible, A is also approximately the mass of the atom in atomic mass unit.

V. Isotopes and their relative abundance

Isotopes are atoms or nuclides of the same chemical element (they have the same number of protons) but a different number of neutrons (and therefore different mass numbers and atomic masses).

$$^{1}_{1}H\ ;\ ^{2}_{1}H\ ;\ ^{3}_{1}H$$

Note:

The chemical properties of two isotopes of the same element are strictly the same because they are determined by the electron sequence, which is the same for both isotopes. In nature, all elements are mixtures of isotopes. So calculating the atomic mass of a chemical element depends on the abundance of each isotope .Abundance is the percentage presence of the isotope in the chemical element. The average is calculated by the following relationship:

$$M = \frac{\sum M_i x_i}{100}$$

VI. Binding and cohesion energy of nuclei

VI.1. Binding energy (E)

This is the energy required to form any nucleus from its nucleons (P + N) according to the following reaction:

$$Z + N \rightarrow {}^{A}_{Z}X \quad \text{avec } E < 0$$

The formation of a nucleus requires negative energy.

VI.2. Cohesive energy (E′)

This is the energy required to destroy a nucleus into its constituents (N + P) according to the reaction:

$${}^{A}_{Z}X \rightarrow Z + N$$

This energy is positive and we can write $E' = -E$.

VI.2.1. Cohesion energy per nucleon

This is the ratio of the cohesion energy of a nucleus to the number of nucleons (A = Z + N).It is generally less than 8.9 MeV for all elements. The ASTON curve represents this average energy as a function of A. This cohesion energy is of the order of / nucleon (1 MeV = 10^6 eV = $1.6*10^{-13}$J).The curve represents a minimum (maximum in absolute value) at A = 60; the corresponding atoms being the most stable being the most stable atoms. Consequently, all the elements will seek to stabilise and approach the zone of maximum stability at around A = 60.

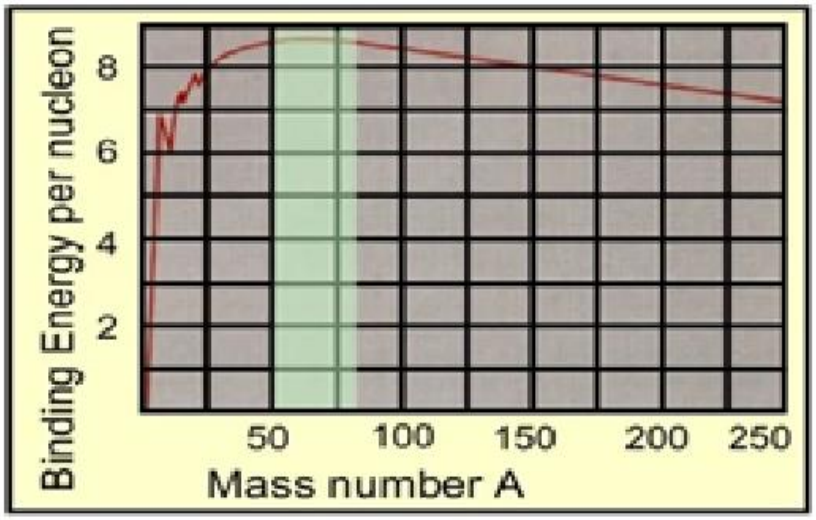


Figure II.8: Binding energy VS Mass number

A < 15: The light atoms combine to form a heavy atom: this is fusion.

A > 200: The heavy atoms will split to form light atoms: this is fission.

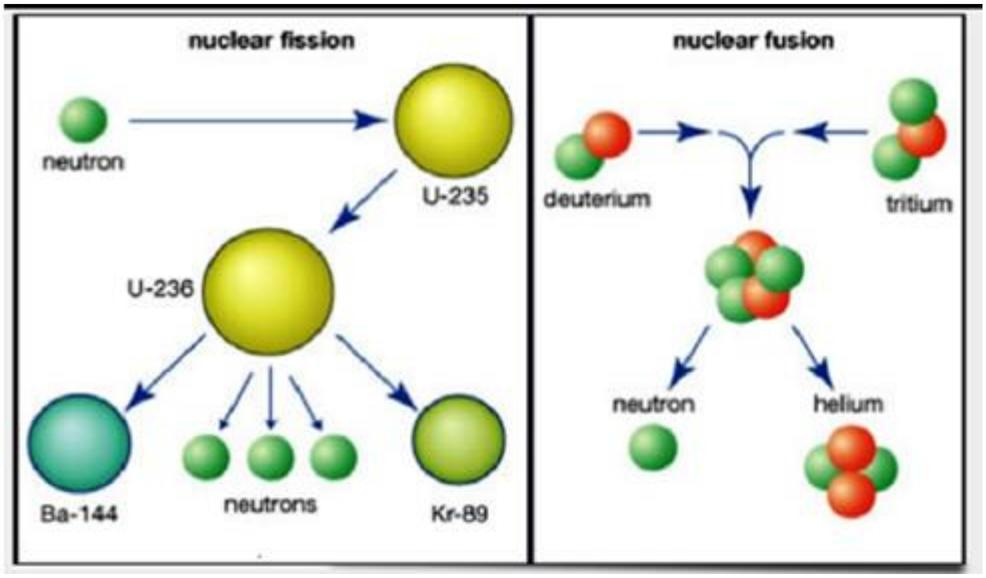


Figure II.9: Fusion and fission reaction

VI.2.2. EINSTEIN's equation

According to the relativity relation, matter and energy are inter-convertible, which means that mass can be transformed into energy and conversely, energy can give mass.

The relationship between energy and mass is given by ENSTEIN's relation (1905):

$$\mathbf{E = m\,C^2}$$

Where C: celerity of light ($3 * 10^{8}$ m/s)

Note:

The mass of the nucleus is always less than the sum of the masses of its constituent's loss of mass Δm which is transformed into energy with:

$$\Delta \boldsymbol{E} = \Delta \boldsymbol{m} * \boldsymbol{C}^2$$

ΔE: cohesive energy

Δm : deficient mass

When creating a core: $\Delta m < 0$

$\Delta \boldsymbol{m} = \boldsymbol{mnoyau} - (\boldsymbol{Z} * \boldsymbol{mp} + \boldsymbol{N} * \boldsymbol{mn})$. We talk about ***binding energy***

When the nucleus decays into nucleons $\Delta m > 0$ $\Delta \boldsymbol{m} = (\boldsymbol{Z} * \boldsymbol{mp} + \boldsymbol{N} * \boldsymbol{mn}) - \boldsymbol{m}_{\textbf{nucleus}}$. We talk about ***cohesive energy***

VI.3. Nucleus stability

Of the 331 naturally occurring nuclides, 284 are stable; the others decompose spontaneously. They are radioactive. The stability of any element is greater the higher the binding energy per nucleon is higher. From A = 210 (Polonium), all nuclides are radioactive. Stability also depends on the number of Z: **N = A - Z**.

The addition of neutrons stabilizes the nuclides by diluting the positive charges of the protons which, being further apart, tend to repel each other less repel each other less. To this end, the ratio between the number of protons and the number of neutrons is the main factor that determines the stability of the atom main factor that determines the stability of a given nuclide.

If $1 \leq Z \leq 20$: the number of protons and neutrons are equal or very close.

If $20 \leq Z \leq 84$: the number of neutrons is greater than the number of protons.

More neutrons are needed neutrons to compensate for the electrostatic repulsion of protons.

If Z ≥ 84: the nuclides are radioactive. The number of neutrons becomes insufficient. The extra neutrons needed for stability can no longer find a place in the nucleus.

CHAPTER III: Radioactivity - nuclear reactions.

I. Natural radioactivity

It was discovered by **Henri BECQUEREL in 1886**. He discovered that uranyl potassium sulphate ($K_2UO_2 (SO_4)_2$) emitted radiation capable of ionizing or printing a photographic plate. This radiation is not affected by any external intervention (temperature, pressure,), which distinguishes it from a chemical reaction. It is a spontaneous nuclear reaction. Heavy nuclei can emit electrons (β-particles) or α particle ($_2^4He$). Less heavy (light) nuclei emit β particles or (electrons).The α and β emission is accompanied by the emission of very energetic photons that make up the γ ray.

Main types of radiation:

I.1. α rays

It mainly concerns heavy elements with atomic number Z ≥ 83.

$$_Z^AX \rightarrow {}_{Z-2}^{A-4}Y + {}_2^4He$$

The α radiation is highly ionizing, very energetic but not very penetrating.

I.2. β^- rays

It concerns unstable isotopes that possess an excess of neutrons. During this emission, a neutron is transformed into a proton according to the reaction below:

$$_0^1\eta \rightarrow {}_1^1P + {}_{-1}^0e$$

During this reaction, the number of protons varies and one element is transformed into another. This is called transmutation.

I.3. β^+ rays

This concerns unstable isotopes with an excess of protons. Such elements will seek to stabilize by increasing N and decreasing Z. For such nuclides, a proton is transformed into a neutron. Proton is transformed into a neutron. At the same time, a positron is ejected from the nucleus. The positron is the antiparticle of the electron; it has the same mass but an opposite charge to the electron.

$$ {}_{1}^{1}P \rightarrow {}_{0}^{1}\eta + {}_{1}^{0}e $$

During this reaction, the number of protons varies and one proton is transformed into another.
It is also a transmutation.

I.4. γ radiation

It appears during α and β emissions. In general, when a nucleus is formed, during disintegration, it does not immediately reach its fundamental state; it is in an excited state. The transition to the ground state releases a photon of the nature of γ radiation.

$$ {}_{Z}^{A}X \rightarrow {}_{Z}^{A}X + \gamma $$

γ radiation is pure electromagnetic radiation, i.e. it has no mass or charge but is highly energetic and has a penetrating power greater than that of α and β particles. Higher penetrating power than α and β particles, but with a lower ionizing power.

II. Artificial radioactivity

II.1. Transmutation reactions

Induced transmutation reactions produce nuclides with a mass number equal to or very close to that of the nuclide used as the target.

$$ {}_{16}^{32}S + {}_{0}^{1}\eta \rightarrow {}_{1}^{1}P + {}_{15}^{32}P \; ; \; {}_{16}^{32}S\,(\eta, p)\,{}_{15}^{32}P $$

(Simplified or sheltered writing)

$$ {}_{7}^{14}N + {}_{2}^{4}He \rightarrow {}_{1}^{1}H + {}_{8}^{17}O \; ; \; {}_{7}^{14}N\,(\alpha, p)\,{}_{8}^{17}O $$

(1st reaction carried out by Rutherford. It led to the discovery of Proton in 1919).

II.2. Nuclear fission

This concerns heavy elements which disintegrate to produce lighter atoms and neutrons which in turn can bombard other neighboring nuclei, causing nuclear fission. Neutrons which in turn can bombard other neighboring nuclei and cause them to fission; this is the nuclear chain reaction.

$$^{235}_{92}U \quad + \quad ^{1}_{0}\eta \quad \rightarrow \quad ^{132}_{51}Sb \quad + \quad ^{101}_{41}Nb \quad + \quad 3\,^{1}_{0}\eta$$

The energy released by this type of reaction is of the order of 200 MeV/atom.

II.3. Fusion reaction

In this type of reaction, two or more light atoms unite to form a heavy nucleus nucleus at high temperature.

During this process, mass is lost and energy is released.

III. Kinetics of radioactive decay

III.1. Energy aspect

During the nuclear reaction, the total number of nucleons and the overall charge are conserved but accompanied by a loss of mass (Δ mm) corresponding to the release of energy given by ***EINSTEIN's*** relation :

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

III.2. Kinetics (law of radioactive decay)

Let the reaction be:

$$A \text{ ------------> } B$$

(B *is not radioactive)*

a	t=0	N_0	
a	t	Nt	N_0 – Nt
a	(t + dt)	$N_0 + dN$	

The experiment showed that the number of atoms $\frac{dN}{dt}$ which decay between t and (t + dt), is proportional to the number of atoms N present at time t, hence:

$$-\frac{dN}{dt} = \lambda N \qquad (1)$$

With:

dN: the variation in the number of radioactive nuclei over time dt

N: designates the number of nuclei present at time t

λ: radioactive or decay constant ($S^{-}1min^{-1}$).

$-\frac{dN}{dt}$: represents the number of particles disintegrated per unit of time.

By integration of equation (1):

$$-\frac{dN}{dt} = \lambda N \quad \text{for } t=0 \text{ we have: } N = N_{0;} \text{ for } t \neq t \text{ we have } N = N_t$$

$$\frac{dN}{dt} = -\lambda N \;\Rightarrow\; \frac{dN}{dt} = -\lambda\, dt$$

$$\int_{No}^{N} \frac{dN}{dt} = \int_{0}^{t} -\lambda\, dt \Rightarrow \ln N - \ln N_0 = -\lambda t$$

$$N_t = N_0\, e^{-\lambda t} \qquad (2)$$

This is the law of radioactive decay.

a. Radioactive half-life

The radioactive half-life is the time after which half of the initial nuclei have undergone decay. It is obtained by replacing in equation (2) t by T and Na by $Na_0/2$. We find:

$$T = \frac{ln2}{\lambda} = \frac{0.69}{\lambda} \qquad (3)$$

Let: T is the time required for N0 ⁄ 2 to disintegrate.

$$(2) \quad \Rightarrow \quad \ln\frac{Nt}{No} = -\lambda t$$

For t =T we have:

$$\ln\frac{No/2}{No} = -\lambda t \quad \Rightarrow \quad -\ln 2 = -\lambda t$$

$$T = \frac{\ln 2}{\lambda}$$

Note

The number of radioactive atoms present is divided by 2 each time a period elapses. At (n) period, the number of nuclei remaining is:

$$N_A = \frac{NAo}{2^n} \qquad (4)$$

The period is a fundamental characteristic of each core. It is independent of

The initial number of atoms

Pressure and temperature.

b. Radioactive activity

This is the average number of disintegrations per unit of time. Simply derive the expression for N_t and taking its opposite (in order to keep a positive quantity). A_0 is the activity of the source at

At an initial time of t = 0 we have $A_0 = \lambda N_0$.

$$A = -\frac{dN}{dt} = \lambda N$$

It can be expressed in: d.p.s, d.p.m or curie (1 Curie = $3.7 * 10^{10}$ dps).This numerical value was chosen so that 1 gram of radium ^{226}Ra has an activity close to 1 curie.

