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The Atomic and Molecular Structure

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Contents

Introduction

This course is primarily designed for first-year undergraduate students in the Physical Measurements department, though it is equally beneficial for those pursuing studies in Alimentary Science. A comprehensive understanding of matter's structure necessitates a solid grasp of Atomistics, the foundational framework for this exploration. We will thoroughly examine key concepts, including classical definitions of the atom, molecule, nucleus, electron, mole, Avogadro's number, and nuclear reactions. These concepts are crucial for establishing a fundamental understanding of chemistry and physics. Following this introduction, we will delve into the electronic configuration of atoms, which describes how electrons are distributed in atomic orbitals. This will lead to an exploration of the periodic classification of elements, including an in-depth look at the periodic table and the recurring properties of elements that arise from their atomic structure.

Additionally, we will define and categorize the various types of chemical bonds—such as ionic, covalent, and metallic bonds—and discuss their significance in determining the properties and behaviors of compounds. A dedicated chapter on hybridization will be included to round out the course, which will elucidate the process by which atomic orbitals mix to form new, equivalent hybrid orbitals. This concept will be tied to the geometry of molecules, illustrating how the arrangement of atoms affects molecular shape and reactivity. By the end of the course, students will have a well-rounded understanding of these fundamental principles, equipping them with the knowledge necessary for advanced studies in both Physical Measurements and Alimentary Science.

Chapter I	Structure Of Matter
Chapter II	Radioactivity and Nuclear Reactions
Chapter III	The Electronic Configuration of Atoms
Chapter IV	Periodic classification and properties of elements
Chapter V	Chemical bonding
Chapter VI	Hybridization And Molecule Geometry

Chapter I

STRUCTURE OF MATTER

I. I. What is matter?

Matter is anything that has mass and occupies volume in space.

The three common physical states of matter

- **Solid:** definite **shape** and definite **volume**..
- **Liquid:** definite **volume** but **no fixed shape**
- The gaseous state has no defined volume or shape; it takes on the volume and shape of its container.

II. Changes of state (phase changes)

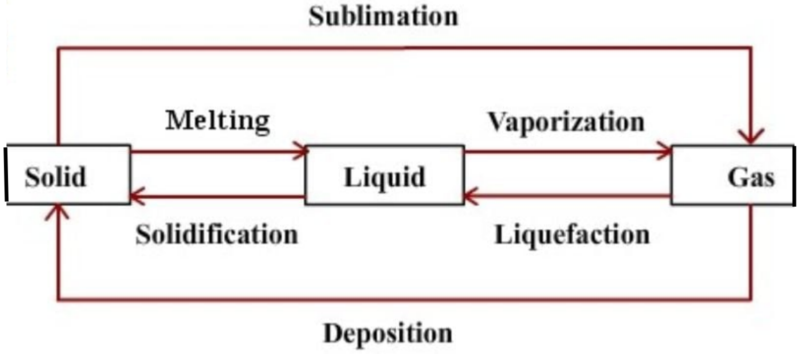
Changes of state are significant physical changes that occur at temperatures that are characteristic of the substance.

Pure iron1538°C (2800°F)

Melting temperature of **water**: 0 °C

Low Carbon Steel: 1425°C - 1540°C

a) Physical change



- Solid → Liquid: **melting**
- Liquid → Solid: **freezing / solidification**
- Liquid → Gas: **vaporization** (evaporation or boiling)
- Gas → Liquid: **condensation / liquefaction**
- Solid → Gas: **sublimation**
- Gas → Solid: **deposition**

b) Chemical change

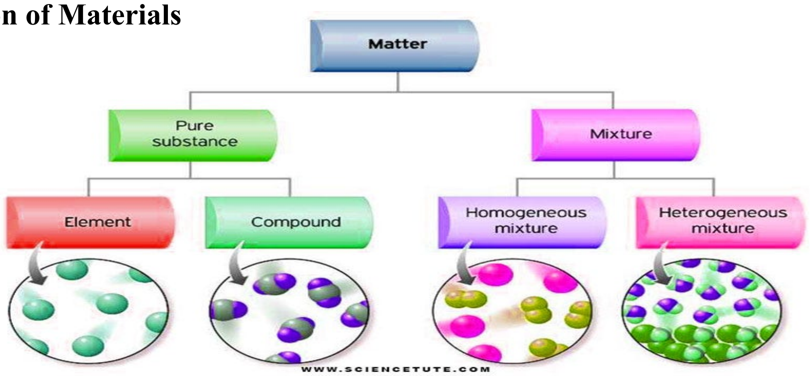
A chemical change is a transformation that changes the nature of a substance using a chemical reaction.

- Gas formation
- Precipitate formation
- Color change
- Energy released (light/heat)

Example: Iron **corrosion**. **Burning** wood.

We can recognize a chemical change through certain indicators

III. Classification of Materials



A) Pure substances

A **pure substance** contains only **one chemical entity** (atom, ion, or molecule). Two types:

- **Element (simple pure substance):** made of one kind of element (Cu, Fe, H_2, O_2…).
- **Compound (pure compound):** made of several elements chemically combined (example: water H_2O).

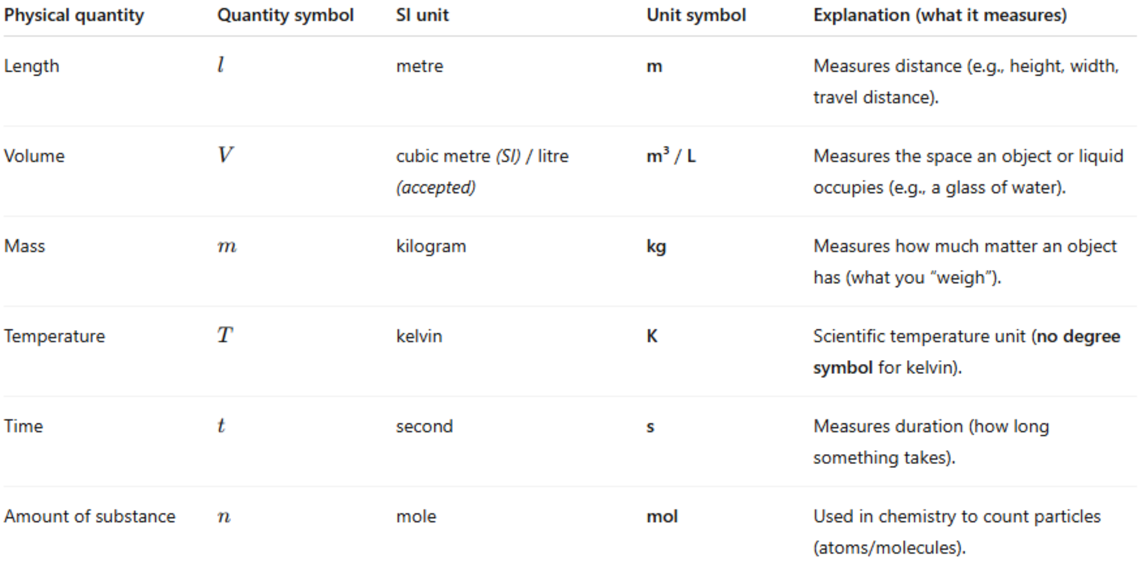
B) Mixtures substances

A mixture **contains** several kinds of chemical entities **mixed together.**

- **Homogeneous mixture:** one visible phase (e.g., salt water).
- **Heterogeneous mixture:** two or more visible phases (e.g., water + oil).

