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Chemistry 1 : Structure of Matter

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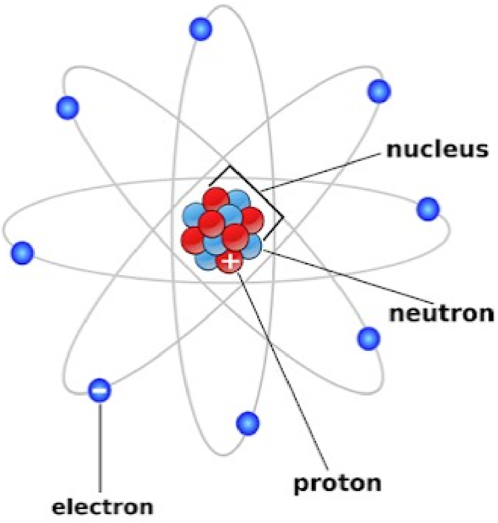

Course for Commun core in sciences and technology

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Table of contents

Introduction

This document on general chemistry, aligned with the LMD system used in Algerian universities, targets first-year students in the common core of technical sciences (ST), material sciences (SM), transport engineering (TR), and related fields. It aims to assist students in navigating the challenges of scientific discourse while ensuring precision. The content summarizes essential knowledge about the structure of matter, a crucial aspect of general chemistry that addresses fundamental concepts of matter.

The document comprises seven chapters:

- Chapter one revisits basic concepts such as states of matter, atoms, molecules, and solutions.
- Chapter two focuses on the atom's essential components and its physical properties, detailing significant experiments (Crookes, J.J. Thomson, Rutherford, Millikan, and Goldstein) that uncovered the electron, proton, and neutron. It concludes with a discussion on atomic structure, isotopes, and their separation and stability.
- Chapter three explains radioactivity and nuclear reactions, including the law of radioactive decay.
- Chapter four reviews atomic description and study according to Bohr's theory, using the hydrogen atom and hydrogen ions as models—and covers related concepts such as the emission spectrum and quantum energy levels.
- Chapter five delves into quantum chemistry, addressing Louis de Broglie's hypothesis, Heisenberg's uncertainty principle, Schrödinger's equation, atomic orbitals, and the electron configuration of multi-electron atoms following the Klechkowski rule.
- Chapter six examines the periodic classification of elements, discussing the principles behind the modern periodic table, chemical families, and the periodicity of physical and chemical properties (atomic radius, ionization energy, electron affinity, electronegativity).
- Chapter seven focuses on chemical bonding, detailing various types such as covalent bonds in Lewis theory, polar covalent bonds, molecular geometry (VSEPR theory), and molecular orbital theory, including the study of polyatomic molecules and hybridization.

  This document reflects my experience teaching the structure of matter in various departments at Frères Mentouri University - Constantine 1.

Chaptre one : Fundamental basics

I

A. Principles and fundamentals

1. Matter

Is anything that takes up space, has volume and mass that can be measured, like water, air, clothes, objects, and more. Matter is made up of very small particles known as molecules, which are a group of even smaller particles called atoms. At the moment, it is believed that matter is made up of tiny particles that cannot be split and do not consist of smaller particles called subatoms.

2. Atom

The smallest part of an element that can take part in reactions without splitting. Atoms of the same element are similar, meaning elements differ from each other based on their atoms. Atoms are represented by one or two letters from their Latin names to distinguish and facilitate their study, like Oxygen atom O, Copper atom Cu, Carbon atom C, Mercury atom Hg. The dimensions of atoms are expressed in Angstrom units where $1A° = 10^{-10}$ m.

3. Molecule

Smallest part of a substance (element or compound). It can exist individually and manifest the properties of the substance.

4. Categories of molecules

- **Single-atom molecules:** These are molecules that contain only one atom, such as the inert gases (Rn, Xe, Kr, Ar, Ne, He), which means it can be said for the symbol: He, the helium atom, or helium molecule, as well as for the rest of the inert gases.

- **Two-atom molecules:** These are molecules that contain only two atoms, which are 7 molecules: I_2, Br_2, Cl_2, F_2, N_2, O_2, H_2.
- **Multi-atom molecules:** These are molecules that contain more than two atoms, such as the ozone molecule O_3, sulfur S_8, phosphorus P_4.

Compound molecules:These are molecules that contain atoms of different types, such as the water molecule H_2O, and the glucose molecule.

5. Physical properties of matter and its classification

a) Physical states of matter

- **Solid State:** Where materials in the solid state are characterized by a specific shape and volume, and materials can be transformed from the solid state to the liquid state in a process known as melting.
- **Liquid State:** Where materials in the liquid state are characterized by taking the shape of the container they are placed in, so they do not have a specific shape, but they have a specific volume. Materials can be transformed from the liquid state to the solid state in a process known as freezing, and from the liquid state to the gaseous state in a process known as evaporation.
- **Gaseous State:** It is a state in which the material does not have a specific volume or shape, and the material can be transformed from the gaseous state to the liquid state in a process known as condensation.

b) Classification of physical corps

Physical corps can be classified into homogeneous materials and others that are heterogeneous. Before delving into the classification, it is necessary to define:

- **System:** It is an isolated piece of the material world. The material in a system can be in different states and these states are phases.
- **Phase:** It is the phase in which the physical and chemical properties are uniform in all samples.
- **Homogeneous material:** Consists of one phase, and all its points have similar properties where its components cannot be distinguished by the naked eye. The material can be simple, compound, or homogeneous solution.
- **Heterogeneous material:** Consists of several phases, where its components can be separated by mechanical methods.

6. Changes in Matter

a) Chemical changes

These are the changes that occur to a substance or group of substances, to produce a new substance or new materials with different properties completely different from the properties of the original materials, such as coal burning, milk going bad, water electrolysis, and many other chemical changes.

b) Physical changes

These are the changes that occur in the state of matter; liquid, solid, or gas, to change its shape and external appearance, and these changes are sometimes related to temperature changes like melting and evaporation, and sometimes do not affect the identity of the substance; such as glass breaking and sugar dissolving in water. **Some physical changes:**

- **Melting:** It is a physical change that occurs in matter, turning it from a solid state to a liquid state by heat, where the heat causes the molecules of the substance to vibrate and break apart which are very tightly bound in the solid state, and the distances between them are short or almost nonexistent in the solid state, and when the substance is heated, the distances between the molecules increase and move away from each other and break apart, to become a liquid substance.
- **Diffusion:** It is a physical change that occurs to a substance in the gaseous state; when gas molecules mix with the air, these molecules spread out and launch into the air taking up a larger volume than before.
- **Compression:** It is a change that occurs to the substance in its gaseous state to turn it into a liquid state, by exposing the gas molecules to pressure; increasing the forces of attraction between them and reducing the distances between them to transform from the gaseous state to the liquid state.

7. Transition between states of matter

Transition between states of matter can occur by heating or cooling.

- **Evaporation:** It's the transition of a substance from the liquid surface from a liquid state to a gaseous state, meaning that the particles of the substance change from a state where the particles are close together and condensed to a state where the particles are more spread out and not condensed.
- **Condensation:** It's a process of transforming a gas into a liquid by cooling, meaning the particles of the substance change from a state where the particles are spread out to a state where the particles are close together and condensed.
- **Freezing:** It's a process of transforming a substance from a liquid to a solid by cooling, meaning the particles of the substance change from a state where the particles are spread out to a state where the particles are close together and condensed.
- **Melting**: It's the state where a substance transitions from a solid state to a liquid state by heating, meaning the particles of the substance change from a state where the particles are close together and condensed to a state where the particles are more spread out and not condensed.

8. Laws of quantity of matter

- **State of solid matter:**

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

  n: Number of moles, **m**: mass, **M**: molar mass
- **Liquid state:**

  n= C×V

  n:Number of moles, C:concentration, V: volum
- **Volume Gas state:**

$$n = \frac{V_g}{V_M}$$

n : number of moles
V_g :Gas volume
V_M :Molar volume

9. Avogadro's law

The same number of gas molecules occupies the same volume V under the same conditions of temperature and pressure; thus, regardless of the gas, it occupies the same volume. This results in the following: The volume occupied by 1 mole of oxygen (O_2) at a pressure of 1 atm and a temperature of 273 kelvin (0 degrees Celsius) with a weight of O_2 equal to 1.43 grams is:

$$PV = nRT \Rightarrow V = \frac{nRT}{P} = 1 \times 0{,}082 \times 273 = 22{,}4\,L$$

or V=32/1.43=22.4L

So, 1 mole of any gas occupies a volume of 22.4 liters under standard conditions and is known as molar volume.

a) Avogadro's number

The number of molecules present in 1 mole of a substance is equivalent to the number of carbon-12 atoms in 12 grams of the isotope carbon. Where:

NA particles = one mole of particles

And the mass of one mole of particles is the molar mass.

N_A atoms = one mole of atoms

$$N_A = 6{,}023 \times 10^{23}\,mol^{-1}$$

Exemple 1

One mole of O_2 molecules contains 6.023 x 10^{23} oxygen molecules.

One mole of O atoms contains 6.023 x 10^{23} oxygen atoms.

Exemple 2

Calculate the number of moles, molecules, copper atoms, and oxygen atoms in a sample of copper oxide with a mass of 1.5 grams

Solution:

$$n_{CuO} = \frac{m}{M} = \frac{1{,}59}{63{,}54} = 0{,}01999\,moles$$

Calculating the number of particles:

$$/\,The\ number\ of\ particles = n_{CuO} \times N_A = 0{,}01999 \times 6{,}02.\,10^{23} = 0{,}12.\,10^{23}\,(particles)\,N_{CuO}$$

Calculating the number of moles:

$$N_{Cu} = N_O = N_{CuO} = 0{,}12.\,10^{23}\,moles$$

10. Atomic weight or Atomic Mass Unit (a.m.u)

It is one-twelfth ($\frac{1}{12}$) the mass of a carbon-12 atom.

Since 1 mol of C atoms have a mass of 12g and N_A mol of atoms=6.022×10^{23}atoms

$$1\,amu=\frac{1}{12}\left(\frac{12\,g}{mol}\right)\left(\frac{1\,mol}{6.022\times10^{23}}\right)=1{,}66\times10^{-24}g=1{,}66\times10^{-27}kg$$

11. Mole

It is the amount of substance that contains Avogadro's number of particles or atoms

-Ways to calculate the number of moles:

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

n:Number of moles, **m**: Weight of material in grams, **M_w**: Molar mass in units g/mol

$$n=\frac{\mathrm{N\ (atomes, molecules)}}{\mathcal{N}_A}=\frac{\mathrm{N}}{6{,}023\cdot10^{23}}$$ ⇒ N= n.N_A:Number of molecules

12. Weight of one atom

$$m'=\frac{M_w}{\mathcal{N}_A}\qquad(g)$$

Weight of one atom

$$1\,\mathrm{amu}=\frac{1}{12}\mathrm{m'}_{^{12}\mathrm{c}}=\frac{1}{12}\times\frac{M_{w(^{12}c)}}{\mathcal{N}_A}=\frac{1}{12}\times\frac{12}{6{,}023\times10^{23}}$$

$$1\ \mathrm{amu}=\ 1{,}66\times10^{-24}\ \mathrm{g}$$

$$1\ \mathrm{amu}=\ 1{,}66\times10^{-27}\ \mathrm{kg}$$

$$m'=\frac{M_w}{\mathcal{N}_A}=M_w\left(\frac{1}{\mathcal{N}_A}\right)\ g$$

$m'=M_w\ amu$

B. Laws of Weight

1. Chemical Formulas

Chemical formulas are symbolic methods that illustrate the elemental composition and the number of atoms in a compound.

- **Empirical formulas (simple form):** provide the simplest ratio between the atoms present in the compound, and can be determined by knowing the mass ratio and atomic masses of the components.

- **Molecular formulas (real):** give the molecular formula of the compound with the actual number of atoms in the compound, and can be determined by knowing its molecular mass.
- **Relationship between the weight percentage and the empirical formula of the compound:** Considering that the empirical formula of a chemical compound represents the number of atoms of the element in one molecule of it, based on this, the empirical formula of the pure compound can be obtained if we know the percentage composition of any molecule's components.

Exemple 1

A chemical compound consists of carbon and oxygen with a weight percentage of 27.28% C. If the compound is pure, what is its empirical formula?

Solution:

Let's assume the compound is C_xO_y.

C ration: C = 27,28 % ⇒ O Ration: O = 100 - 27,28 = 72,72 %

$$\left.\begin{array}{lcl} M_{CxOy} & \longrightarrow & 12x(C) \\ 100\% & \longrightarrow & 27{,}28\%(C) \end{array}\right\} \longrightarrow x = \frac{M\times 27{,}28}{100\times 12} \dots\dots\dots (1)$$

$$\left.\begin{array}{lcl} M_{CxOy} & \longrightarrow & 16y(O) \\ 100\% & \longrightarrow & 72{,}72\%(O) \end{array}\right\} \longrightarrow y = \frac{M\times 72{,}72}{100\times 16} \dots\dots\dots (2)$$

Taking the ratio of $\frac{(2)}{(1)}$ we find:

$$\frac{y}{x}=\frac{M\times 72{,}72}{100\times 16}\times\frac{100\times 12}{M\times 27;28}=2$$

x=1 ⇒ y=2,a linear equationy=2x

Therefore, the primery formula for the compound is:CO_2

Exemple 2

Identify the primery formula and molecular formula of a compound with a mass of 282,88g/mole and its mass centennial composition:O% = 56,36 and = P% 43,64

What is the difference between the primary formula and the molecular formula of the compound and can the two formulas be equal?

Solution:

100 grams of the compound contains 43.36 grams of phosphorus and 56.36 grams of oxygen. Initially, we calculate the number of moles for each element

$$n_P=\frac{m}{M}=1{,}408\,moles$$

$$n_O=\frac{m}{M}=3{,}523\,moles$$

We divide this value by the smallest number, we find 2.5, but the number of atoms in any compound is always an integer, so the correct primary formula is P_2O_5. We compare the primary formula with the molar mass of the compound

$$M_{primary(P_2O_5)}=(31\times 2)+(16\times 5)=142\,g/mol$$

$$M_{real}=283{,}88\,g/mol$$

Therefore:

$$\frac{M_{real}}{M_{primary}}=2$$

Hence, the molecular formula is:

$$(P_2O_5)_2=P_4O_{10}$$

The molecular formula gives the actual number of atoms of each element in the molecule. The primary formula only gives the simplest ratio between the number of atoms of each element. So, the molecular formula is a multiple of the primary formula or equal to it.

2. Weight Percentage

To determine the weight percentage of the components of a pure chemical compound, we follow the steps of the following example:

Find the weight percentage of the components of pure sodium sulfate Na_2SO_4, where:

Na = 23, S = 32, O=16

$$M_{w(Na_2SO_4)}=[(23\times 2)+32+(16\times 4)]=142\,g/mol$$

Na ratio:

$$\left.\begin{array}{lcl} 142g(Na_2SO_4) & \longrightarrow & 46g(Na) \\ x & \longrightarrow & 100\% \end{array}\right\} \longrightarrow x=32{,}4\%$$

O ratio:

$$\left.\begin{array}{lcl} 142g(Na_2SO_4) & \longrightarrow & 46g(O) \\ 100\% & \longrightarrow & y \end{array}\right\} \longrightarrow y=45{,}1\%$$

S ratio:

$$Z=100-(32{,}4+45{,}1) \longrightarrow z=22{,}5\%$$

3. Law of conservation of mass by Lavoisier

The physical and chemical transformations of matter do not lead to the creation or destruction of matter, but only to its rearrangement. (Nothing is lost, nothing is created, everything is transformed

Exemple

$$2\ g\ H_2 + 16\ g\ O_2 \longrightarrow 18\ g\ (H_2O)$$

4. Law of definite proportions (constant) by Proust

When simple or multiple bodies unite to form a compound, this union always occurs in constant weight ratios (meaning the ratios of the union are constant) regardless of the source of the compound or the method of its preparation.

5. Law of multiple proportions by Dalton

When two elements A and B combine to form several chemical compounds, the masses of one of the elements that combine with a fixed mass of the second element in these compounds are in simple multiple ratios to each other.

Exemple 1

In water (H_2O), 16 grams of oxygen combine with 2 grams of hydrogen. In hydrogen peroxide (H_2O_2), 32 grams of oxygen combine with 2 grams of hydrogen. We notice that the ratio (16:32) is a simple ratio (1:2), meaning multiple proportions

Exemple 2

The compounds nitric acid (HNO3), hydrazine (NH_2-NH_2), ammonia (NH_3), and ammonium chloride (NH_4Cl) all contain nitrogen (N) and hydrogen (H). These compounds satisfy the law of multiple proportions.

Solution :

compound	H ration	N ration	H/N ration	
HNO_3	1,6	22,2	0,072	=**1** x 0,072
NH_2-NH_2	12,59	87,41	0,144	= **2** x 0,072
NH_3	17,76	82,24	0,216	=**3** x 0,072
NH_4Cl	7,54	26,32	0,286	= **4** x 0,072

These are multiple ratios, so they satisfy the law of multiple ratios.

C. Solutions

- **Solution Definition**: It is a homogeneous mixture of two or more pure substances in different proportions in such a way that there is no chemical reaction between them.
- **Solvent**: Solvent is the medium in which the solute is dispersed, generally a liquid in which the solution is formed, like H_2O.
- **Solute**: Solute consists of dispersed particles.
- **Solution concentration definition**: It is the amount of the solute in a certain amount of solution.
- **Diluted solution**: It is a solution in which the amount of the solute is low.
- **Concentrated solution**: It is a solution in which the amount of the solute is high.

1. Methods of expressing concentration

a) Weight percentage of the solute or weight percentage concentration

The mass of the solute measured in grams present in 100g of the solution (number of grams of the solute in 100g of the solution).

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

where :

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

You can calculate the mass of the solution if you know the volume of the solution using the relationship:

$$\rho_{sol} = \frac{m_{sol}}{V_{sol}} \Rightarrow m_{sol} = \rho_{sol} \times V_{sol}$$

Where: **ρ** is the density of the solution in g/L

m: is the mass of the solution in g

$$1\ \mathrm{dm}^3 = 1\ \mathrm{L} \quad , 1\mathrm{cm}^3 = 1\mathrm{mL}$$

b) Molar volume

Is the volume of one mole of molecules

Exemple 1

1 mole of water vapor (H_2O) occupies a volume of 22.4 L under standard conditions and 1 mole of liquid water (18g) occupies a volume of 18 ml

c) Mass concentration

Is the mass of the solute present in 1 liter of the solution and is measured in (g/L) units

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

Exemple 2

We dissolve a mass of 3.15 g of sodium chloride in 200 mL of water.

- What is the mass concentration of NaCl?

Solution :

$$C_m = \frac{m}{V} = \frac{3.15 \times 10^{-3}}{200 \times 10^{-3}} = 0.0157\, g/L$$

d) Molarity (M)

Is the number of moles of solute in one liter of the solution and is measured in units: mol/L ; Molarity = number of moles of solute / volume of the solution in liters

$$C \equiv M = \frac{n_{solute}}{V_{sol}\ (L)}$$

Exemple

$n = \frac{m}{M} = \frac{36}{18} = 2\, moles$: Number of moles in 36 g of water :

$n = \frac{V_{CO2}}{V_{molaire}} = \frac{11{,}2}{22{,}4} = 5\, moles$: Number of moles in 11.2 liters of carbon dioxide

e) Molality (m)

number of moles of the solute in 1 kg of the solvent and is measured in units: mol/kg

$$m=\frac{n_{solute}}{m_{solvant(kg)}}=\frac{n_{solute}\times 1000}{m_{solvant(g)}}$$

Remarque

A solution is said to be:

-Decamolar if molarity = 10 m

-Molar if molarity = 1 m

-Decimolar if molarity = 0.1 m

-Centimolar if molarity = 0.01 m

Exemple

We dissolve a mass of 3.15 g of sodium chloride in 200 mL of water.

- What is the molality of NaCl?

Solution :

m=200ml=200g

$$m=\frac{n_{solute}\times 1000}{m_{solvant(g)}}=\frac{m\times 1000}{M\,m_{solvant(g)}}=\frac{3.15}{(23+35.5)0.2}0.269\,g/L$$

f) Normality (N)

We define the normality of an acidic solution in water as the number of moles of the "H_3O^+" ion that can be released by one liter of solution. Similarly, the oxidoreductive normality of a solution corresponds to the number of moles of electrons that can be released by one liter of solution : **N=C×Zeq**

with **Zeq**: this is the number of gram equivalents of H^+ released by an acid, OH^- released by a base, or the number of electrons involved in the case of a redox reaction.

Exemple

A 1M potassium permanganate solution is when there's one mole per liter (1N).

$$MnO_4^{-+8H^{++5e^{-\longrightarrow Mn^{2+}+4H_2O}}}$$

In this case, you can exchange five electrons with one liter, making it a 5N solution.

But if we consider the reaction with :

$$MnO_4^{-+4H^{++3e^{-\longrightarrow MnO_2+2H_2O}}}$$

you can exchange three electrons with one liter, making it a 3N solution.

Exemple

What is the normality of acid in 1 liter of an aqueous solution containing 0.1 mol of HCl and 0.2 mol of H_3PO_4?

Prepare 500 mL of a 0.1N H_2SO_4 solution from a concentrated solution of H_2SO_4 at

98% by mass, with density d=1.84.

Solution :

1.

C_{HCl}=0.2M, $\mathbf{N_{HCl}=C_{HCl} \times Zeq}$ with :

Zeq: it's the number of gram equivalents of H^+ released by an acid, OH^- released by a base, or the number of electrons involved in a redox reaction

$$HCl \longrightarrow H^+ + Cl^- \qquad Zeq=1$$

$N_{HCl}=0.2\times1=\mathbf{0,2\ eqg/L}$

2.

$$N_{H2SO4}=C_{H2SO4}\,.\,Zeq \Rightarrow C_{H_2SO_4}=\frac{N_{H_2SO_4}}{Z_{eq}}=\frac{01}{2}=0,05\,mol/L$$

$$H_2SO_4 \longrightarrow 2H^+ + SO_4^- \qquad Zeq=2$$

$$n=\frac{m}{M}\Rightarrow m=n\times M=C\times V\times M=0,05\times0,5\times98=2,45\,g$$

98 grams of pure H_2SO_4 ⟶ 100 grams of solution.

2.45 grams of pure H2SO4 ⟶ m of H_2SO_4 in the solution.

$$m=\frac{2.45\times100}{98}=2.5\,g$$

$$\rho=\frac{m}{V}\Rightarrow V=\rho\times m=1.84\times2.5=4.625\,mL$$

g) Molar fraction (X)

It's the ratio of the presence of the substance (number of moles n_i) in a mixture of substances (total number of moles of its components n_T).

$$x_i=\frac{n_i}{n_t}, \qquad \sum x_i=1$$

$$x_A+x_B$$

$$\frac{n_A}{n_t}+\frac{n_B}{n_t}=\frac{n_t}{n_t}=1 \qquad ,n=\frac{m}{M}$$

Exemple

We dissolve a mass of 3.15 g of sodium chloride in 200 mL of water

-Calculate the mass fractions of the components in the NaCl solution.

Na (23 g/mol), Cl (35.5 g/mol).

Solution :

$$X_{H_2O}=\frac{n_i}{n_T};n_{H_2O}=\frac{m}{M}=\frac{200}{18}=11.111moles$$

$$X_{H_2O}=\frac{n_{H_2O}}{n_T}=\frac{n_{H_2O}}{n_{H_2O}+n_{NaCl}}=\frac{11.111}{11.111+0.269}=0.976362$$

$$X_{NaCl}=\frac{n_{NaCl}}{n_T}=\frac{n_{NaCl}}{n_{H_2O}+n_{NaCl}}=\frac{0.269}{11.111+0.269}=0.023637$$

Chapter Two: Components of Matter

II

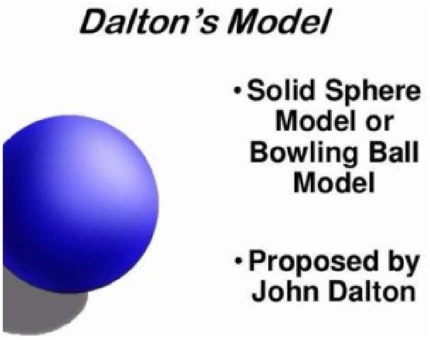
A. Introduction

Scientists conducted experiments to identify the components of matter, working on the composition and separation of materials and found that there are substances that do not break down into simpler substances, they called them elements.

1. Dalton's concept of the atom

It was believed that the external appearance of matter had a stable structure until the scientist "Dalton" came in the early 19th century and proved the opposite, that it is not continuous. He developed his concept of the atom which is based on four points:

1. Matter is made up of atoms.
2. Atoms do not divide into smaller parts.
3. Atoms of the same element are identical.
4. Atoms of different elements differ from each other. It was found that the atom consists of a very dense nucleus carrying a positive charge surrounded by negatively charged electrons.



Dalton's Model

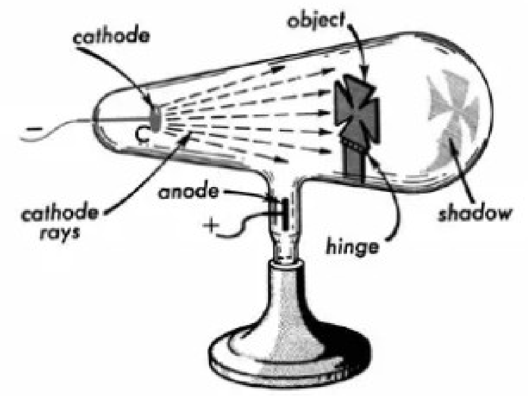
- Solid Sphere Model or Bowling Ball Model
- Proposed by John Dalton

B. Identification of the constituents of the matter

1. Electron

a) William Crookes' electrical discharge experiment (1879)

The English scientist William Crookes in 1870 used a nearly airless tube (because gases do not conduct electricity unless at very low pressure of 0.01 atmosphere) and fixed two metal poles inside connected to a battery. The negative pole is called the cathode, and the positive is called the anode. In the middle, a body in the shape of (+) was fixed. When the electric current was passed, he noticed a green beam emitted, and also found the shadow of the body on the anode. He called the green beam the cathode rays (as they emit from the cathode and this is why the shadow appears on the anode).



b) Thomson's experiment: Determining the ratio |e| /m

To confirm the nature of the cathode rays discovered by Crookes, Thomson conducted his experiment in 1897. When he placed a cathode inside a tube, it produced a vertical electric field on the electrons beam. He noticed that the rays changed direction (deflection of particles towards the positive plate), so he concluded that they are charged particles with a negative charge, not just light radiation (because light is not affected by magnets).

- **Action of the electric field:** The electron beam deflects towards the positive plate of the cathode, meaning upwards, due to the electric force.

  $\vec{F_e} = e\vec{E}$

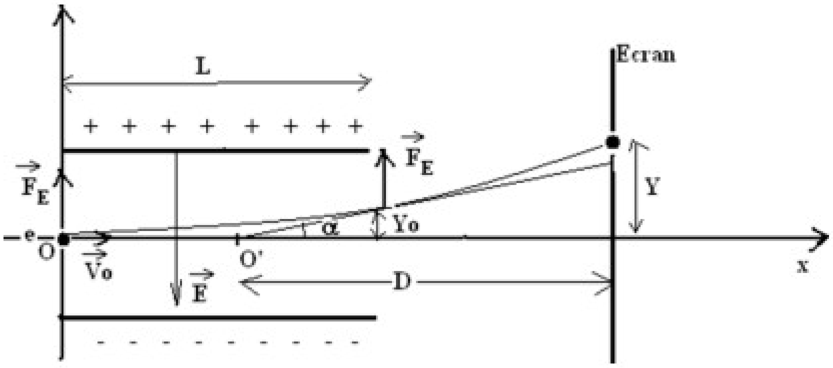
- **Action of the magnetic field:** The electron beam deflects downwards due to the magnetic force.

• Adjust the strength of the electric field and the strength of the magnetic field so that the ray beam takes its horizontal path (initial) and under these conditions:

$$\|\vec{F_e}\| = \|\vec{F_m}\| \Rightarrow eE = e v_0 B$$

$$\Rightarrow v_0 = \frac{E}{B} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1)$$

•the second stage, the magnetic field vector $\vec{B}$ is removed, and then measure the resulting deflection using $\vec{E}$:



Cathode rays inside the electric field are influenced by the electric force $\vec{F}_e = e\vec{E}$, and from the fundamental relationship of dynamics, we have:

$$\vec{F}_e = e\vec{E} = m\vec{\gamma} \Rightarrow \gamma = \frac{eE}{m}$$

Where γ is the acceleration

By applying the force $\vec{F}_e$ on the axis $\vec{Ox}$, we find:

The force applied to the rays in the direction of the axis $\vec{Ox}$ is zero.

$$\left.\begin{aligned} Fe_x &= 0 \\ Fe &= m\gamma_x \end{aligned}\right\} \Rightarrow m\gamma_x = 0 \Rightarrow \gamma_x = 0$$

$$\Rightarrow x = \int_0^t v_0 dt \Rightarrow x = v_0 dt$$

$$\Rightarrow t = \frac{x}{v_0} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (2)$$

By applying the force $\vec{F}_e$ on the axis $\vec{Oy}$, we find:

$$\left.\begin{aligned} Fe_y &= 0 \\ Fe &= m\gamma_y \end{aligned}\right\} \Rightarrow \gamma_y = \frac{eE}{m}$$

$$\gamma_y = \frac{d^2y}{dt^2} = \frac{eE}{m} \Rightarrow \frac{dy}{dt} = v_y = \int_0^t \frac{eE}{m} dt \Rightarrow v_y = \frac{eE}{m}.t$$

$$v_y = \frac{dy}{dt} = \frac{eE}{m}.t \Rightarrow dy = \frac{eE}{m} t\, dt \Rightarrow y = \int_0^t \frac{eE}{m}.t\, dt$$

$$\Rightarrow y = \frac{1}{2}\frac{eE}{m}t^2 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (3)$$

This is the equation of motion of the descended rays when an electric field is applied.

we have :

$$t = \frac{x}{v_0} \Rightarrow y_{(x)} = \frac{1}{2}\frac{eE}{m}\frac{x^2}{v_0^2} \ldots\ldots\ldots\ldots\ldots\ldots\ldots (4)$$

we have :

$$v_0 = \frac{E}{B}$$

$$\Rightarrow y_{(x)} = \frac{1}{2}\frac{eE}{m}x^2\frac{B^2}{E^2}$$

$$\Rightarrow y_{(x)} = \frac{1}{2}\frac{e}{m}x^2\frac{B^2}{E} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(5)$$

This is the general equation for motion with the shape of a segment showing the deflection y for any distance x that the descended rays pass through.

At the end of the electric field: $y = y_0$, $x = l$ by substituting into equation (4) we find:

$$y_0 = \frac{1}{2}\frac{eE}{m}\frac{l^2}{v_0{}^2}$$

$$\Rightarrow \frac{e}{m} = \frac{2\,y_0 v_0^2}{El^2} \ldots\ldots\ldots\ldots(6)$$

or from equation (5) we find:

$$\Rightarrow \frac{e}{m} = \frac{2\,y_0 E}{l^2 B^2} \ldots\ldots\ldots\ldots(7)$$

we have :

$$tg\alpha = \frac{y_0}{\frac{l}{2}} = \frac{Y}{D} \Rightarrow y = \frac{lY}{2D}$$

By substituting into equation (6) we find :

$$\frac{e}{m} = \frac{Y\,v_0^2}{DEl}$$

And by substituting the experimental values (l,B, E, y_0) we can calculate $\frac{e}{m}$, which is independent of the material the ray is made of and the type of gas inside the tube, and thus $\frac{e}{m}$ is a constant value for all materials where:

$$\frac{e}{m} = 1{,}756 \times 10^{11} coulomb/kg$$

Exemple

1. We send a group of electrons with kinetic energy Ec = 4x10^{-14} J between the plates of a capacitor where there is an electric field intensity E. Write the equation for the path inside the capacitor as a function y = f(x) depending on E_c, E, e.
2. If the length of the capacitor plate L= 50 cm and the separation distance between the plates d = 20 cm, and the deviation upon exiting the capacitor is Y_0 = 2 mm, calculate:

- The voltage difference U applied between the plates.
- The angle of deviation α created by the tangent from the midpoint of the lower plate of the capacitor.
- The amount of deviation Y on the screen that is located at a distance of D = 150 cm from the midpoint of the capacitor.

provided: e = 1.6 x 10^{-19} C .

Solution :

Let's assume that the ray tracer on the screen is an extension of interference.

1- Equation of the path inside the capacitor y = f(x) in terms of E_c, E and e.

The incident rays inside the electric field are affected by the electric force:

By projecting the force vector Fe onto the x-axis, we find :

$$t=\frac{x}{v_0}........................(1)$$

By projecting the force vector Fe onto the y-axis, we find :

$$y=\frac{1}{2}\frac{eE}{m}t^2..............................(2)$$

$$We\,have:t=\frac{x}{v_0}\Rightarrow y_{(x)}=\frac{1}{2}\frac{eE}{m}\frac{x^2}{v_0^2}.....................(3)$$

We have also :

$$E_C=\frac{1}{2}mv^2\Rightarrow mv^2=2E_C$$

By substituting into equation (3) we find :

$$y_{(x)}=\frac{1}{4}\frac{eE}{E_c}x^2$$

2- Calculate the voltage difference U applied between the two plates where: L = 50 cm,

d = 20 cm, and y_0 = 2 mm.