IV. Applications of radioactivity

IV.1. Industry

The principle of gamma-graphy is no different from that of X-ray radiography: the image (collected on a photographic plate) of a metal part subjected to γ radiation reveals and detects defects in an organ. All the welds on nuclear reactor vessels are inspected using this method checked using this process. Its main advantages are the fallibility and autonomy of the source (^{60}Co, ^{192}Ir). Betagraphy (using β-radiation) can be used to examine thin objects, check thickness, etc.

IV.2. Medicine and biology

a. Treatment of tumors by irradiation: The γ radiation emitted by a body (cobalt 60, for example) is used to destroy the cells located in the cancerous tumor.

b. Treatment of a tumor by metabolism: Molecules labelled with a β emitter that can be selectively fixed by pathological tissues. Hyperthyroidism is treated in this way.
Hyperthyroidism, thyroid cancer and Vazquez's disease (or polycythemia), using radioactive phosphorus.

c. Scintigraphy Radionuclides are used as tracers: They take part in metabolism in the in the same way as the natural elements with which they are mixed. For example, iodine-131 will be absorbed in the same way as natural iodine. It will therefore be possible to follow the iodine's pathway during its assimilation and monitor the functioning of the thyroid gland, which synthesizes and secretes the iodine-containing hormones responsible for many actions in the body. Iodine hormones, which are responsible for a wide range of cellular actions. We can also study the morphology of an organ made radioactive by fixing a γ or β radioelement. Using various detectors, a true image of the organ can be obtained. Brain surgery makes excellent use of these methods: radioactive phosphorus can be located in tumors that are difficult to distinguish from healthy tissue; the surgeon can then identify the tumor during the operation itself, using Geiger counters. Using special Geiger counters sensitive to β emission.

d. Radioelements are commonly used in chemical analysis: Dosage based on radioactivity is sensitive, simple and fast. Trace elements (10^{-10} mol^{-1}) that cannot be chemically: growth hormones, insulin in the blood, etc.

e. Radio-sterilization: Thousands of items (syringes, dressings, sheets, prostheses, etc.) are sterilized using γ rays, which kill micro-organisms.

IV.3. Agronomy and agri-food

a. Genetic modification: Irradiating plants can cause significant genetic changes. This has resulted in wheat, barley and rice straws that are better adapted to mechanical harvesting and more resistant to lodging.

b. Preservation of foodstuffs: Irradiation γ destroys insects in stored foodstuffs and microorganisms in eggs, meat, etc. microorganisms in eggs, meat, etc. It is also a powerful germ-killing treatment (potatoes).

c. The use of tracers: as led to advances in our knowledge of mineral absorption and transport of minerals. For example, radioactive phosphorus atoms incorporated into a fertilizer will behave in a plant in the same way as stable phosphorus atoms. In this way, the agronomist will be able to track the plant's uptake of the fertilizer and deduce its effectiveness, the most favorable time to apply it and the most effective way to use it on the soil, etc.

V. Dangers of radionuclides

Ejected from the disintegrating nucleus, the particles and photons, whose energy is of the order of the MeV, can pass through inert or living matter. These projectiles collide with the atoms or molecules that make up the matter they pass through. During the impact, the loss of kinetic energy causes ionization or even nuclear reactions. The average distance travelled by a set of particles in a given substance can be defined as the average distance travelled by a set of particles in a given substance as the average distance travelled by these particles before they are stopped. This mean depends on the nature of the particles, their initial kinetic energy and the substance through which through which they pass.

CHAPTER IV: Electronic structure of the Atom

I. Electromagnetic spectrum - wave-corpuscle duality

At the microscopic (atomic) scale, classical physics is inadequate for the study of phenomena. For this reason, a new mechanics was created: quantum mechanics (wave mechanics).

I.1. The wave aspect of light

Certain optical phenomena such as diffraction and diffusion.... interference can only be can only be interpreted if we attribute a wave aspect to light. These electromagnetic waves or light waves propagate in space at a constant speed of the order of 2.99 108 m/s. Each of these waves is characterised by its length or frequency with:

$$\vartheta = \frac{c}{\lambda}$$

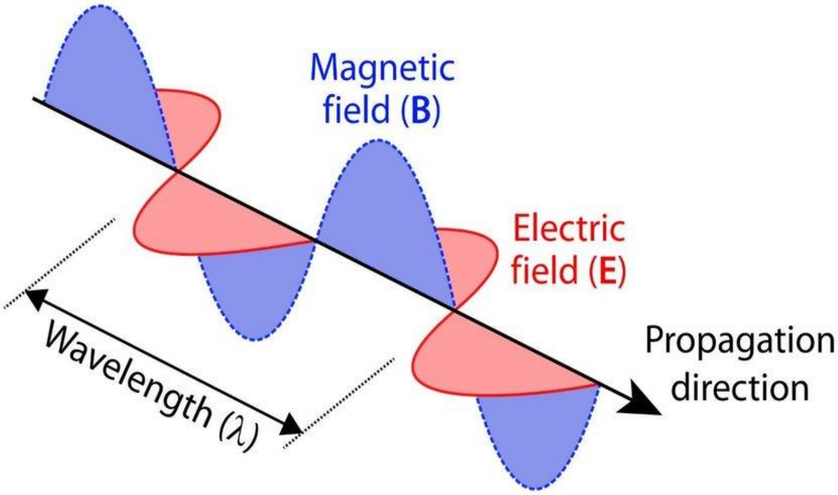


Figure IV.1: Electromagnetic or light wave

Other phenomena are interpreted by wave theory, such as black body radiation (PLANK 1900; quantification of energy) and photo-electricity (EINSTEIN, photons).

Definition: the electromagnetic spectrum is made up of all the light waves where the frequency υ can take all values continuously.

II.2. Corpuscular aspect: photoelectric effect

This effect was discovered by the physicist HERTZ around 1885. The experiment consists of irradiating a by monochromatic light of increasing frequency connected to an electrometer. The electrometer begins to be charged above a frequency ν0; the two arms of the electrometer move apart of the electrometer move apart, indicating the presence of electricity for EINSTEIN, irradiating a metal plate with monochromatic light allowed electrons to be torn off if $\nu = \nu_0$, which is called the threshold frequency characteristic of the metal used. He concludes that light carries grains of matter called quantas, also known as photons. "each carrying an energy E :

$$E = h * \vartheta$$

These photons strike the atoms on the plate and, if they have enough energy, they tear off electrons, producing electricity. This is what constitutes the "photoelectric" effect, i.e. the production of electricity using light, the production of electricity using light.

Note:

According to the mass-energy equivalence relationship, the energy transported by a photon is equal to $m.C^2$ where m is the fictitious mass of the photon (whose rest mass is zero), we have:

$$E = h * \vartheta = m * C^2 = h\frac{C}{\lambda} => \lambda = \frac{h}{m*C}$$

Experiment

If a metal plate is illuminated with light at a frequency ν greater than the threshold frequency threshold frequency ν_0 the extra energy compared with the characteristic energy of the metal
$E_0 = h.\ \nu_0$ is dissipated in the form of kinetic energy taken up by the electrons:

$$E_c = E - E_0 = h\,\vartheta - h\,\vartheta_0 = h * (\vartheta - \vartheta_0)$$

II. INTERACTION BETWEEN LIGHT AND MATTER

Under photoemission, an atom or molecule only absorbs certain frequencies of light. The set of frequencies absorbed is called the absorption spectrum, which constitutes a means of identifying a given atom or molecule. Line positions (electronic transition) are often expressed by the wave number, where:

$$\bar{\vartheta} = \frac{1}{\lambda}$$

The atom is in the ground state if it does not absorb any energy from the external environment. If this is not the case the electron can occupy certain levels designated by (n) (quantum number). The electron can only occupy levels 1, 2, 3, 4 ... which means that the energy is quantised and can only vary by quanta. It can only vary by energy quanta (packets).

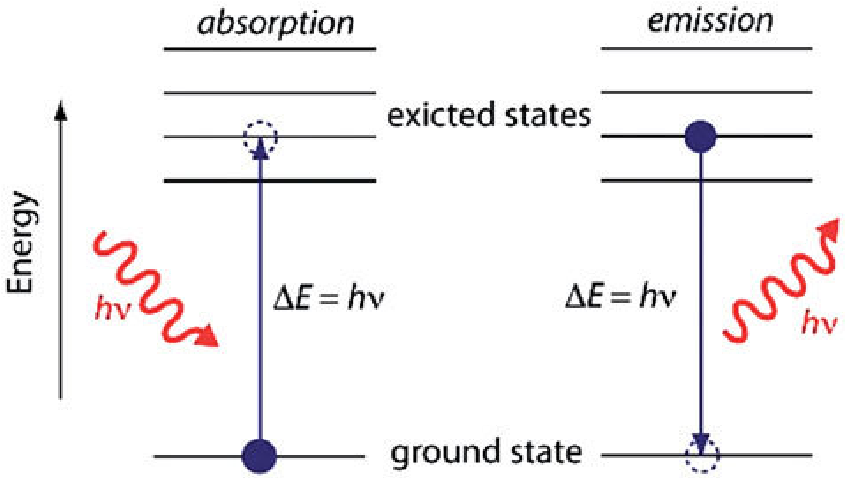


Figure IV.2: Electromagnetic *hv*

Light absorption: If the electron jumps from an orbit of rank n to an orbit of rank m (n<m) such that the atom goes from an En energy to an Em energy, then the atom absorbs radiation of a frequency frequency such that $\Delta E = h * \vartheta$

Light emission: If the electron jumps from an orbit of rank m to an orbit of rank n (m > n) such that the atom goes from an energy Em to an energy En then the atom emits radiation of frequency ν such that $\Delta E = h * \vartheta$.

II.1. HYDROGEN EMISSION SPECTRUM

The hydrogen emission spectrum is obtained by applying an electrical discharge (ddp) to the hydrogen gas hydrogen in a cathode ray tube which causes excitation of the hydrogen atoms. When these atoms return from their excited state to their ground state, they emit electromagnetic radiation. The radiation emitted passes through a prism that selects monochromatic radiation (of the same frequency and wavelength). The spectrum obtained, on the photographic plate, is a spectrum made up of very fine lines of various colors separated by large dark spaces. These spectra were discovered by LYMAN (UV), BALMER (Vis), PASCHEN, BRACKETT, PFUND (IR).

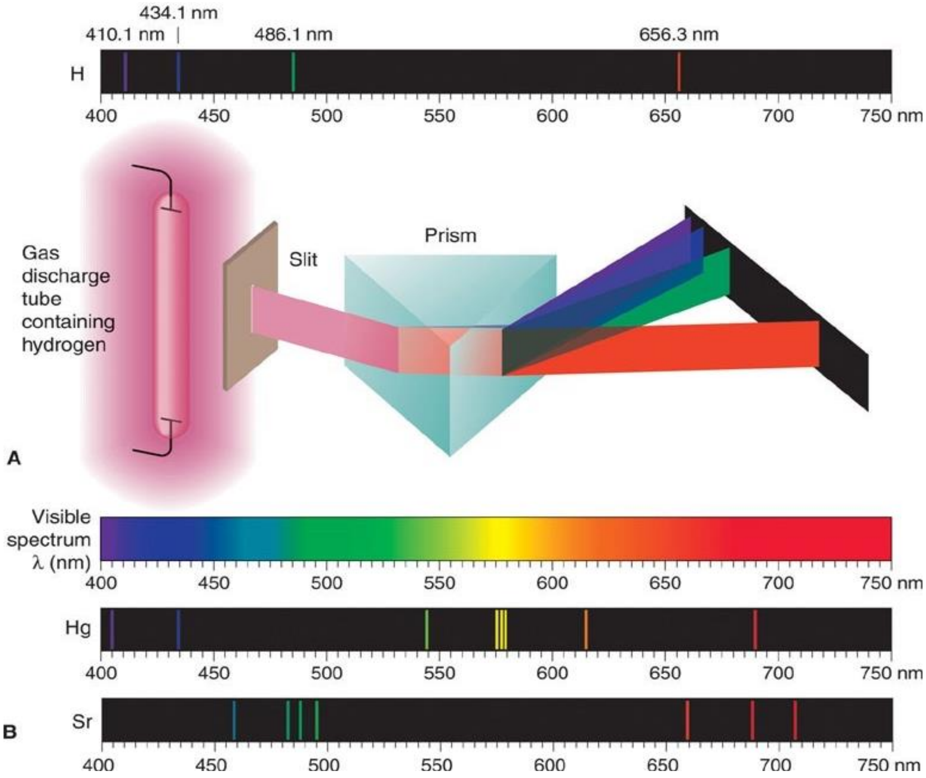


Figure IV.3: The spectrum electromagnetic

*** Note:**

1. Each atom has a characteristic spectrum. For the spectrum studied previously, it is a spectrum of the hydrogen atom and not of the H^2 molecule.
2. Excited atoms emit visible and invisible radiation.
3. The frequencies emitted have well-defined values.
4. All the radiation together makes up the spectrum.

By analysing the light emitted, we can observe a discontinuous spectrum or line spectrum whose wavelengths can be calculated using an empirical formula: ***BALMER-RHYDBERG*** formula.

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

RH: RHYDBERG constant: RH = 10967757.6 m^{-1}.

II.2. CONCEPT OF LINE SERIES

A line series corresponds to all the lines that cause the electron to return to a given level. Each series is named after its discoverer:

1. LYMAN series (UV): n= 1, m = 2, 3, 4, ...
2. BALMER series (visible): n= 2, m = 3, 4, 5, 6, ...
3. PASCHEN series (IR): n= 3, m = 4, 5, 6, ...
4. BRACKETT series (Near IR): n= 4, m = 5, 6, ...
5. PFUND series (Far IR): n= 5, m = 6, 7, 8, ...