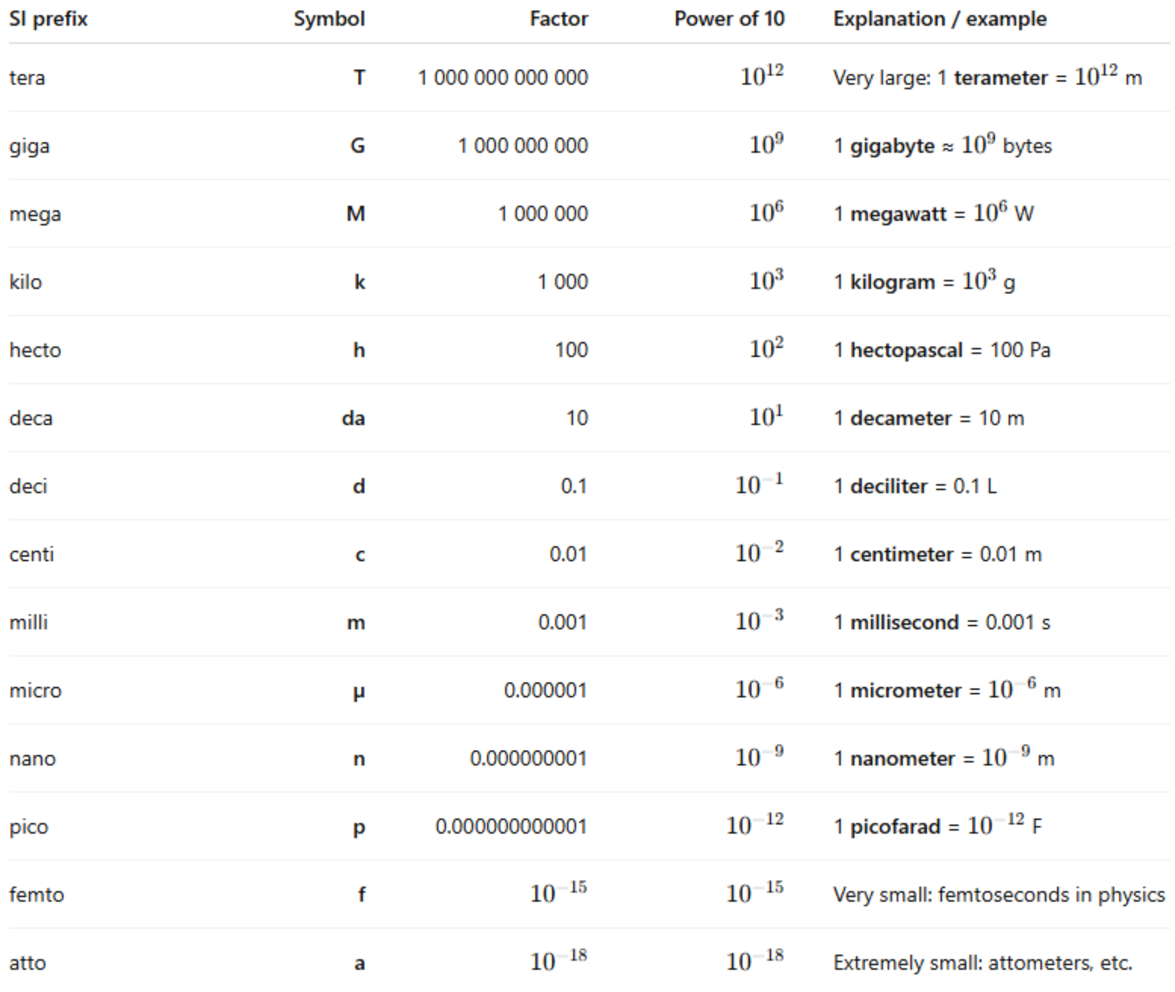
“Phase” = a part that looks uniform. If you can see layers, it’s heterogeneous.

IV. Units and prefixes (SI reminders)



Physical quantity	Quantity symbol	SI unit	Unit symbol	Explanation (what it measures)
Length	l	metre	**m**	Measures distance (e.g., height, width, travel distance).
Volume	V	cubic metre *(SI)* / litre *(accepted)*	**m^3 / L**	Measures the space an object or liquid occupies (e.g., a glass of water).
Mass	m	kilogram	**kg**	Measures how much matter an object has (what you “weigh”).
Temperature	T	kelvin	**K**	Scientific temperature unit (**no degree symbol** for kelvin).
Time	t	second	**s**	Measures duration (how long something takes).
Amount of substance	n	mole	**mol**	Used in chemistry to count particles (atoms/molecules).

To avoid using too many digits to write the values of physical quantities, the prefixes shown in the table below can be used :



SI prefix	Symbol	Factor	Power of 10	Explanation / example
tera	**T**	1 000 000 000 000	10^{12}	Very large: 1 **terameter** = 10^{12} m
giga	**G**	1 000 000 000	10^{9}	1 **gigabyte** ≈ 10^{9} bytes
mega	**M**	1 000 000	10^{6}	1 **megawatt** = 10^{6} W
kilo	**k**	1 000	10^{3}	1 **kilogram** = 10^{3} g
hecto	**h**	100	10^{2}	1 **hectopascal** = 100 Pa
deca	**da**	10	10^{1}	1 **decameter** = 10 m
deci	**d**	0.1	10^{-1}	1 **deciliter** = 0.1 L
centi	**c**	0.01	10^{-2}	1 **centimeter** = 0.01 m
milli	**m**	0.001	10^{-3}	1 **millisecond** = 0.001 s
micro	**μ**	0.000001	10^{-6}	1 **micrometer** = 10^{-6} m
nano	**n**	0.000000001	10^{-9}	1 **nanometer** = 10^{-9} m
pico	**p**	0.000000000001	10^{-12}	1 **picofarad** = 10^{-12} F
femto	**f**	10^{-15}	10^{-15}	Very small: femtoseconds in physics
atto	**a**	10^{-18}	10^{-18}	Extremely small: attometers, etc.

V. Atom, molecule, and Avogadro’s number

- The **atom** is the smallest part of an element that can exist.
- Atoms combine to form molecules, a **molecule** is a union of atoms.
- The **mole** is the unit for measuring the quantity of matter.

The number of atoms contained in a mole is called the *Avogadro Number (AN)*

$$\mathbf{N_A = 6.023\ 10^{23}}$$

VI. Number of moles and molar volume

In chemistry, the **amount of substance** is measured in **moles** (symbol **n**). A mole is a counting unit, like “a dozen,” but much bigger: **1 mole contains 6.022×10236.022 \times 10^{23}6.022×1023** particles (atoms, molecules, or ions).

The **molar mass** (symbol **M**) is the **mass of 1 mole** of a substance. It depends on the chemical formula and is usually expressed in **grams per mole (g/mol)**. For example, if a compound has a molar mass of 18 g/mol, then **1 mole** of that compound has a mass of **18 g**.

$$\mathbf{N=m/M}$$

n: number of moles

m: mass of compound in grams

M: molar mass of the compound in g/mol.

Moles from gas volume (at “normal conditions”)

Under normal conditions of temperature and pressure, one mole of gas molecules always occupies the same volume. This volume is the molar volume (VM):

V_M= 22.4 L/mol

Under these conditions, the number of moles becomes:

n= V/V_M= V/22.4

Example

1. Number of moles contained in 36 g of water :

   n= m_{water}/M_{water} = 18/36= 2 moles

2. Number of moles contained in 11.2 liters of carbon dioxide :

   n= v_{gas}/V_{molar} = 11.2/22.4=0.5 mole

VII. Atomic Mass Unit (a.m.u. or u)

he unit u is defined using the isotope carbon-12 the **u.m.a** or (**u**).

1 u.m.a =1/12 mc=1/NA=1.66 . 10-24 g=1,66 . 10-27 Kg (mc=12/N)

Why carbon-12?

Carbon-12 is stable, common, and easy to use as a reference standard. It provides a reliable “reference atom” for measuring other atomic masses.

Connection between u and the mole (Avogadro’s number)

Avogadro’s number is:

$$N_A=6.022\times1023\ \mathrm{mol}^{-1}$$

- **1 mole** of particles contains N_A particles.

A very useful result links **u** and **grams**:

$$1\ \mathrm{u} \approx 1/N_A\ \mathrm{g}$$

This leads to the numeric conversions:

$$1\ \text{u} \approx 1.66\times10^{-24}\ \text{g} \longrightarrow 1\text{u} \approx 1.66\times10^{-27}\ \text{kg}$$

VIII. Atomic molar mass and molecular molar mass

- Atomic molar mass: is the mass of one mole of atoms.

Ex: M(C)= 12.0 g/mol and M(0) = 16.0 g/mol

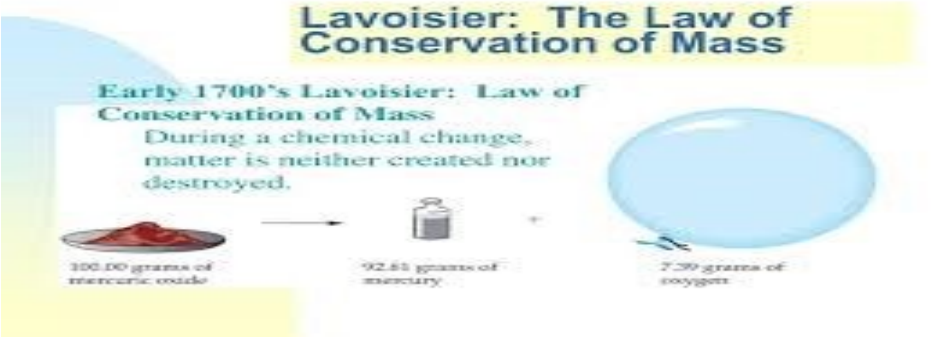
- Molecular molar mass: is the mass of one mole of molecules.

Ex: The molar mass of water H_2O: M(H_2O)= 2.1+16=18 g/mol

IX. Law of conservation of mass (Lavoisier), chemical reaction

"NOTHING IS LOST, NOTHING IS CREATED, EVERYTHING IS TRANSFORMED".