When we leave the electromagnetic coil :

$$E=\frac{U}{d}$$

By substituting (x = L, y = y_0) in (1), we find:

$$y_0=\frac{1}{4}\frac{eU}{E_c d}L^2\Rightarrow U=\frac{4y_0E_cd}{eL^2}\Rightarrow$$

$$U=\frac{4\times(2\times10^{-3})\times(4\times10^{-14})\times(20\times10^{-2})}{1.6\times10^{-19}\times(50\times10^{-2})^2}=1600\,volt$$

3- Calculate the angle of deviation α :

$$tg\,\alpha=\frac{y_0}{\frac{L}{2}}\Rightarrow tg\,\alpha=\frac{2y_0}{L}$$

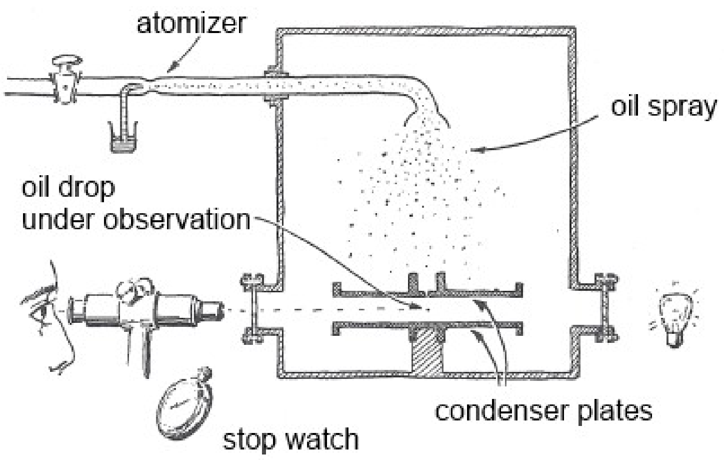
$$tg\,\alpha=\frac{2\times(2\times10^{-3})}{50\times10^{-2}}=0.008\Rightarrow\alpha=0.458^{\circ}$$

4- Calculate the deviation of "y" on the screen from the center of the lens by D=150cm.

$$tg\,\alpha=\frac{2y_0}{L}=\frac{y}{D}\Rightarrow y=\frac{2y_0D}{L}$$

$$\Rightarrow y=\frac{2\times(2\times10^{-3})\times(150\times10^{-2})}{50\times10^{-2}}\Rightarrow y=0.012m=12\,mm$$

c) Millikan Experiment (Determining the electron charge and deduction of its mass)



The Millikan apparatus consists of a capacitor inside a metal chamber placed in a holder or an automatic thermostat. Spray or mist particles pass into the capacitor between the plates where we track their movement through a microscope. The air in the device (inside the metal chamber) is exposed to X-rays, causing it to ionize into ions (free electrons or positive ions) which attach to oil mist particles, giving them an electronic charge. By controlling the electric field intensity, we stabilize the charged oil droplets or particles between the capacitor plates, which remain stationary in the observer's view (choosing the necessary intensity to balance the weight of the mist particles).

So, we have:

$$mg=e_gE.......(1)$$

m:mass of the mist particle or oil droplet

g:gravitational acceleration

E:electric field intensity

In a parallel plate capacitor, we have:

$$E=\frac{V}{d}.......(2)$$

Where:

d:distance between the plates

V:applied voltage between the capacitor plates

From equations (1) and (2):we find

$$e_g=m_gd/V$$

By knowing the mass of the droplet or mist molecule m, we can find the charge e_g (we can find the mass of the molecule by its free fall velocity in air in the absence of an electric field), where Millikan found that

$$e_g=1.60217733\times 10^{-19}c$$

Remarque

1- Millikan found that the charge on an oil droplet (mist) is always equal to or a multiple of the value of the charge e_g, as it is never less than it. This indicates that the molecule can capture one or more electrons and never retains a part of an electron because it is indivisible, resulting in the smallest partial charge being the electron charge.

2- Knowing the ration $\frac{|e|}{m}$ and the elementary charge: $|e|$, it's easy to deduce the mass of the electron.

$\frac{|e|}{m} = 1.759.10^{11}\, Coulombs/Kg = A$ and $|e| = 1.60217733\times 10^{-19} c$

So : $m = \frac{A}{|e|} = \frac{1.759.10^{11}}{1.60217733\times 10^{-19}} = 9.1093897.10^{-31}$

$m_e = 9.1093897.10^{-31} kg = 0.00055\, amu$

i Applications on Malekian experiment

Droplet is subjected to 04 forces which are:

1-Stokes force: (Stochs) : $\vec{F}_S = 6\pi\eta r\vec{v}_0$

2-Electric force: $\vec{F}_E = q\vec{E}$

3- Droplet weight : $\vec{p} = m.\vec{g}$

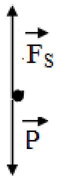
4-Archimedes thrust $\vec{F}_A = m'\vec{g}$ (neglected becauseρ(oil)>>ρ(air)

Whereby:

- Stokes force is opposite to droplet movement
- Archimedes thrust is opposite to droplet weight
- X-rays ionize oil droplets making them charged.

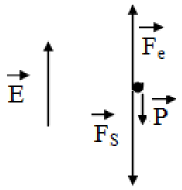
1. In the absence of electric field $\vec{F}_E = 0$, then: droplet falling speed reaches its maximum v_0 and at equilibrium we write:

$$\vec{F}_s + \vec{P} = 0 \quad \Rightarrow F_s = P \quad \Rightarrow 6\pi\eta r v_o = mg \qquad \text{.........(1)}$$



η:constantViscosity of air

2. Under the presence of the electric field $\vec{E}$, the droplet rises and gains a new maximum velocity v'_0. This results in equilibrium:



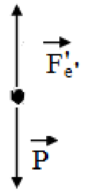
From the relationship: :(1) $r = mg/v_o\pi\eta6$
Therefore results in:

$$q.E = (mg\, v'_o/v_o) + mg \Rightarrow q = mg\times(1 + v'_o/v_o) / E$$

3. We keep the droplet stationary by applying a new electric field $\vec{E}'$ where the droplet acquires a new charge q′, since in this case $\vec{F}_s = 0$ and thus at equilibrium:

$$\overrightarrow{F'_{E'}} + \vec{P} = 0 \quad \Rightarrow \quad F'_{E'} = P$$

$$\Rightarrow q'.E' = m.g \Rightarrow q' = mg/E'$$



By measuring the value of $q - q'$ several times, we get the value of the electron charge which equals:

$$e = -1.602 \times 10^{-19} C$$

Note: Since the droplet is a sphere, then:

$$\begin{Bmatrix} m = \rho V \\ V = 4/3\pi r^3 \end{Bmatrix} => m = 4/3\pi r^3 \rho$$

Exemple

In Millikan's experiment, an oil droplet with mass m and radius r is situated between the parallel plates of a capacitor.

1-The droplet falls freely from a distance of 4 mm in 12.8 seconds.

a-Calculate the radius and mass of the droplet (Archimedes' buoyant force is neglected) ?

2-The droplet becomes charged when an electric field E= 1.8×10^{7} V.m^{-1} is applied. It rises with a speed of 4mm after 16 seconds.

a- Calculate the total charge q, and then deduce the number of charges?

. $\rho = 1{,}26 g.cm^{-3}$, $\eta = 1{,}80\ 10^{-4}$ (MKSA), $g = 9{,}81 m\ s^{-2}$, $e = 1{,}6\ 10^{-19}$ C

Solution :

1- Free fall of the droplet ⟹ the motion is downward.

-The forces acting on the droplet are:

- The force of gravity: P=mg
- The friction force (or Stokes force) F_S The Archimedean thrust is negligible.
- The balance of forces is written: $\sum \vec{F} = \vec{0} \Longrightarrow \vec{P} + \vec{F_S} = \vec{0}$

$$P - F_s = 0 \quad \Longrightarrow mg - 6\pi\eta r v_0 = 0 \Longrightarrow mg = 6\pi\eta r v_0$$

$$on\ a \quad \rho = \frac{m}{V} \Longrightarrow m = \rho V = \rho \frac{4}{3}\pi r^3$$

$$\rho \frac{4}{3}\pi r^3 g = 6\pi\eta r v_0 \qquad \Longrightarrow \quad r = 3\sqrt{\frac{\eta v_0}{2\rho g}}$$

$$\text{N.A} : v_0 = \frac{d}{t} = \frac{4.10^{-3}}{12{,}8} = 3{,}12\,.\,10^{-4} m.s^{-1}$$

$$r = 3\sqrt{\frac{1{,}80\,.\,10^{-4} \times 3{,}12\,.\,10^{-4}}{2 \times 1{,}26\,.\,10^{3} \times 9{,}81}} = 4{,}52\,.\,10^{-6} m$$

$$m = \rho V = \rho \frac{4}{3}\pi r^3 = 1{,}26.10^3 \times \frac{4}{3} \times 3{,}14 \times (4{,}52\,.\,10^{-6})^3 = 4{,}87\,.\,10^{-13} Kg$$

2- The droplet is now moving upwards with a velocity v_1: Under the effect of the electric field E=1.8×10^{7} V.m^{-1} , the forces acting on the droplet are:

-Gravity force p

-Electric force Fe
-Stokes force Fs.
The balance of forces can be written as:

- $\vec{P} + \overrightarrow{F_S} = \overrightarrow{F_e} mg + 6\pi r\eta v_1 = qE$

$$q = \frac{mg + 6\pi r\eta v_1}{E}$$

- N.A : $v_0 = \frac{d}{t} = \frac{4.10^{-3}}{16} = 2{,}5\,.\,10^{-4} m.s^{-1}$

$$q = \frac{4{,}87\,.\,10^{-13} \times 9{,}81 + 6 \times 3{,}14 \times 1{,}80\ 10^{-4} \times 4{,}52\ 10^{-6} \times 2{,}5\,.\,10^{-4}}{1{,}8\ .\,10^{7}} = 4{,}78\ 10^{-19} C$$

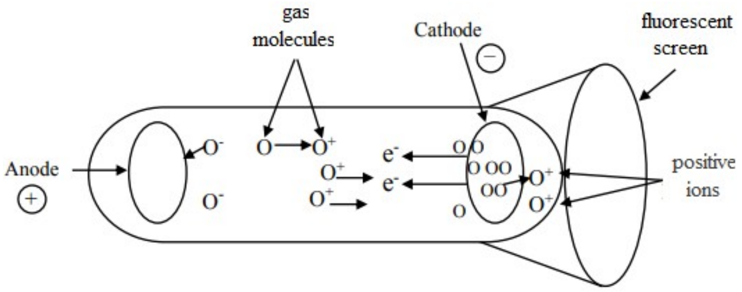
$$q = n.e \Longrightarrow n = \frac{q}{e} = \frac{4{,}78\ 10^{-19}}{1{,}6\ 10^{-19}}. = 2{,}98 \approx 3$$

So the charge q = 3.e

2. Nucleus

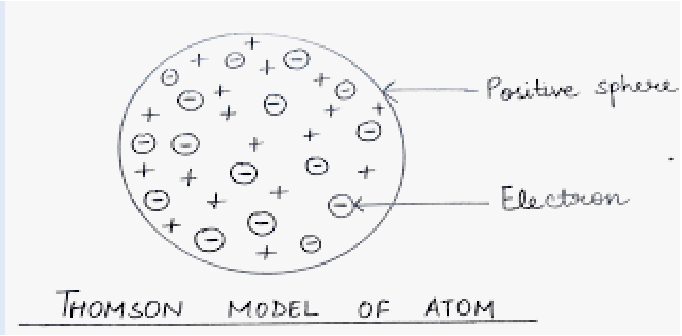
a) Goldstein's experiment (nucleus)

Crok's experiment proved that electrons originate from the descent and move towards the elevator. But Goldstein contradicted in his device the position of the descent and the elevator, so he noticed that there is radiation resulting from particles charged with a positive charge. Therefore, the atom consists of electrons and material charged with a positive charge



b) Thomson model

Since the atom is neutrally charged, Thomson assumed that as long as the atom contained negatively charged electrons, it must contain positively charged particles that make it a neutral atom. Therefore, Thomson modified Dalton's atomic model, suggesting that the atom is not silent but rather a sphere of positive charges with negative electrons dispersed in it.

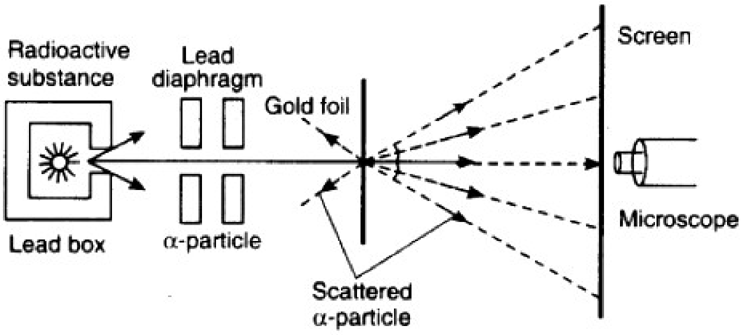


c) Identification of the nucleus (protons and neutrons) : Rutherford-Geiger-Marsden Experiment

The experiment involves bombarding a very thin sheet of metal (Gold) with radiation made up of Helium nuclei (He_2).

Interpretation

Bombarding very thin gold foil with alpha particles, Hans Geiger and Ernest Marsden, then students of Rutherford, observed that a tiny fraction (1 in 100) of these particles were deflected at a high angle as if they were bouncing off a massive obstacle. The impacts were observed in the dark under a microscope on a shining zinc sulfide screen. Rutherford concluded that the atom contained a massive, positively charged core capable of repelling the alpha particles



The three scientists studied the deviation of alpha particles (He^{++}) by directing them onto a gold foil 4.10^{-7}m thick. They found that some of these rays reflect (1 out of 20,000), some also deviate (1%), and most of them get refracted. They concluded from this experiment that there are empty spaces in the atom.

Rutherford found that: there is a part in the atom with high density occupying a very small space where the mass of the atom is concentrated, and this is the part of the rays that got reflected from their path. The penetration of some rays means that most of the atom is empty space, and the deviation of the rays means that they came close to a body with a similar (positive) charge hence they repelled, meaning the nucleus charge is positive. He found that the atom has a significant amount of empty space.

Explaining the deviation of alpha particles:

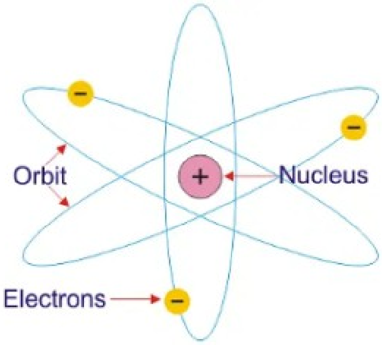
To explain these observed results, Rutherford considers the radius of the nucleus (r_n) as a rigid sphere and the radius of the atom (ra): he finds that:

$r_n = 10^{-14}$ m and $r_a = 10^{-10}$ m.

The deviation of any particle is calculated based on the ratio : $\frac{r_n}{r_a} = 10^4$. This means that the nucleus and atom sizes are far apart (to represent the nucleus, we use a pinhead with a diameter of 1 mm in a spherical perimeter of 10 m diameter which represents the atom). Hence, the probability of collision of the alpha particle with the nucleus is very weak so these particles choose the vacuum and when they come close to the nucleus, a slight deviation occurs. Therefore, the atom consists of a dense nucleus and empty space where electrons exist.

d) Rutherford's Model

The atom is a particle consisting of a small heavy positively charged nucleus containing positive protons, surrounded by a significant amount of empty space, housing negative electrons.



Remarque

Rutherford could not clarify the position of electrons in the empty space around the nucleus. Are the electrons stationary or moving? If they are stationary, why don't they be attracted to the nucleus and immerse in it? If they are moving, why doesn't the atom emit light? It is known that any charged particle moving under the force of attraction must emit light, so Rutherford described the atom as unstable.

3. Proton

The proton was discovered in 1919 by Ernest Rutherford. He noticed that when alpha particles are fired through nitrogen gas, flashes of light indicated the presence of hydrogen nuclei. Rutherford determined that the only place hydrogen could come from was nitrogen, meaning nitrogen must contain hydrogen nuclei. He proposed that the hydrogen nuclei, with an atomic number of 1, are a fundamental element and named them protons, from the Greek word "protos," meaning first.

$$^{14}_{7}N + ^{4}_{2}\alpha \quad \rightarrow \quad ^{17}_{8}O + ^{1}_{1}P$$

The proton is a component of the atom with a positive electrical charge of 1.602 × 10^{-19} coulombs, equal to the negative charge of an electron. The mass of a proton is

$1.672621637 \times 10^{-27}$ kilograms, which is approximately 1800 times the mass of an electron. Physicists use the unit MeV to express the mass of the electron due to the small mass of the proton in kilograms (a very small number that is hard to remember) and this is equal to 938MeV.

4. Neutron

$$^{4}_{2}H_e^{2+} + ^{9}_{4}B_e \quad \rightarrow \quad ^{12}_{6}C + ^{1}_{0}n$$

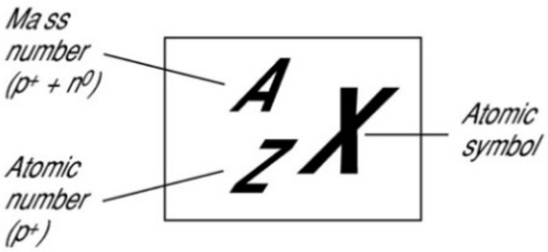
It was believed that the nucleus consisted only of protons until the scientist Chadwick discovered that when he bombarded beryllium atoms (Be) with alpha particles, he observed the formation of carbon atoms and the emission of penetrating and moderate radiation from uncharged particles (not affected by electric or magnetic fields), which were named neutrons. Their characteristics include having no charge (q_N=0) and a mass of 1.0087amu = m_N=$1.67495.10^{-27}$ kg.

C. Basic Components of the Nucleus

The components of the nucleus are called nucleons, which are protons and neutrons. The symbolic notation for an element is as follows: For example:

- The mass number (A) equals the number of nucleons, which is the sum of protons and neutrons.
- The atomic number (Z) equals the number of protons, which is equal to the number of electrons.
- The number of neutrons (N) is the difference between the mass number and the atomic number (N=A-Z).

For **example**: $^{16}_{8}O$, the number of neutrons = 8 = 16-8



1. Isotopes

These are elements that have the same charge number Z and differ in the number of neutrons, meaning the difference in the total mass number.

For **example**: $^{3}_{1}H . ^{2}_{1}H . ^{1}_{1}H$

Remarque

Isotopes have the same chemical properties and differ in physical properties.

a) Average atomic mass

atomic mass of an element is the average mass of a natural mixture of its isotopes, calculated using the following relationship:

$$\bar{M} = \frac{\sum M_i . w_i}{100} = \frac{M_1 w_1 + M_1 w_1 + \cdots}{100} \quad , \qquad \sum w_i = 100\%$$

Wi: Isotope proportion in the mixture.

Mi: Atomic mass of this isotope of the element

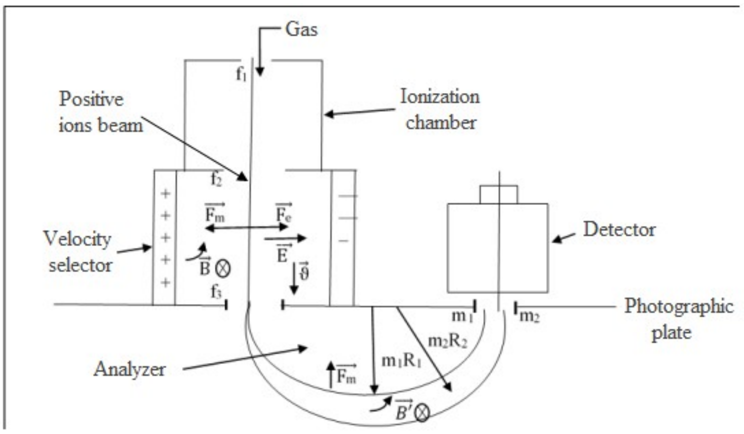
Exemple

Calculate the average mass of the Argon element Ar according to the isotopes 36Ar, 38Ar, 40Ar. The percentages of these isotopes are respectively: 99.6%, 0.0639%, 0.337%.

Solution :

$$M_{Ar} = \frac{0.337 \times 35.968 + 0.063 \times 37.963 + 99.6 \times 39.62}{100} = 39.947$$

b) Isotope separation and mass measurement (mass spectrometry of Bainbridge).



Ionization chamber: It's the source of electrons that bombard the studied material in its gaseous state, causing gas atoms to ionize into M^+ form.

Velocity selector: It's a condenser and a magnet where when ions enter the filter, they are affected by the electric field $\vec{E}$ so they deviate from their original path. By applying a magnetic field perpendicular to the electric field with the same intensity, it corrects the deviation and allows ions to pass through the pole F' towards the analyzer. In this case, it must be:

$$|\vec{F_e}| = |\vec{F_M}|$$

where: For the electric field: $\vec{F_e} = q\vec{E}$

and for the magnetic field: $\vec{F_M} = q v_o \vec{B}$

symbol for the electric field

: symbol for the magnetic field.

Both $\vec{F_M}$ and $\vec{F_E}$ are parallel and different in direction.

We have:

Analyzer: At this point, the ion with mass m is subjected to a magnetic field perpendicular to its path, causing the ion to deflect in a circular path with a radius R where the influencing forces are:

$$|\vec{F_e}| = |\vec{F_M}| \Rightarrow qE = q v_o B \Rightarrow v_o = \frac{E}{B} \ldots..(1)$$

- Constant magnetic force $F_m = qvB_0$

- Central deflecting force $F_C = \frac{mv^2}{R}$

$$|\vec{F_M}| = \vec{F_C} \quad => qvB_o = \frac{mv^2}{R} \quad \Rightarrow \frac{m}{q} = \frac{B_o \times R}{v} \quad , \qquad v = \frac{E}{B}$$

$$\Rightarrow \frac{m}{q} = \frac{BB_oR}{E}$$

For two disintegrations (shapes) with masses m_1 and m_2 appearing on the detector, if the lighter disintegration creates a smaller radius, then:

$$\frac{m_1}{q}=\frac{B B_o R_1}{E}$$

$$\frac{m_2}{q}=\frac{B B_o R_2}{E}$$

Both disintegrations have the same charge, By taking the difference between them, we find:

$$\Rightarrow m_2 - m_1 = \frac{qBB_0}{E}(R_2 - R_1)$$

$$\Rightarrow m_2 - m_1 = \frac{qBB_0}{2E}(D_2 - D_1)$$

$$\Rightarrow \quad \boldsymbol{m_2 - m_1 = \frac{qBB_0}{2E}.d}$$

$$\Rightarrow \quad \boldsymbol{M_2 - M_1 = N_A.\frac{qBB_0}{2E}.d}$$

Exemple

We separate the ions $^{20}Ne^{+}$ and $^{21}Ne^{+}$ using a Bainbridge mass spectrometer. What is the speed of these ions at the exit of the velocity filter, if the distance d between the impact points on the photographic plate is 3cm, with a magnetic induction of 0.2 Tesla

Solution :

The trajectory of ions in the analyzer being circular, we can write:

$$\vec{F}_m=\vec{F}_c$$

$$qvB=m\frac{v^2}{R}\Longrightarrow qB=m\frac{v}{R}$$

With: The mass of a single atom:

So:

The $^{20}Ne^{+}$ ions of atomic mass M_1 ($A_1 = 20$) and charge $q = e$, describe a circumference of radius R_1: $R_1=\frac{M_1}{N_A q}\frac{v}{B}$

The $^{21}Ne^{+}$ ions of atomic mass M_2 ($A_2 = 21$) and charge $q = e$ describe a circumference of radius R_2: $R_2=\frac{M_2}{N_A q}\frac{v}{B}$

$$R_2-R_1=\frac{d}{2}$$

$$\frac{d}{2}=R_2-R_1=\frac{M_2}{N_A q}\frac{v}{B}-\frac{M_1}{N_A q}\frac{v}{B}=\frac{v}{N_A eB}(M_2-M_1)$$

$$\frac{v}{N_A eB}(M_2-M_1)=\frac{d}{2}\Longrightarrow v=\frac{N_A eBd}{2(M_2-M_1)}$$

numerical application :

$$v=\frac{N_A eBd}{2(M_2-M_1)}=\frac{6{,}023.10^{23}\times 1{,}6.10^{-19}\times 0{,}2\times 3.10^{-2}}{2\times(21-20)10^{-3}}=2{,}89.10^{5}\,m.s^{-1}$$

D. Binding and cohesive energy of nuclei

1. Cohesive (binding) energy of the atomic nucleus : Mass defect (mass loss):

the mass of the nucleus measured experimentally using mass spectroscopy is always less than the total mass of the particles that constitute it (protons + neutrons).

The difference is called mass defect or mass deficiency, denoted by the symbol Δm where:

$$\Delta m = Zm_p + (A-Z)\,m_n - M\left({}^{A}_{Z}X\right)$$

$M\left({}^{A}_{Z}X\right)$: Mass of the nucleus measured experimentally

m_n: Mass of the neutron nucleus

m_p: Mass of the proton nucleus

Exemple

Determine the mass loss during the formation of the nucleus of uranium ${}^{235}_{92}U$ from its nucleons. Data: m_p= 1.00728 a.m.u; m_N= 1.00866 a.m.u, m_U = 234.9942 a.m.u.

Solution :

The uranium-235 nucleus ${}^{235}_{92}U$ is made up of 92 protons and 143 neutrons

$$92\,{}^{1}_{1}P + 143\,{}^{1}_{0}n \rightarrow {}^{235}_{92}U$$

Δm = (92× 1.00728 + 143× 1.00866) – 234.9942

Δm = 1,91394 a.m.u.

a) Equivalence: Mass-Energy

The mass loss is due to the formation of the nucleus starting from nucleons, where equivalent energy is released equal to this mass loss according to Einstein's theory:

$$\Delta E = \Delta m . c^2$$

c: speed of light , $c = 3 \times 10^8 m/s$

According to Einstein, the loss of mass is transformed into energy that allows for maintaining the cohesion of the nucleons in the nucleus.

Note: for a given nuclear reaction, is energy released or absorbed ??? To find out, check the sign of ΔE, which depends solely on the sign of Δm since c^2 is always positive.

$$X + Y\,(reactants) \rightarrow Z + M\,(products)$$

The mass defect of the nuclear reaction:

Δm= Σ (Products) − Σ (Reactants).

-If $\Delta m < 0$, it means $\Delta E < 0$, which indicates that energy is released.

-If $\Delta m > 0$, it means $\Delta E > 0$, which means energy is absorbed (consumed).

b) Energy Units : Electron volt

It is the energy of an electron deceived by a quantum jump equal to 1V The electron charge quantum jump (1V) × electron charge = 1eV, where:

$$W = |q|.V = 1{,}6 \times 10^{-19}\,C \times 1V = 1{,}6 \times 10^{-19}\ J \quad (joule)$$

$$1\ MeV = 10^{6}\ eV \quad (Mega\ electronvolt)$$

$$1\ M_{ev} = 1{,}6 \times 10^{-13}\,J$$

$$1\ erg = 10^{-7}\,J$$

$$1\ cal = 4{,}18\,J \quad (calorie)$$

$$1\ Kcal = 10^{3}\ cal$$

Remarque

In the case of microscopic scale, it is preferable to use the electron volt as the energy unit.

$$E_{Fe}(J) = 7.58 . 10^{-11}\,J$$

$$E_{Fe}(ev) = \frac{7.58 \times 10^{-11}}{1.6 \times 10^{-19}} = 4.73 . 10^{8}\,ev$$

$$1\,Mev = 10^{+6}\,ev$$

c) Energy equivalent of the atomic mass unit

it is the equivalent energy of a quantity of 1 a.m.u, where:

$$\Delta m = 1 a.m.u$$

$$1 a.m.u = 1.66.10^{-24} g = 1.66.10^{-27}\ kg$$

$$E_{1a.m.u} = \Delta m \times c^{2} = 1 \times 1.66 \times 10^{-27} \times (3.10^{8})^{2} = 14.94.10^{-11} J$$

$$E_{ev} = \frac{E_J}{1.6.10^{-19}} = 931\,Mev$$

from it :

$$1\,a.m.u = 931\,Mev$$

d) Nuclear binding energy

the energy required to break down the nucleus into its elementary components, protons, and neutrons.

Exemple

Calculate the binding energy of the iron nucleus $^{56}_{26}Fe$

Solution :

$$m_n = (1.00864\ amu), m_p (1.00724\ amu). M(^{56}_{26}Fe) = 55.93754 amu$$

$$\Delta m = 26 \times 1.0072 + 30 \times 1.0086 - 55.9375 = 0.50774\ amu$$

$$\Delta E = \Delta M \times xc^{2} = 0.5077 \times 1{,}66.10^{-27} \times (3.10^{8})^{2} = 7.58.10^{-11} joule$$

e) Nuclear stability

We determine the stability of the nucleus by calculating the average binding energy a Where:

$$a = \frac{E}{A}$$

E:nucleus binding energy
A:nuclear mass number
a:average binding energy (binding energy per nucleon)

Exemple

compare the stability of the iron nucleus $^{56}_{26}Fe$Feand the helium nucleus $^{4}_{2}He$

Solution :

$$M(He^4_2) = 4.0017\ amu\ , \qquad M\left(^{56}_{26}Fe\right) = 55.93754amu$$

$$m_n = (1.00864\ amu), \qquad m_p = (1.00724\ amu).$$

$$\Delta m(He) = 2 \times 1.00724 + 2 \times 1.00864 = 0.299amu$$

$$\Rightarrow\ E_{He} = 0.299 \times 931 = 27.83Mev$$

$$\Delta m(Fe) = 26 \times 1.00724 + 30 \times 1.00864 = 0.5077amu$$

$$\Rightarrow\ E_{Fe} = 0.5077 \times 931 = 473Mev$$

$$a_{He} = \frac{27.83}{4} = 6.95Mev/\text{nucleon}$$

and :

$$a_{Fe} = \frac{473}{56} = 8.44Mev/\text{nucleon}$$

and from it :

$$a_{\mathrm{Fe}} > a_{\mathrm{He}}$$

Thus, iron is more stable than helium

III

Chapter Three: Radioactive Activity and Nuclear Reactions

A. Radioactivity Definition

It's when the internal forces of the nucleus are out of whack and it leads to the emission of ionizing radiation:

- Natural radioactivity discovered in 1898 by Henri Becquerel
- Artificial radioactivity discovered in 1934 by Irène and Fréderic Joliot-Curie
- Radioactivity is the property of an unstable atomic nucleus to spontaneously transform into nuclei of another chemical species, emitting radiation and particles.
- Protons and neutrons are stuck together thanks to a cohesive force called "nuclear interaction," which is usually enough to keep them together. **This is when the nucleus is considered "stable."**
- Some nuclei have too many particles or contain too much energy, so the cohesive force isn't enough to keep the neutrons and protons together. They spontaneously transform, emitting particles without any external intervention. **These nuclei are then considered "unstable." Unstable nuclides are called "radioactive."**

B. Factors affecting radioactive activity

When talking about the radioactive activity of an element, one must discuss the stability of its nucleus. Unstable nuclei are referred to as radioactive nuclei, and they have radioactive activity when the repulsive forces between the nucleons (protons) are greater than the binding forces. Since the nucleus consists of protons and neutrons, we note the following cases in the periodic table:

- If 20 ≥ Z and Z > 1, the elements are stable, and the number of protons is equal to or approximates the number of neutrons.
- If 84 > Z and Z > 20, the nucleus contains more neutrons than protons, causing increased repulsion between the protons, hence decreasing the nucleus's stability.
- If Z ≥ 84, the nuclei are unstable (radioactive) because the number of neutrons increases significantly to the point where there is no longer sufficient space inside the nucleus, leading to instability, known as radioactive activity. The heavy element

Exemple

$$Th^{232}{}_{90} \longrightarrow Ra^{228}{}_{88} \quad + \quad He^{4}{}_{2}$$

Remarque

If the ratio : $\frac{A-Z}{Z} \geq 1.5$, the element in this case is unstable (radioactive).

C. Natural Radiations

Natural radiation consists of 03 types:

1. β Radiations

We have previously mentioned that in case the element is unstable due to a relatively high number of neutrons (the N/Z ratio is high), to mitigate various reactions inside the nucleus, the element automatically attempts to convert neutrons into electrons and protons (electrons are sent outside while protons are retained in the nucleus).