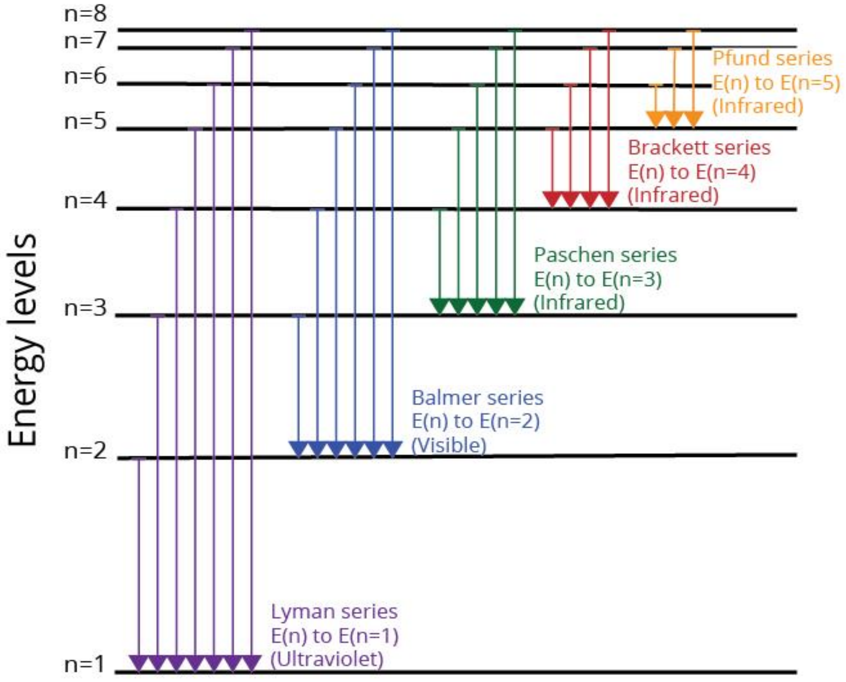


Figure.IV.4: Series of lines

III. CLASSICAL MODELS OF THE ATOM

III.1. RUTHERFORD'S model

According to ***Rutherford***, the electron rotates around the nucleus in a uniform orbit of radius (r). Mechanical stability results from the compensation of the electrostatic forces by the centrifugal forces centrifugal forces due to the rotation of the electron around the nucleus. The model of the hydrogen atom proposed by ***Rutherford*** and ***Perrin*** contradicts experience. With experiment.

This model suggests that	**Experience shows**
1. Spontaneous radiation : An electron moving in an electromagnetic field electromagnetic field radiates energy (electromagnetic wave, classical theory).	1. The hydrogen atom in its ground state does not radiate (the electron remains in its orbit). 2. The hydrogen atom is stable

2. An unstable atom: When the atom radiates, its energy decreases, which leads to a decrease in radius (r) and consequently the fall of the electron on the nucleus. 3. The continuous variation in radius (r) leads to a decrease in energy E and continuous radiation	3. The hydrogen emission spectrum is a line spectrum (discontinuous)

III.2. BOHR's model

BOHR took up ***RUTHERFORD***'s model but based it on the interpretation of the spectrum of hydrogen atom (discontinuous line spectrum). This model is based on the quantum theory (***PLANCK***) according to which the exchange of energy between matter and radiation only takes place in finite quantities through finite quantities. It applies only to the simplest atomic structures, which have only one electron. Only one electron, known as a hydrogenous, such as: H, He^{+}, L, L^{2+}.........

To remedy the inadequacies of ***RUTHERFORD***'s model, ***BOHR*** made two postulates

1^{st} postulate

In BOHR's atomic model, the electron rotates around the nucleus in a uniform circular motion on an orbit of radius (r). Circular motion in an orbit of radius (r). In fact, the electron gravitates on circular orbits called stationary orbits without radiating or emitting energy. Its own energy remains constant as long as it remains in one of these orbits. BOHR arbitrarily postulates that the angular momentum of the electron $\mathbf{m_e.V.r}$ can only take discrete values equal to integer multiples of $h/2\pi$

$$me * V * r = n\,h/2\pi \qquad (5) \text{ with } n = 1, 2, 3,4,.....$$

It follows that only certain values of (r) are allowed.

2nd postulate

A tome only emits or absorbs light radiation when the electron moves from one stationary orbit to another; the corresponding energy is the difference in energy ΔE between the level at which it and the arrival level of the electron

$$\Delta E = E_2 - E_1 = h * \vartheta$$

III.1.2. Radius of stationary orbits

$$(1);\ k * \frac{e^2}{r^2} = m_e \frac{V^2}{r} \Rightarrow r = k * \frac{e^2}{me\, V^2}$$

$$(5);\ m_e * V * r = n \frac{h}{2\pi} \Rightarrow V = \frac{n * h}{2\pi} \frac{1}{me * r}$$

$$V^2 = \frac{n^2\, h^2}{4\pi^2 me^2 r^2} \Rightarrow r = \frac{ke^2}{me} \frac{4\pi^2 me^2 r^2}{n^2\, h^2} \qquad (6)$$

$$r = \frac{4\pi^2 me^2 r^2}{n^2\, h^2}$$

$$With:\ k = \frac{1}{4\pi\varepsilon o}$$

$$r_n = n^2 * a_0\ ;\ r_n = n^2 * 0.521$$

$$a_0 = \frac{h^2 \varepsilon o}{\pi\, me\, e^2} = 0.529\ \hat{A}$$

Is the BOHR radius

III.2.2. Energy of the electron in an orbit:

$$E_T = \frac{k * e^2}{2 * r} = -\frac{e^2}{8\pi\ \varepsilon o\ r}$$

We have: $E_n = \frac{E1}{n^2}$

$E_1 = -13.6\ eV$ $\quad E_n = \frac{-13.6}{n^2} \quad (eV)$

III.2.3. Application to hydrogenoids

BOHR's theory is not general; it applies only to the hydrogen atom and to hydrogenoid ions, consisting of a nucleus of charge (+Z) around which a single electron orbits. A calculation similar to that for hydrogen leads to:

$$r_{\text{hydrogenoid}} = \frac{r_{hydrogen}}{Z}$$

III.2.4. Inadequacy of the BOHR model

The BOHR model (Nobel Prize in 1922) was unable to successfully describe the spectra of poly-electronic atoms. So attempts were made to improve it; SOMMERFILED proposed to complicate the model by using elliptical orbits instead of the simple circular BOHR orbits circular orbits of BOHR (the analogy between the solar system and the elliptical orbits of KEPLER ELLIPTICAL ORBITS). This modification leads to the appearance of two quantum numbers (l, m), but does not this modification led to the appearance of two quantum numbers (l, m), but did not allow large atoms to be described correctly either. This model was abandoned and replaced by the quantum (or wave) model. In other words, BOHR's model could not successfully describe poly-electronic atoms. It does not take into account the effect of attraction of the nucleus on the other electrons. This phenomenon is known as the screen effect.

IV. Model based on wave mechanics

IV.1. Wave-corpuscle duality and De Broglie relation

By analogy with light, DE BROGLIE (1924) postulated that any material particle animated by velocity (V) having a mass (m) could be associated with a wave such that its wavelength wave-length:

$$\lambda = \frac{h}{m*V}$$

This postulate forms the basis of a new mechanics: wave mechanics, which has made it possible to resolve the contradictions and difficulties of classical mechanics.

Remarks:

The DE BROGLIE wave is not generally an electromagnetic wave. It is only electromagnetic only if the particle is a photon.

The particle may be small or large, charged or not (an electron, a nucleus, a ball, a satellite, etc.).

IV.2. Heisenberg's Uncertainty Principle

This principle states that it is impossible to measure simultaneously and accurately the position and the momentum of a corpuscle:

$$\Delta Px = m * \Delta V \qquad p\ (Quantity\ of\ movement) = m * V$$

$$\Delta\ (m * V) * \Delta x \geq \bar{h} \qquad (14)$$

$$\bar{h} = \frac{h}{2\pi}$$

With;

This relationship means that if we can theoretically measure (x) accurately ($\Delta x \rightarrow 0$), then (ΔV) will become large because:

$$\Delta V \geq \frac{\bar{h}}{m * \Delta x}$$

IV.3. One function and Schrödinger equation

Each state of a microscopic system is characterized by a function of coordinates x, y, z, t called the wave function.

This wave function is a mathematical function that characterizes the behavior of a particle at a point M(x, y, z) in space at a time (t) particle at a point M(x, y, z) in space at an instant (t). It is denoted: Ψ (x, y, z, t).It is the square of this function $\Psi 2$ that has physical significance; it represents the probability of the particle's presence of the particle.

IV.3.1. Probability of presence

We call $dP = |\Psi|^2 dV$ the probability of presence of the electron at time (t) in the element of volume dV. For all space:

$$\int_{-\infty}^{+\infty} |\Psi|^2 \, dV = 1$$

The electron is located somewhere in volume V; the Ψ function is then normalized (normalization of wave functions).

IV.3.2. Schrödinger equation

In 1926, ***SCHRÖDINGER*** postulated that the wave function Ψ(x, y, z, t) is a solution of the equation:

$$-\frac{h^2}{8m\pi^2}\left[\frac{\Psi\partial^2}{\partial x^2}+\frac{\Psi\partial^2}{\partial y^2}+\frac{\Psi\partial^2}{\partial z^2}\right] + \Psi E_p = E\Psi$$

Where: m: mass of the particle

Ep (Potential energy) = $-\frac{ZKe^2}{r}$

$$-\frac{h^2}{8m\pi^2}\left[\frac{\Psi\partial^2}{\partial x^2}+\frac{\Psi\partial^2}{\partial y^2}+\frac{\Psi\partial^2}{\partial z^2}\right] + E_p = \text{Hamiltonian}$$

The ***SCHRÖDINGER*** equation can be written in a more condensed form: HΨ = EΨ with:

$$-\frac{h^2}{8m\pi^2}\left[\frac{\Psi\partial^2}{\partial x^2}+\frac{\Psi\partial^2}{\partial y^2}+\frac{\Psi\partial^2}{\partial z^2}\right] + E_p = -\frac{h^2}{8m\pi^2} * \Delta + E_p = -\frac{\bar{h}^2}{2m} * \Delta + E_p$$

With:

$$\bar{h} = \frac{h}{2\pi}\ ;\ E_p = -\frac{ZKe^2}{r}$$

SCHRÖDINGER's equation synthesizes the corpuscular and wave aspects of the microscopic particle wave aspects of the microscopic particle.

a. Wave aspects

For a one-dimensional system, a standing wave whose amplitude is independent of time:

$$\Psi(x) = \Psi_0 cos\,\frac{2\pi x}{\lambda} \qquad (15)$$

b. Corpuscular aspects

According to DE BROGLIE:

$$mV = P = \frac{h}{\lambda} \qquad (16)$$

c. Conservation of energy

$$E = E_c + E_p\,(x) \qquad (17)$$

The combination of these three equations leads to the ***SCHRÖDINGER*** equation. Let's consider the simplest case of a particle moving along an axis (x) in a time-independent potential Ep (x):

$$\Psi(x) = \Psi_0 cos\,\frac{2\pi x}{\lambda}$$

$$\frac{d\Psi}{dx} = -\,\frac{2\pi^{\,2}}{\lambda}\,\Psi_0 sin\,\frac{2\pi x}{\lambda}$$

1st derivative:

$$\frac{d^2\Psi}{dx^2} = -\,\frac{2\pi^{\,2}}{\lambda}\,\Psi_0\,\frac{2\pi}{\lambda}\,cos\,\frac{2\pi x}{\lambda}$$

2nd derivative:

$$\frac{d^2\Psi}{dx^2} = -\,\frac{4\pi^2}{\lambda^2}\,\Psi_0\,cos\,\frac{2\pi x}{\lambda} \qquad (18)$$

But according to DE BROGLIE:

$$M * V = P = \frac{h}{\lambda} \Rightarrow \lambda = \frac{h}{m*V} \qquad (19)$$

From which:

$$E_c = \tfrac{1}{2}\,mV^2 \qquad ; \qquad E = Ec + Ep\,(x)$$

$$2[E_c - E_p(x)] = m.V^2 \qquad (20)$$

Equation:

$$-\frac{h^2}{8\pi^2 m} * \frac{d^2\Psi}{dx^2} + E_p(x) * \Psi(x) = E\,\Psi(x)$$

The unknowns are: E and $\Psi(x)$

The wave function Ψ satisfies the so-called SCHRÖDINGER equation must be:

1. $\Psi(x, y, z)$ must be defined at any point in space;
2. $\Psi(x, y, z)$ must be continuous at all points in space.
3. When (x, y, z) -----□→ , $\Psi(x, y, z)$--□→ 0

IV.4. Results of solving Schrödinger's equation

Schrödinger's equation is written:

$$\frac{h^2}{2m}\Delta - \frac{e^2}{4\pi\varepsilon o r} * \Psi = E\,\Psi \qquad (21)$$

The choice of Cartesian coordinates to study the problem is not appropriate, and because of the spherical symmetry of the atom, we choose spherical coordinates (r, θ, φ)

Where: $x = r.\sin(\theta)\cos(\varphi)$ $0 < x < \infty$

$y = r.\sin(\theta)\sin(\varphi)$ $0 < \theta < \pi$

$z = r.\cos\varphi$ $0 < \varphi < 2\pi$ Or $dv = dx\,dy\,dz = 4\pi r^2 dr$

$$\int_0^{\pi} \sin\theta\, d\theta * \int_0^{2\pi} d\varphi\, r^2 dr = [\cos\theta] * [\cos\rho]\, r^2 dr$$

Note: $\Psi(x, y, z) \rightarrow \Psi(r, \theta, \varphi)$

This is solved by putting the function $\Psi(r, \theta, \varphi)$ as a product of two functions:

$\Psi(r, \theta, \varphi) = R(r).\,Y(\theta, \varphi)$

Solving the equation of $H\Psi = E\Psi$ will only lead to acceptable solutions for certain values of the energy; and given the energy eigenvalues and eigen functions:

H Ψn = En Ψn with n= 1, 2, 3, 4, ...

Each solution of the ***SCHRÖDINGER*** equation has a corresponding eigenvalue, E. For the hydrogen atom, the energy eigenvalues are given by the relation:

$$E_n = \frac{me^2}{8\varepsilon o\, n^{\,2}\, h^2}$$

For $n = 1$ $E_1 = -13.6\ eV$

These differential equations can be solved rigorously. An infinite number of solutions exist. The mathematical conditions for calculating orbitals introduce three integers' n, l, m such that such that:

$$n \in N*; \quad 0 < l \leq n - 1 \quad ; \quad -l < m < +l$$

IV.5. Quantum names and the concept of the atomic orbital

IV.5.1. Quantum numbers

The quantum state of the electron is defined by four quartic numbers:

a. Principal quantum number (n)

This characterizes the level occupied by the electron or the layer it occupies. This layer is sometimes designated by a capital letter.

n = 1 → K layer

n = 2 → L layer

n = 3 → M layer

n = 4 → N layer

b. Secondary (or azimuthal) quantum number (l)

This characterizes the sub-layer occupied by the electron. With $0 < l \leq n - 1$

l = 0 → sub-layer s

l = 1 → sub-layer p

l = 2 → under layer d

l = 3 → under layer f

c. Magnetic quantum number (m) $-l < m \leq +l$

Graphically, this number is represented by a rectangle: we represent as many rectangles as there are possible values of (m).