(Lavoisier 1743-1794)



Lavoisier: The Law of Conservation of Mass

Early 1700's Lavoisier: Law of Conservation of Mass

During a chemical change, matter is neither created nor destroyed.

A balanced chemical equation respects two key principles:

- **Conservation of elements:** during a reaction, atoms are neither created nor destroyed; they are only rearranged. Therefore, each element must appear with the same number of atoms on both sides of the equation.
- **Conservation of mass (Lavoisier's law):** in a closed system, the total mass remains constant, so the mass of the reactants that react is equal to the mass of the products that are formed.

X. Qualitative and Quantitative Analysis of Matter

a) solutions

A **solution** is a **homogeneous mixture** made up of two or more substances. Solutions may exist in the **liquid, solid, or gaseous** state.

- The **solvent** is the substance (most often a liquid) that **dissolves** the other component(s). It is usually present in the **largest amount**.

- The **solute** is the substance (ionic or molecular) that is **dissolved** in the solvent, generally in a **smaller amount**.
- When **water** is the solvent, the mixture is called an **aqueous solution**.

b) concentrations

Concentration expresses the proportion of solute compared with the solvent or the whole solution. Several units are used:

1) Molarity (**C_M**): number of **moles of solute per liter of solution** (mol.L−1)

2) Molality (**C_m**): expresses the quantity of solute contained in 1000g of solvent.(mol.Kg^{-1})

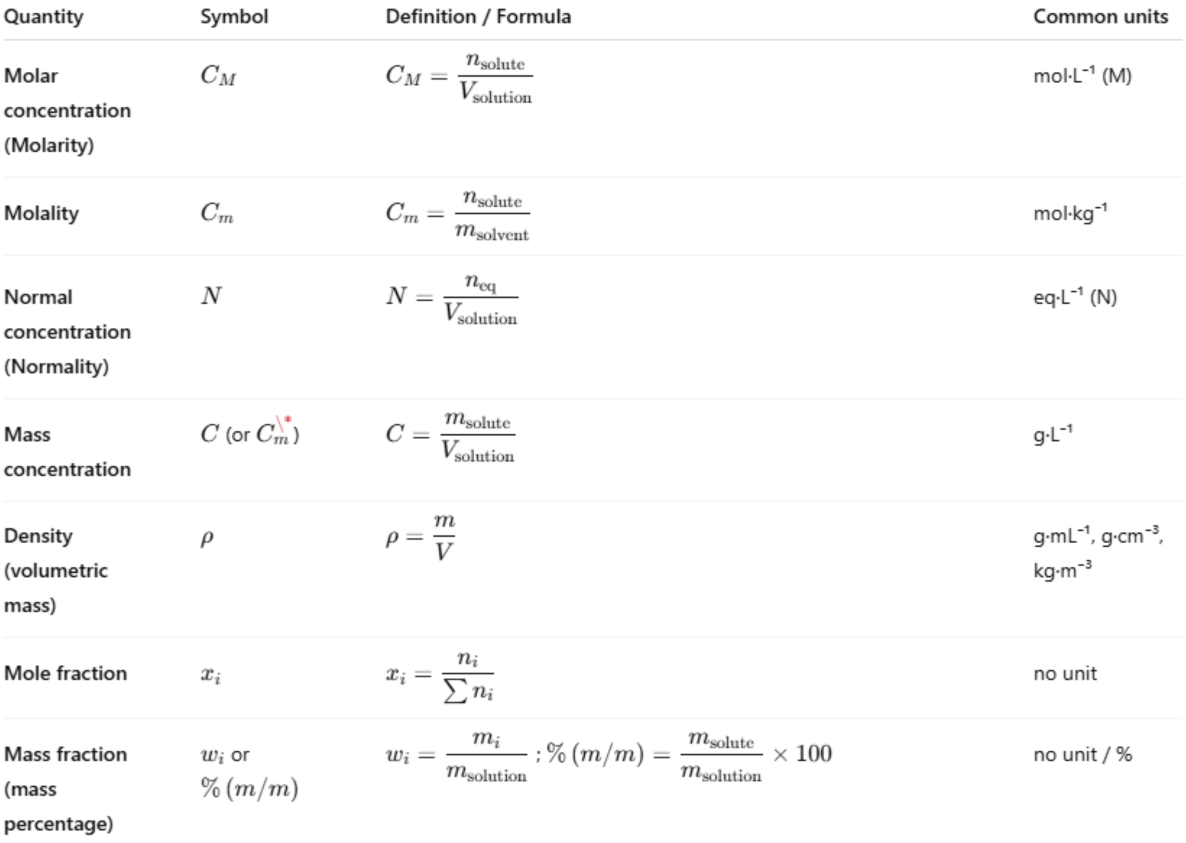
3) Normality (**N**): number of **equivalents of solute per liter of solution** (eq.g/l).

An **equivalent** depends on the reaction and corresponds to one mole of the “active” species involved (such as H_3O^+, OH^-, or e^-).

4) The percentage % of a solution indicates the mass of substance per 100g of solution.

solution. This is a weight-for-weight comparison:

5) The mole fraction (**xi**) indicates the ratio between the number of moles and the total number of moles in the solution.



Quantity	Symbol	Definition / Formula	Common units
Molar concentration (Molarity)	C_M	$C_M = \frac{n_{\text{solute}}}{V_{\text{solution}}}$	mol·L⁻¹ (M)
Molality	C_m	$C_m = \frac{n_{\text{solute}}}{m_{\text{solvent}}}$	mol·kg⁻¹
Normal concentration (Normality)	N	$N = \frac{n_{\text{eq}}}{V_{\text{solution}}}$	eq·L⁻¹ (N)
Mass concentration	C (or $C_m^{\backslash *}$)	$C = \frac{m_{\text{solute}}}{V_{\text{solution}}}$	g·L⁻¹
Density (volumetric mass)	ρ	$\rho = \frac{m}{V}$	g·mL⁻¹, g·cm⁻³, kg·m⁻³
Mole fraction	x_i	$x_i = \frac{n_i}{\sum n_i}$	no unit
Mass fraction (mass percentage)	w_i or $\%\,(m/m)$	$w_i = \frac{m_i}{m_{\text{solution}}}$; $\%\,(m/m) = \frac{m_{\text{solute}}}{m_{\text{solution}}} \times 100$	no unit / %

XI. dilution of an aqueous solution

Diluting an aqueous solution involves reducing its concentration by adding solvent (water).

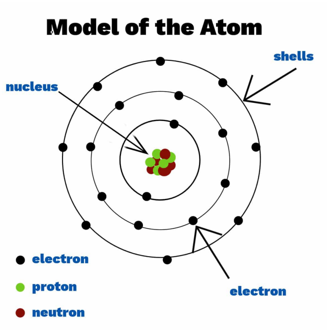
- The initial solution of higher concentration is called **the stock solution**
- The final solution of lower concentration is called the **daughter solution (diluted solution)**.

During a dilution, the quantity of solute is conserved so that we can write :

The problem is to determine the volumes: **Vi**: volume of stock solution to be taken and **Vf**: volume of dilute solution corresponding to that in the volumetric flask.

XII. Notion of Atom, Electron and Nucleus

Atoms differ in structure and mass, and are themselves divided into small parts: electrons and the nucleus (protons + neutrons).



- *The electron*: charged entity (-) is a universal constituent of matter (qé= -1.6 10^{-19} C, m(é) = 9.1 10^{-31} Kg) [Thomson and Mulliken's experiment] (allowed us to determine charge and mass).
- *The nucleus*: the nucleus is made up of stable elementary particles called nucleons, which can take two forms in the free state, neutron and proton.

-*Protons*: are charged particles (+) (qp= +1.6 10^{-19} C, mp=1.673 10^{-27} Kg)

mp ≈ 1836. mé= 1.007 u.m.a

- *Neutrons:* are particles carrying charges (0) (qn= 0 C, mn=1.673 10^{-27} Kg) [Rutherford experiment] (We were able to determine the constituents of the nucleus).

XIII. Identification of components

a- Representation

Each chemical element has its own symbol. It is always written with a capital letter, possibly followed by a small letter: ${}_{Z}^{A}X$

b- Symbolic writing

A is defined as the number of nucleons or mass nbr (protons + neutrons). **Z**: is called the atomic number or number of charges or number of protons (it is also the number of electrons for a neutral atom). **N**: number of neutrons (**N=A-Z**).

c- Isotopes

- These are atoms with the same atomic number (Z) but different mass numbers. An element may have one or more isotopes.
- A number of terms can be defined from the numbers A, Z and N.
- Isotonic: same number of neutrons (N).
- Isobaric: same number of nucleons (A), but different number of protons; the nucleus has approximately the same mass.

d- Isoelectronics : same number of electrons

e- Isotopic composition :

The **average atomic mass** of an element, noted M(X), is the **weighted mean** of the masses of its isotopes, using their **natural abundances** as weights.