Exemple

$${}^{1}_{0}n \rightarrow {}^{1}_{1}P + {}^{0}_{-1}e \dots\dots (B^{-})$$

$${}^{227}_{89}AC \rightarrow {}^{227}_{90}Th + {}^{0}_{-1}e + E$$

and it is :

$${}^{A}_{Z}X \rightarrow {}^{A}_{Z+1}X + {}^{0}_{-1}E$$

Remarque

There is also β+ radiation called positron radiation, consisting of positive electrons produced from the conversion of a proton into a neutron.

$$^{1}_{1}p \rightarrow {}^{1}_{0}n + {}^{0}_{+1}e \ldots \quad (\beta^{+})$$

This type of radiation cannot be obtained except in the industrial field.

2. γ Radiation

The emission of rays accompanied by significant excitation in the nucleus, and to return the nucleus to its ground state, it emits electromagnetic radiation with a very short wavelength (λ<1A°). This electromagnetic radiation has light properties and is a bundle of photons carrying high energy like x-rays.

Exemple

$$^{24}_{82}Pb \rightarrow {}^{24}_{83}Bi + {}^{0}_{-1}e + {}^{0}_{0}\delta + E$$

This radiation does not decrease the atomic number Z or the mass number A of the unstable nucleus, but it decreases the atomic mass due to the reaction by the amount of Δm, which corresponds to the energy.

$$\Delta E = \Delta m \times c^{2} = h.\upsilon = h.c/\lambda$$

Where:

h:Planck's constant $(h = 6.626.10^{-34} j.s)$

λ:Wavelength

υ:Frequency

D. Radioactive Decay Law

The probability of a nucleus undergoing fission is not related to the fission that occurred earlier for a sample to which these nuclei belong, so we say that the nucleus does not "age" or "die without aging". On the other hand, nuclear fission does not affect the behavior of other nuclei in the sample. Therefore, nuclear fission is a probabilistic (random) phenomenon where there is no controlling factor allowing changes in the properties of atomic nuclear fission. The probability of a radioactive nucleus disappearing within a certain period is not related to its age but to the nature of the nucleus.

Exemple

A carbon 14 nucleus that appeared 1000 years ago and another formed five minutes ago have the same probability of disintegrating in the next hour.

We consider a sample containing a number N(t) of radioactive nuclei at a certain moment in time t.

$$A^{*} \quad \rightarrow \quad B(stable)$$

$$t = 0 \quad N_{0} \quad \rightarrow \quad 0$$

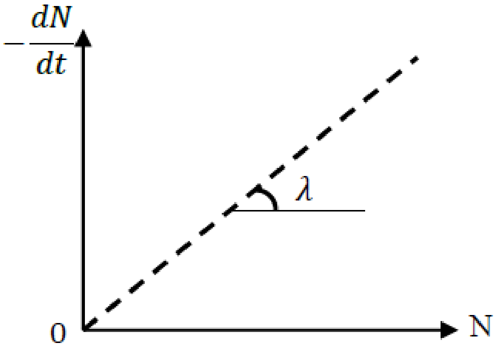
$$t > 0 \quad N_{t} \quad \rightarrow \quad N_{0} - N_{t}$$

The experience indicates that the decay of radioactive atoms is directly proportional to the quantity of unstable atoms (N) existing at a specific time (t). This decay rate is expressed as:

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

Where: $\frac{dN}{dt}$ is the derivative of N with respect to time t.

-λN: with the sign (-), it's the decrease in the number of radioactive particles, the relationship was straightforward:



Where: $-\frac{dN}{dt}$ is directly proportional to the number of nuclei, then:

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

So equation (1) is then a differential equation, the solution of which allows us to obtain the decay law or the decrease law that describes the temporal evolution of the number of radioactive nuclei in a sample.

$$\int_{N_0}^{N} \frac{dN}{N} = -\lambda \int_{t=0}^{t} dt \Rightarrow [\ln N]_{N_0}^{N} = -\lambda [t]_{t=0}^{t}$$

$$\Rightarrow \ln N - \ln N_0 = -\lambda t$$

$$\Rightarrow \ln \frac{N}{N_0} = -\lambda t \Rightarrow \frac{N}{N_0} = e^{-\lambda t}$$

$$\Rightarrow \mathbf{N(t) = N_0 . e^{-\lambda}}$$

This is the law of radioactive decay and applies to all types of radioactive activity (naturally and artificially radioactive nuclei).This law shows that the number of nuclei decreases exponentially with time, where:

N_0 : is the number of radioactive nuclei in a sample at time t = 0

λ: is the radioactive decay constant or activity constant (t^{-1}) (s^{-1}, min^{-1}, h^{-1}, $year^{-1}$.......)

Remarque

The previous relationship can be expressed as follows:

by Substituting $N = -\frac{m.N_A}{M}$ in $N(t) = N_0 . e^{-\lambda}$ becomes:

Mass: $m(t) = m_0 . e^{-\lambda}$

Number of moles: $n(t) = n_0 / \, e^{-\lambda}$

Where m_0 and n_0 are the mass and number of moles of radioactive nuclei respectively in a sample at time t= 0

E. Radiative Activity Law

We express the radioactivity by A, which is the number of decays in a unit of time. The average activity of a source during a period of dt is given by the relationship:

$$-\frac{dN}{dt} = A(t)$$

Assuming that the source consists of radioactive nuclei of one type, we deduce the differential equation. According to relationship (1):

$$\lambda N(t) = A(t)$$

According to the decay law, we obtain the relationship:

$$A(t) = \lambda N_0 . e^{-\lambda t}$$

Therefore, the decay law for the activity of a sample containing only one type of radioactive nuclei is given by the relationship:

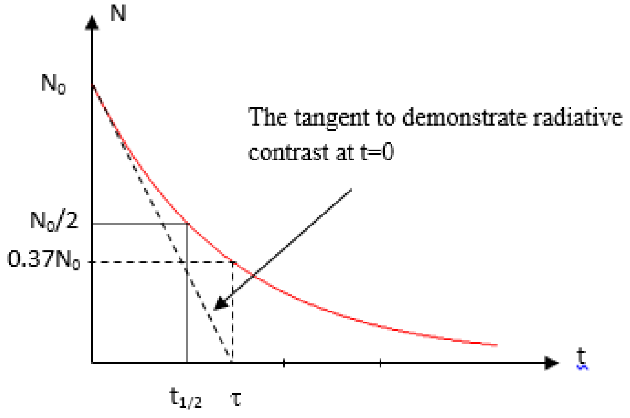
$$\boldsymbol{A(t) = A_0 . e^{-\lambda t}}$$

Where;

$\boldsymbol{A_0 = \lambda . N_0}$: is the initial decay of a sample at time t = 0

1. Radioactive period (τ, T) or Half-life ($t_{1/2}$)

Half-life or decay is the time for which half of the original quantity of radioactive nuclei present in a sample has decayed, meaning half of the quantity remains undecayed $(N = \frac{N_0}{2})$. The half-life time is symbolized by: $t_{1/2}$ and its unit is in seconds.



Time constant (τ): It is the average time for the life of the nucleus where: $\tau = \frac{1}{\lambda}$, and it is measured in seconds (s).

2. Relationship between decay constant (λ) and time constant (τ)

Let t=τ and by substitution in the decay law, it yields:

$$N(t) = N_0 . e^{-\lambda\tau} \Rightarrow N / N_\circ = e^{-\lambda\tau} \Rightarrow ln N/N_\circ = -\lambda\tau$$

From the relationship with half-life: $ln \frac{N_\circ}{2N_0} = -\lambda\tau \Rightarrow ln\, {}^1/_2 = -\lambda t$

$$\Rightarrow - \ln 2 = - \lambda\tau \Rightarrow \boxed{\tau = ln2/\lambda}$$

Définition

Measurement unit: We commonly use the Curie (Ci) as a unit for measuring radioactive activity and also use the Becquerel (Bq) where (1 Ci = 3.7 x 10^{10} dps = 3.7 x 10^{10} Bq).

Definition: The Curie (Ci) is the radioactive activity of one gram of radium (226Ra) and it can be expressed as the number of decays in a unit of time (dps).

F. Abbreviated equations

$${}^{27}_{13}Al + \alpha({}^4_2He) \longrightarrow {}^{30}_{15}P + {}^1_0n$$

$${}^{27}Al(\alpha,n)^{30}P$$

$${}^{227}_{90}Ac \longrightarrow {}^{227}_{90}Th + {}^{0}_{-1}\beta$$

$${}^{227}Ac({}_{-}\beta)^{227}Th$$

$${}^{14}_{7}N + \alpha({}^4_2He) \longrightarrow {}^{17}_{8}O + {}^1_1H$$

$${}^{14}N(\alpha,p)^{17}O$$

Exemple

- Expand nuclear reaction ${}^{56}_{25}Mn(\beta^-)^{56}_{26}Fe$
- It was found that in 7.5 hours, 1 moles of ${}^{56}_{25}Mn$ gives 49g of ${}^{56}_{26}Fe$, Calculate τ of Mn
- Calculate the mass of a sample of manganese (Mn) with an activity 2.106 Ci

Solution:

$${}^{56}_{25}Mn \rightarrow {}^{56}_{26}Fe + {}^{0}_{-1}\beta + \Delta E_N$$

$$1mol\,(Mn)\,56g \rightarrow (Fe)\,49g$$

$$m_0 \qquad m'(resulting)$$

$$m_{remaining} = m_0 - m' = 56 - 49 = 7g$$

$$\boldsymbol{m = m_0 \times e^{-\lambda t}} \Rightarrow \frac{m}{\boldsymbol{m_0}} = e^{-\lambda t} \Rightarrow \mathrm{Ln}\frac{\boldsymbol{m_0}}{m} = \lambda t$$

$$\Rightarrow \lambda = \frac{1}{t} \times Ln\frac{m_0}{m} = \frac{1}{7.5} \times Ln\frac{56}{7}$$

$$\Rightarrow \lambda = 0.277h^{-1}$$

$$\tau = \frac{Ln2}{\lambda} = 2.49h = 8964Sec$$

$$A_0 = \lambda \times N_0 \Rightarrow A_0 = \lambda \times n_0 \times \mathcal{N}_A \Rightarrow A_0 = \lambda \times \frac{m_0}{M} \times \mathcal{N}_A$$

$$\Rightarrow m_0 = \frac{A_0 \times M}{\lambda \times \mathcal{N}_A}$$

$$\lambda = \frac{Ln2}{\tau} \Rightarrow m_0 = \frac{A \times M \times \tau}{\mathcal{N}_A \times Ln2} = \frac{2 \times 10^6 \times 3.7 \times 56 \times 8964}{6.023 \times 10^{23} \times Ln2}$$

$$\Rightarrow m_0 = 0.08899g = 88.99mg$$

G. Nuclear energy calculation

In a nuclear reaction, we observe a change in the mass of the nuclei by an amount Δm where:

$$\Delta m = \sum \text{Product nucleus mass} - \sum \text{Reactant nucleus mass}$$

The energy equivalent to Δm is called nuclear energy and can be calculated based on Einstein's relationship:

$$\Delta E = |\Delta m| \times c^2$$

Exemple

Calculate the nuclear energy when the nucleus of radium (^{226}Ra) transforms into the nucleus of radon (^{222}Rn) Given the nucleus masses as follows:

$$M({}^{222}_{86}Rn) = 222\ .0175amu,\ M({}^{226}_{88}Ra) = 226.254amu,\quad M({}^{4}_{2}He) = 4.003884amu$$

Solution :

We have :

$$\Delta m = (m\,\mathrm{Rn} + m\,\mathrm{He}) - m\mathrm{Ra}$$

$$= (222.0175 + 4.00388) - 226.0254 = -0.0041amu$$

$$\Rightarrow \Delta E = |\Delta m| \times 931.5 = 0.0041 \times 931.5 = 3.8Mev$$

or

$$\Delta E = 0.041 \times (1.66.10^{-27}) \times (3.10^{8})^2 = 0.061.10^{-11}J$$

$$\Rightarrow E_{Mev} = 0.061.10^{-11}/1.6.10^{19} = 3.8Mev$$

H. Natural Radioactivity

It's the study of nuclear reactions that happen between radioactive elements in nature.

Radioactive Family: Let X0 be an unstable element that undergoes a series of reactions to reach a stable element X_n.

$$X_0 \longrightarrow X_1 \longrightarrow X_2 \longrightarrow X_3 \ldots\ldots\ldots \longrightarrow X_n$$

where :X_0 , X_1, X_2, X_3 ....X_n are called the radioactive family.

X_0: is a heavy nucleus representing the beginning of the radioactive series

X_n: is a relatively light nucleus representing the end of the series.

Exemple

$$^{238}_{92}U \xrightarrow{\alpha} {}^{234}_{90}Th \xrightarrow{\beta} {}^{234}_{91}Po \xrightarrow{\beta} {}^{234}_{92}U \xrightarrow{5\,\alpha} {}^{214}_{82}Pb \xrightarrow[4\,\beta]{2\,\alpha} {}^{206}_{82}Pb$$

$$^{238}_{92}U \xrightarrow[6\beta]{8\,\alpha} {}^{206}_{82}Pb$$

Serie	**Beginning of Serie**	**End of Serie**
Thorium	$^{234}_{92}Th$	$^{206}_{82}Pb$
Uranium	$^{235}_{92}U$	$^{207}_{82}Pb$
Uranium	$^{238}_{92}U$	$^{238}_{92}U$
Neptunium	$^{237}_{93}Np$	$^{209}_{83}Bi$

I. Artificial Radioactivity and Nuclear Reactions

We obtain artificial nuclear reactions when we expose nuclei of unstable elements to particles like α, n, e-, p, d or utilize γ radiation.

Artificial nuclear reactions are divided into three types:

-Transmutation reactions

-Fission reactions

-Fusion reaction

1. Transmutation Reactions

These types of reactions allow for the formation of nuclei with mass numbers equal to or close to the mass number of the target nucleus

Exemple

$$^{14}_{7}N \;+\; {}^{4}_{2}He \longrightarrow {}^{17}_{8}O \;+\; {}^{1}_{1}H$$

Remarque

The resulting nuclei can be unstable.

2. Fission Reactions

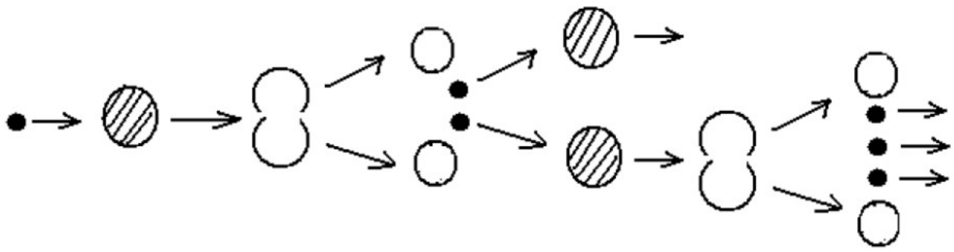
These reactions occur with elements having high mass numbers ($A>200$). Due to weak binding energies, heavy nuclei split into lighter, stable nuclei ($72<A<162$) releasing energy.

Exemple

Bombardment of Uranium nucleus ${}^{235}_{92}U$ with neutrons.

$$
{}^{235}_{92}U \;+\; {}^{1}_{0}n \;\rightarrow
\begin{cases}
{}^{87}_{35}Br + {}^{14}_{7}La + 3\,{}^{1}_{0}n + \mathrm{E} \\
\text{or } {}^{139}_{54}Xe + {}^{95}_{38}Sr + 2\,{}^{1}_{0}n + \mathrm{E} \\
\text{or } {}^{143}_{56}Ba + {}^{90}_{36}Kr + 3\,{}^{1}_{0}n + \mathrm{E}
\end{cases}
$$

In addition to the resulting nuclei, more neutrons are produced capable of initiating further fission reactions, leading to a chain reaction with high energy release culminating in an explosive event, as in a nuclear bomb.



By controlling the fission reaction through absorption of produced neutrons using moderators like graphite, we can harness the energy for practical purposes in daily life, as in nuclear reactors.

3. Fusion Reactions

In these reactions, two light atoms combine to form a heavier nucleus, releasing a high amount of energy. This reaction occurs at temperatures around 50 million degrees Celsius.

Exemple

usion of Deuterium nucleus with Tritium nucleus (Hydrogen bomb)

$$ {}^{2}_{1}H + {}^{3}_{1}He \longrightarrow {}^{4}_{2}He + {}^{1}_{0}n $$

$$ \text{or} \quad {}^{6}_{3}Li + {}^{2}_{1}H \longrightarrow 2\,{}^{4}_{2}He $$

Remarque

Energy released in fusion reactions is greater than that of fission reactions.

J. Radioactive Dating Applications

1. Determining Ages

Carbon $^{14}_{6}C$ is used in dating ancient animals and plants by measuring the remaining ^{14}C content. In the upper layers of the atmosphere (30 km above the Earth's surface), neutrons produced by cosmic rays react with nitrogen to form carbon-14 through the following reaction:

$$^{14}_{7}N + ^{1}_{0}n \rightarrow ^{14}_{6}C + ^{1}_{1}P(^{1}_{1}H)$$

$$^{14*}_{6}C \xrightarrow{[O_2]} {}^{*}CO_2$$

${}^{*}CO_2$ is absorbed through photosynthesis by plants, consumed by animals and humans.

$^{14}_{6}C$ decays according to the following reaction:

$$^{14}_{6}C \rightarrow ^{14}_{7}N + ^{0}_{-1}\beta$$

This reaction is characterized by a half-life: $T = 5568 years$

and a radioactive activity : $A = 15.3\ dpm$

For every 1g of ^{14}C, the decrease in radioactive activity can be used to determine the age of ancient objects.

Exemple

If the radioactive activity of ^{14}C is 1dpm for 1g of ^{14}C, what is the age of an old wooden piece?

Solution :

$$A = \lambda . N$$

$$A_0 = \lambda . N_0$$

$$\ln A/A_0 = -\lambda . t \Rightarrow t = 1/\lambda \ \ln A_0/A.$$

$$t = \tau/\ln 2 \ . \ln A_0/A = 5568/0.693 \times \ln 15.3/1 = 21917.3\ years$$

a) Determining the age of the Earth

The age of the Earth can be calculated by relying on the age of the uranium mine in it, which is based on calculating the amount of lead206pb and 207pb, which are produced from the decay of uranium ^{238}U and ^{235}U respectively.

	^{235}U	$\longrightarrow$	^{207}Pb
$t = 0$	N_0		0
$t = t'$	N		$n = N_0 - N$

We have : $N(t) = N_0 . e^{-\lambda t}$

$$n = N_0 - N = N_0 - N_0 \,.\, e^{-\lambda t} = N_0\,(1 - e^{-\lambda t}) \;\ldots\ldots\ldots\ldots\ldots\ldots(1)$$

$$^{238}U \longrightarrow {}^{206}Pb$$

$$n' = N_0' - N' = N_0' - N_0'.\, e^{-\lambda' t} = N_0'(1 - e^{-\lambda' t})\ldots\ldots\ldots\ldots\ldots\ldots(2)$$

by dividing equation (1) to (2), we find :

$$\frac{n}{n'} = \frac{N_0\left(1 - e^{-\lambda t}\right)}{N'_0\left(1 - e^{-\lambda' t}\right)} \;\ldots\ldots\ldots\ldots\ldots\ldots\ldots (3)$$

And since:

$$\frac{N}{N'} = \frac{N_0\left(1 - e^{-\lambda t}\right)}{N'_0\left(1 - e^{-\lambda' t}\right)} \;\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4)$$

(4) and (3) we get from

$$\frac{n}{n'} = \frac{N_0\left(1 - e^{-\lambda t}\right)}{N'_0\left(1 - e^{-\lambda' t}\right)} = \frac{N}{N'} = \frac{\left(1 - e^{-\lambda t}\right)}{e^{-\lambda' t}} \times \frac{e^{-\lambda t}}{\left(1 - e^{-\lambda' t}\right)}$$

By spectral mass, , $\frac{N}{N'}$ *and* $\frac{n}{n'}$,can be experimentally calculated by substituting into the last relationship, the time t, which is the age of the mine and therefore the age of the Earth, estimated at about 4.54 billion years with a margin of error of 1.

K. The use of radioactivity for therapeutic purposes

Brachytherapy, as the name suggests, was invented by Marie Curie. It is used for cancers, especially gynecological, urological, ENT, or even for brain tumors. The tumors are destroyed by the ionizing radiation created by the radioactive material used. The radioactive sources used in brachytherapy are Cesium 137, Iridium192, and Iodine 125. These three elements deliver high doses of radiation. This method allows the tumor to be irradiated while protecting neighboring organs to the maximum and in some cases avoiding surgical treatments. Once the treatment is completed, the radioactive sources are removed from the patient. For small tumors, brachytherapy is effective in 80 to 90% of cases.

Other Applications of Radioactivity

- **Energy-related:** nuclear power plants for fission, energy source (electricity production).
- **Armament sector:** nuclear missiles, atomic bombs, etc...
- **Biological / geological:** in vivo studies using radioactive markers, dating.
- Radioactive tracers for monitoring various industrial manufacturing processes.
- Carbon 14 for dating ancient objects (up to approximately 40,000 years).

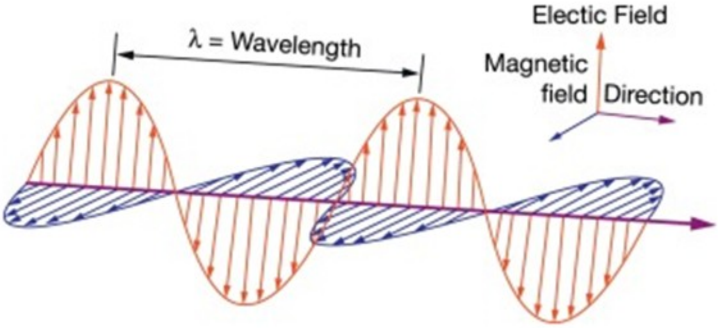
Chapter Four: The electronic structure of atom

IV

A. Electromagnetic Radiation

1. wave nature of light

Light is electromagnetic radiation produced by the combination of electric and magnetic fields and spread with a sinusoidal motion:



All electromagnetic radiation travels at the speed in vacuum, approximately 3.0 × 10^8 m/s and is characterized by a wavelength λ (the distance between two successive amplitudes) and a frequency (rebound), where:

Frequency or pitch∂ : It's the number of waves cut per unit of time (or cycles per second) and it equals the inverse of the period.

$$\partial=\frac{c}{\lambda}=\frac{1}{T}$$

It is measured in S^{-1}

Wave number: It's the number of waves in a unit of length (in one meter or (...cm) and it equals the inverse of the wavelength.

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

It is measured in m^{-1}, cm^{-1}, or $A°^{-1}$.

2. Particle nature of light

Max Planck, the scientist, proposed a very important idea: if light has a wave nature, then this wave carries energy in the form of very small energy units called: energy quanta. This means that the energy transmitted by a light radiation is not continuous, but rather intermittent, and each energy quantum corresponds to energy: $E = h.\partial$

E: energy of a single quantum (J)

∂: frequency of the light wave (Hz)

h: Planck's constant ($h = 6.625\times10^{-34} J.s$)

While the total of these quanta is: $E_n = n\,h.\partial$, where: **n** natural number 1, 2, 3 ...

Einstein generalized the quantum theory by stating that light waves consist of infinitely small particles called photons, and each photon carries energy: $E = h.\partial$

Each photon is a relative particle with negligible mass and neutral charge that moves in a vacuum at the same speed as the wave spreads ($c=3\times10^8$ m/s), possessing energy called a quantum of energy proportional to the optical frequency. Radiations differ from one another in the energy of their photons, where radiation with frequency ∂ carries energy E_{ph} that indeed explains the photoelectric effect.

3. Photoelectric phenomenon

The photoelectric effect, or phenomenon, is the emission of electrons from solid, liquid, and gaseous bodies when they absorb energy from light. The electrons emitted from this phenomenon are called photoelectrons.

a) Emission Mechanism

Photons have a certain energy that corresponds to the frequency of light. In the photoemission process, if an electron in a material absorbs one photon of energy and its energy is greater than the binding energy (work function) of the material, the electron will be emitted. If the photon energy is very low, the electron will not be able to break free from the material. With an increase in the intensity of light, the number of emitted photons increases, leading to an increase in the number of emitted electrons, but it does not increase the energy absorbed for each electron. Therefore, the energy carried by the emitted electron does not depend on the intensity of the incident light, but only on the frequency (energy) of that light.

b) Photoelectric Emissions

For a specific metal, there is a minimum frequency 0 below which no photoelectrons will be emitted when the metal surface is exposed to a frequency lower than that. This frequency is called the threshold frequency, where:

$$E_{ph} = E_0 + E_c \Leftrightarrow h\partial = h\partial_0 + \frac{1}{2}mv^2$$

And then:

$\partial \geq \partial_0$: Electron detachment

$\partial > \partial_0$: Detachment and movement of the electron

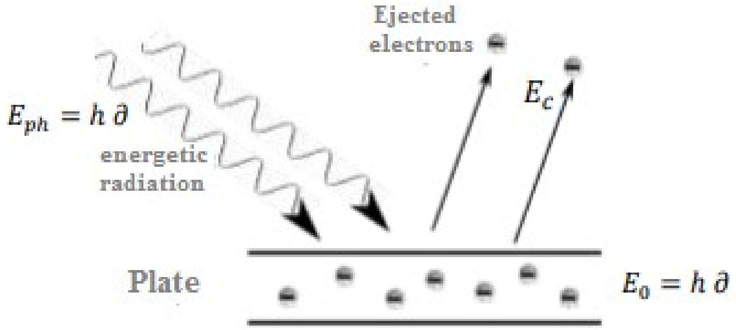
$\partial < \partial_0$: Electron does not detach

When increasing the frequency of the incident beam, while keeping the number of incident photons constant, this will lead to an increase in the photon's energy and consequently an increase in the kinetic energy of the emitted photoelectrons, and thus an increase in the stopping voltage (stopping potential) U0 Where:

$$E_c = e.U_0$$

And the kinetic energy:

$$E_c = \frac{1}{2}mv^2$$



Exemple

An optical radiation with a wavelength of λ = 100 nm falls on a metal surface, causing the emission of electrons from the metal with a kinetic energy EC = 10 eV.

1. Calculate the speed of the emitted electrons.
2. Calculate the threshold energy E0; threshold frequency 0, the threshold period T0, threshold wavelength λ0, and the wave number of the threshold.

   Given: h = 6.62 x 10^{-34} J.s; me = 9.1 x 10^{-31} kg; c = 3 x 10^{8} m/s

   Solution:

$$\lambda = 100nm = 100 \times 10^{-9}m$$

$$E_c = 10eV = 10 \times 1.6 \times 10^{-19}J$$

$$1)\ E_c = \frac{1}{2}mv^2 \Rightarrow v = \sqrt{\frac{2E_c}{m}} = \sqrt{\frac{2\times10\times1.6\times10^{-19}}{9.1\times10^{-31}}} = 1.88 \times 10^6 m/s$$

$$2)\ E_{ph} = E_0 + E_c$$

$$\Rightarrow E_0 = \frac{hc}{\lambda} - E_c = \frac{6.62 \times 10^{-34} \times 3 \times 10^8}{100 \times 10^{-9}} - 10 \times 1.6 \times 10^{-19}$$

$$\Rightarrow E_0 = \frac{3.86 \times 10^{-19}}{1.6 \times 10^{-19}} = 3.86 \times 10^{-19}J = 2.41eV$$

$$3)\ E_0 = h\partial_0 \Rightarrow \partial_0 = \frac{E_0}{h} = \frac{3.86\times10^{-19}}{6.62\times10^{-34}} = 5.8\times10^{14}s^{-1}$$

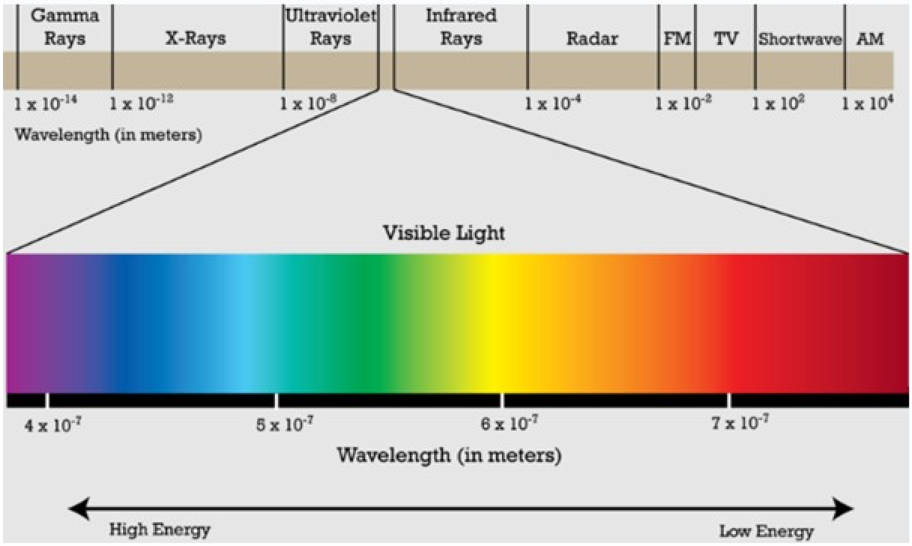
$$4)\ T = \frac{1}{\partial_0} = \frac{1}{5.8\times10^{14}} = 1.72\times10^{-15}s$$

$$5)\ E_0 = \frac{hc}{\lambda_0} \Rightarrow \lambda_0 = \frac{hc}{E_0} = \frac{6.62\times10^{-34}\times3\times10^{8}}{3.86\times10^{-19}} = 5.15\times10^{-7}m$$

$$6)\ \bar{\partial}_0 = \frac{1}{\lambda_0} = \frac{1}{5.15\times10^{-7}} = 1.94\times10^{6}m^{-1}$$

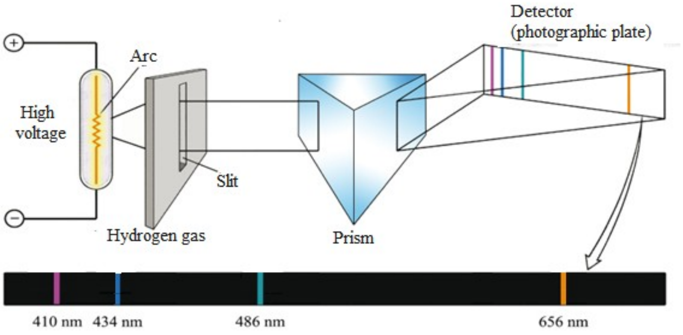
B. Spectrum of electromagnetic radiation

The totality of electromagnetic radiation is called the spectrum, and visible light represents a small part of this spectrum



1. Hydrogen Atom Spectrum (Visible Spectrum)

The atomic spectrum is known to consist of specific and distinct lines, each representing light of a certain frequency, emitted by excited gas atoms. This is called the line spectrum. When an electron transitions from a lower energy level to a higher energy level, it absorbs energy. And when an electron transitions from a higher energy level to a lower energy level, it emits energy in the form of light with a specific frequency and wavelength. This change in energy is considered the basis of the atomic spectrum.



a) Interpretation of the phenomenon

The electrons emitted by the cathode will collide with the molecules of gaseous Hydrogen. Under the influence of these collisions, there is first dissociation of the molecules:

$H_2 \longrightarrow H + H$, then excitation of the atoms: $H + \text{energy} \longrightarrow H^* \text{ (excited)}$, from the excited state the atoms H*(excited) spontaneously return to the ground state: $H^* \text{ (excited)} \longrightarrow H + \text{energy (ground state)}$.

This return to the ground state releases the absorbed energy in the form of light energy to the external environment, which is the principle behind Neon (Ne) and Sodium (Na) lamps.

The pink light emitted by hydrogen is made up of several components; technically, this color is broken down into 4 different monochromatic components (red, turquoise, indigo, and violet).

using a prism. It is concluded that the light emitted by hydrogen is polychromatic, and the 4 radiations obtained constitute the visible spectrum of the hydrogen atom. In addition to these radiations, hydrogen atoms between 500 to 1000 volts, emitting both invisible radiations (Ultraviolet (UV), Infrared (IR)). All these radiations together form the complete spectrum of hydrogen.

2. Spectral line distribution rules

Based on previous experiments and to simplify the meaning of the linear spectrum of hydrogen, we say that when the electron excited in a hydrogen atom returns from higher energy levels to lower energy levels, it loses the energy it gained when it was excited in the form of radiation (linear spectrum). The total spectral lines representing the emission spectrum of the hydrogen atom are called spectral series (where the wavelengths in atomic spectra are located), each group or series of spectral lines is attributed to the sub-orbit that the electron jumps to in the hydrogen atom. For example, a group of lines in the Balmer series, all of which are jumps for the electron from the highest to orbit number 2, and each wavelength in any series can be determined numerically.

a) Balmer series

When studying the spectrum emitted from a hydrogen atom, it was found that these spectral lines appeared to have a specific type of connection to each other. It was natural to formulate an empirical equation that relates their wavelengths. The first to do this was the scientist Balmer, who found that the wavelengths of the spectral lines could be expressed by a simple empirical equation.