These three quantum numbers define a quantum square, which contains two electrons. To distinguish between the two electrons, a fourth spin quantum number (s) is introduced. d. Spin quantum number (s): This characterizes the movement of the electron on itself and can take only two different values ± ½ by convention: $S = +1/2 \uparrow$ and $S = -1/2 \downarrow$

$$S = +\frac{1}{2}\ \boxed{\uparrow} \qquad S = -\frac{1}{2}\ \boxed{\downarrow}$$

IV.5.2. Atomic orbitals

Atomic orbitals are the eigen functions of $H\Psi n = En\Psi n$. Each wave function, solution of the ***SCHRÖDINGER*** equation, is usually called an atomic orbital. An orbital defines both an energy level and the geometry of the region of space in which the electron is located.

Conclusion: The state of an electron is defined by: n, l, m and s

a. S orbital: l = m = 0 Independent of θ and φ. This defines a sphere of radius (r) and centered on the nucleus.

b. Orbital p: l = 1; m = -1, 0, +1 : (p-1, p0, p+1).For an electron in a state described by the orbital (px): the probability is maximum along (x), zero along the axes (y and z) on the nucleus.

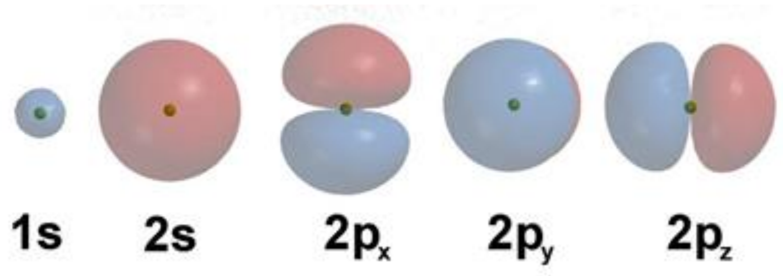


Figure IV.5. Atomic orbitals

V. Polyelectronic atoms in wave mechanics

Consider a poly-electronic atom whose atomic orbitals are defined by $\Psi_{n,l,m}$, to which the energies En, l, m correspond. Corresponding energies $E_{n,\ l,\ m}$. The filling of these orbitals by the Z electrons follows the following rules:

Each sub-layer has its own associated energy level.

Quantum bins in the same sub-layer have the same energy regardless of m and s.

The order of the energy levels of the sub-layers is given by ***KLECHOWSKI's*** rule.

V.1. KLECHOWSKI's rule

The order in which the various layers and sub-layers are filled is in ascending order of energy (n+ l). Hence: 1s / 2s 2p / 3s 3p/ 4s 3d 4p / 5s 4d 5p/ 6s 4f 5d 6p/7s 5f 6d 7p

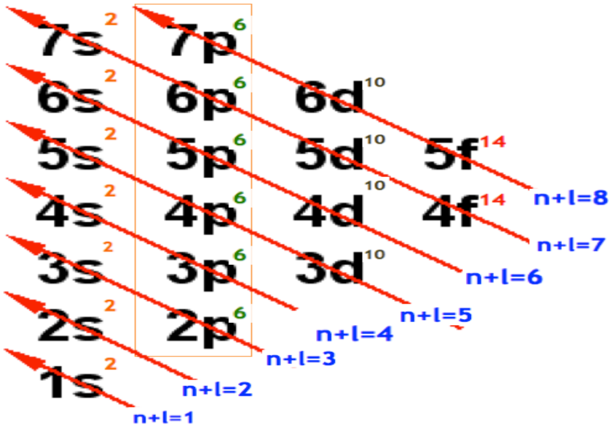


Figure IV.1: *KLECHOWSKI's* rule

Example: comparison between E_{4s} and E_{3d}

E_{4s}= 4 + 0 = 0

E_{3d} = 3 + 2 = 5

V.2. Rules for filling atomic orbitals:

When we want to obtain the electronic configuration of the ground state, we need to know how many electrons must be distributed, and also the number of orbitals that must be filled. Electrons should be distributed and how and where they should be placed. This construction is governed by the principle of edification, which uses the following rules:

a. Principle of stability: the atomic orbitals must be filled in cross-order of their energy, i.e. from the lowest energy to the highest.

b. PAULI's principle: no two electrons in an atom can have the same quantum number (n, l, m) numbers (n, l, m, s), i.e. they cannot have the same quantum state.

c. HUND's rule: in the same sub-layer, the electrons occupy the maximum number of quantum cells.

*Use of quantum dots: The number of quantum dots for a given sub-layer is equal to (m).

Example: sub-layer p: l = 1; m = -1, 0, +1 of which 03 orbital’s ☐☐☐ . For a given (n), the maximum number of electrons is equal to: $2n^2$

Simplified electronic configuration

Rare gas configuration + outer layer

With: rare gas: this is the gas whose atomic number is as close as possible to the atomic number of the element in question while remaining lower than it. The table summarizes some gases:

Noble gas	Symbol	Electron number
Helium	He	2
Neon	Xe	10
Argon	Ar	18
Krypton	Kr	36
Xenon	Xe	54
Radon	Rn	86

Valence layer:

This is the outermost layer occupied by electrons, or the layer with the highest (n). (If an inner sub-layer is not completely filled, this sub-layer is considered to be part of the valence layer). It is this layer that gives the elements their chemical properties.

Valence electrons:

These are the electrons belonging to the valence layer. Electronic structure of ions

Example:

$_{11}$Na: $_{10}$[Ne] $3S^1$

$_{11}$Na+: $_{10}$[Ne] $3S^0$

V.3. Screen effect

V.3.1. SLATER approximation

The SLATER rules make it possible to apply the results of the BOHR model to poly-electronic atoms.

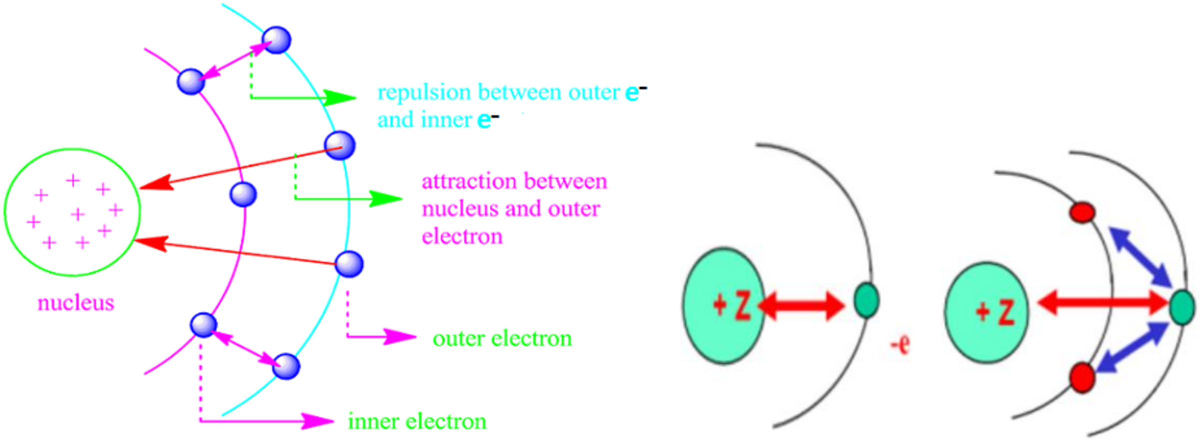


Figure IV.2: Hydroginoide atom and Polyelectronic atom

The other electrons form a screen between the nucleus and the electron being studied.

SLATER model

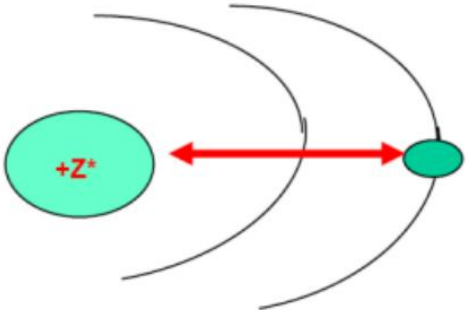


Figure IV.3: Attraction (corrected)

The real charge Z is replaced by a hypothetical charge (Z∗).The effective nuclear charge (Z∗) takes into account both the nucleus-electron attraction and the electron-electron repulsion (shielding effect).electron repulsion (screen effect).

With: $Z* = Z - \sum\sigma$; σ : *screen constant*.

SLATER has stated the rules for expressing this screen effect (σ)

V.3.2. SLATER rules

Write the electronic configuration of the element using the following groups in the following Order:

V.3.2.1. SLATER groups

[1S]; [2 s, 2 p]; [3 s, 3 p]; [2 d]; [4 s, 4 p]; [4 d]; [4 f]; [5 s, 5 p]; [5 d]; [5 f] ...

V.3.2.2. Screen constant values

1. Electron of the same group: σ = 0.35 (except for 1 s where σ = 0.3)

2. Electron from a more external group: the electron is located to the right of the group studied: σ = 0.

3. Electron of a more internal group: the electron is located to the left of the group under study two cases:

a. the electrons of the group immediately below (n-1) have a shielding effect: σ = 0.85

b. the electrons of the innermost groups (n-2), (n-3), (n-4)... have a shielding effect: σ = 1

4. The electron under study belongs to an (nd) or (nf) group:

* The electrons of all the more internal groups (n-1), (n-2), (n-3)... have a screening effect: σ = 1

Summary of shielding constants:

Electron original	**Contribution of other electrons**					
	n-2, n-3,….	**n-1**	**n**			**n+1, n+2,…**
			S, P	**d**	**f**	

S, P	**1**	**0.85**	**0.35**	**0.35**	**0**	**0**
d	**1**	**1**	**1**	**1**	**0**	**0**
f	**1**	**1**	**1**	**1**	**0.35**	**0**

Example: Cl: Z = 17: $1S^2$; $2S^2$ $2p^6$; $3S^2$ $3p^5$

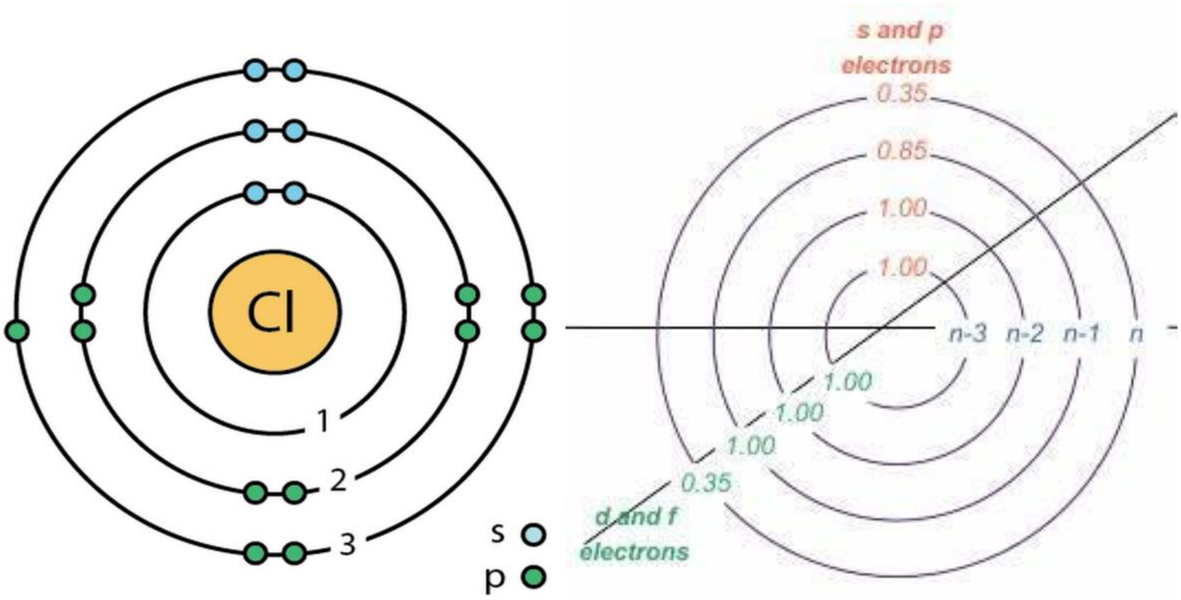


Figure IV.4: SLATER rules

$Z* = 17 - (6 * 0, 35) - (8 * 0, 85) - (2 * 1) = 6,1$

For ions:

$Z* = 17 - (7 * 0, 35) - (8 * 0, 85) - (2 * 1) = 5, 75$

For a hydrogenoid: Bohr.

$$r = a_0 \frac{n^2}{Z}$$

With: $a_0 = 0.529$ Å

For poly-electronic atoms, we replace (Z) by (Z∗) and (n) by (n∗)

$$r = a_0 \frac{n^{*2}}{Z^2}$$

$n^* = 1$ for $n = 1$

$n^* = 2$ for $n = 2$

$n^* = 3$ for $n = 3$

$n^* = 3.7$ for $n = 4$

$n^* = 4$ for $n = 5$

$n^* = 4.2$ for $n = 6$

Ionic radius:

Adding one or more electrons increases the shielding effect and decreases (Z^*) which increases the radius. Anions are therefore always larger than their original neutral atoms. Conversely, if electrons are removed, the shielding effect decreases and therefore (Z^*) increases, which decreases the radius. Cations are therefore always smaller than their original atoms.

Electron addition - - → screen effect ↑ ==> Z^* ↓ ===> r ↑

Electron withdrawal - - → screen effect ↓ ==> Z^* ↑ ===> r ↓

V.3.3. Ionization energy

$$A \rightarrow A^+ + 1e^- \qquad EI_1 = EA^+ + Ee^- - EA$$

The energy of the electron is zero since there has been ionization and the electron is at infinity and no longer interacts with the nucleus.

$Ee^- = 0$ (no interaction with the nucleus).

$$\mathbf{EI_1 = EA^+ - EA}$$

By evaluating the energy of (A) and (A+) we can evaluate the ionization energy by the difference between the two. The total energy of the atom will be evaluated by the sum of the individual energies of the electrons.

CHAPTER V: Periodic Classification of Elements.

I. *MENDELEYEV's* periodic classification

In the XIX (19) th century, only about sixty elements were known. Chemists had found that some elements had relatively similar chemical properties. These elements seemed to form relatively homogeneous families. For example, the halogen family (Fluorine, Chlorine, Bromine and Iodine) or those of the alkali metals (Lithium, Sodium and Potassium). We try to classify the elements in such a way as to show these families. The periodic table as we know it is essentially the work of ***MENDELEIEV***. In 1870 he published a table in which the elements were roughly classified in order of atomic masses. In addition, elements with similar properties were classified in the same column. To ensure that his classification took families into account, he did not hesitate to reverse the order of certain elements and to leave some cells empty. He thought that the missing elements. He described in advance the properties that these elements should have. These elements were discovered later and they did have the properties he had predicted.