If the element X has isotopes 1,2,…,n with:

- isotopic masses: M1,M2,…,MnM_1, M_2, \dots, M_nM1,M2,…,Mn
- natural abundances: nτ1,τ2,…,τn (in %)

then:

$$M(x) = \frac{M1\tau 1 + M2\tau 2 + \mathrm{M3}\tau 3 + \cdots \ldots . + \mathrm{Mn}\tau\mathrm{n}}{100}$$

Equivalently (if abundances are written as fractions xix_ixi where

$$\sum \mathrm{xi} = 1$$

$$M(x) = \sum_{i}^{n} MiXi$$

Where:

- M(X) = average atomic mass of element X
- τi = natural abundance of isotope i (in %)
- Mi = atomic mass of isotope i

TUTORIAL N° 01

Exercise 01

These include oxygen (O2), silver (Ag), cooking salt (NaCl), mineral water, seawater, oil and sugar water.

a) Indicate which are in the pure state and which are in a mixture.

b) Which bodies are simple and which are compound?

c) Classify them into homogeneous and heterogeneous mixtures, indicating the number of phases.

Exercise 02

1. Calculate the number of moles in the following cases:

a- 5 g gold M(Au) = 197g/mol b- 1 mg silver M(Ag) = 107g/mol

c- 1 kg of carbon M(C)= 12g/mol d- 0.5 kg of silicon M(Si) = 28 g/mol e- 4.48 litres of nitrogen gas (N2); M(N) = 14g/mol

2. Calculate the mass (or volume) contained in :

a- 0.2 moles of iron b- 4 moles of sodium chloride

c- 30 moles of dihydrogen (D) d- 0.6 moles of sulphuric acid (H2SO4).

Exercise 03

1. The non-equilibrium equation for the following reaction is given: C + CuO→ Cu + CO2

a) Balance the reaction

b) Calculate the molecular or atomic molar masses of all the reactants and products.

c) 18 g of carbon are reacted. What is the mass of copper obtained at the end of the reaction?

2. Calculate the quantity of substance contained in :

a.1.6 g methane (CH_4) /

b. 1.7 g ammonia (NH_3) /

c. 4.4 g carbon dioxide (CO_2).

3. What mass is contained in :

a.0.2 moles of ethane (C_2H_6) /

b.2.5 moles of sulphuric acid (H_2SO_4).

Exercise 04

Balance the following reactions to obey the first law:

1. $Al + S \longrightarrow Al_2S_3$
2. $C + O_2 \longrightarrow CO_2$

3. $Fe + O_2 \longrightarrow Fe_2O_3$
4. $PbO + C \longrightarrow Pb + CO_2$
5. $C_3H_8 + Cl_2. \longrightarrow C + HCl$

Exercise 05

Here is the equation that represents this reaction: $S(s)+ O_2(g) \rightarrow SO_2(g)$.

a) What is the molar mass of sulfur dioxide?

b) If combustion of the sulphur produces 48 g of sulphur dioxide, what was the initial mass of sulphur?

c) How much oxygen is needed to burn 100 g of sulphur?

Exercise 06

Dissolve 12g KOH in 250ml water.

Calculate the number of moles of KOH dissolved, the molality, molarity, normality and mole fraction of KOH.

Given that: the density of water is 1kg/l and M(K) = 39g/mol.

Exercise 07

100 mL of aqueous diiodine solution (I2) with a concentration of 5.0 x 10-2 mol.L-1 is available.

What volume of stock solution should be used to prepare 50.0 mL of dilute diiodine solution with a concentration of 1.0.10-2mol.L-1?

Exercise 08

Nitric acid has a molecular weight of 63g/mol.

a- Calculate the molar concentration of a concentrated commercial solution of 90% nitric acid, with a density of 1.482 g/cm3.

b- What is the volume of this concentrated commercial solution needed to prepare one litre of
1 M nitric acid?

c- What is the volume of this concentrated commercial solution needed to prepare 15 ml of
0.1 M nitric acid?

Exercise 09

a- Numbers can be entered in the three positions A, Z, and q on the X symbol of an element. What exactly does each of these mean?

b-What is the number of protons, neutrons and electrons present in each of the following atoms or ions?

${}^{19}_{9}F \quad {}^{24}_{12}Mg \quad {}^{79}_{34}Se^{-2}$

c- Four nuclides A, B, C and D have nuclei composed as shown below:

	A	B	C	D
Number of protons	21	22	22	20
Number of neutrons	26	25	27	27
Mass Number.	47	47	49	47

Are there any isotopes among these four nuclides?

Exercise 10 :

What is the number of protons, neutrons, and electrons that make up the following structures?

${}^{12}_{6}C$ ${}^{13}_{6}C$ ${}^{14}_{6}C$ ${}^{16}_{8}0$ ${}^{16}_{8}O^{-2}$ ${}^{27}_{13}Al^{+3}$ ${}^{56}_{26}Fe^{+3}$ ${}^{40}_{20}Ca^{+2}$

Exercise 11:

Draw up a list of isobars and isotones of the following nucleons:

^{15}O; ^{14}N; ^{13}C; ^{12}B; ^{17}O; ^{15}N; ^{16}O; ^{18}F; ^{17}F.

Exercise 12 :

a- Calculate the atomic mass of natural chlorine, knowing that it is made up of 75.4% of the 35Cl isotope and 24.6% of the 36Cl isotope.

M (^{35}Cl) = 34.967420 g and M (^{36}Cl) = 36.96560 g

b- Carbon in its natural state (C=12.011) contains 98.89% carbon 12. Calculate the atomic mass of the isotope carbon 13. two isotopes 12C and 13C. Knowing that

Exercises Solutions

Exercise 01: Classification of Matter

These include oxygen (O_2), silver (Ag), cooking salt (NaCl), mineral water, seawater, oil and sugar water.

a) Pure state or mixture

Pure substances (Pure state)

- Oxygen (O_2) - A pure element consisting of only O_2 molecules
- Silver (Ag) - A pure element consisting of only Ag atoms
- Cooking salt (NaCl) - A pure compound with a fixed chemical composition

Mixtures

- Mineral water - Contains water and dissolved minerals (salts, ions)
- Seawater - Contains water and dissolved salts (primarily NaCl, $MgCl_2$, etc.)
- Oil - When considering oil and water mixture, it forms a mixture
- Sugar water - Contains water and dissolved sugar

b) Simple or compound bodies

Simple substances (Elements)

- Oxygen (O_2) - An element composed of only one type of atom (oxygen)
- Silver (Ag) - An element composed of only one type of atom (silver)

Compound substances

- Cooking salt (NaCl) - A compound composed of sodium and chlorine atoms in a fixed ratio (1:1)

Note: The mixtures (mineral water, seawater, oil, sugar water) are neither simple nor compound substances. They are combinations of multiple substances and therefore classified as mixtures.

c) Classification into homogeneous and heterogeneous mixtures

Homogeneous mixtures (1 phase)

A homogeneous mixture has a uniform composition throughout with no visible boundaries between components.

- Mineral water - One liquid phase; dissolved minerals are uniformly distributed
- Seawater - One liquid phase; dissolved salts are uniformly distributed
- Sugar water - One liquid phase; dissolved sugar is uniformly distributed

Heterogeneous mixtures (Multiple phases)

A heterogeneous mixture has a non-uniform composition with visible boundaries between different phases.

- Oil and water - Two distinct liquid phases (immiscible liquids); oil does not dissolve in water, creating a visible separation

Note: If "oil" refers to pure oil alone (not mixed with water), it would be considered a pure substance in the liquid state (1 phase), not a mixture.