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

Where: $n \in N > 2$ and R_H: Rydberg'sonstant$\left(R_H = 1.09768 \times 10^7 m^{-1}\right)$

i Laws of series Distribution

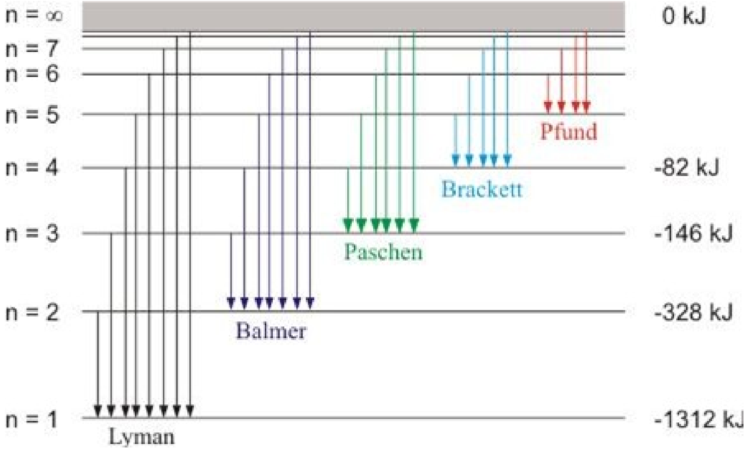
Redberg made a great effort in 1896 to express a series by Morse, and found that it is better to use the inverted wavelength (known as the wave number) in mathematical relationships instead of the wavelength as follows:

$$\bar{\delta}=\frac{1}{\lambda}=R_H\left(\frac{1}{n_1^2}-\frac{1}{n_2^2}\right)$$

And it is suitable for calculating the wavelengths of all spectral lines in all spectral regions.

If $n_2 > n_1$, then for each value of n_1, there corresponds a series of spectral lines (the orbit to which the transition ends), and for each value of n_2, there corresponds a line in this series (the orbit from which the transition begins). In this way, the boundaries of any series in the spectrum (electron transitions in a hydrogen atom) can be calculated.

1. **Lyman series:**
   Located in the UV (ultraviolet) range (97.25 – 121.57) nm, this series is known for its values:
   $n_1=1$ and $n_2= 2,3,4..........\infty$
2. **Balmer Series:**
   It is located in the visible spectrum in the range of (434.1 – 656.3) nm, and is defined by the following natural numbers:
   $n_1=2$ and $n_2= 3,4,5..........\infty$
3. **Bachen Series :**
   It is situated in the near infrared (IR) domain in the renge of (1094 − 1875) nm, and is defined by the following natural numbers:
   $n_1=3$ and $n_2= 4,5,6..........\infty$
4. **Brakett series:**
   It is located in the medium infrared field in the range of (2630 − 4050) nm, and is defined by the following natural numbers.
   $n_1=4$ and $n_2 =5,6,7..........\infty$
5. -**Pfund series:**
   It is located in the infrared region in the range of (7400 − ∞) nm, and is defined by the following natural numbers:
   $n_1=5$ and $n_2=6,7,8..........\infty$



These experimental relationships were what gave Niels Bohr the necessary evidence to develop the first concept of the hydrogen atom

Exemple

1- Calculate the first line in the Lyman's series.

$$\bar{\delta}=R_H\left(\frac{1}{n_1^2}-\frac{1}{n_2^2}\right)=R_H\left(\frac{1}{1_1^2}-\frac{1}{2_2^2}\right)=\frac{3}{4}R_H m^{-1}$$

So the first line in the Lyman series

$$\bar{v}=\frac{3}{4}R_H m^{-1}$$

2- Calculate the final line e in Lyman's series:

$$\bar{\partial}=R_H\left(\frac{1}{n_1^2}-\frac{1}{n_2^2}\right)=R_H\left(\frac{1}{1_1^2}-\frac{1}{\infty_2^2}\right)=R_H=\frac{1}{\lambda_\infty}\Rightarrow\lambda_\infty=\frac{1}{R_H}$$

3. Release energy calculation

When we know the value of the wave number for a certain line, we can calculate the energy emitted from a hydrogen atom using the following relationship:

$$\Delta E = h.\,\partial$$

Where : **h** Planck's constant ($h = 6{,}62.10^{-34}$J.s)

$$\Delta E = h.\,\partial = h.c/\lambda = h.c.\bar{\partial}$$

4. Spectrum of hydrogen-like ions (Hydrogenoids)

We call hydrogen-like ions all atoms that carry Z protons in their nucleus and have one electron orbiting around it, or they are atoms that lose their electrons and only retain one electron, and the relation will be :

$$\bar{\partial}=\frac{1}{\lambda}=R_H Z^2\left(\frac{1}{n_1^2}-\frac{1}{n_2^2}\right)$$

Exemple

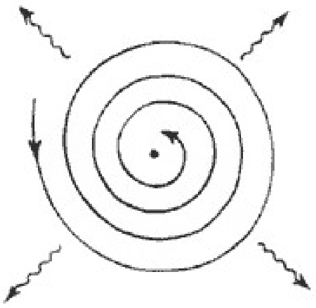
${}_2He^+$, ${}_3Li^{+2}$, ${}_4Be^{+3}$

5. Critical of the Rutherford model

According to the classical theory, the electron in its orbit around the nucleus will continuously emit electromagnetic radiation because it moves in a circular path. This means that it constantly loses energy until it loses it completely, resulting in the orbit being spiral as shown in the opposite figure. Eventually, the electron will collide with the nucleus and the atom will disappear, contradicting the stability of atoms for the following reasons:

1- This phenomenon has not been experimentally observed.

2- The electron's energy continuously decreases, so the emitted radiation should be continuous. However, experiments have shown that the radiation emitted by the hydrogen atom is not continuous.



C. Quantum theory of hydrogen and hydrogen-like systems :Bohr'satomic model

Bohr attempted to create a comprehensive model of atomic structure, drawing on Rutherford's idea of the atom and Max Planck's concepts of quantization and the emission of photons. He presented his model of the hydrogen atom, which proposed that an electron orbits the nucleus in circular orbits. He also suggested a set of dynamic hypotheses for the atom.

1. Bohr'satomic model

Bohr attempted to create a comprehensive model of atomic structure, drawing on Rutherford's idea of the atom and Max Planck's concepts of quantization and the emission of photons. He presented his model of the hydrogen atom, which proposed that an electron orbits the nucleus in circular orbits. He also suggested a set of dynamic hypotheses for the atom.

a) First postulate

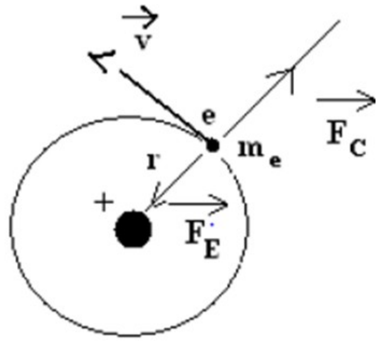
Electrons orbit around the nucleus (proton) in a continuous circular path without emitting energy (contrary to Rutherford's nuclear theory, which suggests that electrons move around the nucleus in a spiral path until they eventually fall onto the nucleus due to the gravitational attraction between the nucleus and the electron). To remain in its orbit, the centrifugal force must balance with the electrostatic attraction between the nucleus and the electron (Coulomb's attraction forces), meaning that:

$$\sum \vec{F} = \vec{0}$$

The electron is influenced by two forces:

A- Coulomb's law of attraction

$$F_E = \frac{K|q.q'|}{r^2} = \frac{KZe^2}{r^2}$$



Where :

$$K = \frac{1}{4\pi\varepsilon_0} = \quad 9.10^9\ \mathrm{m}^{-1}$$

ε_0 : Vacum permitivity

B- Force centrifuge:

$$F_c = \frac{m_e v^2}{r}$$

In order for the electron to continue orbiting around the nucleus without falling onto it, it must be:

$$\vec{F_E} = \vec{F_C}$$

$$\frac{KZe^2}{r^2} = \frac{m_e v^2}{r}$$

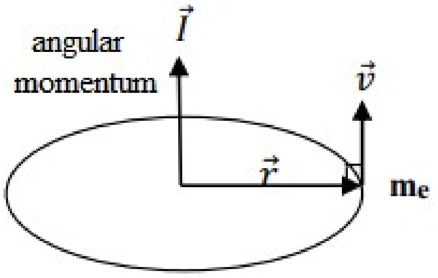
$$\Rightarrow \frac{KZe^2}{r} = m_e v^2$$

And from that, we get the expression for kinetic energy:

$$E_c = \frac{1}{2}m_e v^2 = \frac{1}{2}\frac{KZe^2}{r}$$

b) Second postulate

An electron of a hydrogen atom or a hydrogen-like ion can only move in circular orbits where its angular momentum L or angular momentum for the nucleus in multiples of the complete value of h (Planck's constant):



$$\vec{I} = \vec{r}\,\Lambda\,\vec{p} \quad \Rightarrow \vec{I} = \vec{r}\,\Lambda\, m_e\vec{v}$$

$$\|\vec{I}\| = \|\vec{r}\|.\, m_e \|\vec{v}\|.\sin(\vec{r},\vec{v}) \qquad , \qquad \vec{r} \perp \vec{v}$$

$$\Rightarrow \|\vec{I}\| = r.\, m_e v.\sin\left(\frac{\pi}{2}\right)$$

and :

$\mathrm{I} = \mathrm{n}\frac{h}{2\pi}$ (n=1,2,3,4,........∞)

Quantization condition (energy and angular momentum quantization):

$$\Rightarrow m_e v\, r = n\frac{h}{2\pi}$$

c) Third postulate

The third assumption states that the energy of the electron in its orbit is a constant value and it does not emit electromagnetic radiation while rotating around the nucleus.

1. The electron must exist in specific locations along its circular path because each orbit holds a specific energy and this energy must be defined and quantized according to the Planck theory.
2. The electron's energy changes when transitioning from one allowed orbit to another (from an initial state with energy E_i to a final state with energy E_f), leading to the emission or absorption of a specific amount of energy.

$$\Delta E = \left|E_f - E_i\right| = h\,\partial$$

d) Determining the radius of the hydrogen and hydrogen-like atom orbits

Assuming that an electron is stable in a circular orbit with a radius rn and a speed vn, the electrostatic attraction force (Coulomb attraction) is equal to the centripetal force, which leads to the second assumption:

$$\frac{KZe^2}{r_n} = m_e v^2 \ldots\ldots\ldots (1)$$

By multiplying both sides by m_e and using the quantization condition:

$$\frac{n^2h^2}{4\pi^2{r_n}^2} = m_e^2v^2 \ldots\ldots\ldots\ldots\ldots (2)$$

From equations (1) and (2), we find:

$$\frac{KZm_ee^2}{r_n} = \frac{n^2h^2}{4\pi^2{r_n}^2}$$

$$\Rightarrow \qquad \boldsymbol{r_n = \frac{h^2}{4\pi^2KZm_ee^2}\times n^2}$$

where: n = 1, 2, 3, ...

In the case of the hydrogen atom where Z=1 and for the orbit n=1 :

$$r_1 = \frac{h^2}{4\pi^2KZm_ee^2}$$

$$r_1 = \frac{(6{,}62\,.10^{-34})^2}{4(3{,}14)^2(9.10^9)(9{,}1\,.10^{-31})(1{,}6\,.10^{-19})^2}$$

$$= 0{,}528.\ 10^{-10} = 0{,}528A^o$$

This is the Bohr radius for the first circular orbit.

$$=> \qquad \boldsymbol{r_n = r_1 \times \frac{n^2}{Z}}$$

where :n = 1 , 2 , 3 , ...

Therefore, according to the Bohr theory of the hydrogen atom, the electron is present in the following orbits: $r_n = r_1$, $4r_1$, $9r_1$, ...

e) Determining the speed of the electron in the orbit n

According to the quantization condition:

$$m_ev_nr_n = n\frac{h}{2\pi} \Rightarrow v_n = \frac{nh}{2\pi m_er_n}$$

By substituting the term rn in the previous relationship, we find:

$$v_n = \frac{nh.4\pi^2KZm_ee^2}{2\pi m_e.h^2.n^2}$$

$$\boldsymbol{\Rightarrow v_n = \frac{2\pi KZe^2}{h}\times\frac{1}{n}}$$

In the case of the hydrogen atom H (Z=1)and when n=1 (the speed of the electron in the first Bohr orbit), we find:

$$v_1 = \frac{2\pi K e^2}{h} = \frac{2\times(3{,}14)\times 9.10^9\times(1{,}6.10^{-19})^2}{6{,}62.10^{-34}} = 2.18.10^6 \text{ m/s}$$

$$\Rightarrow \quad v_n = v_1 \times \frac{Z}{n}$$

v_n: the velocity of the electron in the orbit n

f) Defining the total energy term for the electron in the orbit n

The total energy En for the electron in orbit (n) equals the sum of kinetic energy and potential energy, meaning the total energy equation looks like:

$$E_T = E_C + E_P$$

$$E_P = \int_r^{\infty} F_C dr = \int_r^{\infty} \frac{KZe^2}{r^2} dr = KZe^2 \int \frac{dr}{r^2}$$

$$\Rightarrow E_P = KZe^2\left[\frac{1}{r}\right] = KZe^2\left[\frac{1}{\infty} - \frac{1}{r}\right]_r^{\infty} = -\frac{KZe^2}{r}$$

$$-\frac{KZe^2}{r} \quad \Rightarrow E_T = E_C + E_P = \frac{KZe^2}{2r} = -\frac{1}{2}\frac{KZe^2}{r}$$

By substituting the term r in the relationship E_T we find:

$$E_T = -\frac{KZe^2 4\pi^2 m_e e^2 KZ}{2\,h^2 n^2}$$

$$\Rightarrow E_T = -\frac{2K^2Z^2e^4\pi^2 m_e}{h^2n^2}$$

Exemple

In the case of the hydrogen atom and in orbit 1 and Z=1 (the energy of the electron in the first orbit of the hydrogen atom, representing the binding energy):

E_{1H} = - 13.58 eV

$$E_n = \frac{E_{1H}\times Z^2}{n^2}$$

Thus, we can write the allowed energy levels for the hydrogen atom with the following relationship:

$$E_n = -E1,\ -E1/4, \ldots\ldots$$

Remarque

By using the third hypothesis, we can calculate the energies and frequencies of potential transitions. If an electron in the initial state with energy level E_{n1} transitions to a final state with energy level E_{n2}, the emitted photon energy is given by the following relationship:

$$\Delta E = E_{n2} - E_{n1} = h.\,\partial = h.c/\lambda = h.c.\bar{\partial}$$

We have:

$$E_{n1} = -\frac{2K^2Z^2e^4\pi^2m_e}{h^2} \times \frac{1}{n_1^2}$$

$$E_{n2} = -\frac{2K^2Z^2e^4\pi^2m_e}{h^2} \times \frac{1}{n_2^2}$$

$$\Rightarrow \Delta E = E_{n2} - E_{n1} = -\frac{2K^2Z^2e^4\pi^2m_e}{h^2} \times \left(\frac{1}{n_2^2 - n_1^2}\right)$$

$$\Rightarrow \bar{\partial} = -\frac{2K^2Z^2e^4\pi^2m_e}{c.h^3} \times \left(\frac{1}{n_2^2} - \frac{1}{n_1^2}\right)$$

In accordance with the Balmer relationship, we find:

$$\bar{\partial} = Z^2 R_H\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

$$R_H = \frac{2\pi^2K^2m_ee^4}{c\,h^3} = \frac{2\times(3,14)^2(9\times10^9)^2\times(9.1.10^{-31})\times(1,6.10^{-19})^4}{(3.10^8)\times(6,62.10^{-31})^3}$$

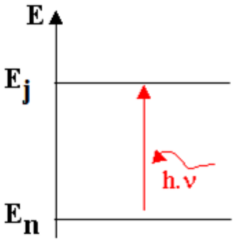
$$\Rightarrow \qquad R_H = 1.0974 \times 10^7\ m^{-1}$$

While the experimental value is equal to:

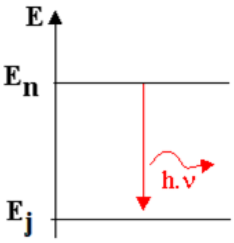
R_{exp} = (109677.576 + 0,012) cm^{-1}

2. Interpretation of the absorption and emission spectrum of hydrogen and its like

Bohr, in his theory, was able to provide an explanation for the lines seen in the hydrogen spectrum. The radiant energy absorbed by the atom causes the electron to move from a lower energy level (small value of n) to a higher energy level (large value of n), and then the radiant energy is emitted (in the form of photons) when the electron returns back to the ground level. The movement of the electron from one level to another is like a tennis ball moving up or down the stairs, where the ball moves from one step to another but never stays in between levels.



absorption spectrum



emission spectrum

We get the emission or absorption spectrum when the electron moves from an orbit of rank **n_i** to an orbit of rank **n_j** where **i>j**, meaning the electron goes from a high energy orbit to a lower energy orbit, emitting a quantum of energy or a photon of light as shown in the figure .

The energy difference between the orbits is represented by ΔE, allowing us to know the emitted radiation as follows: Emission Spectrum:

$$\text{Emission spectrum}: \Delta E = \left| E_{n_j} - E_{n_i} \right|$$

We get absorption spectrum when a hydrogen atom or hydrogen-like ion absorbs energy in the form of radiation, causing the electron to move from energy level **n_i** to energy level **n_j**, where **$j>i$**. The frequency of absorbed radiation can be calculated using the following relationship:

$$\text{Adsorbsion spectrum}: \Delta E = \left| E_{n_j} - E_{n_i} \right|$$

Exemple

What is the energy absorbed by a hydrogen atom corresponding to the first line of the Lyman series and what is the wavelength of the absorbed radiation?

Solution:

$n_1 = 1$, $n_2 = 2$

$$\Delta E = |E_2 - E_1| \quad , E_n = E_{1H} \times Z^2/n^2$$

$$E_1 = E_{1H} \times (1)^2/(1)^2 = E_{1H} \ , E_2 = E_{1H} \times (1)^2/(2)^2$$

$$\Delta E = |E_2 - E_1| = \left| E_{1H}\frac{1}{4} - E_{1H} \right| = \left| -\frac{3}{4}E_{1H} \right| = \frac{3}{4}(13{,}54) \approx 10{,}2024 \text{ eV}$$

Calculating the wavelength:

$$\Delta E = h \times \partial = h.c/\lambda = \frac{6{,}62.10^{-34} \times 3.10^{8}}{10{,}20 \times 1{,}6.10^{-19}} 1216{,}9\, A^o \approx 1{,}2169.10^{-7} \text{ m}$$

3. Basic condition and the excited state - Ionization Energy

The relationship of the radius $r_n = r_1 \times \dfrac{n^2}{Z}$ shows the increasing values of the radii halves with the increase of n, as well as the total energy.

$$r_1 > r_2 > r_3 \ldots . > r_\infty$$

$$E_1 > E_2 > E_3 \ldots . > E_\infty$$

With Z > 1 in state of hydrogen-like ions

- **Standard state:**

  The electron in a hydrogen atom and hydrogen-like atoms, in the absence of any external force, occupies the most stable orbit corresponding to the smallest energy value, which is the orbit characterized by **n=1**. We can say that the atom is in its basic state.

- **Excited state (unstable state):**

  When an electron absorbs energy **$\Delta E = h\partial$** and jumps to an orbit with higher energy than the initial orbit, we say that the atom is excited, meaning unstable.

  -Transition to orbit 2 corresponds to the first excited state

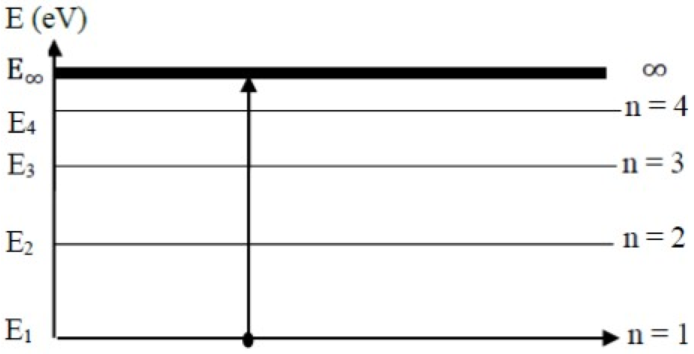
  -Transition to orbit 3 corresponds to the second excited state... and so on.

- **Ionization Energy:**
  It is the energy required to remove the electron from orbit **n** to infinity, denoted by **E_i** (ionization).

$$\Delta E_i = E_\infty - E_i = -E_i$$

$$\Delta E_i = -E_{1H} \times Z^2/n^2$$

The ionization energy of a hydrogen atom in the ground state is: **ΔE_i = 13.54 eV**



4. Bohr's Theory Shortcomings

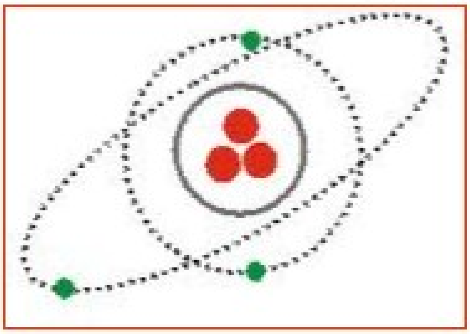
Bohr found weaknesses in the Bohr model, such as:

- Bohr interpreted that the electron transition from one level to another, for example from n=3 to n=2, gives a single spectral line, while spectroscopy shows that this spectral line consists of several closely spaced spectral lines, indicating the presence of multiple energy levels for each quantum number n.
- The difficulty of applying the Bohr model to multi-electron atoms because calculating the spectra of these atoms is very complex due to electron shielding.
- Assume that the electron orbits in specific orbits and in a single plane around the nucleus, which means that the hydrogen atom is flat, contradicting later proof that the atom is solid.
- Assume that the electron is a material particle and does not consider the wave nature of electrons.
- Assume that both the position and speed of the electron can be accurately determined at the same time, which is practically impossible because the measuring device used will change the position or speed.
- Bohr did not consider the possibility of the electron exceeding the fixed orbits he defined and the possibility of it being in an area around this fixed orbit.

D. Sommerfeld Atomic Model

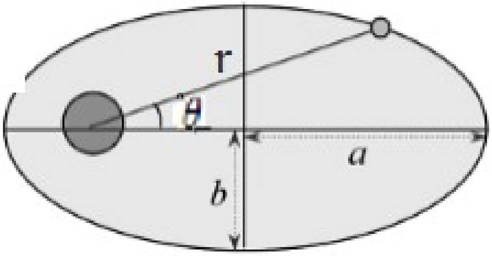
Introduction:

Bohr's theory had a great advantage in explaining the hydrogen atom and its semi-derivatives by using the concept of quantization while maintaining the laws of classical mechanics, but it failed to explain the spectra of other atoms. The first modifications to the Bohr model were made by Sommerfeld, who introduced additional quantization conditions, taking into account that spectral lines are split into several lines (with slightly different λ) if there is light emission in a magnetic field (the Zeeman effect). Based on that, a new shape is generated from the Bohr atom, which consists of spherical (closed) electronic orbits that can have noncentral non-circular (eccentric) sub-orbits, subject to an additional quantized number, which is the secondary quantum number **ℓ**.



Sommerfeld assumed that the electron's orbit around the nucleus is an ellipse, with the nucleus located at one of its foci, making Bohr's circular orbits a special case.

Therefore, the location of the electron is determined by the distance between the nucleus and the electron r and the angular angle θ, and they are constantly changing during the electron's movement.

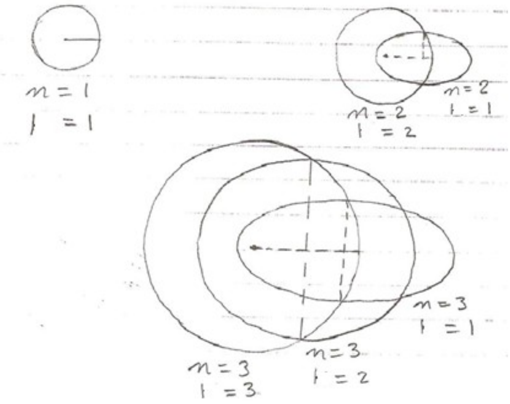


$$\oint P_r dr = n_r \hbar$$

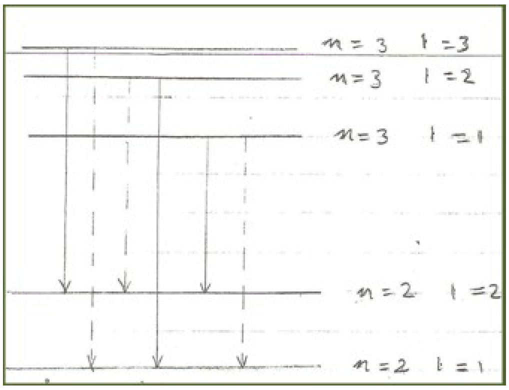
$$\oint P_\theta dr = n_\theta \hbar$$

Where n_r: the semi-quadratic quantum number and the axial quantum number. Solving these equations shows that the half-length of the major axis a of the ellipse is determined by the principal quantum number n, while the length of the minor axis b depends on the secondary quantum number **ℓ**, where: **1 ≥ ℓ ≥ 0** (an integer)

$$\frac{a}{b} = \frac{n}{l+1}$$



When an electron moves from an energy level with quantum number n=3 to a lower energy level with n=2, there will be 3 resulting spectral lines.



So, the principal quantum number n alone is not enough to distinguish this pattern, which is why we consider other quantum numbers.

Remarque

In the Bohr model, the angular angle θ changes, while the distance r is constant

1. principal quantum number n

Is the sum of the azimuthal quantum number and the magnetic quantum number. Therefore, when n=1, then: And also when n=2, then: , , for circular orbit

$$n = n_r + n_\theta$$

$$n = 1, 2, 3, \ldots\ldots$$

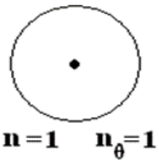
$$n_r = 0, 1, 2, \ldots\ldots$$

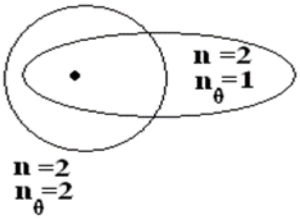
$$n_\theta = 1, 2, 3, \ldots\ldots.$$

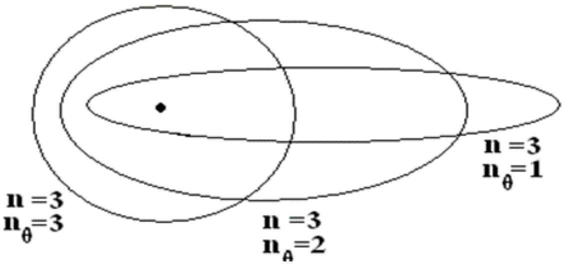
Therefore, when :n=1 ⇒ $n_r = 0$ and $n_\theta = 1$

And also when : n=2 ⇒ $n_r = 1$, $n_\theta = 1$ for elliptical orbit
$n_r = 0$ $n_\theta = 2$ for circular orbit

And when n=3, there are three possible orbits for the electron.







2. Secondary quantum number ℓ

Is used to determine sublevels of energy in each principal energy level, and it determines their number. Sublevels are the real levels in the atom where:

-In the case of circular orbit where a = b, we have

$$\frac{a}{b} = \frac{n}{\ell + 1} \Rightarrow n = \ell + 1$$

=> ℓ = n – 1, which is the maximum value for the secondary quantum number and corresponds to circular orbit

As for the lowest value, it corresponds to the 1s state: 1s : ℓ=0

$$\Rightarrow \quad 0 \leq \ell \leq n\text{-}1$$

-Each principal energy level contains a number of sublevels equal to n.

-The sublevel symbols are **s, p, d, f.**

- Scientist "Sommerfeld" discovered sublevels when he found that a single spectral line consists of several sublines by using a more accurate spectroscope than the Bohr spectroscope.

-The **first level K** consists of one sublevel which is 1s.

-The **second level L** consists of two sublevels which are 2s and 2p.

-The **third level M** consists of three sublevels which are 3s, 3p, 3d.

-The **fourth level N** consists of four sublevels which are 4s, 4p, 4d, 4f.

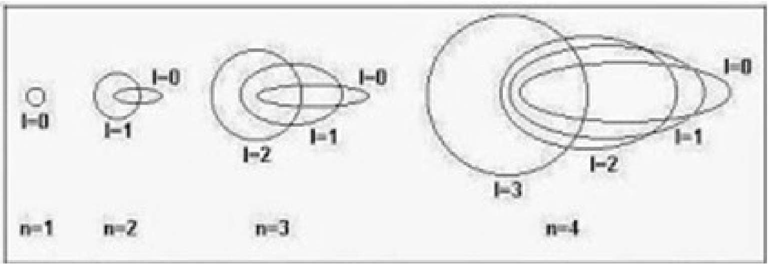
And so on for the fifth, sixth, and seventh levels, similar to the fourth level. Where :

$$\ell = 0 \Rightarrow \text{s (orbit)}$$

$$\ell = 1 \Rightarrow \text{p (orbit)}$$

$$\ell = 2 \Rightarrow \text{d (orbit)}$$

$$\ell = 3 \Rightarrow \text{f (orbit)}$$



Exemple

Let the main quanta number of the layer be 3. What are the corresponding sublayers for this layer?

Solution:

ℓ= {0,1,2}

When :

ℓ=0 ⇒ Under the layers (the most flat sp shape)

ℓ=1⇒ Under the layerp (the less flat shape)

ℓ=2⇒ Under the layerd (the shape takes a circular form)

Sommerfeld model found limited success:

- Did not predict the correct number of lines for the exact structure of the spectral line
- Did not provide any information on the relative intensities of the spectral lines
- Did not shed light on how electrons are distributed in the atom
- Could not explain some experimental results such as the Zeeman effect and the Stark effect

E. Magnetic quantum number m_ℓ (Zeeman effect)

Zeeman effect is a phenomenon of the splitting of spectral lines from a source under the influence of a constant magnetic field into several lines (separation of spectral lines, i.e., photons imply separation in energy levels in the presence of a magnetic field). For example, if we have an atom with an emission spectrum wavelength of 400 nm, when exposed to an external magnetic field, we observe a splitting in the spectral lines, meaning the appearance of an additional line on the sides of the original line with the value of 399 nm and 401 nm.

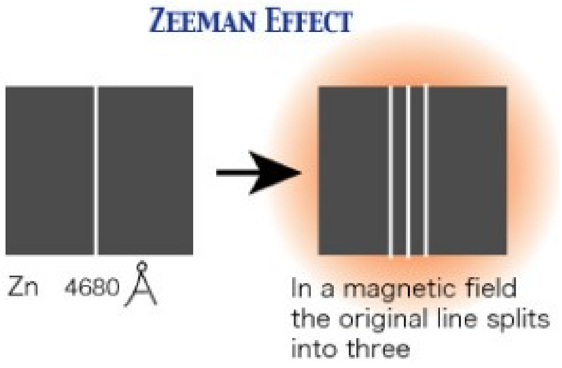
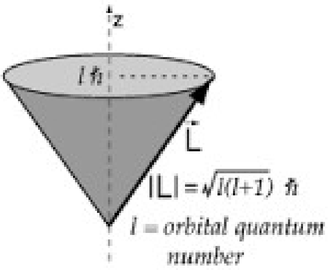


Figure 1. Splitting of the zinc 4680Å line in a magnetic field due to the Zeeman effect.

The following figure represents the rotation of the electron around the nucleus, where the loop represents the path of the electron around the nucleus (L), and the axis represents the angular momentum direction of the electron's orbit around the nucleus.

The axis of rotation is vertical if the level of rotation of the ring is parallel to the surface of the earth. But if the axis makes an angle with the vertical to the surface, then the axis will rotate around the vertical to the surface in a path shaped like a cone



According to the theory of quantization, the orbital angular momentum of the electron is allowed to take specific angles only, meaning it's constrained in space. L represents the direction of the orbital angular momentum, and is calculated based on the equation:

$$L = \sqrt{\ell(\ell+1)\hbar}$$

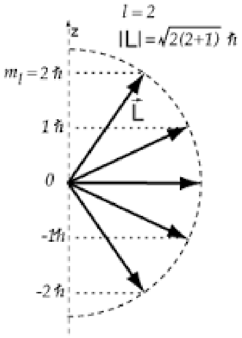
The secondary quantum number is denoted as ℓ,

The magnetic quantum number is denoted as mℓ ,which determines the direction of angular momentum relative to an imaginary axis LZ, and is given by the relationship :

$L_z = m_\ell \hbar$

For values of mℓ, if ℓ = 1 then mℓ can be 1, 0, or -1; and if ℓ = 2 then mℓ can be +2, +1, 0, -1, or -2.

The range for **m_ℓ** values is **+ℓ to -ℓ : + ℓ ≥ mℓ ≥ -ℓ**, indicating the angular momentum direction is confined depending on the quantum number.