II. Modern periodic classification

Today, chemical elements are arranged in ascending order of atomic number. Atoms with the same number of electrons on their outer layer are in the same column. Atoms with the same number of occupied electron layers are on the same line called the period. This classification is done in a table with seven (7) rows (period) and 18 columns (groups or sub-groups).

III. Construction principles

III.1. Period

There are seven (7) periods of different lengths. There is a simple relationship which can be used to find the number of elements (x) that a complete period of radius (n) can contain: For n odd.

$$x = \frac{(n+1)^2}{2}$$

For n even

$$x = \frac{(n+2)^2}{2}$$

III.2. Blocks

The elements are placed in three blocks:

Block (s): corresponds to the filling of the sub-layer (ns) of the nth layer.

Block (p): fills the sub-layer (np) of the nth layer.

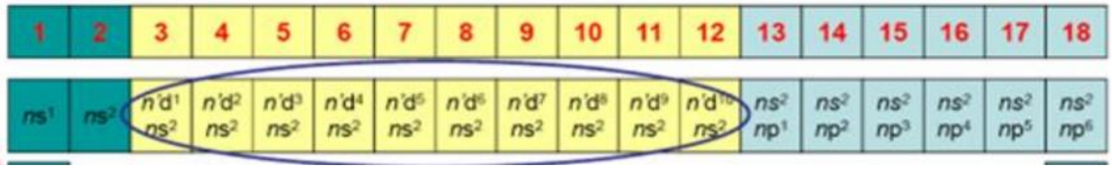
Block (d): fills the sub-layer ((n-1) d of the nth layer.

Block (f): fills the sub-layer ((n-2) f of the nth layer. In this block

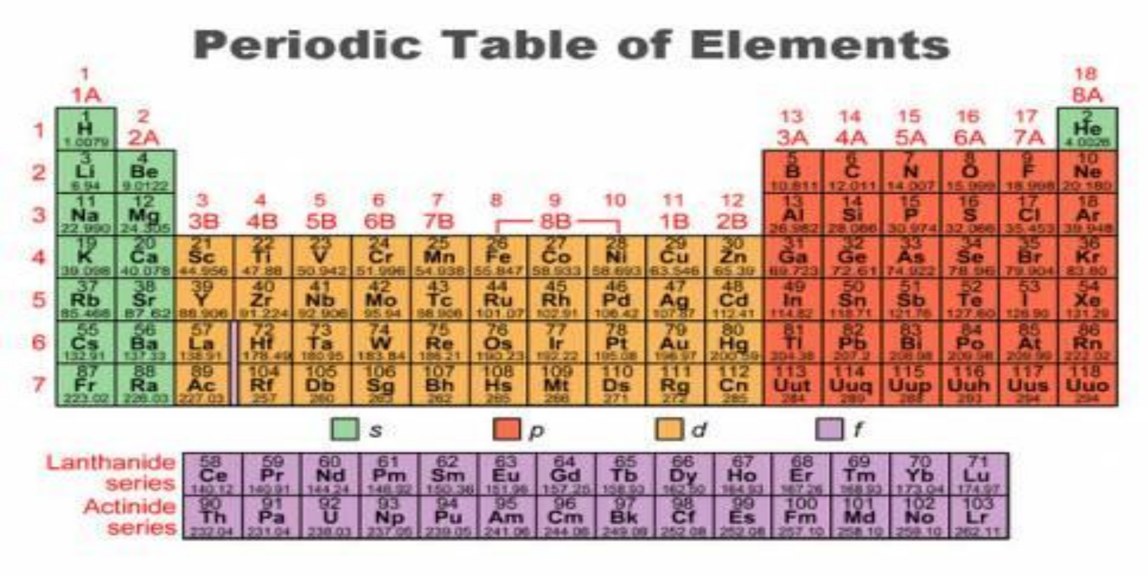
There are two families:

Lanthanide families: corresponding to the filling of the sub-layer (4f)

Actinide families: corresponding to the filling of the sub-layer (5f)



1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
ns^1	ns^2	$n'd^1$ ns^2	$n'd^2$ ns^2	$n'd^3$ ns^2	$n'd^4$ ns^2	$n'd^5$ ns^2	$n'd^6$ ns^2	$n'd^7$ ns^2	$n'd^8$ ns^2	$n'd^9$ ns^2	$n'd^{10}$ ns^2	ns^2 np^1	ns^2 np^2	ns^2 np^3	ns^2 np^4	ns^2 np^5	ns^2 np^6



Periodic Table of Elements

	1 1A	2 2A	3 3B	4 4B	5 5B	6 6B	7 7B	8	9 8B	10	11 1B	12 2B	13 3A	14 4A	15 5A	16 6A	17 7A	18 8A
1	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Uuq	115 Uup	116 Uuh	117 Uus	118 Uuo

🟩 s 🟥 p 🟧 d 🟪 f

Lanthanide series	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
Actinide series	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

Figure V.1: Periodic Table of elements

III.3. Chemical groups

Columns form chemical groups with similar properties, i.e. the same external structure. They are denoted by Roman numerals from **I** to **VIII**. There are two types of sub-group: A and B such as:

a. Sub-group A: Has an external structure (the valence electrons are the electrons of the s and p sub-layers). In this case, the chemical groups are noted: $\mathbf{I_A}$ a $\mathbf{VIII_A}$.
This group includes the following families:
The family of alkalis with an electronic structure (nS1) except for hydrogen (column 1).
The alkaline earth family with electronic structure (nS2) (column 2).
The halogen family, electronic structure (nS2 np4) (column 16).
The halogen family with electronic structure (nS1 np5) (column 17).

b. Sub-group B: the structure of the outer layer is (nS2 (n-1) dx) these are the elements belonging to columns 3 to 7 and 11 and 12. They are called ***transition elements***.

III.4. Rare or noble gases

These are elements found in column 18 (VIIIA). These elements are present in very small in the atmosphere and are not very reactive. They are characterized by sub-layers (S and p) that are which gives them greater stability.

III.5. Metals and non-metals

Most of the elements on the periodic table are metals. They occupy the left-hand side of the table. Metals tend to form cations (give up electrons)

$$\text{Mg} \text{ ---------}\rightarrow \text{Mg}^{+2} + 2\ e^{-}$$

Non-metals occupy the right-hand side of the table. They tend to form anions (capture electrons). Between the two types, there are metalloids that exhibit both metallic and non-metallic behavior. They are called semiconductors (boron, silicon, arsenic, antimony, tellurium, and astatine).

Conclusion

Elements are classified in ascending order of atomic number. In a line or period we classify elements belonging to the same layer. In the same column, elements with the same external electronic structure or the same number of valence electrons. All the elements in the sand block are in sub-group A; the elements in the block whose sub-layer is incompletely filled are the transition metals and the B sub-group.

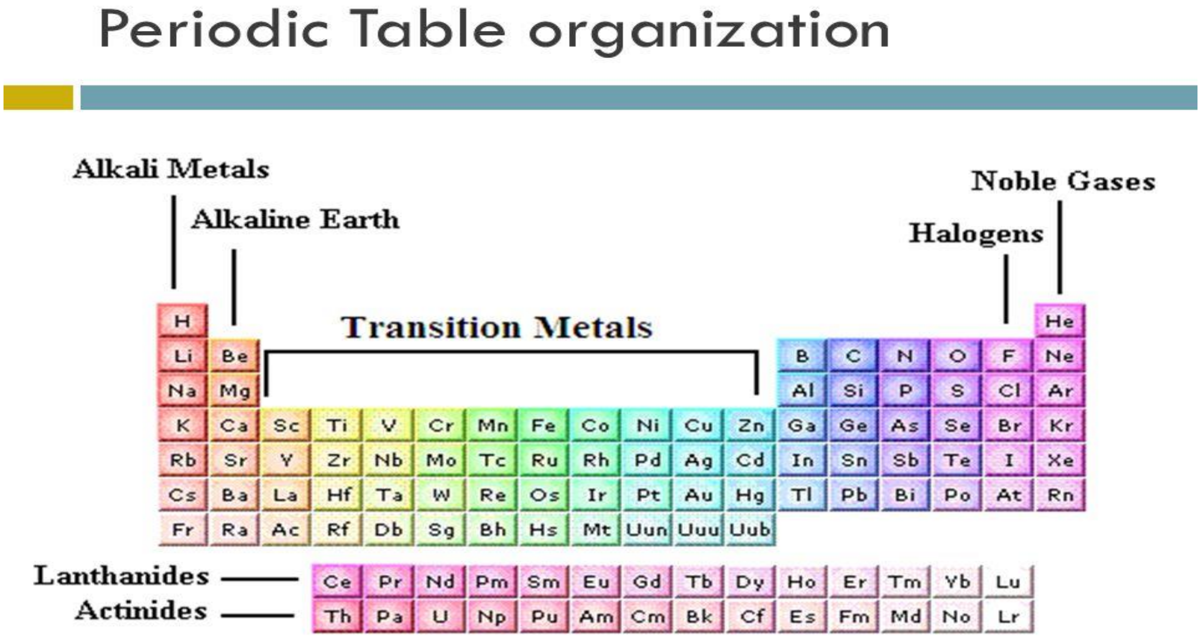


Figure V.2: Periodic Table Organization

IV. Evolution of the periodicity of the physico-chemical properties of elements

IV.1. Atomic radius(R)

Following a period, the radius decreases from left to right (I_A----→ V_{IIIA})

The cation (electron loss) has a smaller radius than the neutral atom.

The anion (electron gain) has a larger radius than the neutral atom.

IV.2. Ionization energy (IE)

This is the energy required to extract electrons from an atom. The ionization energy increases from the left to the right of the periodic table, because the further to the right you go, the greater the number of electrons that can be extracted. The number of electrons increases (Z increases), the attraction between nucleus-electron increases and the electrons will be more attached to the nucleus. Therefore, to remove them from the atom, we need to provide more energy, so the ionization energy increases over the same period. Following the same column, the ionization energy decreases from top to bottom, because the further down you go, the greater the number of ions downwards, the more layers there are, the further and the electrons are from the nucleus and the attraction between nucleus and electron decreases, and consequently the ionization energy decreases.

IV.3. Electron affinity (EA)

This is the energy involved in the addition of an electron to the neutral gaseous atom. This addition produces a negative ion according to the diagram:

A + 1e- → Gas + energy or electronic affinity

Electronic affinities are not easy to measure. Several methods exist, the most common is to measure the ionization energy of the negative ion.

$$A^{-}\text{gas} + \text{energy or electronic affinity} \rightarrow A\ \text{gas} + 1e^{-}$$

Since these two equations are inverses of each other, we have:

Ionization energy = electron affinity in absolute value in general, electronic affinities tend to increase with Z over a period of time since halogens have the highest electron affinities.

Note:

For nble gases, very low electron affinities are to be expected because here an extra electron would have to occupy an electron cloud where n is greater than n of these valence electrons, so it would not be well retained by the nucleus. The ionization energy of ion A- ion, i.e. the electron affinity of A, will vary as the ionization energy of the ionized atom.

IV.4. Electronegativity

This represents the ability of an element in a molecule to acquire a negative charge. It is a qualitative description of electron sharing in a chemical bond between two different atoms. The electronegativity of an atom is not apparent when it is isolated, but only when it chemical bond with another element. Three different scales are used to measure this tendency of atoms to attract electrons to greater or lesser extent electrons:

a. PAULING scale

This is the most commonly used scale. In this scale, the difference in electronegativity between two elements is evaluated by the relation.

$$(x_A - x_B)^2 = \Delta_{(eV)} = E_{A-B} - \sqrt{E_{A-A} - E_{B-B}}$$

b. MULLIKEN scale

For MULLIKEN, electronegativity is the arithmetic mean between the energy of first ionization energy and the electro-affinity of the element:

$$x_m = \frac{1}{2}(EI_1 + EA)$$

c. ALLRED and ROCHOW scale

Electronegativity is the force of attraction between an atom and an electron separated from the nucleus of that atom by a distance equal to the atom's covalent radius. by a distance equal to the atom's covalent radius.

$$x = \frac{0.35 * Zeff^2}{r^2} + 0.744$$

CHAPTER VI: Chemical bonds.

I. The covalent bond in LEWIS theory

The term "bond" refers to all the interactions involved in holding atoms together to form stable molecules.

Considerations:

The stronger the chemical bond, the greater the energy required to break it;

The system formed is stable when its energy is minimal;

When two atoms unite, the system formed (molecule) has a lower energy than that of the two isolated atoms that of the two isolated atoms;

The electrons of the atoms involved in the bonds are the electrons of the layers or valence electrons.

Rare gases are the most stable elements; their structure corresponds to a minimum of energy; and from this we can deduce **the octet rule**.

The octet rule an atom or ion with an electronic structure similar to that of rare gases, that is, 08 electrons in the valence shell, will be very stable. In other words: "to form a stable whole, atoms tend to exchange electrons in such a way as to acquire the electronic configuration of rare gases.

I.1. Valence layer

This is the outermost layer occupied by electrons (the layer with the highest n). If an inner sublayer is not completely filled, this sublayer is considered to be part of the valence layer part of the valence layer. It is this layer that gives the elements their chemical properties.

Valence electrons: are the electrons belonging to the valence layer.

I.2. The different types of bond

a. Covalent bond: this results from the formation of a pair of electrons with opposite spins belonging to both atoms.

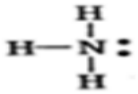
b. Dative bond or covalent coordination bond: this is a covalent bond between two atoms where the two electrons shared in the bond come from the same atom.

c. Ionic bond: this is formed between ions with opposite signs (purely ionic bonds do not exist. This is the limit of the covalent bond.

d. Polarized bond: this is a partially covalent bond. It is considered to be between two elements of different electro-negativity.

I.3. LEWIS diagram (covalent bond model): This model is convenient for represent the molecule simply. It considers only the valence electrons that actually participate in the bonds in the bonds. The covalent bond is symbolised by a dash.