Exercise 02 :

1. Calculate the number of moles

Formulas:

- n = m/M (for solids/liquids)
- n = V/22.4 (for gases at STP)

Problem	Calculation	Answer
a) 5 g Au	5 ÷ 197	**0.0254 mol**
b) 1 mg Ag	0.001 ÷ 107	**9.35×10^{-6} mol**
c) 1 kg C	1000 ÷ 12	**83.33 mol**
d) 0.5 kg Si	500 ÷ 28	**17.86 mol**
e) 4.48 L N_2	4.48 ÷ 22.4	**0.2 mol**

2. Calculate the mass (or volume)

Formulas:

- m = n × M
- V = n × 22.4 (for gases at STP)

Problem	Molar Mass	Calculation	Answer
a) 0.2 mol Fe	56 g/mol	0.2 × 56	**11.2 g**
b) 4 mol NaCl	58.5 g/mol	4 × 58.5	**234 g**
c) 30 mol H_2	2 g/mol	30 × 2	**60 g** or **672 L**
d) 0.6 mol H_2SO_4	98 g/mol	0.6 × 98	**58.8 g**

Key Molar Masses Used

- Fe = 56 g/mol
- NaCl = 23 + 35.5 = 58.5 g/mol
- H_2 = 2 g/mol
- H_2SO_4 = 2(1) + 32 + 4(16) = 98 g/mol
- Molar volume (STP) = 22.4 L/mol

Exercise 03:

1. Chemical Reaction: $C + CuO \rightarrow Cu + CO_2$

a) Balance the Reaction

Unbalanced: $C + CuO \rightarrow Cu + CO_2$

Balanced equation:

$$2CuO + C \rightarrow 2Cu + CO_2$$

b) Molar Masses of Reactants and Products

Substance	Composition	Molar Mass
C (Carbon)	1 × 12	**12 g/mol**
CuO (Copper oxide)	63.5 + 16	**79.5 g/mol**
Cu (Copper)	1 × 63.5	**63.5 g/mol**
CO_2 (Carbon dioxide)	12 + 2(16)	**44 g/mol**

c) Mass of Copper Obtained from 18 g of Carbon

Given: 18 g of C

Step 1: Calculate moles of C

$$n(\mathrm{C}) = \frac{m}{M} = \frac{18}{12} = 1.5 \text{ mol}$$

Step 2: Use stoichiometry from balanced equation: 1 C → 2 Cu

$$n(\mathrm{Cu}) = 1.5 \times 2 = 3.0 \text{ mol}$$

Step 3: Calculate mass of Cu

$$m(\mathrm{Cu}) = n \times M = 3.0 \times 63.5 = 190.5 \text{ g}$$

Answer: 190.5 g of copper

2. Calculate the Quantity of Substance (Number of Moles)

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

a) 1.6 g of methane (CH_4)

Molar mass: $M(CH_4) = 12 + 4(1) =$ **16 g/mol**

$$n = \frac{1.6}{16} = 0.10 \text{ mol}$$

Answer: 0.10 mol

b) 1.7 g of ammonia (NH_3)

Molar mass: $M(NH_3) = 14 + 3(1) =$ **17 g/mol**

$$n = \frac{1.7}{17} = 0.10 \text{ mol}$$

Answer: 0.10 mol

c) 4.4 g of carbon dioxide (CO_2)

Molar mass: $M(CO_2) = 12 + 2(16) =$ **44 g/mol**

$$n = \frac{4.4}{44} = 0.10 \text{ mol}$$

Answer: 0.10 mol

3. Calculate the Mass Contained In

Formula: $m = n \times M$

a) 0.2 moles of ethane (C_2H_6)

Molar mass: M(C_2H_6) = 2(12) + 6(1) = **30 g/mol**

$$m = 0.2 \times 30 = 6.0 \text{ g}$$

Answer: 6.0 g

b) 2.5 moles of sulphuric acid (H_2SO_4)

Molar mass: M(H_2SO_4) = 2(1) + 32 + 4(16) = **98 g/mol**

$$m = 2.5 \times 98 = 245 \text{ g}$$

Answer: 245 g

Exercise 04:

1. $2\text{Al} + 3\text{S} \rightarrow \text{Al}_2\text{S}_3$

2. $\text{C} + \text{O}_2 \rightarrow \text{CO}_2$

3. $4\text{Fe} + 3\text{O}_2 \rightarrow 2\text{Fe}_2\text{O}_3$

4. $2\text{PbO} + \text{C} \rightarrow 2\text{Pb} + \text{CO}_2$

5. $\boldsymbol{C}_3\text{H}_8 + 4\text{Cl}_2 \rightarrow 3\text{C} + 8\text{HCl}$

Exercice 05 :

Reaction Equation

$$\text{S(s)} + \text{O}_2\text{(g)} \rightarrow \text{SO}_2\text{(g)}$$

a) Molar mass of sulphur dioxide (SO_2)

$$M(\text{SO}_2) = M(\text{S}) + 2 \times M(\text{O})$$

$$M(\text{SO}_2) = 32 + 2(16) = 32 + 32 = 64 \text{ g/mol}$$

b) Initial mass of sulphur for 48 g SO_2 produced

Mass of SO_2 = 48 g

Initial mass of S

Calculate moles of SO_2

$$n(\text{SO}_2) = \frac{m}{M} = \frac{48}{64} = 0.75 \text{ mol}$$

Use stoichiometry from balanced equation (1:1 mole ratio)

$$n(\text{S}) = n(\text{SO}_2) = 0.75 \text{ mol}$$

Calculate mass of S

$$m(\text{S}) = n \times M = 0.75 \times 32 = 24 \text{ g}$$

Answer: 24 g of sulphur

c) Oxygen needed to burn 100 g of sulphur

Given: Mass of S = 100 g

Mass of O_2 required

Calculate moles of S

$$n(\text{S}) = \frac{m}{M} = \frac{100}{32} = 3.125 \text{ mol}$$

Use stoichiometry (1:1 mole ratio: S : O_2)

$$n(\text{O}_2) = n(\text{S}) = 3.125 \text{ mol}$$

Calculate mass of O_2

$$m(\text{O}_2) = n \times M = 3.125 \times 32 = 100 \text{ g}$$

100 g of oxygen

Exercise 06:

Given Data

- Mass of KOH = 12 g
- Volume of water = 250 mL = 0.250 L
- Density of water = 1 kg/L
- Molar mass: M(K) = 39 g/mol, M(O) = 16 g/mol, M(H) = 1 g/mol
- **M(KOH) = 39 + 16 + 1 = 56 g/mol**

1. Number of Moles of KOH

$$n(\text{KOH}) = \frac{m}{M} = \frac{12}{56} = 0.214 \text{ mol}$$

Answer: 0.214 mol (or 3/14 mol)

2. Molality (m)

Formula: $m = \frac{n_{\text{solute}}}{m_{\text{solvent (kg)}}}$

Mass of solvent: 250 mL × 1 kg/L = 0.250 kg

$$m = \frac{0.214}{0.250} = 0.857 \text{ mol/kg}$$

Answer: 0.857 mol/kg (or ≈ 0.86 mol/kg)

3. Molarity (M)

Formula: $M = \frac{n_{\text{solute}}}{V_{\text{solution (L)}}}$

Assuming solution volume ≈ 250 mL = 0.250 L:

$$M = \frac{0.214}{0.250} = 0.857 \text{ mol/L}$$

Answer: 0.857 mol/L (or ≈ 0.86 M)

4. Normality (N)

Formula: $N = n_{\text{equivalents}} \times M$

For KOH (strong monoprotic base with 1 OH^- group):

- n(equivalents) = 1

$$N = 1 \times 0.857 = 0.857\ \text{N}$$

Answer: 0.857 N (or ≈ 0.86 N)

5. Mole Fraction of KOH (X_KOH)

Formula: $X_{\text{KOH}} = \frac{n_{\text{KOH}}}{n_{\text{total}}}$

Step 1: Calculate moles of water

$$n(\text{H}_2\text{O}) = \frac{m}{M} = \frac{250}{18} = 13.89\ \text{mol}$$

Step 2: Total moles

$$n_{\text{total}} = 0.214 + 13.89 = 14.10\ \text{mol}$$

Step 3: Mole fraction

$$X_{\text{KOH}} = \frac{0.214}{14.10} = 0.0152$$

Answer: 0.0152 (or ≈ 1.52%)

Exercise 07 :

Given Data

- Stock solution volume available: 100 mL
- Stock concentration: $C_1 = 5.0 \times 10^{-2}$ mol·L⁻¹
- Desired solution volume: $V_2 = 50.0$ mL
- Desired concentration: $C_2 = 1.0 \times 10^{-2}$ mol·L⁻¹

Dilution Calculation

Formula: $C_1V_1 = C_2V_2$

Solve for V_1 (volume of stock solution needed):

$$V_1 = \frac{C_2 \times V_2}{C_1}$$

$$V_1 = \frac{(1.0 \times 10^{-2}) \times 50.0}{5.0 \times 10^{-2}}$$

$$V_1 = \frac{0.5}{0.05} = 10.0\ \text{mL}$$

Answer: 10.0 mL of stock I_2 solution is needed

Exercise 08:

Given Data

- Molecular weight of HNO_3: M = 63 g/mol
- Commercial solution: 90% HNO_3 by mass
- Density of commercial solution: ρ = 1.482 g/cm³

a) Molar Concentration of 90% HNO_3 Solution

Calculate mass of solution in 1 L

$$\text{Mass of 1 L} = 1.482\ \text{g/mL} \times 1000\ \text{mL} = 1482\ \text{g}$$