When a charged object moves in a circular orbit (like an electron), it generates an orbital magnetic moment μ that is inverse to the orbital angular momentum L, given by the formula **$\mu_{orbital}$**

$$\mu_{orbital} = \frac{-e}{2m_e} L$$

The energy gained by the electron from the magnetic field to change its direction is calculated using :

$$U(\theta) = -\mu \cdot B$$

which leads to :

$$U=\frac{e}{2m}L_zB = m_\ell\frac{e\hbar}{2m}B$$

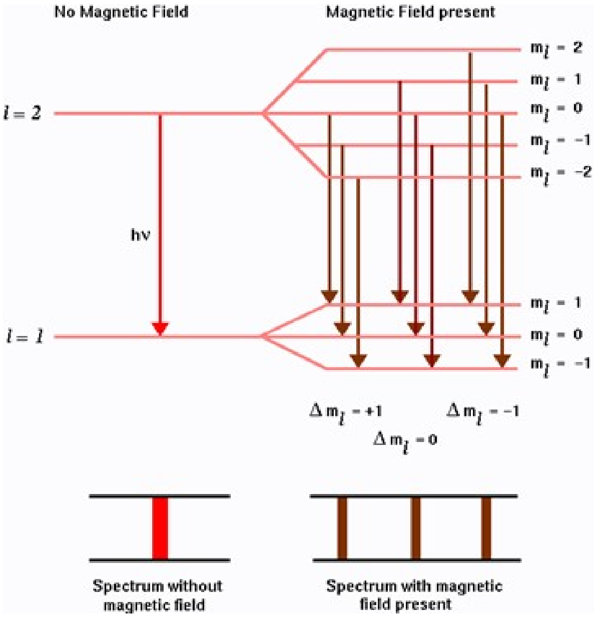
This shows an increase in energy for each specific level characterized by the magnetic quantum number **m_ℓ**.

By substituting constants into the equation, we find :

$$\Delta E = m_\ell\frac{e\hbar}{2m}B = m_\ell\,\mu_B\,B$$

where **μ_B** represents the Bohr magneton.

This indicates that when an atom is exposed to a magnetic field, its energy levels separate from each other based on the magnetic quantum number **m_ℓ** and magnetic field, resulting in emitted spectral lines dependent on **m_ℓ**. This was experimentally proven by Zeeman, showing a separation in spectral lines when atoms are subjected to a magnetic field.



Remarque

The rule governing the transfer of electrons between energy levels is:

$$\Delta\ell=\pm1, \neq 0$$

$$\Delta m_\ell=0, \pm1$$

Exemple

For **n = 1**: $\ell = 0$; $m_\ell = 0$ → 1s

For **n = 2**:

a) $\ell = 0$; $m_\ell = 0$ → 2s

b) $\ell = 1$; $m_\ell = \{-1, 0; +1\}$ → 2p

For **n = 3**:

a) $\ell = 0$; $m_\ell = 0$ → 3s

b) $\ell = 1$; $m_\ell = \{-1, 0, +1\}$ → 3p

c) $\ell = 2$; $m_\ell = \{-2, -1, 0, +1, +2\}$ → 3d

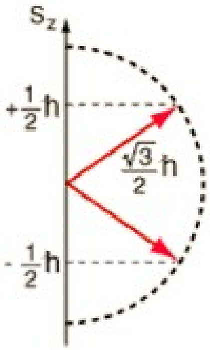
For **n = 4**:

a) $\ell = 0$; $m_\ell = 0$ → 4s

b) $\ell = 1$; $m_\ell = \{-1, 0, +1\} \rightarrow 4p$
c) $\ell = 2$; $m_\ell = \{-2, -1, 0, +1, +2\} \rightarrow 4d$
d) $\ell = 3$; $m_\ell = \{-3, -2, -1, 0, +1, +2, +3\} \rightarrow 4f$

F. Quantum number of the electron spin or self-spin m_S (Stern and Gerlach experiment)

In this experiment, scientists observed that when a sample of silver is exposed to a magnetic field, there is a doubling of the silver atom beams in two equal values. One set of silver atoms above the Z-axis direction positive and another set below the Z-axis direction negative.

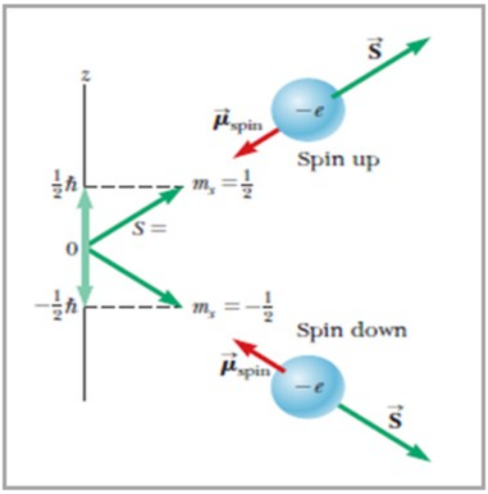


The reason for this separation in the groups is due to an additional motion that was not taken into account, and by calculating the magnetic torque field responsible for displacing hydrogen atoms, it was found that this magnetic torque is much greater than the magnetic torque resulting from the electron motion around the nucleus (the electron can be imagined as a charge spinning around its axis in addition to the orbital motion of the electron orbit) and therefore the responsible for displacement is another and greater magnetic torque value from the orbital magnetic torque. This torque was the spin magnetic torque resulting from the electron motion around itself (spin motion). There are two cases for this motion either clockwise or counterclockwise and this is why two sets of atoms were obtained on the experiment slide. It was found that the spin angular momentum valueS can be calculated with the following equation

$$S = \sqrt{s(s+1)}\hbar$$

The direction of the spin angular momentum in the Z-axis direction is quantified by **m_s**, which is called the spin quantum number or self-spin, **hence the angular momentum of the electron ms takes two directions +1/2 and -1/2 based on the electron spin direction**:

$$S_Z = m_s\hbar = \pm\frac{1}{2}\hbar$$



The magnetic spin of the electron is given by the equation :

$$S = \sqrt{\frac{1}{2}\left(\frac{1}{2}+1\right)}\,\hbar = \frac{\sqrt{3}}{2}\hbar$$

And it is responsible for the results of the Stern Gerlach experiment.

Through this experiment, it was observed that it proved an important concept, the correctness of the quantization principle, however, the results also confirm that there is a missing link and that there is a fundamental motion that was not predicted, which is the electron spin around itself.

Chaptre five : Wave mechanics

V

Bohr's theory, despite its importance, has remained unable to explain the structure of multi-electron atoms. That's why a more comprehensive theory was introduced, relying on new concepts for the wave properties of matter. The movement of electrons cannot be determined by specific orbits, but rather complex movements that can be explained by combining the wave properties of electrons and calculating the probabilities of their presence in these orbits

A. Wave-particle duality

Previous experimental phenomena and results have shown without a doubt that electromagnetic radiation (light) has wave-like properties in some experiments and particle-like properties in others. The scientist Planck assumed in 1900 that light is a quantum phenomenon. This means that electromagnetic radiation consists of light particles called photons, each carrying a bundle of energy represented by a body called a quantum. For radiation with a frequency **∂**(sec^{-1}), the energy of a single quantum is given by the relationship:

$$E = h.\partial \ (Joule)$$

Where : **h** represents Planck's constant and its value in the international system is 6.625×10^{-34} J.S , And the energy of the photon derived from Einstein's theory of relativity is given by the relationship:

$$E = m.c^2$$

Where **E** is the energy of the quantum or the photon, **m** is the mass of the photon, and **c** is the velocity of light. Combining these two relationships leads to obtaining the following relationship:

$$h.\partial = \mathrm{m.c}^2 = \frac{hc}{\lambda} \quad => \quad \lambda = \frac{\boldsymbol{h}}{\boldsymbol{mc}}$$

This statement clearly expresses the duality of matter and wave.

B. De Broglie hypothesis

De Broglie assumed that material bodies have a dual property, meaning that matter with mass can have wave-like properties under certain conditions in addition to being a particle. Therefore, De Broglie generalized the previous statement to every particle with relative mass m and moving at speed v, characterized by a wavelength λ:

$$\lambda = \frac{h}{mv} = \frac{h}{P}$$

λ: Wave nature

P : Momentum or amount of motion: Particle nature

If an electron is subjected to acceleration resulting from a potential difference U, the accompanying wave is:

$$E_c = \frac{1}{2}mv^2 = eU \Rightarrow m^2v^2 = 2mU \Rightarrow mv = \sqrt{2m_eU} = P$$

$$\lambda = \frac{1}{2}mv^2 \Rightarrow \boldsymbol{\lambda} = \frac{\boldsymbol{h}}{\sqrt{\boldsymbol{2m_eU}}}$$

Exemple

Calculation of the wavelength associated with:

An electron with a kinetic energy of 54 eV:

Using the De Broglie relation: λ = h / mv with kinetic energy

$$E_{kinetic} = \frac{mv^2}{2} \Rightarrow \lambda = \mathrm{h}/(2m.Ec)^{1/2}$$

$$\mathrm{N.A:}\ \lambda = 6.62 \times 10^{-34}/[2 \times (9.109 \times 10^{-31}).(54 \times 1.6 \times 10^{-19}]^{1/2} = \mathbf{0.1668} \times \mathbf{10^9}\boldsymbol{m} = \mathbf{1.67°}\boldsymbol{A}$$

C. Heisenberg's principle of uncertainty (skepticism)

The principle of uncertainty (skepticism) by Heisenberg states that it is impossible to measure two physical properties of an object at the same time with greater accuracy than Planck's constant h. For example, if we want to measure the position and momentum of an electron at the same time, there must be an error in measuring one of them because the measurement used for one of these properties must disturb the system, leading to an error in measuring the other property. This can be explained as follows:

The photon used to determine the electron's position must be a high-energy photon with a small wavelength, which, according to the Compton effect, can change the electron's position and momentum (**p=mv**) when it collides with the electron to determine its position, thus increasing the uncertainty in its momentum. At the same time, if a long-wavelength photon is used to determine its momentum, this wavelength cannot determine the electron's position, leading to an increase in uncertainty in the position because

$\Delta x = \lambda$. The essence of what Heisenberg assumed is represented by the following equation:

$$\Delta p \times \Delta x \geq \hbar$$

Where : $\hbar = h/2\pi$, Δx represents the error in position, and $\Delta p = m\times \Delta v$ represents the error in momentum.

Exemple

Calculate the absolute uncertainty on the speed of the electron moving at a speed v=2200m/s and the uncertainty on the position is ±2A° , We have :

$$\Delta p \times \Delta x \geq \hbar \Rightarrow m_e \Delta v \times \Delta x \geq \hbar$$

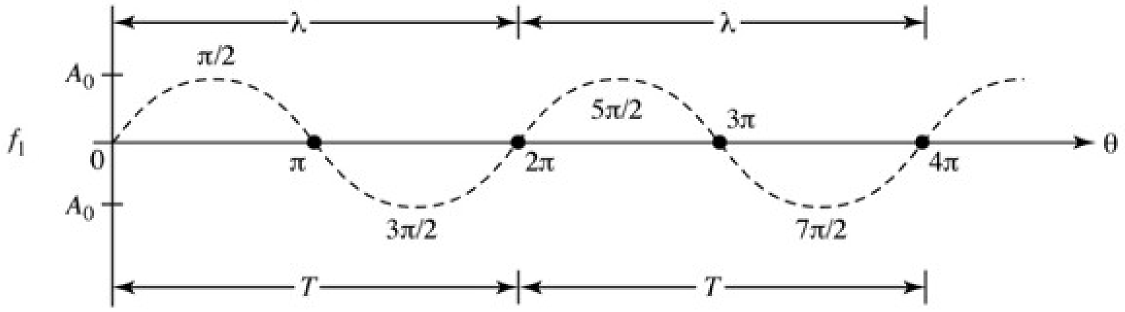
$$\Rightarrow \quad \Delta v = \frac{\hbar}{m_e \Delta x} = \frac{6{,}62\ .\ 10^{-34}}{9{,}1\ .10^{-31} \times 2\ .10^{-10}} = 3637.10^{3} m/s$$

$$\Delta v_{electron} = |2200 \pm 3637.10^{3}|\, m/s$$

This result is rejected because it does not comply with Heisenberg's uncertainty principle, leading us to search for a new idea to determine the probability of the electron's position around the nucleus, thus replacing classical mechanics with wave mechanics.

D. Wave propagation equation in one direction x

1. Oscillatory motion equation



$$\phi(x,t) = a \sin 2\pi\left(\partial t - \frac{x}{\lambda}\right)$$

Where φ represents the wave function that depends on the position x and time t; λ is the wavelength; ∂ represents the frequency and λ is the wavelength.

We calculate the partial derivatives (1) and (2) with respect to the position x

$$\frac{d\Phi}{dx} = -\frac{2\pi a}{\lambda} cos2\pi\left(\text{vt} - \frac{x}{\lambda}\right)$$

$$\Phi''(\text{x}) = \frac{d^2\Phi}{dx^2} = -\left(\frac{2\pi}{\lambda}\right)^2 a\ cos2\pi\left(\text{vt} - \frac{x}{\lambda}\right)\ldots\ldots\ldots\ldots\ldots..(1)$$

We calculate the partial derivatives (1) and (2) with respect to the time t

$$\frac{d\Phi}{dt} = 2\pi\text{va}\ cos2\pi\left(\text{vt} - \frac{x}{\lambda}\right)$$

$$\Phi''(\text{t}) = \frac{d^2\Phi}{dt^2} = -(2\pi v)^2 sin\ 2\pi\left(\text{vt} - \frac{x}{\lambda}\right)\ldots\ldots\ldots\ldots\ldots..(2)$$

By dividing (1) by (2) we find:

$$\frac{\frac{d^2\Phi}{dx^2}}{\frac{d^2\Phi}{dt^2}} = \frac{-\left(\frac{2\pi}{\lambda}\right)^2 a}{-\left(\frac{2\pi}{\lambda}\right)^2 a} = \frac{1}{(\lambda v)^2}$$

If the oscillatory motion is optical (electromagnetic), it is in the form **c = vλ** so we get:

$$\frac{d^2\Phi}{dx^2} = \frac{1}{c^2} \times \frac{d^2\Phi}{dt^2}$$

E. Schrodinger equation

We have the equation :

$$\Psi = \text{a}\sin(2\pi\ \lambda)\text{x}$$

Where: **Ψ** represents the wave function at a fixed time (wave function capacity change function); **λ** is the wavelength and **x** represents the segment of the axis along which the wave is spreading.

$$\frac{d\Psi}{\text{dx}} = \frac{2\pi\text{a}}{\lambda}\cos\left(\frac{2\pi}{\lambda}\right)\text{x}$$

$$\frac{d^2\Psi}{\text{dx}^2} = -\frac{4\pi^2\text{a}}{\lambda^2}\sin\left(\frac{2\pi}{\lambda}\right)\text{x}$$

$$\Rightarrow \qquad \frac{d^2\Psi}{\text{dx}^2} + \left(\frac{4\pi^2}{\lambda^2}\right)\Psi = 0$$

From De Broglie's equation:

$$\lambda^2 = \frac{h^2}{(mv)^2}$$

The total energy relationship is written as follows:

$$\text{E} = \text{T} + \text{U} \Rightarrow \text{T} = \text{E} - \text{U} = \frac{1}{2}mv^2$$

From the previous relationship and substitution, we get:

$$\lambda^2 = \frac{h^2}{m^2v^2} = \frac{h^2}{2m(\frac{1}{2}mv^2)} = \frac{h^2}{2mT} = \frac{h^2}{2m(E-U)}$$

By substitution into the previous differential equation we find:

$$\frac{d^2\Psi}{dx^2} + \frac{8\pi^2 m(E-U)}{h^2}\Psi = 0$$

$$\Rightarrow \quad \frac{d^2\Psi}{dx^2} + \frac{8\pi^2 m}{h^2}\Psi(E-U) = 0$$

This is the general Schrödinger equation

By generalizing the equation in space:

$$\frac{d^2\Psi}{dx^2} + \frac{d^2\Psi}{dy^2} + \frac{d^2\Psi}{dz^2} + \frac{8\pi^2 m}{h^2}\Psi(E-U) = 0$$

We put:

$$\frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2} = \nabla^2(\text{Laplacien})$$

We substitute in the previous equation:

$$\boldsymbol{\nabla^2\Psi + \frac{8\pi^2 m}{h^2}(E-U)\Psi = 0}$$

The Schrödinger equation represents the fundamental principle in wave mechanics, meaning that everything we experimentally observe regarding a particle must satisfy this equation.

1. Another form of the Schrödinger equation

We have:

$$\nabla^2\Psi + \frac{8\pi^2 m}{h^2}(E-U)\Psi = 0$$

$$\Rightarrow \quad \nabla^2\Psi + \frac{8\pi^2 m}{h^2}E\Psi - \frac{8\pi^2 m}{h^2}U\Psi = 0$$

$$\Rightarrow \quad \nabla^2\Psi + \frac{8\pi^2 m}{h^2}E\Psi = \frac{8\pi^2 m}{h^2}U$$

$$\Rightarrow \quad \frac{8\pi^2 m}{h^2}E\Psi = \left(\frac{8\pi^2 m}{h^2}U - \nabla^2\right)\Psi$$

By division by $\frac{8\pi^2 m}{h^2}$:

$$E\Psi = \left(U - \frac{h^2}{8\pi^2 m}\nabla^2\right)\Psi$$

By setting:

$\mathrm{H} = \mathrm{U} - \frac{\mathrm{h}^2}{8\pi^2\mathrm{m}}\nabla^2$ and calling H the Hamiltonian operator

We get:

$$\mathrm{E}\Psi = \mathrm{H}\Psi$$

Which is the simplified Schrödinger equation.

In the case of one direction:

$$\mathrm{H} = \mathrm{U} - \frac{\mathrm{h}^2}{8\pi^2\mathrm{m}}\frac{\mathrm{d}^2}{dx^2}$$

To simplify at the beginning, we will try to deal with the equation in one direction only

$$\mathrm{E}\Psi(\mathrm{x}) = \left(\mathrm{U} - \frac{\mathrm{h}^2}{8\pi^2\mathrm{m}}\frac{\mathrm{d}^2}{dx^2}\right)\Psi(\mathrm{x})$$

This equation describes the total energy of a moving particle determined by its position **x**, and the value in the brackets can be understood as a factor affecting the wave function **Ψ**, resulting in a constant multiplied by the function itself. This equation is known as the Schrödinger equation in the form of the distinctive energy equation. The values of energy **E** at which the Schrödinger equation has acceptable solutions are called the distinctive or eigenvalues. Therefore, the Schrödinger equation determines the energy levels that an electron can occupy in a hydrogen atom, from which the corresponding wave function **Ψ** for each level is known. These energy levels are characterized by a set of quantum numbers from which we can construct a comprehensive model of the hydrogen atom. For example, an electron orbits a proton under the influence of Coulomb potential, and we want to know the shape of the orbit it follows and also the energy of the electron in each orbit. The energy may be discrete (separated), meaning there are specific values of energy allowed, known as eigenvalues, each of which corresponds to a specific eigenfunction.

2. Probability of finding the particle in the whole space

The function **Ψ** doesn't have any direct physical meaning, it just classifies the wave associated with the electron, but its square Ψ^2=Ψ 〚 ×Ψ 〛 ^* (*means the complex function's companion), indicating the probability of the electron's presence in a specific space around the nucleus. The electron cloud distribution (electron density) is given by :

$$\mathrm{dp} = |\Psi^2(x,t)|.\,\mathrm{dv} = \Psi(\mathrm{x,t})\Psi^*(\mathrm{x,t})\ .\mathrm{dv}$$

where ; **dp** represents the probability of the particle being within the volume **dv**. The areas with high electron cloud density are the most likely regions for electron presence, and vice versa.

$$\rho(x{,}t) = \frac{\mathrm{dp}}{\mathrm{dv}} = |\Psi^2(x,t)|$$

The probability of particle presence in the entire space, representing the sum of probabilities of the particle's presence in all contiguous volume elements around each other in the infinite space, can be at most (1=100%) written as:

$$\int_0^1 \mathrm{dp} = \int_{-\infty}^{+\infty} |\Psi^2(x,t)|.\,\mathrm{dv} = \int_{-\infty}^{+\infty} \Psi(\mathrm{x,t})\Psi\ (\mathrm{x,t})\ .\mathrm{dv} = 1$$

This is called the normalization condition.

The wave function that satisfies the normalization condition must:

- Be single-valued, meaning each specific position corresponds to a unique value of the wave function only, giving a probability of one for the particle's presence.

- Be continuous, as well as its derivatives, because if the function is not continuous (i.e., there is a break in the function somewhere), the particle becomes undefined in the region of the break.
- The function must be defined at every point and its values cannot be infinite because the probability of the particle's presence becomes infinite, which is not physically acceptable.

a) Probability of electron existence

The function $\psi^2 = r^2|R_{n\ell}(r)|^2$ tells us about the electron density (cloud) or the probability of finding an electron at a certain point in space P with coordinates (r , θ, φ). For example, for the **s¹** orbital:

The probability density of finding an electron at a significant distance from the nucleus between r and dr is: $P(r) = \left|\psi_{1,0,0}\right|^2 d\tau$

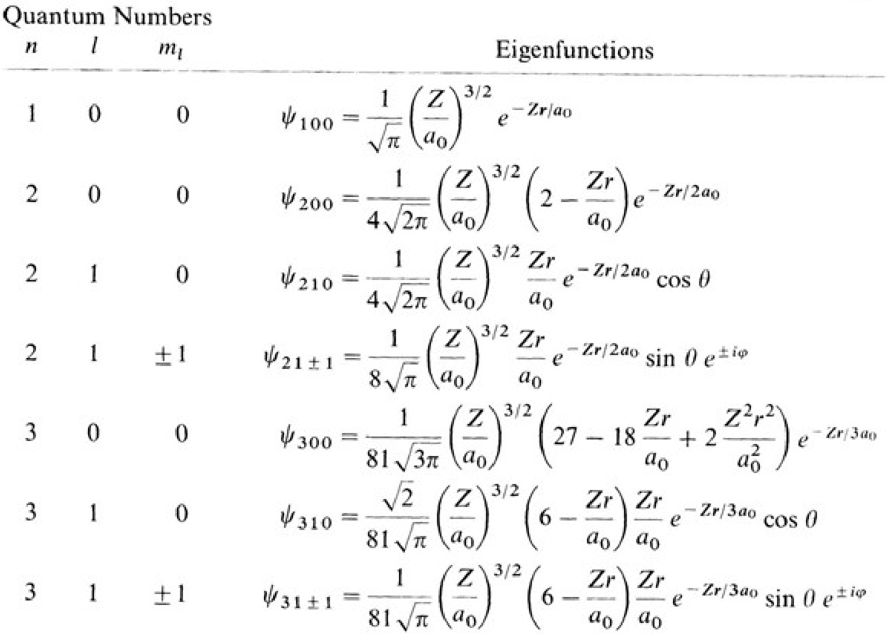
Where dτ is the volume of a circle with radius r and thickness **dr**:

$$d\tau = 4\,\pi^2 dr$$

Then :

$$P(r) = 4\,\pi^2 \left|\psi_{1,0,0}\right|^2$$

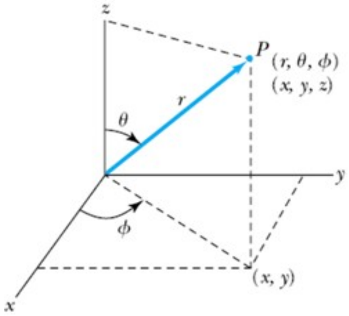
Among the solutions to the Schrödinger equation for the hydrogen atom and its analogues are:



Quantum Numbers			
n	l	m_l	Eigenfunctions
1	0	0	$\psi_{100} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$
2	0	0	$\psi_{200} = \frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\left(2-\frac{Zr}{a_0}\right) e^{-Zr/2a_0}$
2	1	0	$\psi_{210} = \frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{Zr}{a_0} e^{-Zr/2a_0}\cos\theta$
2	1	±1	$\psi_{21\pm1} = \frac{1}{8\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{Zr}{a_0} e^{-Zr/2a_0}\sin\theta\, e^{\pm i\varphi}$
3	0	0	$\psi_{300} = \frac{1}{81\sqrt{3\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\left(27-18\frac{Zr}{a_0}+2\frac{Z^2r^2}{a_0^2}\right) e^{-Zr/3a_0}$
3	1	0	$\psi_{310} = \frac{\sqrt{2}}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\left(6-\frac{Zr}{a_0}\right)\frac{Zr}{a_0} e^{-Zr/3a_0}\cos\theta$
3	1	±1	$\psi_{31\pm1} = \frac{1}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\left(6-\frac{Zr}{a_0}\right)\frac{Zr}{a_0} e^{-Zr/3a_0}\sin\theta\, e^{\pm i\varphi}$

Where: $a_0 = \frac{h^2}{4\pi^2 me^2} = 0{,}529A^0$ (It's the same as the Bohr radius)

3. Solving the Schrodinger equation for the hydrogen atom



$$x = r\sin\theta\cos\varphi$$
$$y = r\sin\theta\sin\varphi$$
$$z = r\cos\theta$$

where :

$$r \leq 0 \text{ and } r = \sqrt{x^2 + y^2 + z^2}$$
$$0 \leq \theta \leq \pi$$
$$0 \leq \varphi < 2\pi$$

The potential energy of the electron under the influence of the nucleus electric field:

$$U = -\frac{Ze^2}{4\pi\varepsilon_0 r^2}$$

and hence the Schrodinger equation becomes as follows:

$$\left(-\frac{Ze^2}{4\pi\varepsilon_0 r^2} - \frac{h^2}{8\pi^2 m}\nabla\right)\Psi(x,y,z) = E\Psi(x,y,z)$$

The problem we face when trying to solve the last equation is that we cannot separate the variables **x,y,z** from each other due to the presence of **r** in the potential energy, so we resort to transferring the issue from the Cartesian coordinates system with its variables **x,y,z** to the spherical coordinates system with its variables **r, θ, φ**. And we write the total function **Ψ**, which depends on the three variables **r, θ, φ** in the form of the product of three sub-functions, each of which depends only on one variable:

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

4. Special values of energy

Mathematical calculations showed that in order for the solutions to this equation (radial function) to be physically acceptable, the value of energy must be replaced by:

$$E_n = -\frac{13{,}6}{n^2}Z^2$$

Where n: the principal quantum number (must be an integer and positive, i.e., **n∈N**).

It is the same expression of energy that we obtained using the Bohr model, which is fundamentally based on energy quantization.

5. Special functions and quantum numbers

The special functions **ψ** or atomic orbitals are solutions to the Schrodinger equation, where for each value **n** corresponds to **n^2** a function or orbital. The special wave function Ψ is written in the form of the product of the function representing the radial part **$R_{n\ell}$ (r)** (only related to r) and the function **$Y_{\ell\, m}$(θ,φ)** representing the angular part (only related to **φ** and **θ**) as follows:

$$\Psi_{n\ell m}(r,\theta,\varphi) = \underbrace{R_{n\ell}(r)}_{\text{Radial part}}.\underbrace{Y_{\ell m}(\theta,\varphi)}_{\text{Angular part}}$$

It is characterized by the quantum numbers **n, ℓ, m**

n : is the principal quantum number and defines the electron shell, where : $n \in \mathbb{N}$

ℓ : is the secondary quantum number and defines the symmetry type of atomic orbitals (stations), where :

$$\ell \in [\![1-n;0]\!]$$

Exemple

ℓ = 0 →spherical symmetry

ℓ > 0 →axial symmetry

m_ℓ: The magnetic quantum number tells us about the orientation in space and its geometric shapes:

$$m_\ell \in [\![-\ell;+\ell]\!]$$

Fondamental

Conclusion :

We conclude that the solutions to the Schrödinger equation confirm all the results and conclusions reached by Bohr with the hydrogen atom, which can all be summarized into one equation, the Schrödinger equation

6. Atomic orbital (AO)

An orbital is a volume or a region of space near the nucleus, where the probability of finding the electron is very high (about 95%, for example). It depends on the wave function ψ of the electron determined by the Schrödinger equation using the orbital approximation

a) Spatial representation of atomic orbitals

It is impossible to represent the atomic orbital **Ψ** unless we separately represent the radial part of the function **R(r)** (which changes with **r**) and the angular part $\Theta(\theta).\Phi(\varphi)$ (which changes with **θ** and **φ**) that represents the area.

Since the function **Ψ** itself has no direct physical meaning but its square **Ψ^2** indicates the probability of finding the electron in a specific space surrounding the nucleus, it is important, for the study of its variations in space, to represent at each point $|\Psi^2|$ and in the same way the variations of both $R^2(r)$and $\Theta^2(\theta).\Phi^2(\varphi)$The area of the function is given by the relation:

$$\rho = R^2(r).\Theta^2(\theta).\Phi^2(\varphi)$$

At every point in this area, the probability density of finding an electron is the same, **ρ**.

The electron cloud decreases in density as we move away from the nucleus, and we can determine a specific volume of this cloud, for example, 95%, meaning that within this volume, there is a 95% chance of finding the electron. This volume represents the probability space of finding the electron, and the area of this volume is given by the equation:

$$r = f(\theta,\varphi)$$

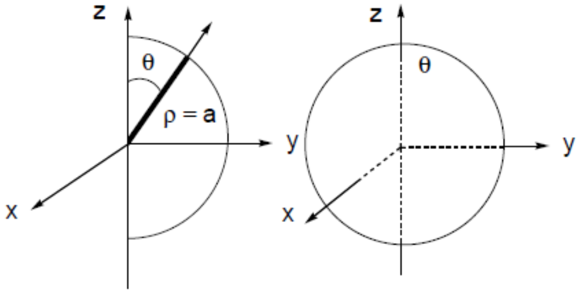
i representation of orbitals Ψ_{ns}

When it comes to the radial part **R(r)**, for each value of n corresponds to one orbit **Ψ_{ns} (ℓ=0)** or station n: the **Ψ** function **$Y_{\ell m}(\theta,\varphi)$** as the angular part.

the angular part **$Y_{\ell m}(\theta,\varphi)$** for ψ function remains constant and is given according to the results of solving the Schrödinger equation with the relationship :

$$Y_{\ell m}(\theta,\varphi) = \frac{1}{2\sqrt{\pi}} = a$$

If we plot a graph in the plane that includes the angle **φ (φ =п/2**, the plane yOz), we obtain a half circle for **п < θ < 0**. And in generalizing in space, this half circle transforms into a sphere with a radius of **a** as the angle φ changes from **0 to 2п** (spherical symmetry).



The function **s** takes the same positive value no matter which direction we change.

ii Representation of orbitals For the function Ψ_{np}

When **ℓ = 1**, there are three types of p orbitals, which consist of **2 lobes** that are symmetrical around the nucleus and are oriented along the corresponding axis. (**m = 1, 0, -1**) ⇒ **OA (Px, Py, and Pz** respectively for the x, y, and z-axes).

Let's consider the atomic orbital **Ψ_{np} (m=0)** , according to the solutions of Schrodinger equation, the angular part **$Y_{\ell m}(\theta,\varphi)$** of **Ψ** is written as:

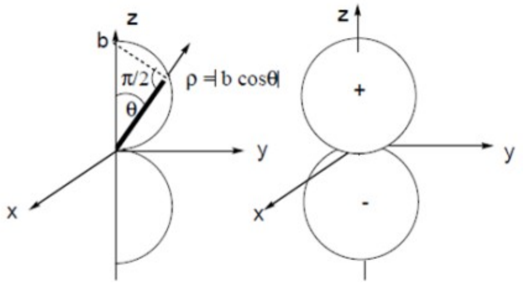
$$Y_{\ell m}(\theta,\varphi) = \left|\frac{\sqrt{3}}{2\sqrt{\pi}} cos\theta\right| = b|cos\theta|$$

Where : **b = 0,489**

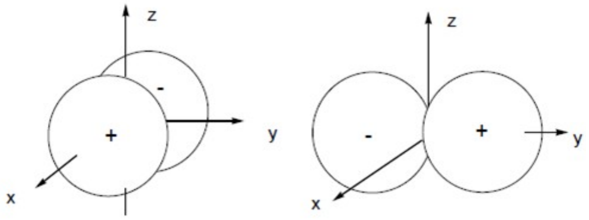
in the plane yoz, when the angle **θ** changes from **0 to п**, we get 02 half circles with b radius, So these two half circles become 02 spheres , in general in space when **θ** changes from 0 to 2п, and symmetrical with respect to the xoy plane, and are directed towards the axis z .

Thus, the angular component function Yℓm(θ,φ) becomes positive when θ changes from 0 to п/2 (half space), and negative when θ changes from п/2 to п.

The function **Ψ_{pz}** has the greatest absolute value in z, and disappears on the plane **xOy** at the point 0 (where the probability of the electron's existence in both directions is zero), at this plane the spheres directed along the axis z are opposite and symmetrical.



Similarly, we represent the other two functions Ψ_{py} and Ψ_{px}



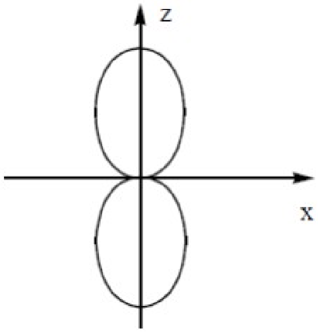
Since the square of the function Ψ only has a physical meaning (probability of electron presence) it is necessary to represent the angular part square curve $Y^2_{\ell m}(\theta,\varphi)$.