Example:



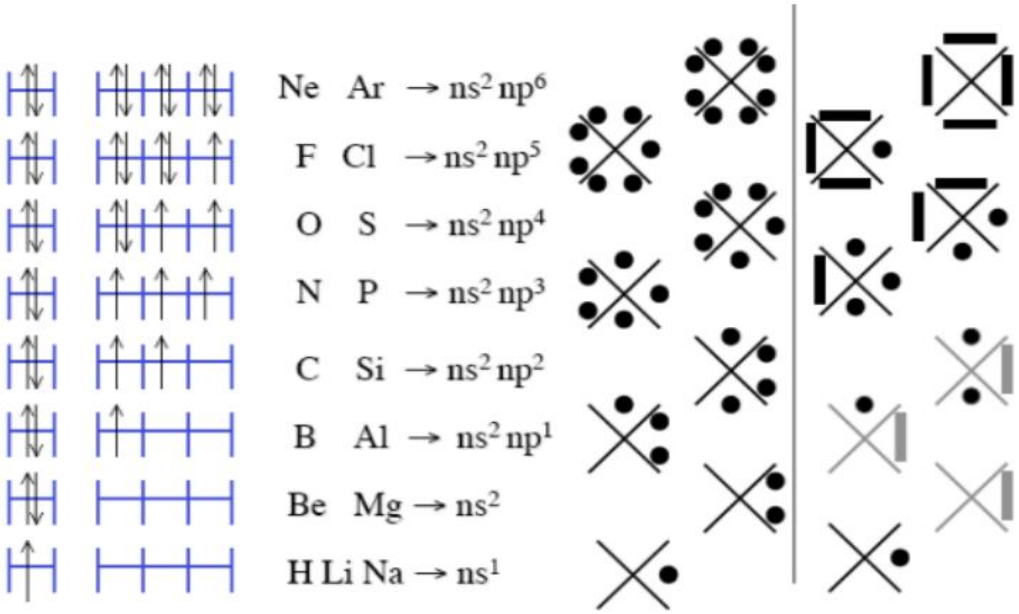


Figure VI.1: LEWIS diagram of atom.

Note:

Excited states are indicated by superscript stars (*). The number of stars corresponds to the number of excitations. All the excitations considered increase the atom's valence of the atom. It is sometimes interesting to decrease the valence. This is possible by the reverse mechanism. Instead of unpairing doublets to obtain single electrons, it is necessary to is possible to pair single electrons to obtain doublets and thus reduce the valence.

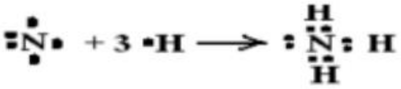
Examples:

1) H_2 $H\ (Z=1)\ :\ 1s^1\ \boxed{\uparrow}$ $\boxed{\uparrow}\ H\ (Z=1)\ :\ 1s^1 :$ **•H**

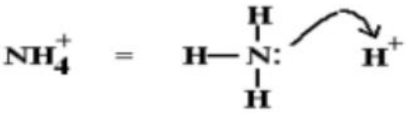
Representing molecules:

H•—•H

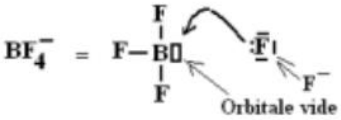
2) NH_3: $N\ (Z=7) : 1s^2\ 2s^2 2s^3$ $\boxed{\downarrow\uparrow}\boxed{\uparrow}\boxed{\uparrow}\boxed{\uparrow}$



3) NH_4^+ : $NH_3 + H^+ \dashrightarrow NH_4^+$; BF_4^- : $BF_3 + F^- \dashrightarrow BF_4^-$



;



It can happen that two atoms are joined together by several bonds at the same time. (Multiple bonds). There are only 03 types of bond: single, double and triple.

Notions of valence excitations of atoms:

To obtain the diagram of molecules according to LEWIS, the fundamental state is not sufficient for all possibilities. The Lewis diagram to obtain the desired bonds more easily. These modifications correspond to the creation of excited states. In the Lewis model, it is the single electrons that form the chemical bonds.

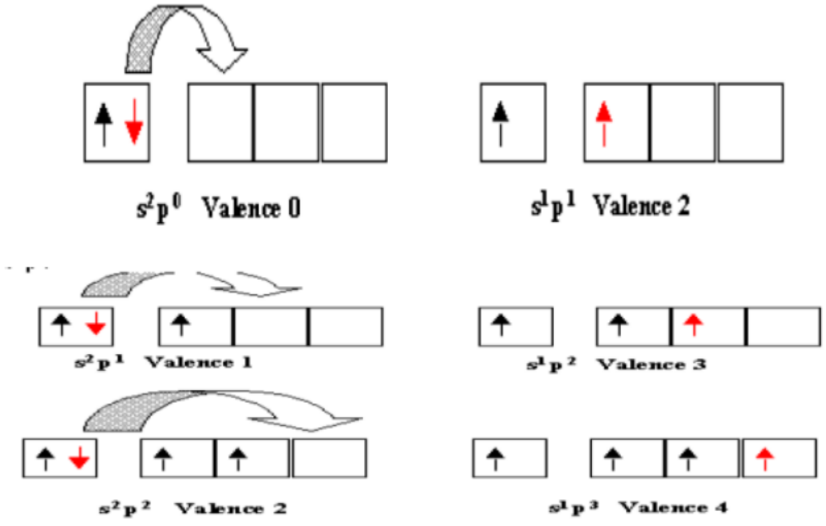
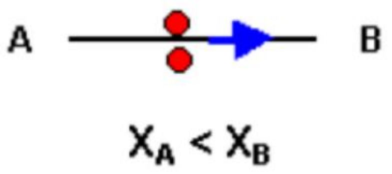


Figure VI.2: LEWIS diagram of chemical bands.

II. Polarized covalent bond, dipole moment and the partial ionic nature of the bond

When the bond is formed by atoms of the same species (A2, X3,...) there is a symmetrical distribution of the electronic cloud ensuring the covalent bond. Symmetrical distribution of the electron cloud ensuring the covalent bond. The bond is then non-polar. When the bond is not symmetrical, the most electronegative atom receives an excess of electrons and acquires a negative positive charge. Conversely, the other atom loses electrons and acquires a positive charge. The molecule is considered to be an electric dipole and the bond is said to be polarized.



This polarized bond has a dipole moment which is a vector quantity characterized by: A direction: that of the bond;

Direction: from pole (+) to pole (-);

Intensity: U = q * d; q: electric charge, d: distance separating the two charges.

II.1. Iconicity of connections:

The iconicity of a bond is expressed by its iconicity percentage. This is given by the relation

$$CI = \frac{\mu_{exp}}{\mu_{the}} * 100 = \frac{qd}{ed} * 100 = \frac{q}{e} * 100$$

III. Geometry of molecules

V.S.E.P.R or GELLESPIE methods this is a simple way of predicting the geometric shape of molecules from their **LEWIS diagram**. V.S.E.P.R stands for Valence Schell Electronic Pairs Repulsion of the Valence Layer. Gillespie is based on the distribution of electronic doublets around a central nucleus and their repulsion. Depending on the number of doublets around the central nucleus, we obtain several geometric shapes of the molecule.

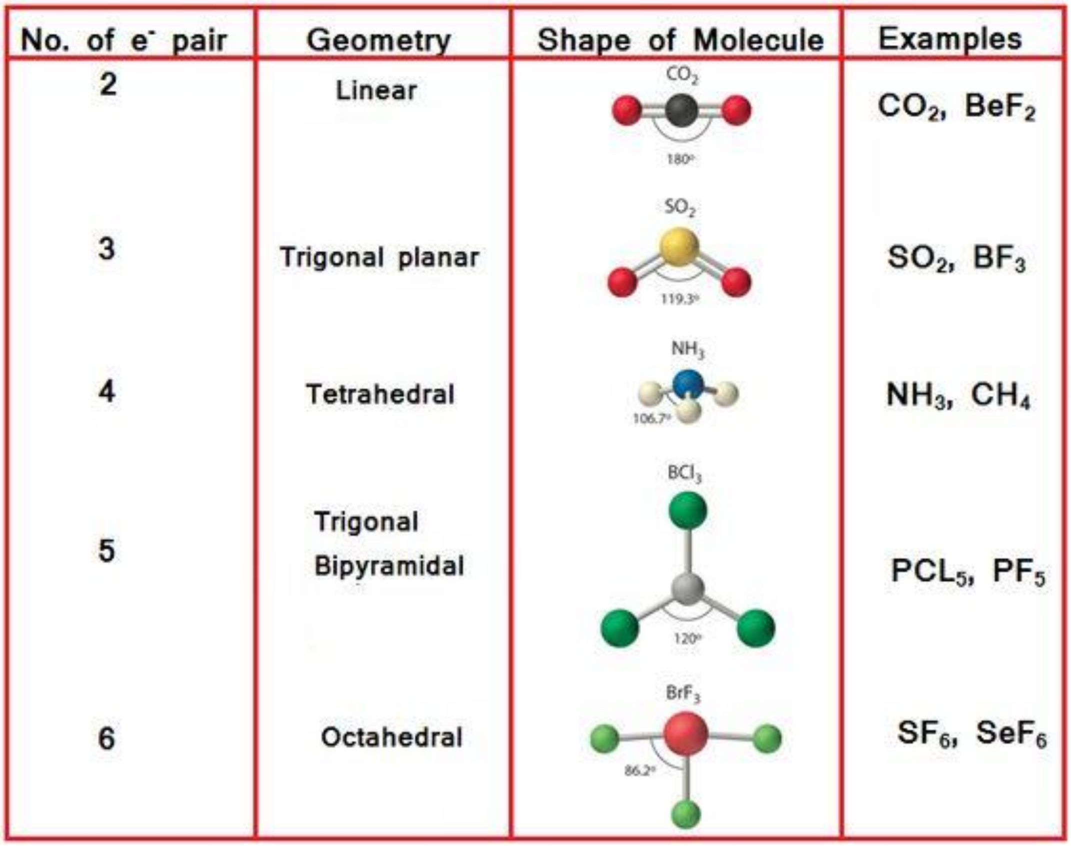
Two doublets will be placed at either end of a diameter of the sphere. The pattern of repulsion is a straight line.

Three doublets will be positioned on an equatorial plane of the sphere, in directions corresponding to those of an equilateral triangle 120° apart.

Four doublets will be placed on the surface of the sphere, in directions corresponding to those of a tetrahedron at 109.5° to each other.

Five doublets will be placed on the surface of the sphere, in directions corresponding to those of a pyramid with a triangular base. The first three are at 120° to each other on an equatorial plane. The other two will be placed on either side of this plane.

Six doublets will be placed on the surface of the sphere, in directions corresponding to those of a pyramid or octahedron, with the first four placed at the vertices of a square.



No. of e⁻ pair	Geometry	Shape of Molecule	Examples
2	Linear	CO_2 180°	CO_2, BeF_2
3	Trigonal planar	SO_2 119.3°	SO_2, BF_3
4	Tetrahedral	NH_3 106.7°	NH_3, CH_4
5	Trigonal Bipyramidal	BCl_3 120°	PCL_5, PF_5
6	Octahedral	BrF_3 86.2°	SF_6, SeF_6

Figure VI.3: V.S.E.P.R or GELLESPIE methods.

Determining the geometry

A molecular model will be described by the following form: $\mathbf{AX_nE_m}$

Where: A is the central atom,

n: denotes the number of binding doublets

m: denotes the number of non-bonding doublets

The geometry of the molecule can therefore be predicted as a function of n+m.

n+m = 2 Linear form $\alpha = 180°$ Triangular form

n+m = 3 triangular shape $\alpha = 120$

n+m = 4 tetrahedral shape $\alpha = 120°$

n+m = 5 Bipyramid shape with triangular base α = 90° and 120°.

n+m = 6 Octahedron shape α = 180°

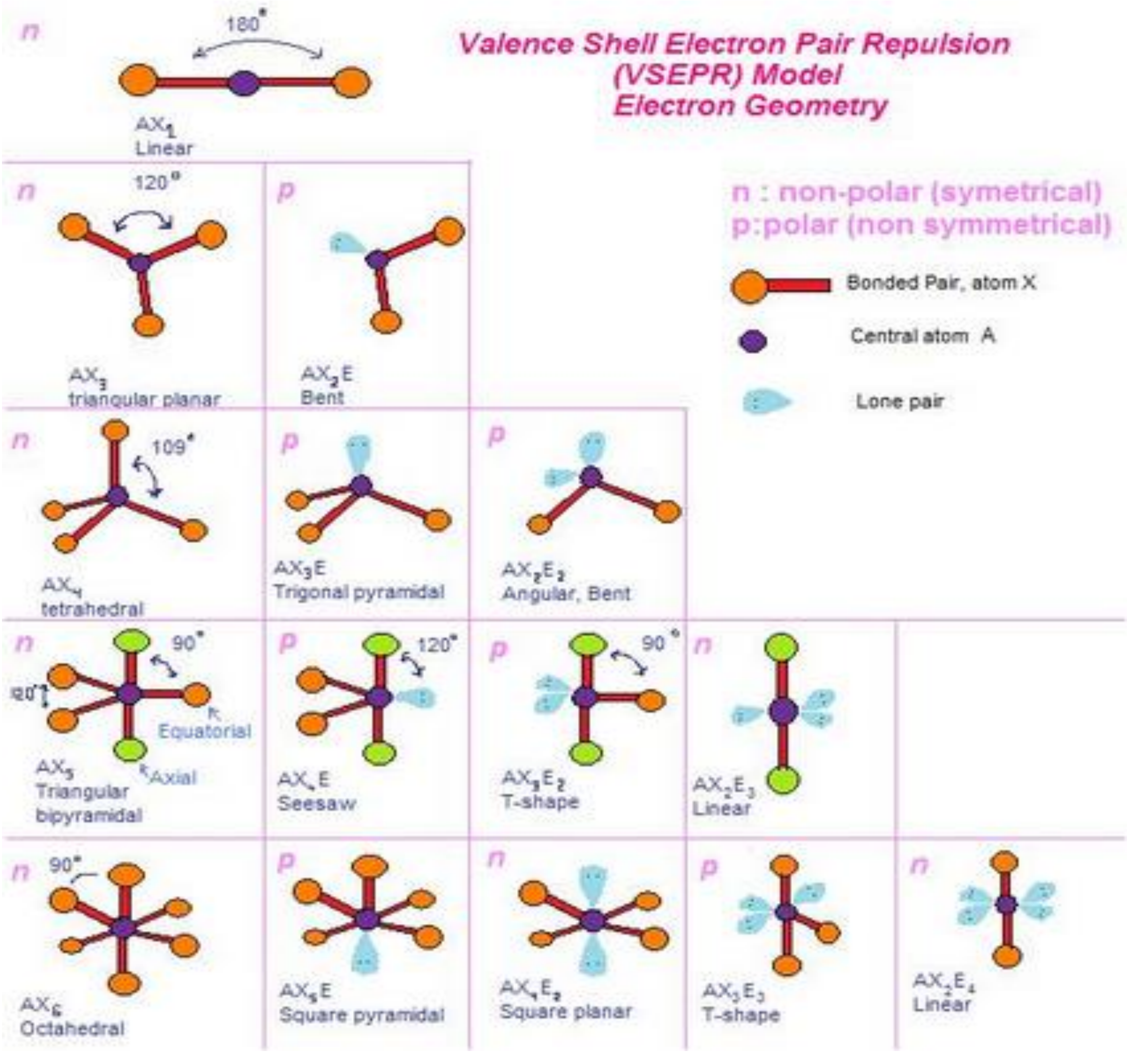
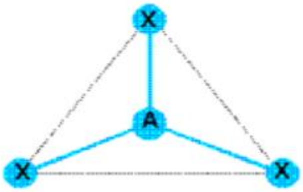


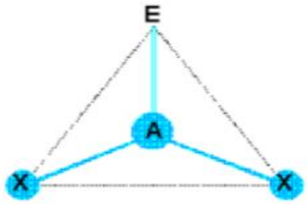
Figure VI.4: Molecular model geometry.