Calculate mass of HNO_3 (90% by mass)

$$\text{Mass of HNO}_3 = 0.90 \times 1482 = 1333.8\ \text{g}$$

Calculate moles of HNO_3

$$n(\text{HNO}_3) = \frac{1333.8}{63} = 21.17\ \text{mol}$$

Calculate molarity

$$M = \frac{21.17\ \text{mol}}{1\ \text{L}} = 21.17\ \text{M}$$

Answer: ≈ 21.2 M (or 21 mol/L)

b) Volume of Stock Solution for 1 L of 1 M HNO_3

Formula: $C_1V_1 = C_2V_2$

Given:

- C_1 = 21.2 M (concentrated solution)
- C_2 = 1.0 M (desired dilute solution)
- V_2 = 1.0 L = 1000 mL (desired volume)

Calculate V_1:

$$V_1 = \frac{C_2 \times V_2}{C_1} = \frac{1.0 \times 1000}{21.2} = 47.2\ \text{mL}$$

Answer: ≈ 47–48 mL of concentrated HNO_3

c) Volume of Stock Solution for 15 mL of 0.1 M HNO_3

Formula: $C_1V_1 = C_2V_2$

Given:

- C_1 = 21.2 M (concentrated solution)
- C_2 = 0.1 M (desired dilute solution)
- V_2 = 15 mL (desired volume)

Calculate V_1:

$$V_1 = \frac{C_2 \times V_2}{C_1} = \frac{0.1 \times 15}{21.2} = 0.0708\ \text{mL}$$

Answer: ≈ 0.07 mL (or 70 µL) of concentrated HNO_3

Exercise 09 :

Part a) Nuclear Notation: A, Z, and q

In the nuclear symbol notation $^{A}_{Z}X^{q}$, the three positions have the following meanings:

Position A (Mass Number)

- **Definition**: Total number of nucleons in the nucleus
- **Calculation**: A = Number of protons + Number of neutrons
- **Location**: Superscript on the upper left of the element symbol
- **Significance**: Identifies the specific isotope of an element

Position Z (Atomic Number)

- **Definition**: Number of protons in the nucleus
- **Key Property**: Z uniquely identifies the element (determines which element it is)
- **Electrons in neutral atom**: electrons = Z
- **Location**: Subscript on the lower left of the element symbol
- **Significance**: Defines the chemical properties and element identity

Position q (Net Charge)

- **Definition**: Electric charge of the ion
- **Positive charge (+)**: Indicates loss of electrons (cation)
- **Negative charge (-)**: Indicates gain of electrons (anion)
- **Location**: Superscript on the upper right of the element symbol
- **Neutral atoms**: No charge shown (q = 0)
- **Significance**: Shows ionization state of the atom

Part b) Protons, Neutrons, and Electrons

General Formulas

The relationships for calculating particles in atoms and ions:

- **Number of protons** = Z (atomic number)
- **Number of neutrons** = A − Z (mass number minus atomic number)
- **Number of electrons** = Z − q (atomic number minus charge)
  - For neutral atoms (q = 0): electrons = Z
  - For positive ions (q = +n): electrons = Z − n
  - For negative ions (q = −n): electrons = Z + n

Worked Examples

Example 1: $^{19}_{9}F$ (Fluorine-19, neutral atom)

- **Protons**: 9
- **Neutrons**: 19 − 9 = 10
- **Electrons**: 9

Example 2: $^{24}_{12}$Mg (Magnesium-24, neutral atom)

- **Protons**: 12
- **Neutrons**: 24 − 12 = 12
- **Electrons**: 12

Example 3: $^{79}_{34}Se^{-2}$ (Selenide ion, -2 charge)

- **Protons**: 34
- **Neutrons**: 79 − 34 = 45
- **Electrons**: 34 + 2 = 36 (gained 2 electrons due to -2 charge)

Part c) Isotopes Among Four Nuclides

Data Summary Table

Property	**Nuclide A**	**Nuclide B**	**Nuclide C**	**Nuclide D**
Number of protons (Z)	21	22	22	20
Number of neutrons	26	25	27	27
Mass Number (A)	47	47	49	47
Element	Scandium (Sc)	Vanadium (V)	Vanadium (V)	Calcium (Ca)

Analysis of the Four Nuclides

Comparing atomic numbers (Z values):

- **Nuclides B and C**: Both have Z = 22 (both are Vanadium atoms)
  - B has 25 neutrons (A = 47)
  - C has 27 neutrons (A = 49)
  - Different number of neutrons despite same Z
- **Nuclide A**: Z = 21 (Scandium)
  - Different from B and C
- **Nuclide D**: Z = 20 (Calcium)
  - Different from B, C, and A

Nuclides B and C ARE isotopes of each other because:

- Same number of protons: Z = 22
- Different number of neutrons: 25 versus 27
- Different mass numbers: A = 47 versus A = 49

- Both are Vanadium isotopes:

Exercise 10 :

For each nuclide, the number of particles is determined using the nuclear notation $^{A}_{Z}\mathrm{X}^{q}$:

- **Protons** = Atomic number Z
- **Neutrons** = Mass number A minus atomic number Z (i.e., $A - Z$)
- **Electrons** = Atomic number Z corrected by the ionic charge q
  - For a positive charge: subtract the charge from Z
  - For a negative charge: add the charge to Z
  - For neutral atoms: electrons = protons = Z

Solutions

Nuclide	Protons	Neutrons	Electrons	Notes
$^{12}_{6}\mathrm{C}$	6	6	6	Neutral atom
$^{13}_{6}\mathrm{C}$	6	7	6	Neutral atom; isotope of $^{12}\mathrm{C}$
$^{14}_{6}\mathrm{C}$	6	8	6	Neutral atom; isotope of $^{12}\mathrm{C}$
$^{16}_{8}\mathrm{O}$	8	8	8	Neutral atom
$^{16}_{8}\mathrm{O}^{2-}$	8	8	10	Anion with 2 extra electrons
$^{27}_{13}\mathrm{Al}^{3+}$	13	14	10	Cation; lost 3 electrons
$^{56}_{26}\mathrm{Fe}^{3+}$	26	30	23	Cation; lost 3 electrons
$^{40}_{20}\mathrm{Ca}^{2+}$	20	20	18	Cation; lost 2 electrons

Exercise 11:

Isobars are nuclides with the same mass number (A) but different atomic numbers (Z). They have different numbers of protons and neutrons.

Isotones are nuclides with the same number of neutrons (N) but different atomic numbers (Z) and mass numbers (A).

The relationship is: $N = A - Z$ (neutron number = mass number − atomic number)

Data for Each Nuclide

First, let's determine the atomic number, mass number, and neutron number for each nuclide:

Nuclide	Z	A	$N = A - Z$
$^{15}\mathrm{O}$	8	15	7
$^{14}\mathrm{N}$	7	14	7
$^{13}\mathrm{C}$	6	13	7
$^{12}\mathrm{B}$	5	12	7
$^{17}\mathrm{O}$	8	17	9

^{15}N	7	15	8
^{16}O	8	16	8
^{18}F	9	18	9
^{17}F	9	17	8

Key atomic numbers:

- Boron (B) = 5
- Carbon (C) = 6
- Nitrogen (N) = 7
- Oxygen (O) = 8
- Fluorine (F) = 9

Isobars (Same Mass Number A)

Isobars with $A = 12$

- ^{12}B ($Z = 5, N = 7$)

Note: Only one nuclide with $A = 12$ *in the list.*

Isobars with $A = 13$

- ^{13}C. ($Z = 6, N = 7$)

Note: Only one nuclide with $A = 13$ *in the list.*

Isobars with $A = 14$

- ^{14}N ($Z = 7, N = 7$)

Note: Only one nuclide with $A = 14$ *in the list.*

Isobars with $A = 15$

- ^{15}O ($Z = 8, N = 7$)
- ^{15}N ($Z = 7, N = 8$)

These are isobars because both have $A = 15$ (same mass number) but different atomic numbers and neutron numbers.

Isobars with $A = 16$

- ^{16}O ($Z = 8, N = 8$)

Note: Only one nuclide with $A = 16$ *in the list.*

Isobars with $A = 17$

- ^{17}O ($Z = 8, N = 9$)
- ^{17}F ($Z = 9, N = 8$)

These are isobars because both have $A = 17$ (same mass number) but different atomic numbers and neutron numbers.

Isobars with $A = 18$

- ^{18}F ($Z = 9, N = 9$)

Note: Only one nuclide with $A = 18$ in the list.

Isotones (Same Number of Neutrons N)

Isotones with $N = 7$

- ^{15}O ($Z = 8, A = 15$)
- ^{14}N ($Z = 7, A = 14$)
- ^{13}C ($Z = 6, A = 13$)
- ^{12}B ($Z = 5, A = 12$)

These are all isotones because they all have $N = 7$ neutrons but different atomic numbers and mass numbers.