As for the oerbital s, there spherical form remains unchanged. And for the orbital **p** be:

$$\rho = Y_{\ell m}(\theta,\varphi) = \left|\frac{\sqrt{3}}{2\sqrt{\pi}} cos\theta\right|^2 = b^2|cos^2\theta|$$

And thus the shape of the two spheres becomes a geometric shape of two equal and symmetrical lobes because:

$b = 0,489 < 1$



7. Generalization of multi-electron atoms

In the case of an atomic system composed of q electrons in addition to the nucleus, the Schrödinger equation is written as:

$$E\Psi = H\Psi$$

Where :

$$H = -\frac{h^2}{8\pi^2 m_N}\nabla^2 - \sum_j \frac{h^2}{8\pi^2 m_e}\nabla_j{}^2 + U$$

The first part of the equation is neglected in front of the second part because the nucleus mass mN is much larger than the electron mass m_e.

The potential energy U is given by the relationship:

$U = \frac{KZe^2}{r}$

And from it, the Schrödinger equation is written in the case of multi-electron atoms, for example, the helium atom:

$$\nabla_1{}^2\Psi + \nabla_2{}^2\Psi + \frac{8\pi^2 m}{h^2}(E + \frac{K2e^2}{r_1} + \frac{K2e^2}{r_2} - \frac{K2e^2}{r_{12}})\Psi = 0$$

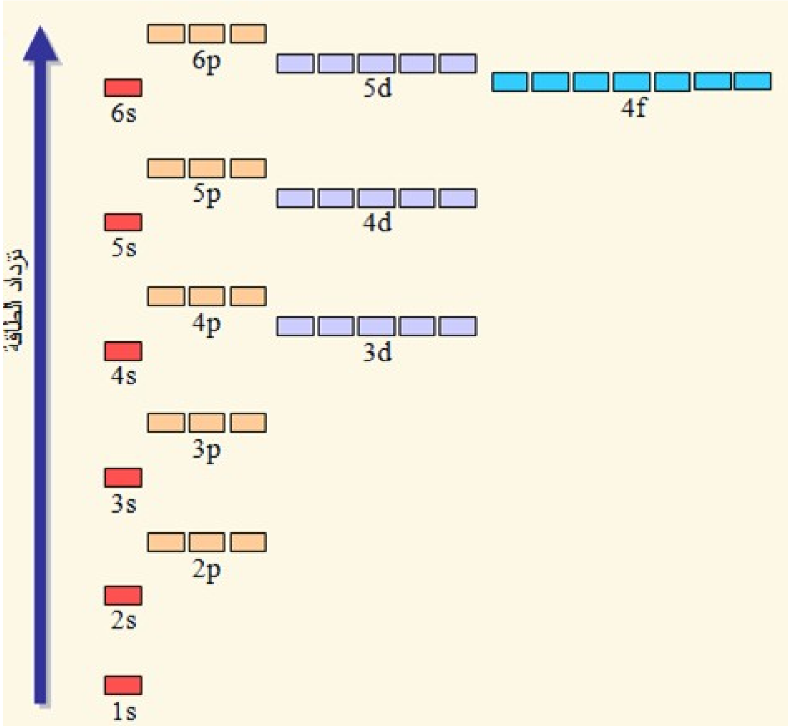
Where: r1 and r2 are the distances between electrons 1 and 2 from the nucleus, and r12 is the distance between the electrons. The difficulty in solving lies in the factor $\mathbf{r_{12}}$ because the relationship between the electrons is unknown, so in order to solve this complex equation, we resort to approximate methods

8. Solutions to the equation

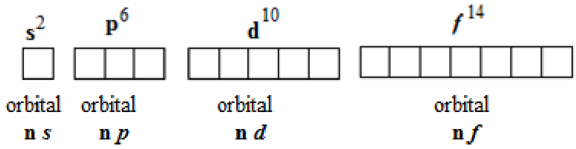
Special functions: Atomic orbitals in the case of multi-electron atoms retain the same characteristics as atomic orbitals in the case of hydrogen and its analogues.

Eigenvalues of energy: In the case of hydrogen and its analogues, the energy of atomic orbitals in a specific layer is equal because it is associated with the principal quantum number n

(E =f (n)), so we say that the energy levels are degenerate. However, in the case of multi-electron atoms, the energies of atomic orbitals in a specific layer do not have the same value because they change depending on the principal quantum number n and the secondary quantum number ℓ **(E =f (n, ℓ))**. Therefore, the arrangement of the energy levels of these orbitals follows the increasing order of **(n + ℓ)**.



Atomic orbitals in the case of multi-electron atoms are approximate solutions that allow placing electrons in quantized energy levels as shown in the figure.



Remarque

In the case of equal sum **(n+ ℓ)** for two level, the level with the smaller **n** must have the smaler energy .

It's notable, for example, that the energy below the level **3d** is higher than the energy below the level **4s**, despite the presence of 3d in the third main energy level and **4s** in the fourth main energy level. Therefore, the arrangement of sub-level occupation by electrons is not necessarily according to the quantum number system, but is arranged according to the actual progression in increasing their energies, so that the atom contains the least possible amount of energy, thus achieving the greatest possible stability and steadiness.

F. Principles governing the electronic structure of an atom

1. Definition of electronic configuration

Definition of electronic configuration:

The electronic configuration refers to how electrons are distributed among the various atomic orbitals, following specific rules known as filling rules.

Notations used for electronic configuration :

To express the electronic configuration of an element, two types of notations are used:

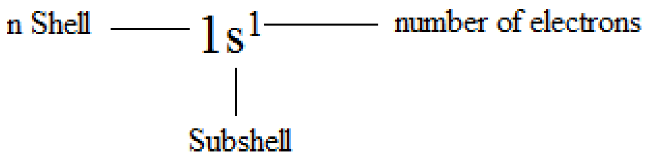
Quantum box notation: Here, the subshells are represented by boxes, also called quantum chambers, and an electron is depicted with an up arrow ↑ if it has a spin number of $s = +1/2$, and a down arrow ↓ if it has a spin number of $s = -1/2$. For the **s** orbital, there is **one box**. For the **p** orbital, there are **three boxes**. For the **d** orbital, there are **five boxes**. For the **f** orbital, there are **seven boxes**.

Values of ℓ and the corresponding quantum boxes:

The magnetic quantum number m defines the number of orientations in space that an electron can take when it's under the influence of a magnetic field. It characterizes the quantum boxe occupied by the electron. **$-l \le m \le +l$**:

m value	0	-1, 0, 1	-2, -1, 0, 1, 2	-3, -2, -1, 0, 1, 2, 3
boxes presentation	☐	☐☐☐	☐☐☐☐☐	☐☐☐☐☐☐☐

spdf notation: for hydrogen, which has only one electron, it is written as **$1s^1$**, which we read as one **s** one.



The electronic configuration of atoms is defined by 4 quantum numbers.

n: principal quantum number: It defines the shell. The energy of the electron depends on n.

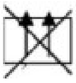
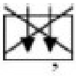
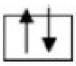
ℓ: secondary or azimuthal quantum number: it's an integer that ranges from 0 to n-1. It defines the subshells **s, p, d, f**. It determines the shape and symmetry of the orbitals (s, p, d, forbitals, etc.)

m_ℓ: magnetic quantum number: It takes values between -l and l (including the values of **-ℓ** and **+ℓ**). For a value of m, there are **(2ℓ+1)** values of m corresponding to it. It determines the orientation of the orbitals in space.

m_s: spin quantum number: The spin quantum number is defined as the angular momentum (or spin) of the electron. **s = -1/2** or **+1/2** (2 directions of rotation of the electron on itself).

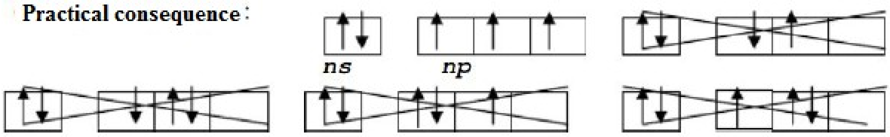
G. Rules for arranging orbitals

1. **Pauli Exclusion Principle:** This rule states that it is impossible for two electrons in the same atom to have the same sets of four quantum numbers. So if electrons in the first three quantum numbers agree, each must have a different spin from the other. In other words, each orbit must only be occupied by two electrons, provided that they have opposite spins (opposite in direction).

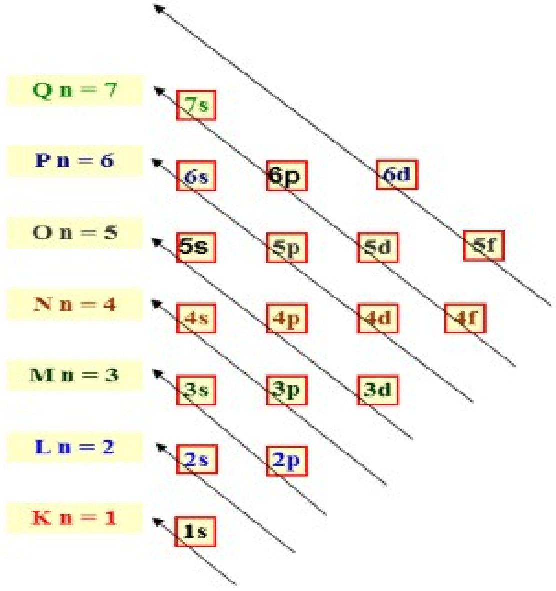




2. **Hund's Rule:**
This rule states that the most stable way to distribute electrons for the electrons occupying the same subshell is to occupy them parallelly first to achieve the maximum possible number of unpaired electrons and do not start pairing until there is no other option in front of them.
Based on the above, we can establish the following rules for how to distribute electrons in different subshells and atomic orbits. These rules are:
   - For each main shell with the value n, there are also n subshells, i.e., for shell **n = 2**, there are two subshells which are **2s** and **2p**.
   - Each subshell with value l contains a number of **(2ℓ + 1)** orbitals, for example, the p subshell contains 3 orbitals.
   - There cannot be more than two electrons in each atomic orbit and hence, the maximum number of electrons in each subshell is twice the number of its orbitals.
   - The maximum number of electrons in each main shell can be determined according to the relationship **$2n^2$**.

Practical consequence :



3. **Aufbau Principle (KLECHKOWSKI rule):**
Known as the building-up principle in German, it states that as the atomic number increases, the number of protons and electrons also rises, filling orbitals according to their increasing energy. The rule dictates that orbitals fill in order of increasing (n+l); for equal (n+ ℓ) values, they fill in order of increasing n and decreasing l. This results in the electron configuration of a multi-electron atom's ground state.



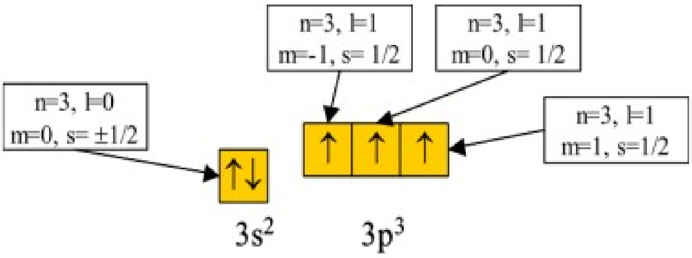
Exemple

What are the quantum numbers associated with the valence electrons of phosphorus and calcium?

Solution:

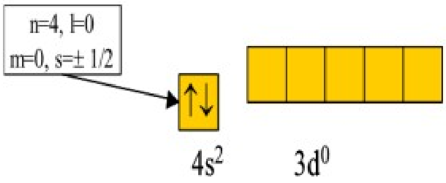
- **P: [Ne] $3s^2$ $3p^3$** 5 valence electrons

3p electrons are in 3 orbitals with different m values **(-1, 0, 1)**, with spins of the same sign. 3s electrons are in the same orbital with opposite spins



- **Ca : [Ar] $4s^2$**

4s electrons in the same orbital with opposite spins



H. Representation of electronic structure

1. Electronic distribution

It's a description of how electrons are distributed in the orbits of an atom or how atomic subshells are filled with electrons. The composition or electronic distribution refers to the way electrons are distributed in the orbits of the atom. The process involves gradually filling the subshells in each electron shell starting from the lowest energy. This is because in its stable state, an atom is in its lowest possible energy state. The nucleus is the center of the atom and electrons revolve around it in specific energy levels known as electron shells represented by the symbols f, d, p, s. These, in turn, are divided into subshells apart from the first shell, symbolized by s, p, d, f.

Exemple

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

$_{26}\text{Fe} : 1s^2\ 2s2\ 3p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^6$

Remarque

The electronic distribution can be abbreviated by replacing the filled secondary layers with the symbol of the noble gas that corresponds to it, preceding the studied element in the periodic table.

Exemple

$_{11}\text{Na} : 1s^2\ 2s^2\ 3p^6\ 3s^1 \equiv_{10} |\text{Ne}|\ 3s^1$

$_{26}\text{Fe} : 1s^2\ 2s^2\ 3p^6\ 3s^2\ 3p6\ 4s^2\ 3d^6 \equiv_{18} |\text{Ar}|\ 3d^6\ 4s^2$

a) Valence Electrons

These are the electrons that occupy subshells that come after the noble gas configuration in the electronic distribution of the studied element.

Exemple

$_{26}\text{Fe} : 1s^2\ 2s^2\ 3p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^6$

To become : $_{26}\text{Fe} : 1s^2\ 2s^2\ 3p^6\ 3s^2\ 3p^6\ 3d^6\ 4s^2$

Exemple

$_{14}\text{Si} : 1s^2\ 2s^2\ 3p^6\ 3s^2\ 3p^2 \equiv_{10}[\text{Ne}]\ 3s^2\ 3p^2$

Remarque

The valence electrons are the ones that determine the chemical properties of a specific element because they are involved in the formation of chemical bonds.

-The layers that include the valence electrons are called the outer electron structure. As for the electrons that occupy the filled layers, they form the electron configuration of noble gases with core electrons.

2. Electronic Configuration

Is the rearrangement of electronic distribution according to the increasing principal quantum number n.

Exemple

$_{26}\text{Fe} : 1s^2\ 2s^2\ 3p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^6$

To become : $_{26}\text{Fe} : 1s^2\ 2s^2\ 3p^6\ 3s^2\ 3p^6\ 3d^6\ 4s^2$

3. Electronic structure of ions

To find the electronic structure of ions with multiple electrons, we first write the electronic configuration of the atom, then we remove electrons from the outermost layers.

Exemple

${}_{20}Ca^{+2}$, ${}_{26}Fe^{+2}$, ${}_{26}Fe^{+3}$

${}_{20}Ca$: $1s^2\ 2s^2\ 3p^6\ 3s^2\ 3p^6\ 4s^2$

${}_{20}Ca^{+2}$: ${}_{18}$ [Ar]

becomes:

${}_{26}Fe$: $1s^2\ 2s^2\ 3p^6\ 3s^2\ 3p^6\ 3d^6\ 4s^2$

${}_{26}Fe^{2+}$: ${}_{18}$[Ar] $3d^6$

Chaptre six : Periodic table of elements

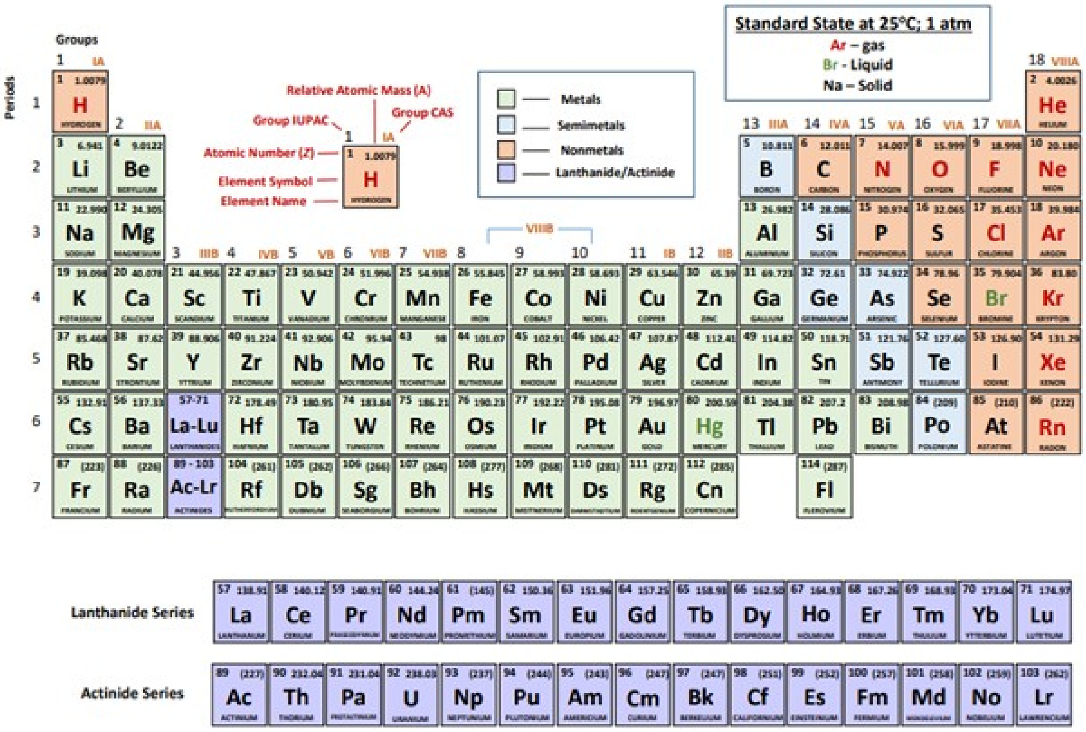
VI

A. History

In the 19th century, only about sixty elements were known. Chemists noticed that some elements had relatively similar chemical properties. These elements seemed to form fairly homogeneous families. For example, the halogen family (Fluorine, Chlorine, Bromine, and Iodine) or the alkali metals (Lithium, Sodium, and Potassium). So, the goal was to classify the elements in a way that would highlight these families. The periodic classification as we know it is largely thanks to MENDELEIEV. In 1870, he published a table where the elements were mostly arranged in order of atomic mass. Moreover, elements with similar properties were placed in the same column. To ensure his classification reflected the families, he didn't hesitate to swap the order of some elements and left some boxes empty. He believed that the missing elements would be discovered later. He even described the properties that these elements should have. Eventually, these elements were discovered, and they did indeed possess the predicted properties

B. Modern periodic table

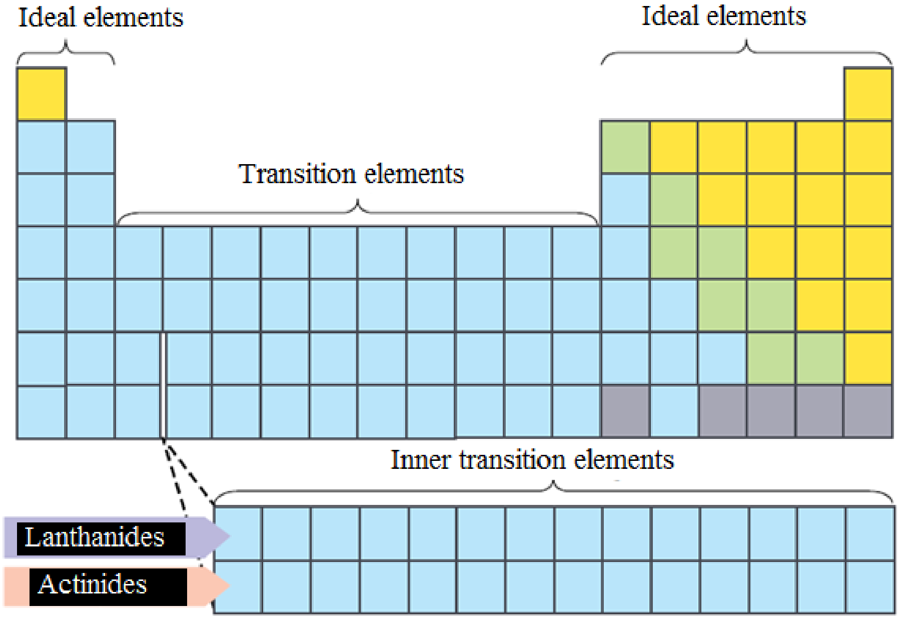
The modern periodic table that is currently used by chemists was invented by the scientist Deming in 1923. In this table, the elements are arranged according to their increasing atomic numbers. The elements are placed in seven numbered periods (1-7) based on the number of electron energy levels they have and the electrons they contain. A period is a horizontal row in the periodic table that contains elements whose properties gradually change in a predictable manner. The periodic table also consists of 18 vertical columns called groups, each column containing a group or family of elements with the same valence electron number. Each group includes elements that share similar physical and chemical properties.



C. Periodic Table Regions

The modern periodic table can be divided into regions as shown in the following figure. It includes the first region, which consists of groups 1 and 2, and groups 13 to 18. This region is called the group of ideal elements and includes metals, non-metals, and metalloids. Elements in groups 3 to 12 are called transition elements and are all metals. There are also inner transition elements located below the periodic table, such as the lanthanides and actinides, with one following element 57, which is lanthanum, and the other following element 89, which is actinium.

Note: Lanthanides and actinides are placed below the table to avoid it becoming too wide.



The table also includes four regions: (s, p, d, f). Representative Elements Group

1. Ideal Elements Group

- **s group elements**

  This group includes the first two columns IA and IIA, with each column having two electrons and ending with a distribution of ns.
- **p group elements :**

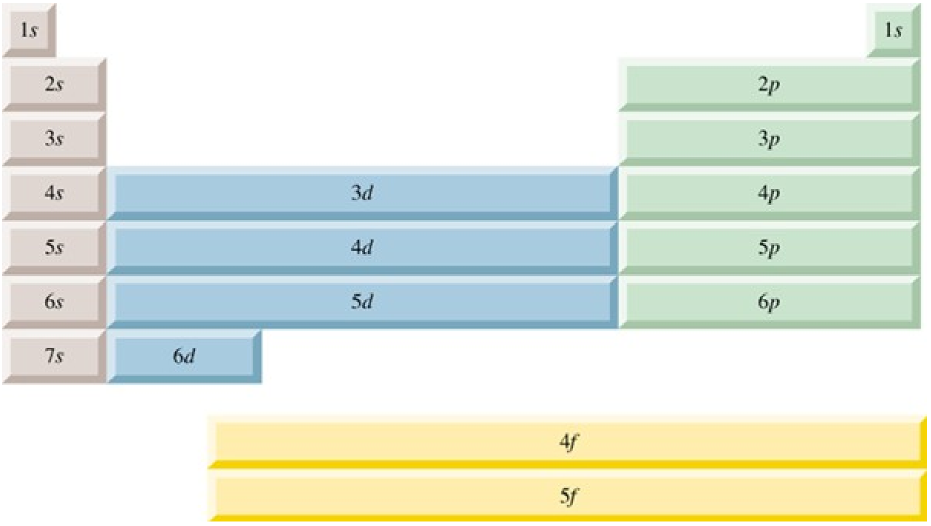
  This includes the third, fourth, fifth, sixth, seventh, and eighth columns (from **III_A** to **$VIII_A$**), except for helium, with each column having six electrons and ending with a distribution of np.

2. Transition Elements Group

- **d group elements :**

  This includes columns from **I_B** to **$VIII_B$**, with each column having ten electrons and ending with a distribution of **(n-1)d**.
- **f group elements :**

  This includes fourteen columns, with each one having fourteen electrons and ending with a distribution of **(n-2) f**, where n represents the cycle number, which are the lanthanides and actinides groups.



D. Periodic table is divided into :

1. Periodic table periods (lines)

The periodes are the horizontal rows in the table where there are 7 lines in the table. The elements of each line agree on the principal quantum number n for the outer electron layer (valence electrons) and express the line number and start the filling of electrons from the sub-layer s and end with the sub-layer p except for the first line, for

Exemple

example ;

$_{19}$K :$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^1$.

$_{20}$Ca: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2$.

First period:

This period includes two elements, Hydrogen and helium, and their electronic configuration is **$1s^1$, $2s^1$** respectively. Thus, the first energy level K fill has been filled (where the principal quantum number is **n=1**) in the element **Helium**.

Second period:

The period starts with the element **Lithium** and its configuration is **$1s^2\ 2s^1$**, where a single electron enters the second energy level with **n=2**, including eight elements where the paths are filled with electrons from one element to another, ending with **Neon** gas and its configuration **$1s^2\ 2S^2\ 2P^6$**. Thus, the second energy level has been completely filled with eight electrons in the element **neon**.

Third period:

It is similar to the second period, starting with the element **Sodium** where an electron enters the third energy level **M** where **n=3**, and the configuration is **$1s^2\ 2s^2\ 2P^6\ 3s^1$**, continuing to fill the third energy level with electrons from one element to another, ending the line with **Argon** gas and its configuration **$1s^2\ 2s^2\ 2P^6\ 3s^2\ 3P^6$**. Since this level can hold 18 electrons, the period ends, and the 3 d paths in the third shell are empty.

Fourth period:

This period starts with the element **Potassium**, and the inner electron does not enter the third energy level where **3d** paths are empty. However, the electron will enter the shell of the fourth energy level **N** where **n = 4**, and the configuration is : **$1S^2\ 2S^2\ 2P^6\ 3S^2\ 3P^6\ 4S^1$**. Following **Potassium** is the element **Calcium**, and the electron also enters the **4s** path, and the **Calcium** configuration is :**$1S^2\ 2S^2\ 2P^6\ 3S^2\ 3P^6\ 4S^2$**. Moving to the third element in this line, **Scandium**, it resumes filling the paths with electrons in the third energy level in **3d** paths that are empty, continuing to fill them with ten electrons as we transition from **Scandium** with a configuration of **$4S^2\ 3d^1$** to the element **Zinc** with a configuration of **$4S^2\ 3d^{10}$**, thus filling the third energy level with eighteen electrons. The ten elements from **Scandium** to **Zinc** are called the first transition elements. In the next element, **Gallium**, the filling of electronic paths in the fourth energy level in the **4P** path is resumed, so the configuration of **Gallium** is : **$4S^2\ 3d^{10}\ 4P^1$** and the filling of the **4P** paths continues with six electrons in the successive elements, ending the line with **Krypton** gas and its configuration **$4S^2\ 3d^{10}\ 4P^6$**, noting that the fourth energy level still contains completely empty **4f, 4d** paths of electrons

Fifth period:

similar to the previous period. The period starts with the fifth energy level **O** where **n=5** while the **4d and 4f** orbitals remain empty in the fourth energy level. The period starts with the element **Rhobidium** with a configuration of **$5S^1$**, followed by the element **Stronium** with a configuration of **$5S^2$**. In the next element, **Yttrium**, the filling stops in the fifth energy level and the outer electron enters through the fourth energy level in the **4d** orbitals with a configuration of **$5S^2\ 4d^1$**, filling the **4d** orbitals with ten electrons starting from **Yttrium** up to **Cadmium** with a configuration of **$5S^2\ 4d^{10}$**. These elements are called the second transition series. In the next element, **Indium**, the filling stops in the fourth energy level and the **4f** orbitals remain empty. The filling of the fifth energy level orbitals resumes with electrons, where the outer electron in **Indium** enters the **5P** orbitals, which are filled with six electrons. The fifth period ends with **Xenon** and a configuration of **$5S^2\ 4d^{10}\ 5P^6$**, with the **5d** and **5f** orbitals remaining empty in addition to the **4f** orbitals.

Sixth period:

The period begins by occupying the **6P** energy shell paths where **n= 6** and the period starts with the element **Cesium** and its configuration **$6S^1$** and the element **Barium** and its configuration **$6S^2$**. In the next element, which is **lanthanum**, the outer electron enters the fifth energy shell in empty **5d** paths and its configuration is : **$6S^2\ 5d^1$** where the appearance of the third transitional element series begins, then the filling stops in the **5d** paths in the next element. The outer electron enters the fourth energy shell in empty **4f** paths that continue to be filled with fourteen electrons, resulting in a series of 14 elements called the first inner transition series known as the **lanthanides** series. This series starts with the element **Cerium** and its configuration **$6S^2\ 5d^1\ 4f^1$** and the last element of this series is the element **Lutetium** and its configuration

$6S^2\ 5d^1\ 4f^{14}$. After this series ends, the filling of the fifth energy shell resumes, where **5d** paths are filled to their full capacity of ten electrons, representing the third transition series starting with the element **Hafnium** and its configuration **$6S^2\ 4f^{14}\ 5d^2$** and ending with the element mercury and its configuration **$6S^2\ 4f^{14}\ 5d^{10}$**. The sixth periode ends with six elements, where the **6P** paths are filled with six electrons, starting with the element **Thallium** and its configuration **$6S^2\ 4f^{14}\ 5d^{10}\ 6P^1$** and ending with **Radon** gas and its configuration $6S^2\ 4f^{14}\ 5d^{10}\ 6P^6$.

Seventh Period:

The period begins with the element **Francium** where the filling of the 7th energy level **Q** with electrons begins with a configuration of **$7S^1$**, followed by the element Radium with a configuration of **$7S^2$**. Similar to the previous period, the filling in the 7th energy level stops and continues in the 6th energy level where the filling of the **6d** orbitals in **Actinium** with a configuration of **$7S^2\ 6d^1$** starts. The filling of the 6d orbitals stops, and the appearance of the fourth element occurs in the series of transition metals where the filling of the **5f** orbitals starts, leading to a series of 14 elements known as the **Actinides** series or the second inner transition series starting from **Thorium** with a configuration of **$7S^2$ $6d^1$ $5f^1$**, then **Protactinium** with a configuration of **$7S^2$ $6d^2$ $5f^2$**, and ending with Nobelium with a configuration of **$7S^2$ $6d^1$ $5f^{14}$** .

a) Exceptions to Klechkowski's rule (Anomalous elements)

These are elements that have an electron distribution that deviates from the Aufbau principle, where the d subshell is either half-filled or fully filled (saturated), making the element more stable.

There are 22 anomalous elements in the periodic table when the shell is more stable.

The element keeps its normal position.

Exemple

Cu, Ag, Au have a real configuration of **s^1 d^{10}** according to Klechkowski, instead of **d^9 s^2**, so they still stay in column 11 and don't move to column 12. f-block: a **d** electron is placed before the **f** electrons appear :

$24Cr: 18[Ar]4S^2 3d^4 \longrightarrow Cr: 18[Ar]4S^1 3d^5$

$29Cu: 18[Ar]4S^2 3d^9 \longrightarrow Cu: 18[Ar]4S^1 3d^{10}$

$36[Kr]5S^2 4d^3 \longrightarrow Nb: 36[Kr]5S^1 4d^4$

$42Mo: 36[Kr]5S^2 4d^4 \longrightarrow Mo: 36[Kr]5S^1 4d^5$

$36[Kr]5S^2 4d^6 \longrightarrow Ru: 36[Kr]5S^1 4d^7$

$36[Kr]5S^2 4d^7 \longrightarrow Rh: 36[Kr]5S^1 4d^8$

$36[Kr]5S^2 4d^8 \longrightarrow Pd: 36[Kr]4d^{10}$

$47Ag: 36[Kr]5S^2 4d^9 \longrightarrow Ag: 36[Kr]5S^1 4d^{10}$

$54[Xe]6S^2 4f^{14} 5d^8 \longrightarrow Pt: 54[Xe]6S^1 4f^{14} 5d^9$

$79Au: 54[Xe]6S^2 4f^{14} 5d^9 \longrightarrow Au: 54[Xe]6S^1 4f^{14} 5d^{10}$

$86[Rn]7S^2 5f^{14} 6d^8 \longrightarrow 110Ds: 86[Rn]7S^1 5f^{14} 6d^9$

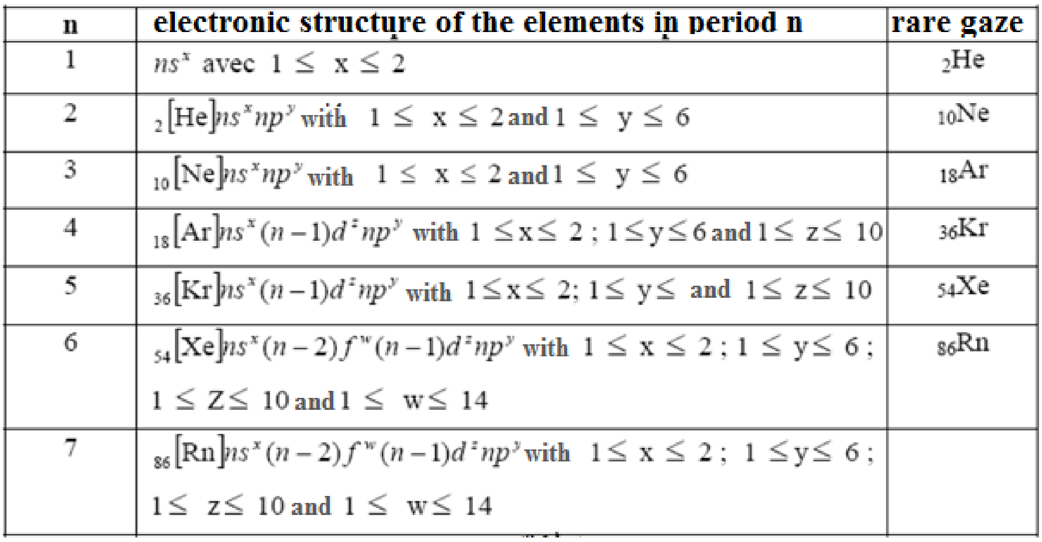
$111Rg: 86[Rn]7S^2 5f^{14} 6d^9 \longrightarrow 110Ds: 86[Rn]7S^1 5f^{14} 6d^{10}$

2. Periodic table columns (groups)

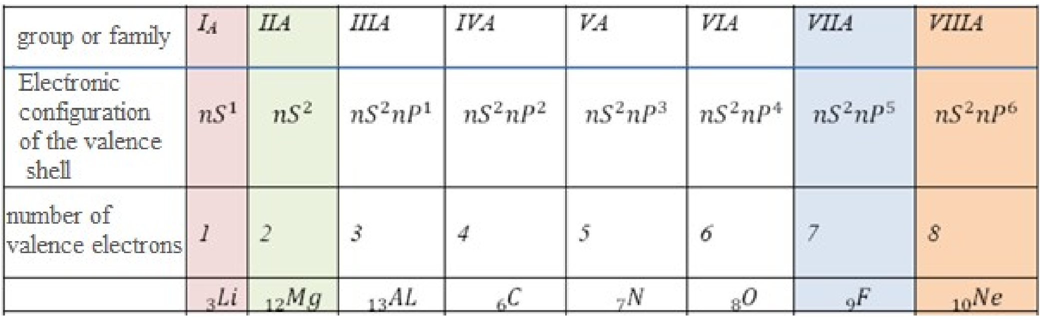
there are 18 columns, each consisting of elements with the same number of electrons in the outermost shell (valence electrons). They are divided into eight subgroups A and eight subgroups B, each numbered from I to VIII. Subgroup VIIIB consists of columns 8, 9, and 10 and is called the triads.