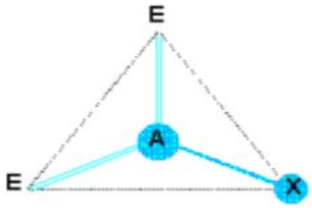
a. <u>n+m = 3</u>

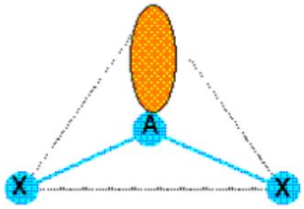
Figure of repulsion: Equilateral triangle

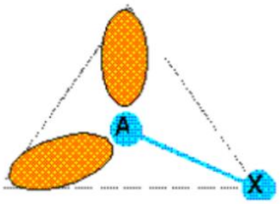
Molecular types: AX3 - AX2E - AXE2











The AX3 molecule is indeed a flat triangular molecule.

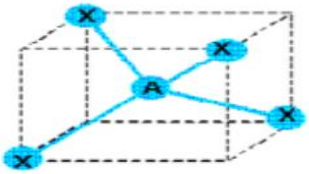
The AX2E molecule will be V-shaped with an angle of 120°.

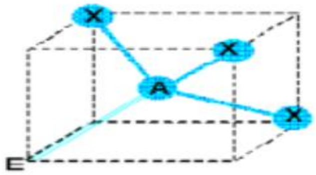
The molecule AXE2 will be linear.

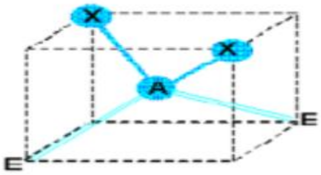
b. <u>n+m = 4</u>

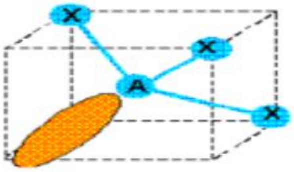
Figure of repulsion: Tetrahedron

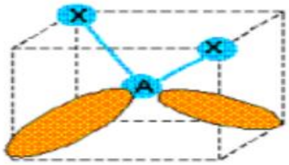
Molecular types: AX4, AX3E, AX2E2, AXE3











IV. Chemical bonding in the quantum model

IV.1 Molecular orbital theory (LCAO method)

In the atom, each electron is described by an atomic orbital Ψ. In the molecule, each electron will be described by a wave function which is a molecular orbital. The theory of molecular is based on the following principles, which are similar to those for atoms.

Note: it is possible to solve the Schrodinger equation rigorously for a single-electron system, but the problem is much more difficult than for a hydrogen atom with a single-electron system. But the problem is much more difficult than for the hydrogen atom because of the loss of spherical because of the loss of spherical symmetry, and the calculations are considerably more involved.

a. Formation and nature of bonds

In the Lewis model, the bond resulted from the pooling of an electron doublet between two atoms. This simple idea remains broadly valid in the quantum model, in which the chemical bond results from the overlapping of two atomic orbitals to give two electron orbitals. Chemical bond results from the overlapping of two atomic orbital's to give two molecular orbitals. There are two types of overlap that will lead to two different types of bond bonds. In this section we will only look at bonds involving p-type atomic orbitals.

b. Energy aspect:

The complete solution of the Schrödinger equation leads to the value of the energies of the two Molecular orbitals. We find that the energy of the bonding orbital is lower than that of the separate atoms, which corresponds to stabilization. Conversely, the anti-bonding orbital has a higher energy, which corresponds to destabilization.

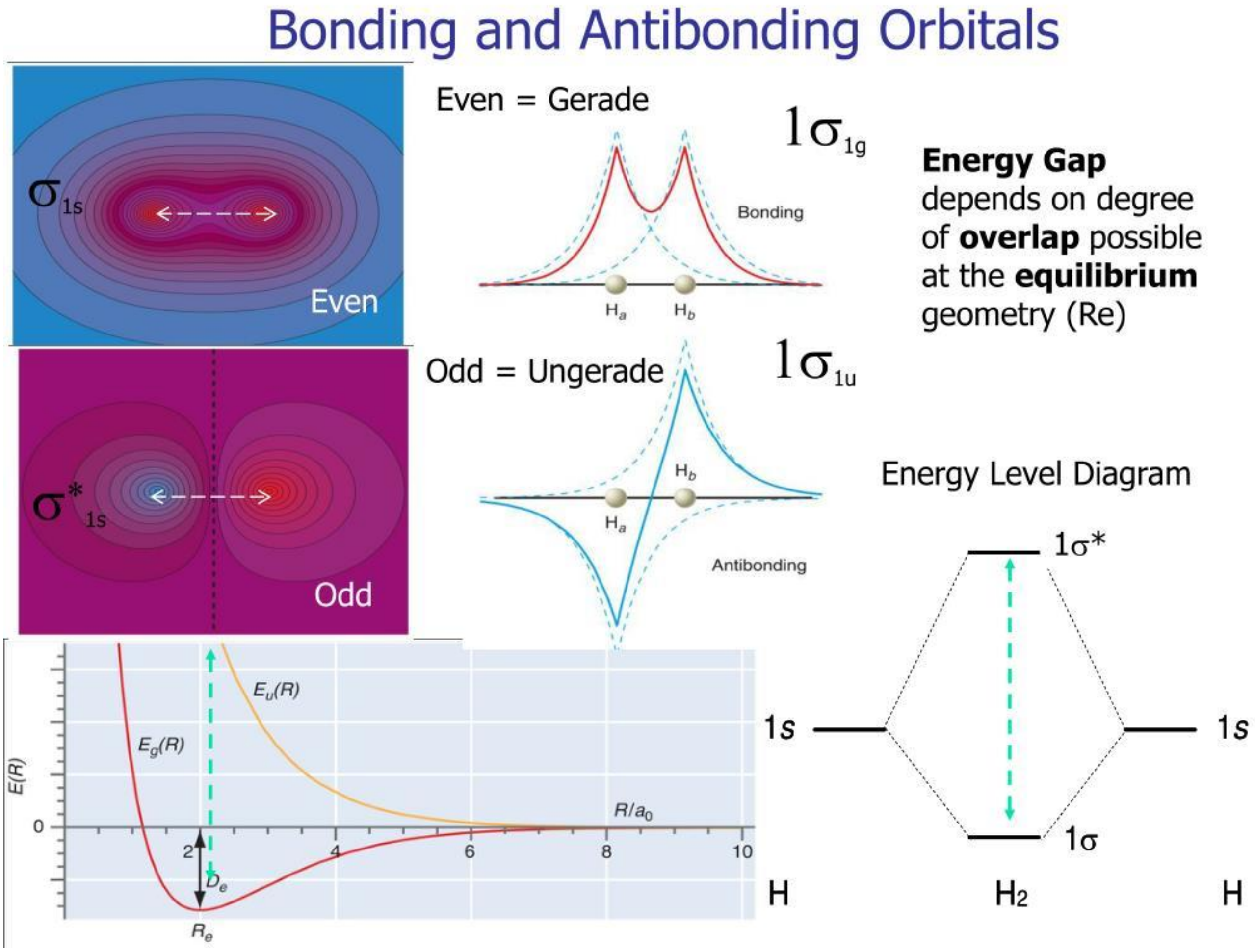


Figure VI.5: Bonding and Anti-bonding orbitals.

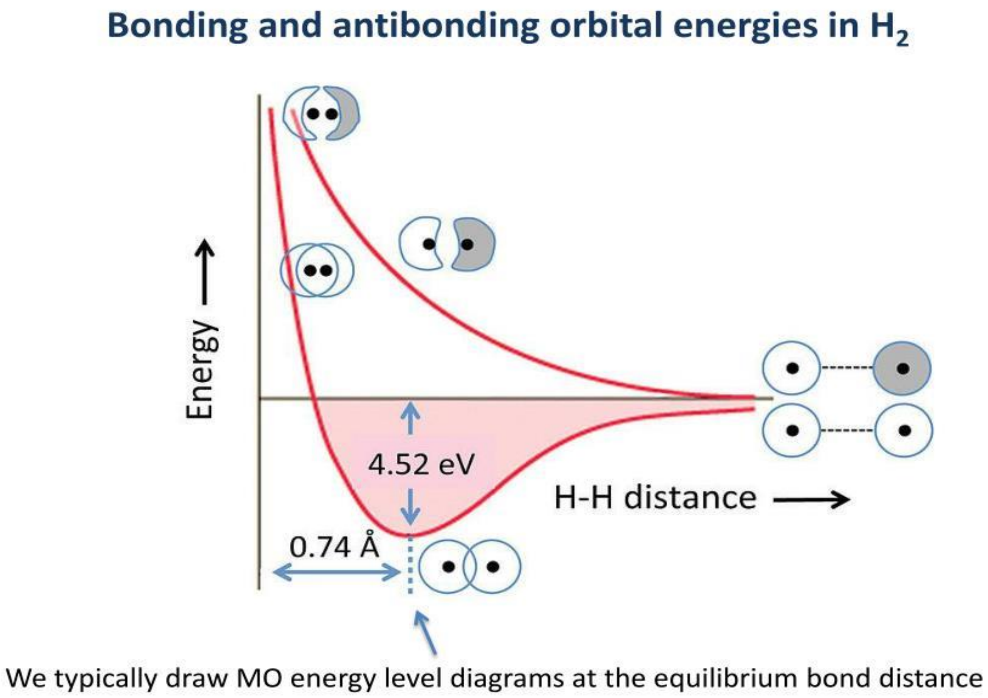
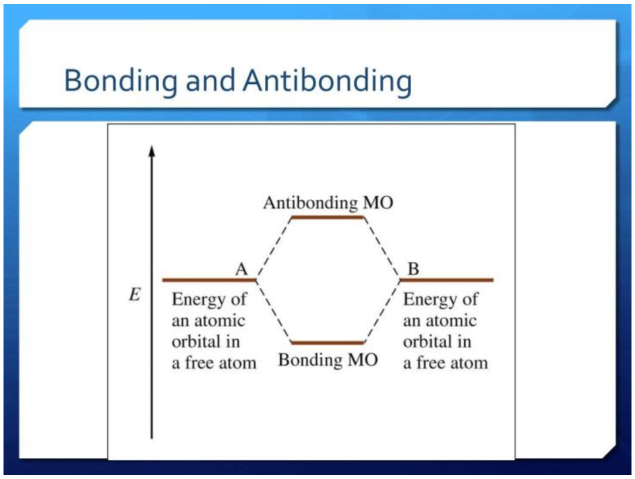


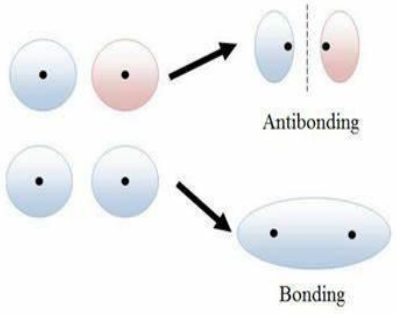
Figure VI.6: Bonding and Anti-bonding orbital energies in H_2.

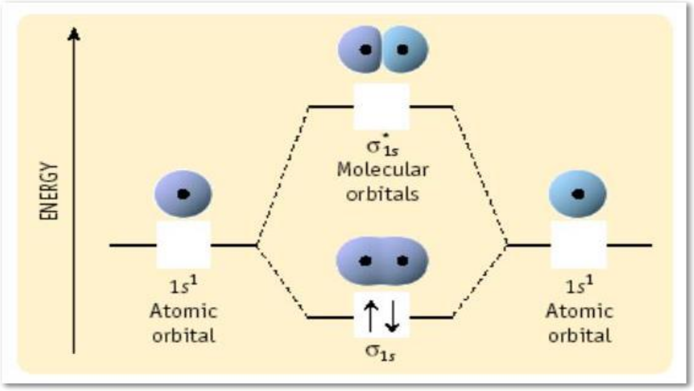
IV.2. Generalization to homo-nuclear diatomic molecules

The results obtained for the H_2 molecule are generalized to the other diatomic molecules homonuclear diatomic molecules He_2, Li_2, Be_2, B_2, C_2, N_2, O_2, F_2 and Ne_2.The He_2 molecule: the atomic orbitals (A.O.) to be considered are the 1s orbitals of He occupied by two electrons since the configuration of the atomic orbitals is the same by two electrons, since the configuration of He is $1S_2$. The diagram will be identical to that obtained for H_2.


Bonding and Antibonding

Molecular Orbital Theory



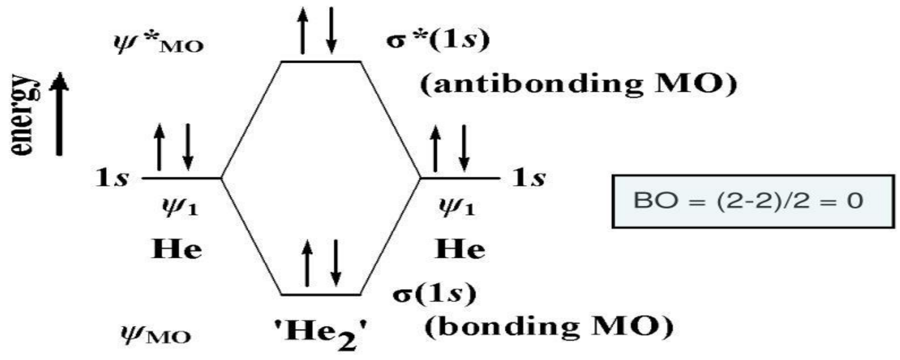


1. # MO’s = # atomic orbitals used.
2. Bonding MO is lower in energy than atomic orbitals. Antibonding MO is higher.
3. Electrons assigned to MO’s of higher and higher energy.