Isotones with $N = 8$

- ^{15}N ($Z = 7, A = 15$)
- ^{16}O ($Z = 8, A = 16$)
- ^{17}F ($Z = 9, A = 17$)

These are all isotones because they all have $N = 8$ neutrons but different atomic numbers and mass numbers.

Isotones with $N = 9$

- ^{17}O ($Z = 8, A = 17$)
- ^{18}F ($Z = 9, A = 18$)

These are isotones because both have $N = 9$ neutrons but different atomic numbers and mass numbers.

Relationship	Nuclides
Isobars ($A = 15$)	^{15}O , ^{15}N
Isobars ($A = 17$)	^{17}O , ^{17}F
Isotones ($N = 7$)	^{15}O , ^{14}N , ^{13}C , ^{12}B
Isotones ($N = 8$)	^{15}N , ^{16}O , ^{17}F
Isotones ($N = 9$)	^{17}O , ^{18}F

Exercise 12:

Part a) Atomic Mass of Natural Chlorine

Problem Statement

Calculate the atomic mass of natural chlorine, knowing that it is made up of:

- 75.4% of the ^{35}Cl isotope with mass $M(^{35}\text{Cl}) = 34.967420$ g/mol

- 24.6% of the ^{36}Cl isotope with mass $M(^{36}\text{Cl}) = 36.96560$ g/mol

Solution

The average atomic mass is calculated as a weightel average based on the fractional abundance of each isotope:

$$\text{Atomic mass} = \sum (\text{fractional abundance} \times \text{isotopic mass})$$

Given data:

- Fraction of ^{35}Cl: $f_1 = 75.4\% = 0.754$
- Fraction of ^{36}Cl: $f_2 = 24.6\% = 0.246$
- Mass of ^{35}Cl: $M_1 = 34.967420$ g/mol
- Mass of ^{36}Cl: $M_2 = 36.96560$ g/mol

Calculation:

$$\text{Atomic mass(Cl)} = (0.754)(34.967420) + (0.246)(36.96560)$$
$$= 26.3617 + 9.0957 = 35.4574 \text{ g/mol}$$

Answer: The atomic mass of natural chlorine is approximately **35.46 g/mol** (or 35.46 amu).

Note: This value is consistent with the accepted atomic weight of chlorine (≈ 35.45), confirming our calculation.

Part b) Atomic Mass of ^{13}C

Carbon in its natural state has an atomic weight of 12.011 g/mol and contains 98.89% of the ^{12}C isotope. Calculate the atomic mass of the isotope ^{13}C, knowing that natural carbon consists of only two isotopes: ^{12}C and ^{13}C.

Using the same weighted average formula, we can rearrange to solve for the unknown mass of ^{13}C:

$$\text{Atomic mass} = (f_{12})(M_{12}) + (f_{13})(M_{13})$$

Given data:

- Average atomic weight of natural carbon: 12.011 g/mol
- Fraction of ^{12}C: $f_{12} = 98.89\% = 0.9889$
- Fraction of ^{13}C : $f_{13} = 1.11\% = 0.0111$
- Exact mass of ^{12}C: $M_{12} = 12.000$ g/mol (by definition)
- Unknown mass of ^{13}C: $M_{13} = ?$

Setting up the equation:

$$12.011 = (0.9889)(12.000) + (0.0111)(M_{13})$$

Solving for M_{13}:

First, calculate the contribution from ^{12}C:

$$(0.9889)(12.000) = 11.8668$$

Substitute back:

$$12.011 = 11.8668 + (0.0111)(M_{13})$$

Rearrange to isolate M_{13}:

$$12.011 - 11.8668 = (0.0111)(M_{13})$$

$$0.1442 = (0.0111)(M_{13})$$

$$M_{13} = \frac{0.1442}{0.0111} = 12.99 \approx 13.00 \text{ g/mol}$$

Answer: The atomic mass of the isotope ^{13}C is approximately **13.00 g/mol** (or 13.00 amu).

Note: This value is consistent with the accepted mass number of ^{13}C, which is 13 by definition. The slight difference from 13.0 accounts for the binding energy differences in the nucleus (mass defect).

Chapter II

Radioactivity and nuclear reactions

I-Introduction

Radioactivity is a natural occurrence wherein specific unstable atomic nuclei spontaneously convert into more stable nuclei through the emission of radiation. This radiation manifests in several forms, including alpha particles, beta particles, and gamma rays, and is associated with the release of energy.

Antonio Henri Becquerel (left), Pierre Curie, Marie Curie (right). Date Unknown. Nobel Prize.

The discovery of radioactivity occurred in 1896, when French physicist Henri Becquerel (1852–1908) was investigating phosphorescent substances. He noted that uranium salts could discolour photographic plates even in the absence of light, demonstrating that uranium emits invisible radiation independently. This constituted a significant scientific advancement as it demonstrated that atoms are not invariably stable and can generate energy autonomously.

Pierre Curie and Marie Curie further expanded upon Becquerel's research by conducting a more in-depth examination of uranium minerals. In 1898, two new elements with exceptionally powerful radioactive emissions were found.

Polonium, commonly denoted by the isotope ^{212}Po

Radium is commonly denoted by the isotope ^{226}Ra

Their findings validated that radioactivity is an atomic characteristic associated with the nucleus, rather than a chemical reaction. This discovery created the basis of nuclear physics and opened the way to many scientific and medical applications.

II- Natural radioactivity

Natural radioactivity consists of the spontaneous decomposition of certain so-called radioactive elements **(N/Z>1.51),** which appear unstable and give rise to real transmutations called (*DESINTEGRATIONS*). The emission of radiation always accompanies this transformation of a radioactive nucleus.

a- The stability and instability of the nucleus :

- A stable nucleus is a nucleus that retains the same composition indefinitely.
- An unstable or radioactive nucleus is a nucleus that spontaneously disintegrates, producing a different nucleus and emitting either :

- An α (*alpha*) particle

- An electron (${}_{-1}e$) is radioactive (${}_{-1}\beta$) if the nucleus contains too many neutrons (*negatons*).

- A radioactive proton (${}_{(+1)}e$) (${}_{+1}\beta$) if the nucleus contains too many protons (*positrons*).

- And sometimes a very energetic electromagnetic radiation (γ) called (*Gamma*).

b- Different types of radiation

We use the device from **WILSON**'s experiment to identify the different types of radioactive radiation: we observe three types of radiation: (α), (β), and (γ).

- **The α (alpha) particles.**

- These are positive particles, helium nuclei, written symbolically as ***Ion He^{2+}*.**

- These particles are ejected at high-speed $\boldsymbol{v} \approx 2x10^{7}$m/s.

- The particles are directly ionizing but not very penetrating.

- They are stopped by a sheet of paper and a few centimeters of air

- They penetrate the skin to a depth of just a few micrometers.

- They are not harmful to the skin. However, they are dangerous if absorbed internally.

The general equation. $${}_{Z}^{A}X^{*} \longrightarrow {}_{Z-2}^{A-4}Y + {}_{2}^{4}\alpha + {}_{0}^{0}\gamma$$

Example : $${}_{88}^{226}Ra \longrightarrow {}_{86}^{222}Rn + {}_{2}^{4}\alpha + {}_{0}^{0}\gamma$$

The radiation (α) is highly ionizing but not very penetrating (the particles (α) are stopped by a sheet of paper)

- **The β (beta) particles.**

A distinction is made between:

-The **β**$^{-}$ particles are electrons: Mass: $\mathbf{m_e}$=9.1x10^{-31}kg; Charge: **e**=-1.60x10^{-19}C

- The **β** particles^{+} which are positrons (antiparticle of the electron); Mass: $\mathbf{m_e}$=9.1x10^{-31}Kg
Load: **e**=+1.60x10^{-19}C.

- The particles are emitted at high velocity **v**≈2.8x10^{8}m/s.

- They are more penetrating but less ionizing than **α particles**.

- They penetrate the skin to a depth of just a few millimeters.

- They are dangerous for the skin.

The general equation $^{A}_{Z}X^{*} \longrightarrow {}_{Z+1}^{A}Y + {}_{-1}^{0}\beta + {}_{0}^{0}\gamma$

$$^{A}_{Z}X^{*} \longrightarrow {}_{Z-1}^{A}Y + {}_{+1}^{0}\beta + {}_{0}^{0}\gamma$$

Example: $^{234}_{91}Pa \longrightarrow {}^{234}_{92}U + {}_{-1}^{0}\beta$; $^{15}_{8}0 \longrightarrow {}^{15}_{7}N + {}_{-1}^{0}\beta$

Rq: β radiation is not very ionizing but penetrates (through a 0.4 mm thick lead plate).