Subgroup A:

there are eight columns, numbered from **I_A** to **$VIII_A$**, including the elements **s** and **p**. The electronic structure for the valence electrons is in the form **nS^x** and **nS^x nP^y**, where **x** and **y** are the valence electrons.



n	electronic structure of the elements in period n	rare gaze
1	ns^x avec $1 \leq x \leq 2$	$_2He$
2	$_2[He]ns^xnp^y$ with $1 \leq x \leq 2$ and $1 \leq y \leq 6$	$_{10}Ne$
3	$_{10}[Ne]ns^xnp^y$ with $1 \leq x \leq 2$ and $1 \leq y \leq 6$	$_{18}Ar$
4	$_{18}[Ar]ns^x(n-1)d^znp^y$ with $1 \leq x \leq 2$; $1 \leq y \leq 6$ and $1 \leq z \leq 10$	$_{36}Kr$
5	$_{36}[Kr]ns^x(n-1)d^znp^y$ with $1 \leq x \leq 2$; $1 \leq y \leq$ and $1 \leq z \leq 10$	$_{54}Xe$
6	$_{54}[Xe]ns^x(n-2)f^w(n-1)d^znp^y$ with $1 \leq x \leq 2$; $1 \leq y \leq 6$; $1 \leq Z \leq 10$ and $1 \leq w \leq 14$	$_{86}Rn$
7	$_{86}[Rn]ns^x(n-2)f^w(n-1)d^znp^y$ with $1 \leq x \leq 2$; $1 \leq y \leq 6$; $1 \leq z \leq 10$ and $1 \leq w \leq 14$	



group or family	I_A	IIA	IIIA	IVA	VA	VIA	VIIA	VIIIA
Electronic configuration of the valence shell	nS^1	nS^2	nS^2nP^1	nS^2nP^2	nS^2nP^3	nS^2nP^4	nS^2nP^5	nS^2nP^6
number of valence electrons	1	2	3	4	5	6	7	8
	$_3Li$	$_{12}Mg$	$_{13}AL$	$_6C$	$_7N$	$_8O$	$_9F$	$_{10}Ne$

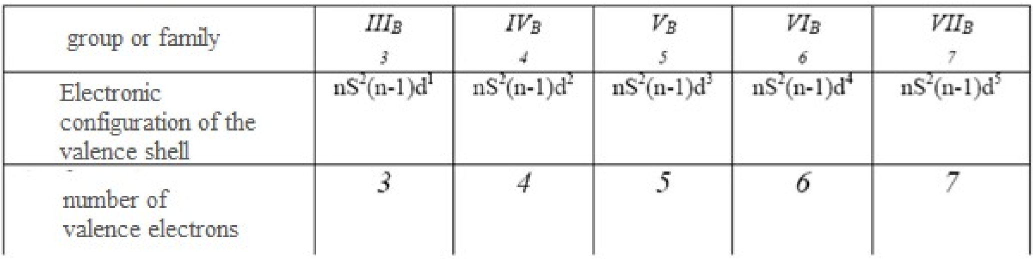
Exemple

$_{37}$Rb: $_{36}$[Kr] $5s^1$: 1 valence electron, so **Rb** belongs to group I and subgroup A.

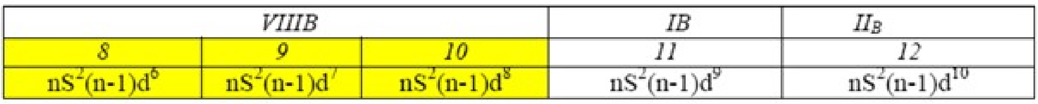
$_{33}$As: 18[Ar] $3d^{10}$ $4s^2$ $4p^3$: 5 valence electrons, so As belongs to group V and subgroup A.

Subgroup B:

there are eight columns, numbered from **I_B to $VIII_B$**, including the element d. The electronic structure for the valence electrons is in the form **nS^x $(n-1)d^y$**, where **x** and **y** represent the valence electrons and the sum **(x + y)** of the electrons will indicate the group of the element.



group or family	III_B 3	IV_B 4	V_B 5	VI_B 6	VII_B 7
Electronic configuration of the valence shell	$nS^2(n\text{-}1)d^1$	$nS^2(n\text{-}1)d^2$	$nS^2(n\text{-}1)d^3$	$nS^2(n\text{-}1)d^4$	$nS^2(n\text{-}1)d^5$
number of valence electrons	3	4	5	6	7



VIIIB			IB	II_B
8	9	10	11	12
$nS^2(n\text{-}1)d^6$	$nS^2(n\text{-}1)d^7$	$nS^2(n\text{-}1)d^8$	$nS^2(n\text{-}1)d^9$	$nS^2(n\text{-}1)d^{10}$

Exemple

$_{40}$Zr : $1S^2$ ....$5S^2$ $4d^2$: (x + y) = 4 ⇒ 4 valence electrons,

Zr : belongs to group IV and subgroup B ⇒ IV_B

When : $8 \leq x + y \leq 10$, the corresponding elements will belong to group $VIII_B$ (the triads).

Exemple

$_{26}$Fe: $1S^2$ ....$3d^6$ $4S^2$ ⇒ group $VIII_B$
$_{27}$Co: $1S^2$ ....$3d^7$ $4S^2$ ⇒ group $VIII_B$
$_{45}$Rh: $1S^2$ ....$5S^2 4d^7$: x + y = 9 valence electrons ⇒ group $VIII_B$.

- When (x + y) > 10

$(n - 1)d^{10}$ ns^1 ⇒ group I_B, as in Au: $1S^2$ .... $5d^{10}$ $6S^1$ (I_A)
$(n - 1)d^{10}$ ns^2 ⇒ group II_B, as in Hg: $1S^2$ .... $5d^{10}$ $6S^2$ (II_A)

a) Main Groups

There are 8 main groups referred to as groups.

First main Group: Known as the alkali metals, these elements are active, and their activity increases as we go down starting with the element hydrogen, which has only one valence electron

Exemple

$_1$H: $1s^1$

$_3$Li:$1s^2\ 2s^1$

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

Second main Group: Known as the alkaline earth metals, they have two valence electrons

Exemple

$_4$Be : $1s^2\ 2s^2$

$_{12}$Mg : $1s^2\ 2s^2\ 2p^6\ 3s^2$

Seventh main Group: Elements of this group are called halogens; they are active elements, with chlorine being the most famous, containing seven valence electrons

Exemple

$_9$F: $1s^2\ 2s^2\ 2p^5$.

$_{17}$Cl: $1s^2\ 2s^2\ 2p^6\ 3s^2 3p^5$.

Eighth main Group: Elements of this group are called noble gases, owning 8 valence electrons, meaning their outer shell is full except for Helium, which has 2 valence electrons, hence these are stable elements

Exemple

$_2$He : $1s^2$.

$_{10}$Ne: $1s^2\ 2s^2\ 2p^6$.

$_{18}$Ar: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$

E. Criteria for chemical recognition

Metals give cations, and their oxides are basic. For example: Mg gives Mg^{2+} and $MgO + H_2O$ forms $Mg(OH)_2$.

Non-metals give anions, and their oxides are acidic. For **example**: S gives S_2- and SO_2 + H2O® forms H_2SO_3. The "border" isn't sharply defined: metalloids (semiconductors) used in electronics (Si, Ge, As, Sb) fall somewhere in between metals and non-metals.

- **Metallic character:**

  It's the ability to easily lose outer electrons (with less energy), Indeed, the element is trying to acquire the closest noble gas configuration to itself. The outer orbitals contain fewer than 4 electrons, like calcium 20Ca: ....$4s^2 \rightarrow Ca^{2+} + 2e^-$. Nonmetals, on the other hand, tend to attract electrons: $O + 2e^- \rightarrow O^{2-}$, with outer s and p orbitals having $\geq 4\ e^-$.
- **Sanderson's Rule:**

  An element is metallic if the number of electrons in its highest n shell is less than or equal to its period number. (Except for H and Ge).

Exemple

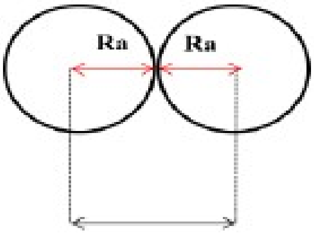
Mg: $Z = 12 = 10 + 2 \Rightarrow$ (Ne) $3s^2$, 2 electrons in n=3 and belongs to period 3 => 2 < 3 ⇒ Mg is a metal.

Bi: $Z = 83 = 54 + 15 \Rightarrow$ (Xe) $4f^{14}\ 5d^{10}\ 6s^2\ 6p^3$, 5 electrons in n=6 and belongs to period 6 => 5 < 6 ⇒ Bi is a metal.

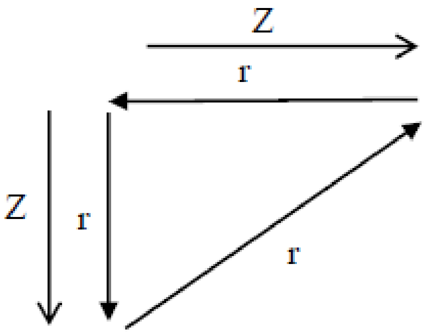
F. Properties in the periodic table (R_a)

1. Atomic radius

It is half the distance between the centers of two identical atoms in a diatomic molecule.



1. Atomic radius decreases in each period as we move from left to right. This is because as we move to the right of the table, the number of atoms increases, which increases the number of protons in the nucleus accompanied by an increase in the number of electrons. However, they occupy the same principal level, so the nucleus attracts these electrons more, causing the atomic radius to decrease **(Z↗, r↘)**.
2. Atomic radius increases within each group as we move down the table. This is due to the increase in the number of principal levels as we move down the table, resulting in less nucleus attraction to electrons and an increase in the atomic radius **(Z↗, n↗, r↗)**.



Remarque

The atomic radius of an element is given by the relationship:

$$r = \frac{n^2}{Z_{eff}}.a$$

With **Z_{eff}**: effective charge and **a_0 = 0.53Å** Bohr radius.

Exemple

Table: example of elements from the same period (the third period n=3).

Elements of the third period.	Na	Mg	Al	Si	P	S
Z	11	12	13	14	15	16
Atomic radius r (Å)	1,9	1,6	1,43	1,32	1,28	1,27

Throughout a column Z↗ and n↗ ⇒ volume↗ so the electron cloud increases and r↗.

Table: example of elements in the same column (column n 14, group IV_B).

Elements	C	Si	Ge	Sn	Pb
Z	6	14	32	50	82
Atomic radius r (Å)	0,914	1,32	1,37	1,62	1,75

Exemple

For the atom of 3Li: Let's calculate the atomic radius of the Li atom and the ionic radius of the Li+ ion.

Li atom: We start with the electronic configuration of lithium:

$_3$**Li**: $1s^2\ 2s^1 2p^0$

n= 2, $Z_{eff} = Z - \sigma\ (2s)$.

σ (2s) = 0x0,35 + 2x0,85 =1,7 ⇒ Z_{eff} = 3-1,7 = 1,3.

$$r(Li) = \frac{2^2}{1,3}.0,53 = 1,630\ \text{Å}$$

$3Li^{+}: 1s^2\ 2s^0 2p^0$

$n = 1,\ Z_{eff} = Z - \sigma\ (1s).$

$\sigma\ (1s) = 1x0{,}30 = 0{,}30 \Rightarrow Z_{eff} = 3 - 0{,}30 = 2{,}7.$

$$r(Li^{+}) = \frac{1^2}{2{,}7} . 0{,}53 = 0{,}196\ Å$$

$r(Li^{+})$ $= 0{,}196$ Å.

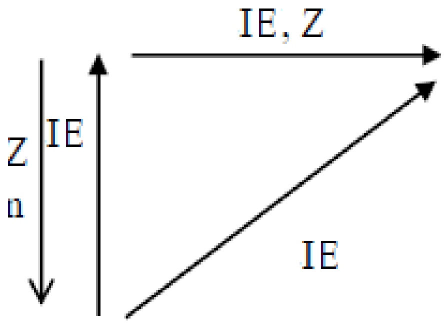
2. Ionization energy (IE)

It is the energy required to remove an electron from a single atom in the gaseous state.

$$A + \text{energy} \longrightarrow A^{+} + e^{-}$$

Ionization energy varies in the table as follows:

1. Ionization energy increases in each period as we move from left to right. This is because the smaller atomic radius leads to increased nucleus attraction to electrons making it difficult to remove an electron.
2. Ionization energy decreases within each group as we move down the group. This is due to the increase in atomic radius, resulting in less nucleus attraction to electrons and making it easier to remove an electron. Noble gases have the highest ionization energy due to their stability, making it difficult to remove electrons from stable atoms



Remarque

We define energy as follows:

- First ionization (IE_1) is the energy required to remove the least tightly held electron from the nucleus.

  $I_{E1} = E(A^{+}) - E(A).$

  $$K(g) \longrightarrow K^{+}\ (g) + 1\ e + I_{E1}$$

- 2nd ionization: IE_2 energy needed to remove the 2nd electron.

  $I_{E1} = E(A^{++}) - E(A^{+}).$

  $$K^{+}(g \longrightarrow K^{+2}\ (g) + 1\ e + I_{E2}$$

3. Electronegativity (E_n)

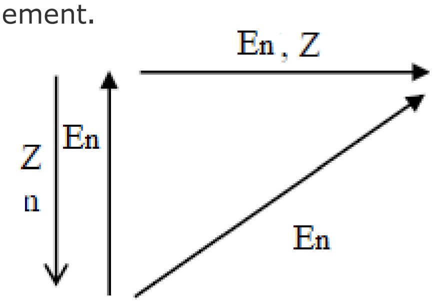
It is the atom's ability to attract shared electrons towards it when bonding with another atom.

$A_{(g)} + B_{(g)} \longrightarrow A^{+}_{(g)} + B^{-}_{(g)}$, it's said that B is more electronegative than A

The trend of electronegativity in the periodic table is as follows:

1- Electronegativity increases as we move from left to right in a period, except for noble gases with zero electronegativity. This is due to the decrease in atomic radius leading to increased nucleus attraction to electrons, making it easier to attract electrons.

2- Electronegativity decreases as we move down a group. This is because of the increase in atomic radius leading to decreased nucleus attraction to electrons, making it harder to attract electrons. The most electronegative element F is considered the Fluorine element.

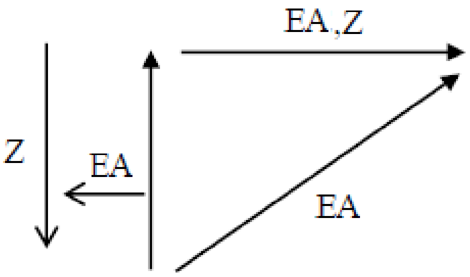


4. Electron Affinity (tendency to capture electrons)-E.A

Just as ionization energy is a good measure of the ability of an atom to transform into a positive ion, electron affinity gives a good measure of the ability of an atom to transform into a negative ion.

$$X + e^{-} \longrightarrow X^{-} + E.A$$

The electron affinity represents the energy released when a neutral gas-phase atom gains an electron to form a negative ion. Electron affinity measures how well the atom bonds with an additional electron. Electron affinity decreases vertically in the periodic table from top to bottom and increases horizontally from left to right. This can be explained by the change in atomic size, where the size increases when moving down a group causing the nucleus attraction forces to decrease, hence the decrease in electron affinity. On the other hand, moving from left to right in a period causes the atomic size to decrease, leading to increased nucleus attraction forces for electrons, thus increasing the electron affinity. The electron affinity for inert gases is zero because they have a stable valence electron configuration, where there is no availability for an additional electron.



Exemple

Arrange the following elements in each series according to their increasing radius: $_{11}$Na; $_{19}$K; $_{37}$Rb.

Solution:

The valence layer increases from top to bottom. As a result, the attraction between the outer electron and the nucleus gets weaker, and the atomic radius increases from Sodium to Rubidium. $r_{Na} < r_K < r_{Rb}$

Chapter Seven: Chemical Bonds

VII

Except for the noble gases (the last column of the periodic table), which are single atoms, all atoms can contribute to chemical bonds, forming molecules and/or solid or liquid substances. Furthermore, even the "inert" gases eventually condense at very low temperatures (or under high pressure). To classify bonds, the fundamental concepts are bond energies (or inversely: bond dissociation energies) and the electronegativity of atoms involved in chemical bonds. There are two types of bonds: strong and weak bonds.

1. **Strong bonds**:
   To break strong bonds, it is necessary to provide dissociation energies ranging from 200 to 500 kilojoules per mole of the bond (roughly 50 to 100 kilocalories per mole or about 2 to 5 electron volts per bond). There are four types of strong bonds:
   - Covalent (sharing) bond – Lewis representation
   - Ionic bond
   - Coordinate covalent or polar covalent bond (dipole moment)
   - Metallic bond
2. **Weak bonds**:
   There are four types of weak bonds:
   - Hydrogen bonds
   - Van der Waals bonds

A. Bond Energy

It is the energy released from all free atoms when they bond together, and it is a negative factor. Therefore, the dissociation energy, which is the minimum energy required to break this bond, is its opposite and is positive. A chemical bond forms between two atoms if the resulting system (molecule) is more stable and has lower energy than the two separate atoms. For example, the bond energy for the molecule H_2 (H-H) is 431 kilojoules / mole. The dissociation energy is thus 431 kilojoules / mole.

$2H \rightarrow H_2$: $\Delta E = -431$ kJ/mol = -103 kcal/mol= -4.47 eV

$H_2 \rightarrow 2H$: $\Delta E = 431$ kJ/mol = 103 kcal/mol= 4.47 eV

Just to let you know, this energy is three times lower than the energy required for separating an electron from a proton in its ground state, which needs an ionization energy of 13.6 volts

B. Strong Bonds

To break strong bonds, it is necessary to provide dissociation energies estimated between 200 and 500 kilojoules per mole of the bond (roughly 50 to 100 kilocalories per mole or about 2 to 5 electron volts / bond).

- If the electronegativity difference is **$0 < \Delta\chi \leq 0.5$**, the bond is considered non-polar covalent.
- If the electronegativity difference is **$0.5 < \Delta\chi \leq 1.9$**, the bond is considered polar covalent or ionic covalent. (It is an intermediate bond between non-polar covalent and ionic bonds).
- If the electronegativity difference is **$\Delta\chi > 1.9$**, the bond is ionic.

Complément : Polar covalent and ionic bonds

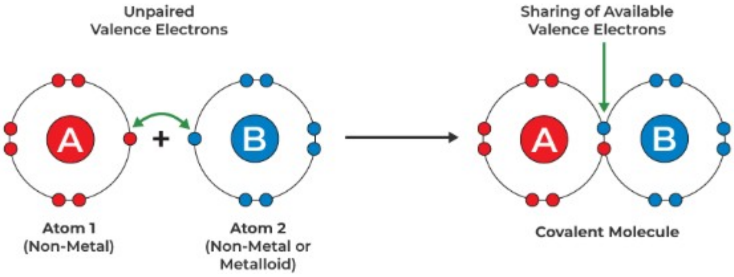
Polar covalent bonds occur when a highly electronegative element combines with a less electronegative element (0.5> electronegativity difference >7). This leads to the electron density being pulled towards the atom with high electronegativity in an uneven manner for the electron charge between the shared atoms in the bond. When the electronegativity difference exceeds 1.7, the bond becomes covalent ionic, such as in the molecule H2O. Due to the high electronegativity of O, the electrons in the O-H bond are attracted to the O atom. Therefore, we say that these bonds (covalent) are polar (partially ionic), and we indicate the positive charge $\delta+$ on H and the negative charge on O ($\delta<1$).

1. Covalent bond

The covalent bond between two non-metal atoms A and B is the sharing of two electrons. Each atom provides one valence electron. There are three types of covalent bonds:

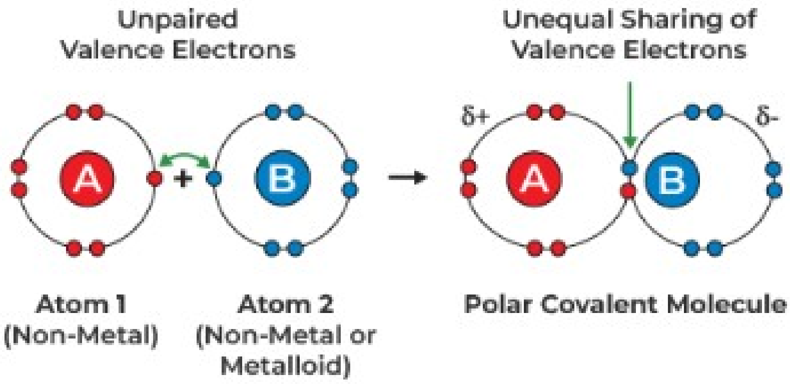
a) Perfect covalent bond

Normal means it's a sharing of two unpaired electrons and a perfect bond between two atoms of the same electronegativity.



b) Polar covalent bonds

This type of covalent bond occurs when the electronegativity of the combining atoms differs, leading to unequal electron sharing. Electrons are attracted to the more electronegative atom, with an electronegativity difference greater than zero but less than 2. Consequently, the shared electron pair is closer to that atom. For instance, molecules that form hydrogen bonds exhibit this unbalanced electrostatic potential, where hydrogen interacts with electronegative atoms like fluorine, nitrogen, or oxygen.

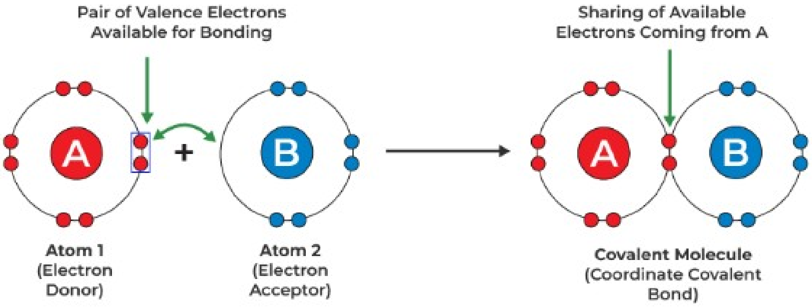


we indicate the positive charge δ+ on H (A)and the negative charge on O (B)(δ<1).

c) Coordination or dative covalent bonds

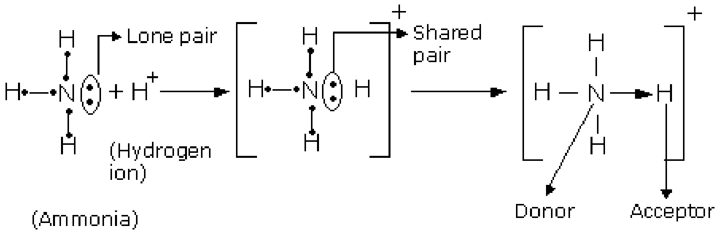
In this type of bond, one atom, known as the donor, provides a pair of electrons to another atom, the acceptor, which has an empty orbital. The less electronegative atom acts as the donor in this dative bond, represented by an arrow pointing from the donor to the acceptor.

Complément



Exemple

Formation of Ammonium ion



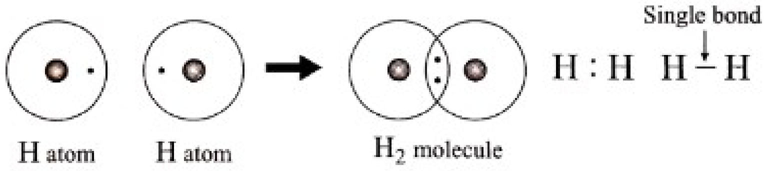
Formation of HCl molecule

2. Ionic Bonding – Lewis Representation

Ionic bonding is a type of chemical bonding that occurs between atoms with dissimilar electronegativities, where one atom donates one or more electrons to another atom resulting in an attraction that holds the resulting molecule together. Atoms tend to contribute or share electrons in a way that fills their electron shell. This bond is always stronger than other forces (bonds) between molecules, such as hydrogen bonding. The Lewis representation of an ionic bond describes the number of electron pairs shared between the atoms forming the bond. The most common type of ionic bond is the single bond, where only one pair of electrons is shared. Bonds with more than one pair of electrons are called multiple ionic bonds. Sharing two pairs of electrons is called a double bond, and sharing three pairs is called a triple bond. An example of a double bond is nitrous acid (between N and O), and an example of a triple bond is hydrogen cyanide (between C and N).

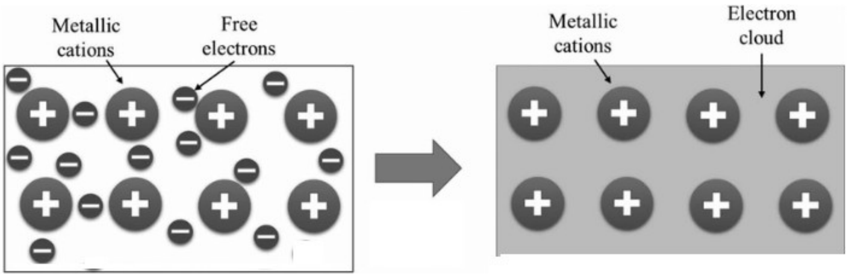
Exemple

H_2 molecule



3. Metallic bonding

Involves atoms that have a low number of electrons in their outer shell, which is the case with metals. These electrons are loosely held to the nucleus and can be easily removed. The atoms then become positive ions. The electrons that have been removed from the atoms are shared among all these atoms, forming an "electron cloud" that keeps everything together. This is why a metal can conduct electrical energy.



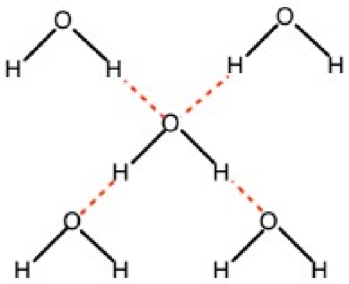
C. Weak Bonds

1. Hydrogen Bonds

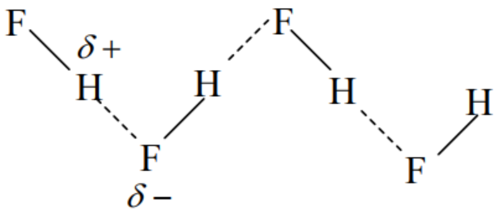
This type of non-chemical bond (van der Waals forces) exists in polar covalent molecules containing a hydrogen atom with an electronegativity of 2 and a small-sized atom with high electronegativity such as fluorine, oxygen, and nitrogen with electronegativities of 4, 3.04, 3 respectively. Similar to dipole-dipole attraction, hydrogen bonding arises from the attraction between the hydrogen atom (positive pole +δ) in one molecule with one of the atoms with high electronegativity mentioned above (negative pole δ-) in another molecule. Therefore, this bond is a specific case of dipole-dipole attractions and is often represented by a dashed line between the hydrogen atom in one part and the atom of one of the above-mentioned elements in another part, as shown in the following

Exemple

Water molecule H_2O



Hydrogen fluoride molecule HF



2. Van der Waals Bonds

Van der Waals bonds are usually extremely weak (e.g. He, Ne, Ar - gases or liquids or solids) but can be stronger in some cases (solid iodine I2 which is a type of graphite bond). These bonds cause condensation of all molecules or atoms in a liquid or solid at low temperatures, and this condensation occurs when there are no stronger bonds. Additionally, inert gases like : H_2, O_2, N_2, F_2, Cl_2, etc., condense due to van der Waals bonds between the molecules.

Van der Waals bonds are formed through the attraction process between permanent dipole-dipole pairs (polar molecule state).

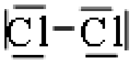
D. Lewis Representation of an Atom or Molecule

Octet Rule (The Eight Rule):

This rule is based on the assumption that atoms forming molecules must be surrounded by at least 8 electrons or 4 pairs of electrons to achieve maximum stability. Atoms seek to achieve the electronic distribution of the nearest noble gas (ns2np6) in the periodic table, making it easy to predict the most stable ion of elements in groups s and p in the periodic table. This rule does not apply to elements with different electronic structures far from noble gases (groups d and f and column 14).

Exemple

in the molecule Cl_2, the octet rule is fulfilled as each chlorine atom is surrounded by four pairs of electrons.



General method for drawing Lewis structures :

It's a way to draw the shape of a molecule, showing the arrangement of valence electrons and the number of bonds in the molecule. Free electrons are represented by dots, single bonds by two dots or a line, double bonds by four dots or two lines, and triple bonds by six dots or three lines. A Lewis structure can be drawn for any molecule with covalent bonds or for complexes with coordinate bonds.

1- Identify the central atom (the atom with the lowest electronegativity and the highest valence).

2- Calculate the valence electrons for each element.

2- Calculate the total number of valence electrons in the molecule.

3- Connect the central atom to the other atoms with covalent bonds (each two dots or a short straight line represents a covalent bond, which is a pair of electrons and is called bonding electrons).

4- Subtract the number of bonding electrons from the total number of valence electrons, and distribute the remaining on the outer atoms so that each atom has eight electrons, except for hydrogen, which only gets two electrons.

6- The remaining valence electrons are added to the central atom as non-bonding electrons. 7- If the number of electrons on the central atom is less than eight, non-bonding electron pairs are used to form double bonds between the central atom and the outer atoms.

Important notes when drawing Lewis structure:

1- The central atom is written first.

2- If the molecule is a negatively charged ion (Anion), we add to the valence electrons a number equal to the charge of the ion.

3- If the molecule is a positively charged ion (Cation), we subtract from the valence electrons a number equal to the charge of the ion.

4- We start by placing valence electrons (forming bonds) on the molecule's atoms, where each hydrogen atom takes two electrons, and any other atom will have its share of eight electrons.

Exemple

Draw the Lewis structure of ammonia NH_3

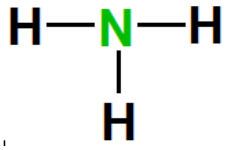
Solution:

1- The central atom is nitrogen.

2- Valence electrons: H = 1, N = 5.

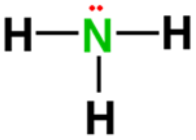
3- Total valence electrons = (3 x 1) + 5 = 8.

4- The central atom is connected to the other atoms by single covalent bonds.



Number of bonding electrons = 6

Difference = 8-6 = 2 placed in the form of non-bonding pairs on the central atom



Exemple

Draw the Lewis structure of carbon dioxide CO_2

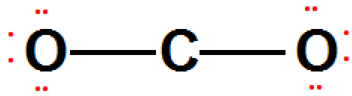
Solution:

1- Central atom carbon

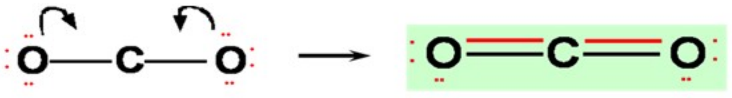
2- Valence electrons = (2×6) +4 = 16

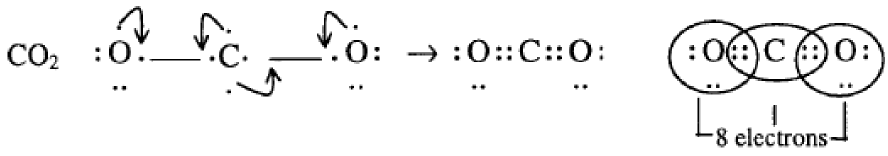
3- Formation of covalent bonds

4- Difference between bonding electrons and total valence electrons = 16-4=12 distributed on the outer atoms (oxygen) so that each gets 8 electrons.