Bond order = 1/2 [# e- in bonding MOs
- # e- in antibonding MOs]

Figure VI.7: Molecular orbital theory.

The non-existent He_2 molecule
(bond order = 0)



The MO diagram for the He_2 molecule is similar to that for the H_2 molecule, but we see that the energy drop of the pair of electrons in the $\sigma 1s$ orbital is negated because the other pair in the $\sigma^* 1s$ rises in energy by an equal amount. There is thus no net stabilization, and so the He_2 molecule does not exist.

Calculation of the bond index: nl = 1/2 (2 - 2) = 0

The bond index is zero, which means that no bond is formed between the two helium atoms. Helium atoms. This fact is confirmed by experiment; helium is an inert gas that does not form molecules. If we take into account the fact that $\Delta E^* > \Delta E$ we can even see that He2 is less stable than the two separate Helium atoms, the formation of a molecule would correspond to a destabilization and the molecule cannot exist.

IV.3. Polyatomic molecules or atomic orbital hybridization theory

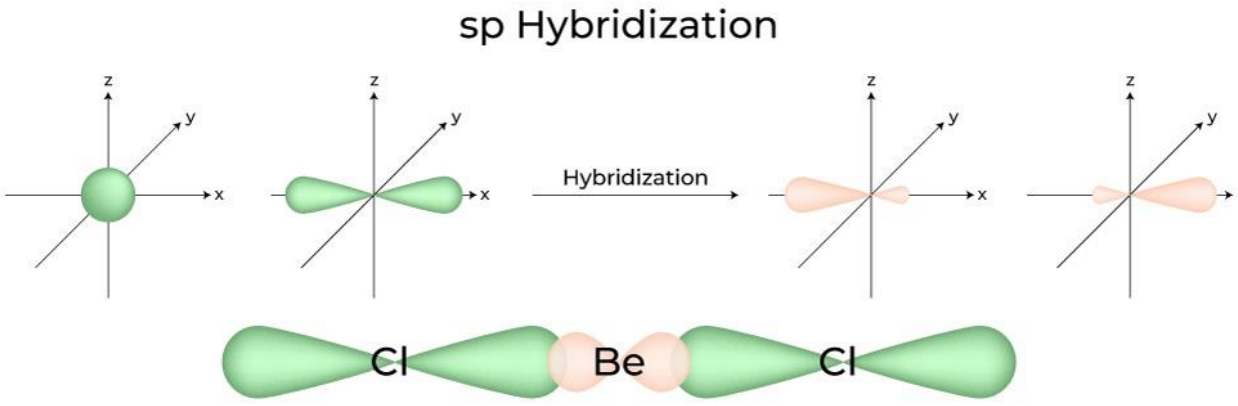
The case of molecules with more than two atoms is of course more complex than that of diatomic molecules. The main additional difficulty consists in bringing the molecular geometry into play geometry. The use of normal atomic orbitals does not explain the different geometric forms of molecules shapes of molecules with identical atomic orbitals. To overcome this difficulty, we turn to the notion of hybridization of atomic orbitals. It can be shown mathematically (and we will admit it) that any linear combination of two or more wave functions or more wave functions that are solutions of the Schrödinger equation is itself a solution of this Schrödinger equation. It is this mathematical property that forms the basis of the technique of hybridization of atomic orbitals.

We are not going to go into the details of this mathematical technique, but we will simply illustrate its interest. We start by identifying the atomic orbitals involved in the bonds under consideration. An each atomic orbital is assigned a mathematical function and its own geometric shape. The actual geometric shape of the molecule is determined either experimentally or by applying the V.S.E.P.R. method. The geometry of the bonds in the molecule is therefore known (the angle between them). We then mathematically determine the linear combination of the initial atomic orbitals, which will lead to new orbitals called hybrid orbitals whose geometric shape corresponds to the actual shape of the molecule under study. This mathematical sleight of hand then allows us to explain the formation of molecular orbitals by overlap of these hybrid atomic orbitals.

There are three types of hybridization suitable for describing the geometry of molecules:

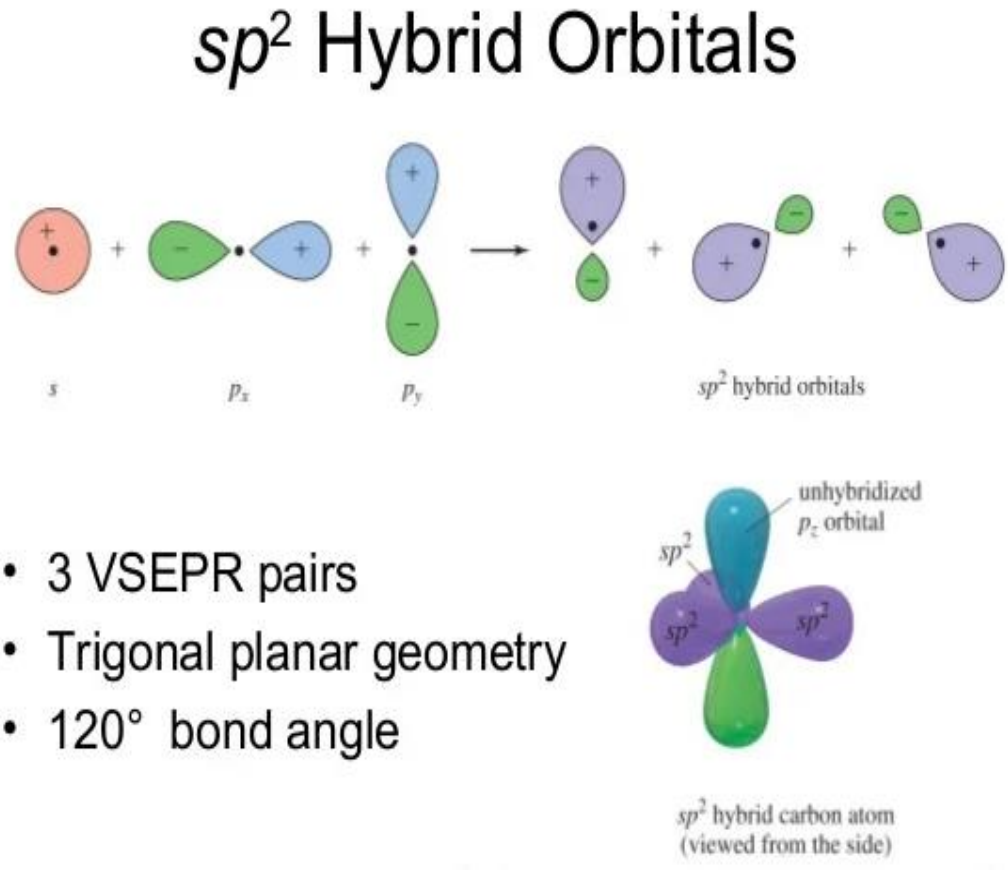
IV.3.1. sp hybridization (linear or diagonal):

This first form of hybridization corresponds to a mixture of the s orbital and a p orbital, with the other two remaining unchanged (hence the name sp). Such a mixture replaces two of the by two collinear hybrids pointing along a straight line. These two functions are therefore well suited to describing linear molecules such as $BeCl_2$, acetylene, HCN...



IV.3.2. sp^2 hybridization (trigonal)

This corresponds to a mixture of the s orbital and two p orbitals, the third remaining unchanged (Hence the name sp2). Such a mixture replaces three of the initial functions with three hybrids pointing towards the vertex of an equilateral triangle. They are therefore well suited to description of planar molecules such as boron derivatives or double-bonded compounds such as ethylene such as ethylene, formaldehyde (H_2CO)...

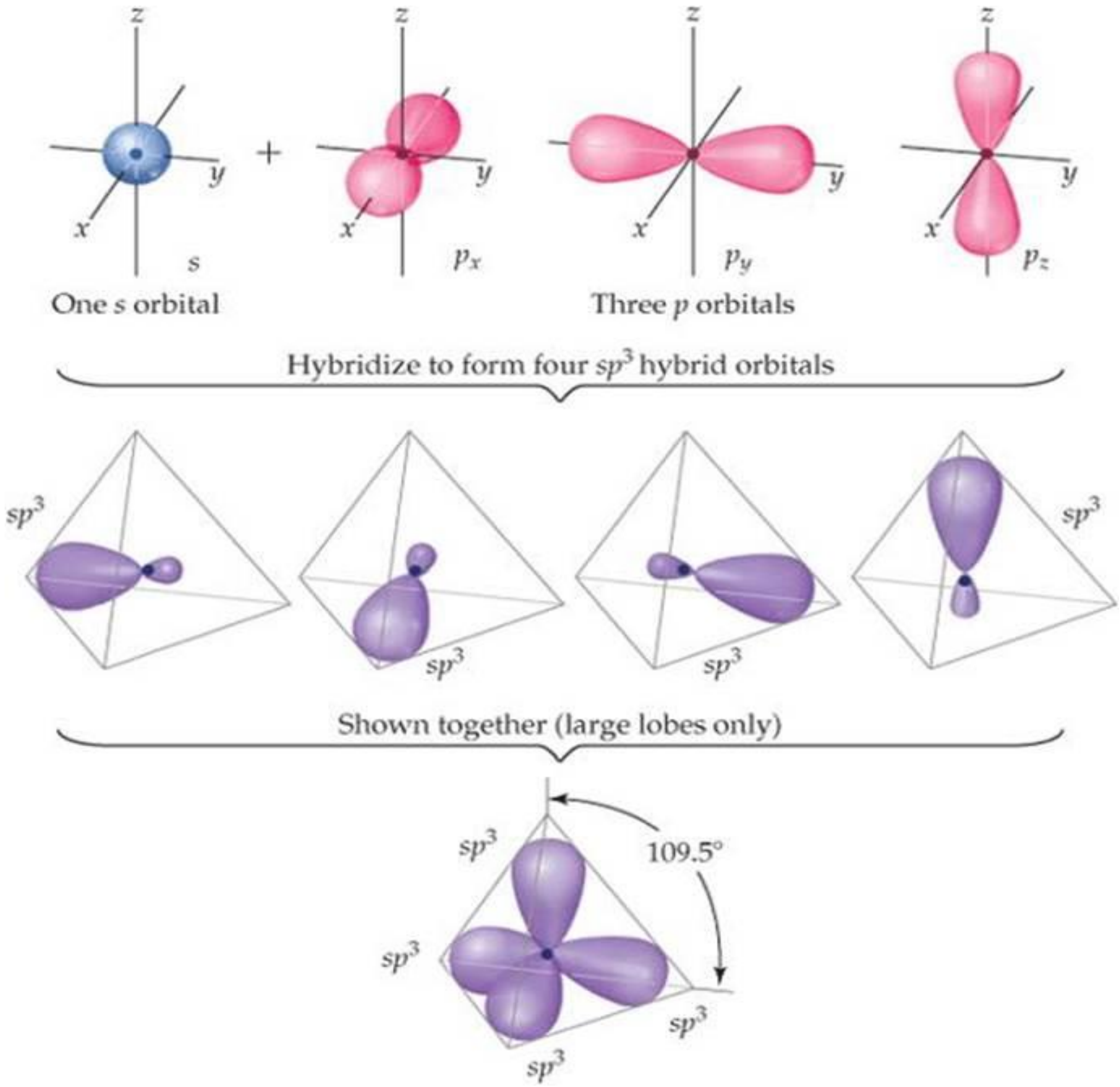


sp^2 Hybrid Orbitals

- 3 VSEPR pairs
- Trigonal planar geometry
- 120° bond angle

IV.3.3. sp^3 hybridization:

This hybridization corresponds to a mixture of the s orbital and the three p orbitals (hence the name sp3). Such a mixture replaces the four initial functions with four hybrids pointing towards the vertex of a tetrahedron. These new functions are therefore perfectly suited to the approach described. Above and can be applied to all molecular structures involving atoms in a tetrahedral environment. Let's take the example of the carbon atom and the oxygen atom.


z
y
x
s
+
p_x
p_y
p_z
One s orbital
Three p orbitals
Hybridize to form four sp^3 hybrid orbitals
sp^3
Shown together (large lobes only)
109.5°

REFERENCES

- Chemguide.co.uk, (2015). atomic orbitals. Retrieved 28 September 2015, from http://www.chemguide.co.uk/atoms/properties/atomorbs.html
- Chemwiki.ucdavis.edu, (2015). Atomic orbitals. Retrieved 27 September 2015, from http://chemwiki.ucdavis.edu/@api/deki/files/8855/Single_electron_orbitals.jpg
- Chemwiki.ucdavis.edu, (2014). 6.9: Electron Configurations and the Periodic Table - Chemwiki. Retrieved 2 October 2015, from http://chemwiki.ucdavis.edu/?title=Textbook Maps/General Chemistry Textbook Maps/Map: Brown, LeMay, %26 Bursten %22Chemistry: The Central Science%22/06. Electronic Structure of Atoms/6.9: Electron Configurations and the Periodic Table
- Jha, A. (2013), What is Heisenberg's Uncertainty Principle? The Guardian. Retrieved 27 September 2015, from http://www.theguardian.com/science/2013/nov/10/what-is-heisenbergs-uncertainty-principle
- Mpcfaculty.net, (2015). Complete Electron Configurations. Retrieved 30 September 2015, from http://www.mpcfaculty.net/mark_bishop/complete_electron_configuration_help.htm
- Nano.gov. (2015), what is Nanotechnology? | Nano. Retrieved 5 November 2015, from http://www.nano.gov/nanotech-101/what/definition
- Wwu.edu, (2015). Stardust. Retrieved 27 September 2015, from http://www.wwu.edu/skywise/a101_dust.html
- Atkins, Peter and Julio de Paula. Physical Chemistry for the Life Sciences. New York: Oxford University Press, 2006.
- Chang, Raymond. Physical Chemistry for the Biosciences. USA: University Science Books, 2005.
- Gore, Michael. Spectrophotometry & Spectrofluorimetry. New York: Oxford University Press, 2000.

- Price, Nicholas and Dwek, Raymond and Wormald, Mark. Principles and Problems in Physical Chemistry for Biochemists. R. G. Ratcliffe. New York: Oxford University Press, 1997.
- Irwin H. Segel, Biochemical Calculations (How to Solve Mathematical Problems in General Biochemistry), 2nd edition, John Wiley & Sons, 1975 http://www.nist.gov/pml/div685/grp03/spectrophotometry.cfm