5- For carbon to get 8 electrons, form double bonds with the oxygen atoms.





E. Molecular Geometry - VSEPR Theory

The Lewis model provides a convincing explanation of the basic mechanisms of bonding and bond-breaking. However, it does not explain the magnetic properties of molecules or molecular ions, nor does it provide information about the direction and geometric shape of bonds, and the difference between σ and π bonds.

1. VSEPR Method Principle

VSEPR theory (Valence Shell Electron Pair Repulsion), also known as Gillespie's theory, aids in predicting the geometry of polyatomic structures around a central atom. This theory allows us to:

- Anticipate permanent electrostatic dipole moments, which contribute to the cohesion of matter (such as Van der Waals and Keesom forces).
- Examine the chemical reactivity of organic molecules, which is closely tied to the geometry around a carbon atom.

a) VSEPR Theory Overview

VSEPR theory, also known as Gillespie theory, explains how atoms (X) bonded to a central atom (A), along with non-bonding electron pairs (E), arrange themselves in space to minimize electronic repulsions between all electron pairs in the valence shell of the central atom. This allows predictions about the molecular geometry surrounding the central atom. The molecule adopts a shape that minimizes repulsions (R) between pairs (P) of valence electrons (E) by maximizing the distance between bonding and non-bonding electron pairs around the central atom. This theory applies to molecules or ions of the type:

$\mathbf{AX_nE_m}$

Where:

A: represents the central atom;

X: any atom bonded to A;

n: number of bonds;

E: any non-bonding pair (NBP) of the central atom A;

m: number of NBPs.

The sum **(n+p)**, known as the total number of pairs, provides information about the basic geometry of the molecule.

So depending on **n+m**, we predict the molecule's geometry.

n+m=2 linear shape $\alpha=180°$

n+m=3 triangular shape $\alpha=120°$

n+m=4 tetrahedral shape $\alpha=180°$

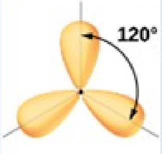
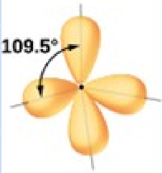
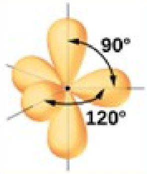
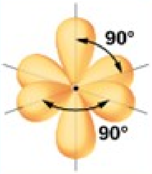
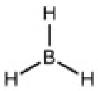
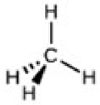
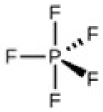
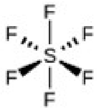
n+m=5 triangular bipyramidal shape $\alpha=90°$ and 120°

n+m=6 octahedral shape $\alpha=180°$

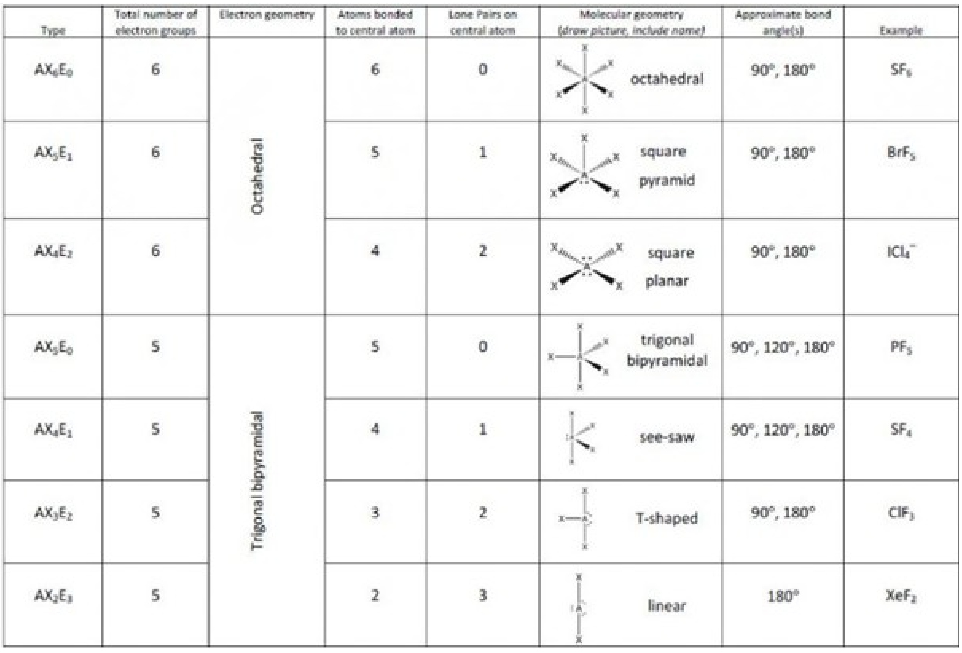
Exemple

Lewis structure for H_2O would show:

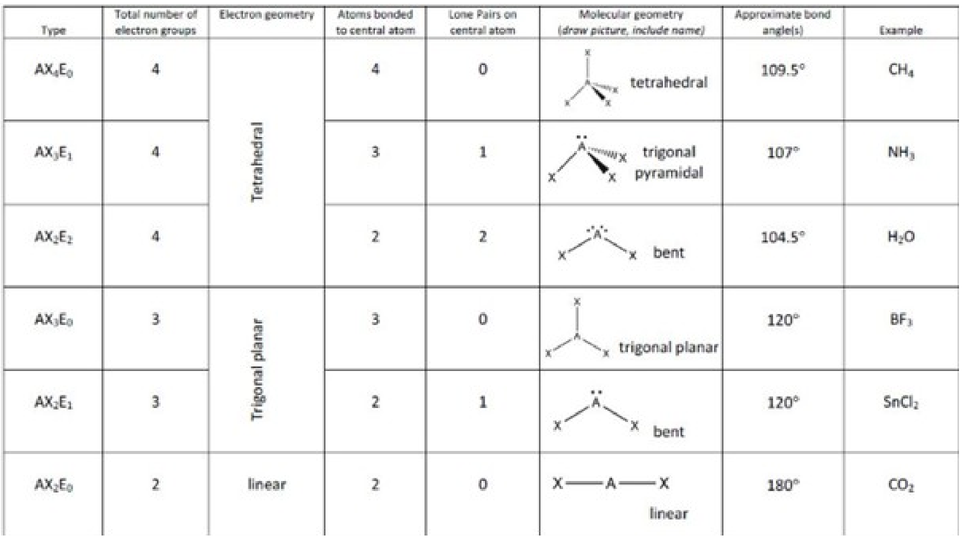
There are 4 pairs (2 unshared) around O, which will experience mutual repulsions and give the molecule a spatial configuration ($\alpha > 90°$), resulting in a tetrahedral shape:

Number of regions	Two regions of high electron density (bonds and/or unshared pairs)	Three regions of high electron density (bonds and/or unshared pairs)	Four regions of high electron density (bonds and/or unshared pairs)	Five regions of high electron density (bonds and/or unshared pairs)	Six regions of high electron density (bonds and/or unshared pairs)
Spatial arrangement					
Line-dash-wedge notation	H—Be—H				
Electron pair geometry	Linear; 180° angle	Trigonal planar; all angles 120°	Tetrahedral; all angles 109.5°	Trigonal bipyramidal; angles of 90° or 120° An attached atom may be equatorial (in the plane of the triangle) or axial (above or below the plane of the triangle).	Octahedral; all angles 90° or 180°

The following figure shows the ideal molecular geometries based on electron-pair arrangements for various combinations of lone and bonding pairs. To improve clarity, we include a typical wedge and dash representation for each combination, as these can often be confusing. Although there are various correct ways to rotate the molecule and position the wedges and dashes, these specific depictions were chosen for their simplicity. VSEPR theory suggests that molecular and electron-pair geometries are the same in the absence of lone pairs. In this context, A represents the central atom, X denotes a peripheral atom, and E indicates an unshared electron pair.



Type	Total number of electron groups	Electron geometry	Atoms bonded to central atom	Lone Pairs on central atom	Molecular geometry (*draw picture, include name*)	Approximate bond angle(s)	Example
AX_6E_0	6	Octahedral	6	0	octahedral	90°, 180°	SF_6
AX_5E_1	6		5	1	square pyramid	90°, 180°	BrF_5
AX_4E_2	6		4	2	square planar	90°, 180°	ICl_4^-
AX_5E_0	5	Trigonal bipyramidal	5	0	trigonal bipyramidal	90°, 120°, 180°	PF_5
AX_4E_1	5		4	1	see-saw	90°, 120°, 180°	SF_4
AX_3E_2	5		3	2	T-shaped	90°, 180°	ClF_3
AX_2E_3	5		2	3	linear	180°	XeF_2



Type	Total number of electron groups	Electron geometry	Atoms bonded to central atom	Lone Pairs on central atom	Molecular geometry (*draw picture, include name*)	Approximate bond angle(s)	Example
AX_4E_0	4	Tetrahedral	4	0	tetrahedral	109.5°	CH_4
AX_3E_1	4		3	1	trigonal pyramidal	107°	NH_3
AX_2E_2	4		2	2	bent	104.5°	H_2O
AX_3E_0	3	Trigonal planar	3	0	trigonal planar	120°	BF_3
AX_2E_1	3		2	1	bent	120°	$SnCl_2$
AX_2E_0	2	linear	2	0	X—A—X linear	180°	CO_2

F. Covalent bond in the quantum model

For atoms, solving the molecular Schrodinger equation gives wave functions that describe the behavior of electrons in the molecule. This equation can only be accurately solved in the simplest cases, such as the case of the hydrogen molecule H_2. For molecules or other multi-electron atoms (atoms with more than one electron orbiting around them), approximate methods are used to solve it.

1. Physical side of bonding

Chemical bonding occurs through the combination of atomic orbitals, leading to the formation of atomic orbitals. There are two different types of orbital combinations that correspond to two different types of bonds: σ bonds and π bonds.

a) Head-on overlap (sigma type bond)

Sigma bonds result from a head-on overlap between the orbitals involved, resulting in narrower orbitals. Sometimes the electrons in the sigma bond are referred to as "sigma electrons". This type of overlap is specific to s and p-type atomic orbitals and leads to the formation of a sigma (σ) bond.

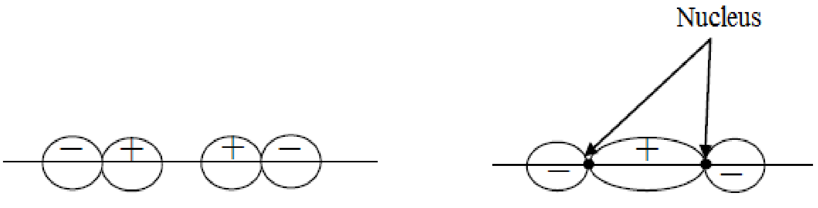
i S type

$$ns + ns \rightarrow \sigma ns + \sigma ns^*$$

Bonding molecular orbital σs type s-s

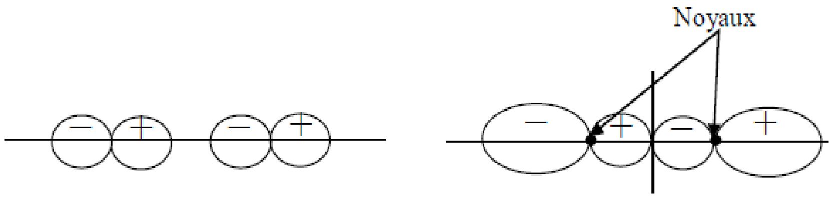
Antibonding molecular orbital σs

ii nPz type



AO(P_z) AO (P_z)

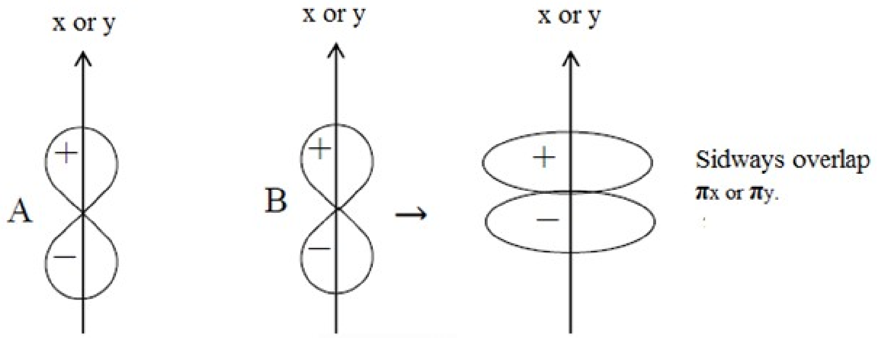
Bonding molecular orbital σ_z



Antibonding molecular orbital σ_z^*

b) b) Side overlap (π type bond)

This type of bond involves side overlap of p-type atomic orbitals, leading to the formation of a π bond.



Sigma (σ)bonds differ from π bonds in that sigma bonds are stronger than pi (π) bonds.

2. Mathematic side :L.C.O.A Theory in Chemistry

This theory is an approximate solution to the Schrödinger equation, which involves a linear combination of atomic orbitals, meaning the sum of atomic wave functions or their differences. The wave function for diatomic molecules like H_2 looks like this:

$$\psi = C_a\psi_a + C_b\psi_b$$

Where **ψ** is the molecular wave function, and ψa and ψb are atomic wave functions, while Ca and Cb are adjustable factors. According to the approximate **L.C.O.A** theory, the bond only concerns the united atoms and has a specific length and energy related to those united atoms. For example, in the hydrogen molecule H_2:

- The electron of atom **H_A** occupies the **$1S_A$** atomic orbital, represented by the wave function **ψ_A**.
- The electron of atom **H_B** occupies the **$1S_B$** atomic orbital, represented by the wave function **ψ_B**.
- In the electron bond **H_A-H_B**, they occupy a molecular orbital. They are represented by the wave function **ψ_{AB}**, which is a linear combination of the **ψ_A** and **ψ_B** wave functions. The **ψ_{AB}** wave function is written as:

$$\psi_{AB} = a\psi_A + b\psi_B$$

In reality, only the wave function squared has physical significance (electron probability). The electron probabilities are as follows:

-Near A: $a^2\psi_A^2$

-Near B: $b^2\psi_B^2$

-Between A and B (the bond): $2ab\psi_A\psi_B$

Due to symmetry, atoms A and B serve the same role, so there's no valid reason to say the electron is near A or B, and vice versa.

Thus, the probability of an electron being near A is equal to the probability of it being near B, with no distinction between them. Therefore:

$$a^2 = b^2 \;\Rightarrow\; b = \pm a$$

$$\psi_{AB} = a\psi_A + b\psi_B = a\psi_A \pm \psi_B$$

There are two solutions for the ψ_{AB} function:

-If: **b = + a**

$$\psi_{AB} = a\psi_A + b\psi_B = a(\psi_A + \psi_B)$$

-If: **b = - a**

$$\psi_{AB} = a\psi_A - b\psi_B = a(\psi_A - \psi_B)$$

Both equations are solutions to the Schrödinger equation and allow us to obtain two molecular orbitals from two atomic orbitals.

The function $\Psi_L = a(\psi_A + \psi_B)$ is called the bonding function because it corresponds to an increase in electron probability between atoms A and B, leading to bond formation.

Conversely, the function $\mathrm{AL}\Psi_{AL} = a(\psi_A - \psi_B)$is called the antibonding function because it corresponds to a decrease in electron probability between atoms A and B, preventing bond formation.

In cooperative bonding, a shared electron pair is obtained by combining two atomic orbitals, each containing an electron (high probability of finding the electron in the shared region).

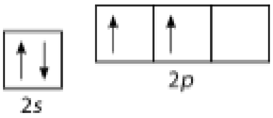
G. Hybridization of Atomic Orbitals

1. Hybridization for Single Bonds (sp^3 Hybridization)

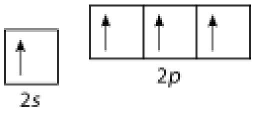
In this type, hybridization occurs between one s orbital and three p orbitals, resulting in four sp3 hybrid orbitals with the same shape and energy, distributed in space to form a regular tetrahedral angle. The atom is at the center of the tetrahedron, and the angles between the hybrid orbitals are 109.5 degrees.

Exemple

Consider the carbon atom in the methane (CH_4) molecule. An isolated carbon atom has an electron configuration of $1s^2$ $2s^2$ $2p^2$, meaning that it has two unpaired electrons in its 2p orbitals, as shown below.



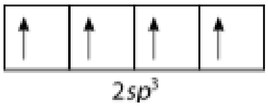
According to the description of valence bond theory so far, carbon would be expected to form only two bonds, corresponding to its two unpaired electrons. However, methane is a common and stable molecule that contains four equivalent C−H bonds. One way to account for this might be to promote one of the 2s electrons to the empty 2p orbital.



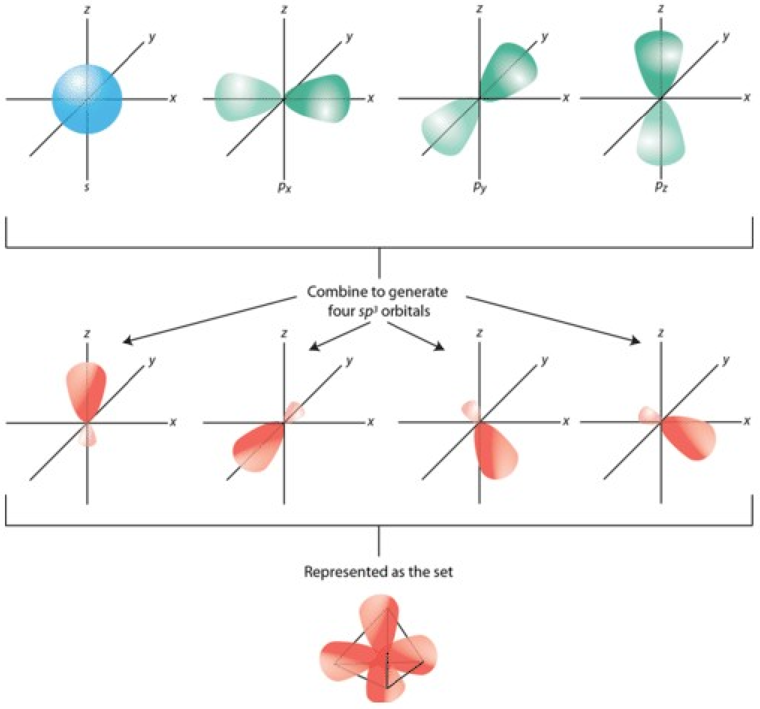
Now, four bonds are possible. The promotion of the electron “costs” a small amount of energy, but recall that the process of bond formation is accompanied by a decrease in energy. The two extra bonds that can now be formed result in a lower overall energy, and, thus, a greater stability, for the CH_4 molecule. Carbon normally forms four bonds in most of its compounds.

The number of bonds is now correct, but the geometry is wrong. The three p orbitals (p_x, p_y, p_z) are oriented at 90° angles relative to one another. However, as we saw in our discussion of **VSEPR theory**, the observed H−C−H bond angle in the tetrahedral CH_4 molecule is actually 109.5°. Therefore, the methane molecule cannot be adequately represented by simple overlap of the 2s and 2p orbitals of carbon with the 1s orbitals of each hydrogen atom.

The single 2s orbital hybridizes with the three 2p orbitals to form a set of four hybrid orbitals, called sp^3 hybrids.



The sp3 hybrids are all equivalent to one another. Spatially, the hybrid orbitals point toward the four corners of a tetrahedron (Figure below).

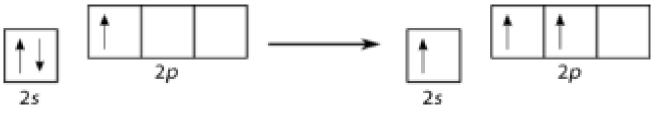


2. Hybridization of a double bond (sp^2 hybridization)

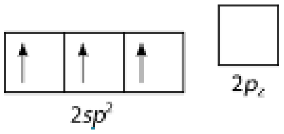
In this type, a mixing occurs between an S-type orbit with two P-type orbits to form three new hybrid orbits of equal energy and the same shape, varying in space at the level of a surface triangular equilateral. The orbits are directed towards the vertices of the triangle, and the angle between each pair of orbits is 120 degrees.

Exemple

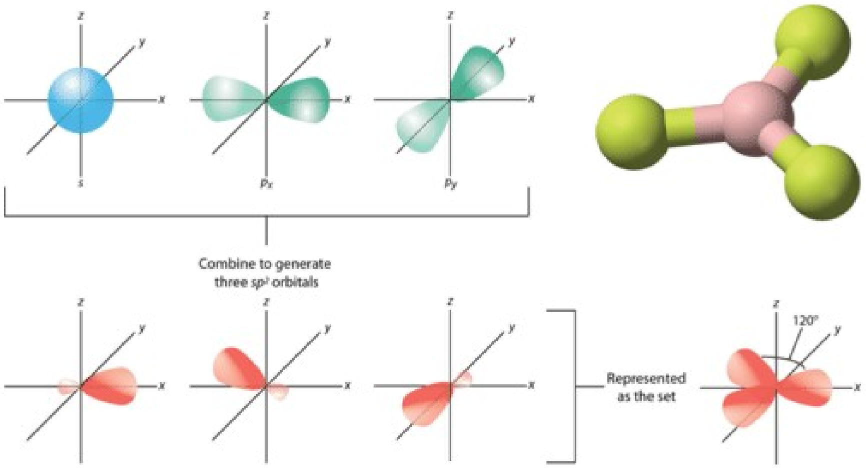
Boron trifluoride (BF3) is predicted to have a trigonal planar geometry by VSEPR. First, a paired 2s electron is promoted to an empty 2p orbital.



This is followed by hybridization of the three occupied orbitals to form a set of three sp^2 hybrids, leaving the $2p_z$ orbital unhybridized. The choice of which p orbital to leave unhybridized is arbitrary, but $2p_z$ is conventionally chosen in the case of sp^2 hybrids



The geometry of the sp^2 hybrid orbitals is trigonal planar, with the large lobe of each orbital pointing toward one corner of an equilateral triangle (Figure below). The angle between any two of the hybrid orbital lobes is 120°. Each can bond with a 2p orbital from a fluorine atom to form the trigonal planar BF_3 molecule.



3. Hybridization for triple bond (sp hybridization)

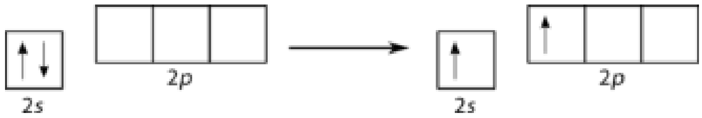
Or linear hybridization, in this type the mixing occurs between one s orbital and one P orbital, and it is called sP hybridization and the angle between the two orbitals is 180 degrees.

Example: Formation of acetylene gas from carbon and hydrogen after hybridizing the carbon orbitals.

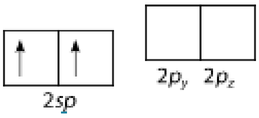
The carbon atom contributing to the formation of a triple bond needs to hybridize one 2s orbital and one 2p orbital to form two hybrid orbitals called ps. The s and p orbitals are linear and there are two orbitals perpendicular to these orbitals which are $2p_y$ and $2p_z$.

Exemple

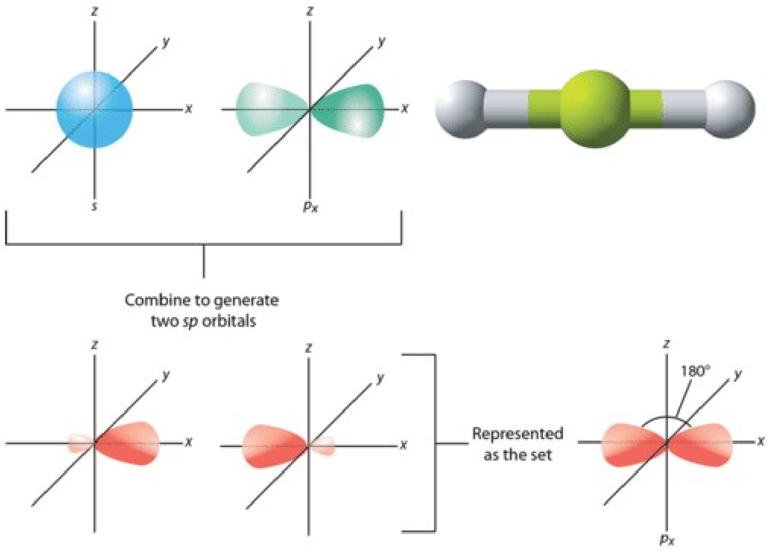
A beryllium hydride (BeH_2) molecule is predicted to be linear by VSEPR. The beryllium atom contains only paired electrons, so it must also undergo hybridization. One of the 2s electrons is first promoted to an empty 2p orbital.



The occupied orbitals are then hybridized, and the result is a pair of sp hybrid orbitals. The two remaining p orbitals (arbitrarily chosen to be p_y and p_z) do not hybridize and remain unoccupied.



The geometry of the sp hybrid orbitals is linear, with the large lobes of the two orbitals pointing in opposite directions along one axis, arbitrarily defined as the x-axis (Figure below). Each can bond with a 1s orbital from a hydrogen atom to form the linear BeH_2 molecule.



4. Hybridization of d orbitals

Elements in the third period and beyond are capable of expanding their octet to form molecules with either trigonal bipyramidal or octahedral electron domain geometries. In order to accomplish this, the previously unoccupied orbitals in the d sublevel of the central atom are involved in the hybridization process.

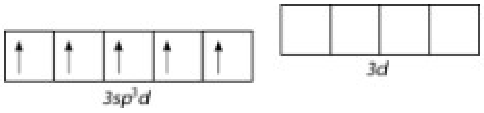
a) Hybridization sp^3d

This hybridization combines three atomic p orbitals and one atomic d orbital to create five sp^3d hybrid orbitals arranged in a pyramidal shape. Three orbitals lie in a plane with 120-degree angles between them, while two perpendicular orbitals form a 180-degree angle. These hybrid orbitals direct towards the corners of a trigonal bipyramid.

Exemple

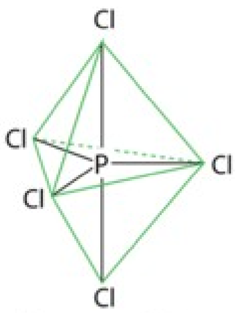
Phosphorus pentachloride (PCl_5) has a trigonal bipyramidal shape and electron domain arrangement, with one electron transitioning from the 3s orbital to fill an empty 3d orbital.

The hybridization happens with one s orbital, three p orbitals, and one d orbital. The combination of these five hybrid orbitals is known as sp^3d hybrids.

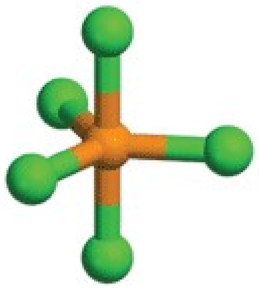


The five hybrid sp^3d orbitals overlap with the 3p orbital of each chlorine atom, forming the five covalent bonds in PCl_5. The figure below shows the shape and orientation of the sp^3d hybrid orbital sets.

sp^3d orbitals



Trigonal-bipyramidal Structure

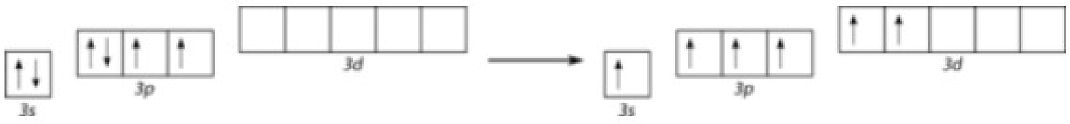


b) Hybridization sp^3d^2

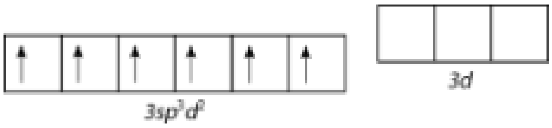
This hybridization results from the combination of an s atomic orbit and 3 p atomic orbits and 2 d atomic orbits to give six equivalent hybrid orbits of the sp^3d_2 hybridization, which takes on an octahedral shape. This hybridization occurs in molecules of the type AX_6, AX_5E, or AX_4E_2.

Exemple

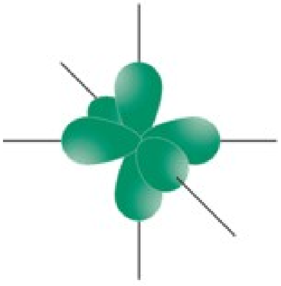
Sulfur hexafluoride (SF_6) has a molecular shape that's octahedral. Here, one 3s electron and one 3p electron are bumped up into two empty 3d orbitals



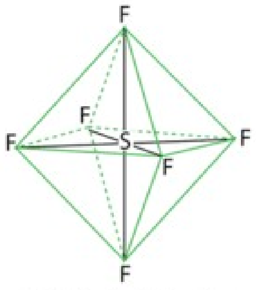
Theh now happens with one s orbital, three p orbitals, and two d orbitals. The resulting set of six equivalent orbitals is known as sp^3d^2 hybrids.



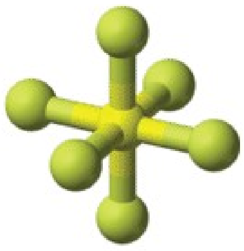
The overlap of the six hybrid sp^3d_2 orbitals with the 2p orbital of each fluorine atom results in the six covalent bonds of SF_6. Other molecular geometries derived from an octahedral electron domain geometry (square pyramidal, square planar) also exhibit this type of hybridization. The figure below shows the shape and orientation of the sp^3d^2 hybrid orbital sets.



sp^3d^2 orbitals



Octahedral Structure



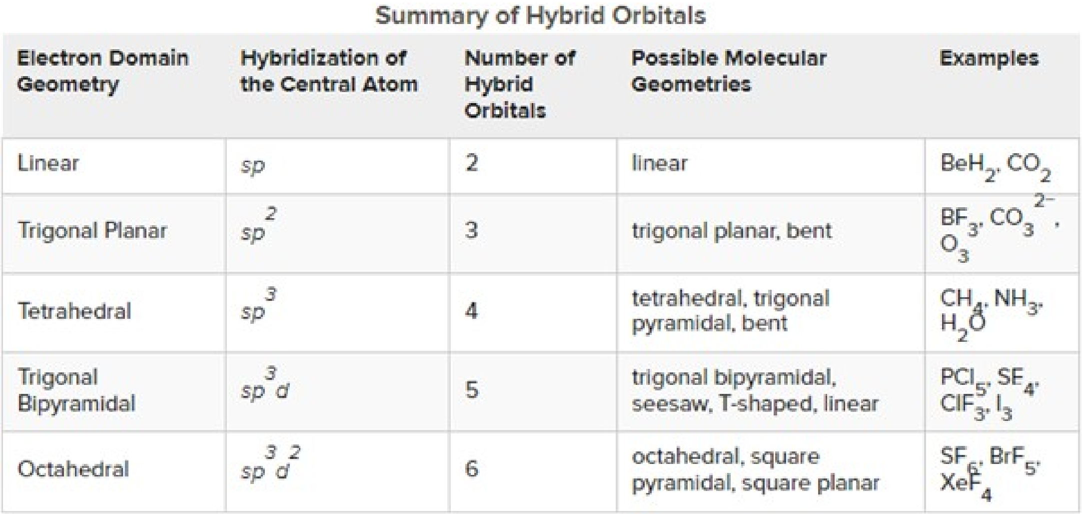
5. Conclusion

Hybridization can be summarized in three steps:

1. Draw the Lewis electron-dot structure of the molecule.
2. Apply VSEPR theory to predict the electron domain and molecular geometries.

3. Associate the electron domain geometry with the corresponding hybridization of the central atom.

Below are the possible hybridizations along with examples.



Summary of Hybrid Orbitals

Electron Domain Geometry	Hybridization of the Central Atom	Number of Hybrid Orbitals	Possible Molecular Geometries	Examples
Linear	sp	2	linear	BeH_2, CO_2
Trigonal Planar	sp^2	3	trigonal planar, bent	BF_3, CO_3^{2-}, O_3
Tetrahedral	sp^3	4	tetrahedral, trigonal pyramidal, bent	CH_4, NH_3, H_2O
Trigonal Bipyramidal	sp^3d	5	trigonal bipyramidal, seesaw, T-shaped, linear	PCl_5, SF_4, ClF_3, I_3
Octahedral	sp^3d^2	6	octahedral, square pyramidal, square planar	SF_6, BrF_5, XeF_4

Conclusion

In closing, and as a summary of what's been presented in this publication, I can say that the course on the structure of matter, aimed at first-year students in technical sciences, material sciences, and transport engineering, among others, is one of the most important courses in chemistry. This is due to its emphasis on the general concepts needed by students in their academic journey. I divided the course into seven chapters: the first chapter is about revisiting some basic concepts in chemistry; the second covers the essential elements of matter; the third describes the process of radioactivity; the fourth reviews the description and study of the atom; the fifth discusses quantum chemistry; the sixth is dedicated to the periodic classification of elements; and the seventh focuses on chemical bonding.

Finally, I hope this publication is comprehensive and well-structured, serving as a reliable reference for both students and teachers alike.