- **γ (gamma) radiation.**

It accompanies the emission of **α**, **β**$^{+,}$ and **β**$^{-}$ particles.

- It consists of an electromagnetic wave with a very short wavelength ($\lambda \approx 10^{-12}$mand$\nu \approx 10^{20}$Hz).
- Radiation is made up of photons traveling at the speed of light and with zero mass.
- They are not directly ionizing, but they are highly penetrating.
- They can penetrate up to 20cm of lead.
- By interacting with the atoms of the substances they pass through, they can give rise to electrons, which are ionizing.

The general equation $^{A}_{Z}X^{*} \longrightarrow {}^{A}_{Z}X + {}_{0}^{0}\gamma$

Example: $^{14}_{7}N + {}_{-1}^{0}\beta \longrightarrow {}^{15}_{8}N + {}_{0}^{0}\gamma$

III. The law of radioactive decay (emission)

Radioactive decay is a **spontaneous** process that follows a **first-order law**. This means that the number of nuclei that decay per unit time is **proportional to the number of radioactive nuclei still present**.

We consider the simple transformation: X∗ (unstable)⟶X (stable, non-radioactive)

The equation:

	$X^* \longrightarrow$	X (Non Radioactive)
	Unstable	**Stable**
T=0	N_0	0
T	Nt	N_0-Nt

Numbers of nuclei over time

- At =0: radioactive nuclei: N0 the stable nuclei formed is 0
- At time t: radioactive nuclei remaining: Nt the stable nuclei formed is N0−Nt

Variation during a short time interval

During a very small time interval dt, a number dN of radioactive nuclei disintegrate. Therefore:

- the number of unstable nuclei decreases from Nt to Nt−dN,
- the number of stable nuclei increases by the same amount dN.
  - The following equation gives the decay rate: $-dN/dt=\lambda$

λ: radioactive constant.

$$(-dN)\,/\,dt = \lambda N \Longrightarrow -\int_{N_0}^{N_t} dN/_{N} = \lambda \int_{t_0}^{t} dt \Longrightarrow LnN]_{N_0}^{N_t} = -\lambda t \Longrightarrow \ln N_t - \ln N_0 = -\lambda t$$

$\ln N_0$ = constante

$\ln N_t/N_0 = -\lambda t$ ou $\ln N_0/N_t = \lambda t$ other expression $N_t = N_0\, e^{-\lambda t}$ or $N_0 = N_t\, e^{\lambda t}$

Rather than indicating the decay rate by its radioactive constant, it is simpler to give the half-life $t_{1/2}$.

N_t: represents the average number of undisintegrated nuclei or nuclei remaining at the time (t).

N_0: represents the average number of undisintegrated nuclei or nuclei remaining at the time (t=0).

λ, called the **decay constant** (or **radioactive constant**), is a value that is **specific to each radioactive nuclide**. It measures the **likelihood of decay per unit time** and depends only on the **nature of the nucleus**. It is expressed in **inverse time units**, for example: s^{-1}, min^{-1}, h^{-1}, $year^{-1}$, etc.

IV – Radioactive Half-Life ($T_{1/2}$)

This is the time after which half the sample (unstable nuclei) has disintegrated.

at $t=T_{1/2} \Rightarrow N_t = N_0/2$ (unstable nuclei have decayed and $N_0/2$ stable nuclei have formed).

$\Rightarrow \ln N_0/N_t = +\lambda t$ à $t = T = t_{1/2}$, $N_t = N_0/2 \Rightarrow \ln N_0/N_0/2 = \lambda t$

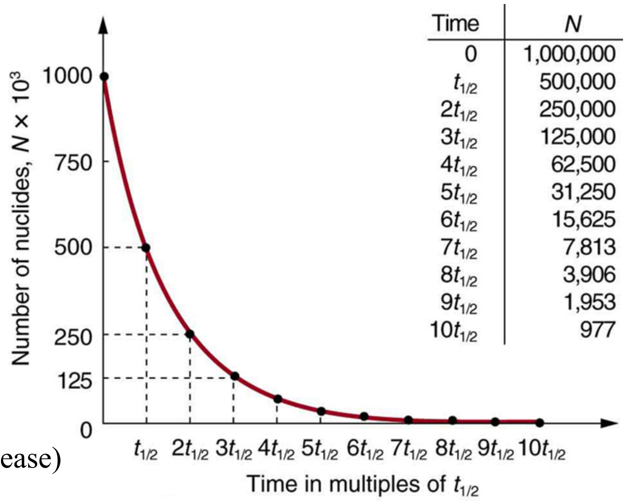
$\Rightarrow \ln 2 = \lambda t$ et $t_{1/2} = \ln 2/\lambda$ ou bien $\lambda = \ln 2/t_{1/2}$

[T] varies as a function of seconds.

V- Radioactive activity (A)

This is the number of radioactive nuclei that disintegrate per unit of time. It is also the instantaneous speed of unstable nuclei (proportional to the number of unstable nuclei that have not disintegrated).

$-dN/dt = A$ and $A = \lambda N$ (the sign (-) indicates a decrease)



Time	N
0	1,000,000
$t_{1/2}$	500,000
$2t_{1/2}$	250,000
$3t_{1/2}$	125,000
$4t_{1/2}$	62,500
$5t_{1/2}$	31,250
$6t_{1/2}$	15,625
$7t_{1/2}$	7,813
$8t_{1/2}$	3,906
$9t_{1/2}$	1,953
$10t_{1/2}$	977

at (t=0) ⇨ $N_t = N_0$ ⇨ $A(0)=\lambda N_0$ (A_0 the initial activity)
at time (t) ⇨ $- dN/N = \lambda\, dt$ and $A=\lambda N$ ⇨ $A(t) = A(0)\, e^{-\lambda t}$ or $A_0=A(t)e^{\lambda t}$

A: expressed as disintegration per unit time dp(t) [dps (sec) or dpm (min).......]

And also the radioactive activity expressed in (1Ci= 1Curie), the curie corresponds to the activity of 1g of Radium-226 per second.

- The decay of radium-226 produces an alpha particle and gamma radiation according to:

$${}_{88}^{226}Ra \longrightarrow {}_{86}^{222}Rn + {}_{2}^{4}\alpha + {}_{0}^{0}\gamma$$

Given that the half-life of ${}^{226}Ra$ is about **1580 years**, we can calculate the activity corresponding to **1 curie**.

Convert the half-life to seconds

$T_{1/2}=1580\times365\times24\times60\times60\approx4.9826\times10^{10}$ s

Calculate the decay constant

$\lambda=\ln2/T_{1/2} \approx 0.693/\ 4.9826x10^{10} \approx 1.385\times10^{-11}\ s^{-1}$

Determine the number of nuclei in 1 g of Ra-226

$$N = \frac{1}{226}N_A = \frac{6.023x10^{23}}{226} = 2.665x10^{21\,nucleide}$$

Calculate the activity

$A=\lambda N=(1.385\times10^{-11})(2.665\times10^{21})\approx3.69\times10^{10}$ disintegrations/s

Therefore:

1 Ci≈3.69×1010 dps (dps = disintegrations per second)

VI- Artificial Radioactivity and Nuclear Transformations

A **nuclear reaction** is a transformation that affects the **nucleus** of an atom. Unlike chemical reactions (which involve electrons), nuclear reactions can change:

- the **atomic number** Z (nature of the element),
- the **mass number** A (number of nucleons),

  and they are usually accompanied by a large release (or absorption) of energy.

Common nuclear processes include:

- **Radioactive decay** (spontaneous): α, β−, β+, γ
- **Nuclear fission**: a heavy nucleus splits into smaller nuclei + neutrons + energy
- **Nuclear fusion**: light nuclei combine to form a heavier nucleus + energy

a) Transmutations

Nuclear transmutations are nuclear reactions in which the nucleus of an atom is transformed into a different nucleus, producing new nuclides. This usually happens when a target nucleus is bombarded by particles (such as neutrons, protons, or alpha particles).

After bombardment, the original nucleus is modified and the products formed generally have mass numbers that are close to that of the initial nucleus, because the reaction involves adding or removing only a few nucleons.

Example:

${}^{27}_{13}\mathrm{Al} + {}^{4}_{2}He \longrightarrow {}^{30}_{15}P + {}^{1}_{0}n$ we note $({}^{27}Al(\alpha, n){}^{30}P)$

b) Nuclear fission reaction (splitting)

Nuclear fission is the process in which a heavy nucleus (high mass number) splits into two lighter nuclei of medium mass after being struck by a projectile, most often a **neutron**.This reaction produces:

- two fission fragments (medium-mass nuclei),
- several free neutrons,
- and a large amount of energy**.**

Example

$${}^{235}_{92}U + {}^{1}_{0}n \longrightarrow {}^{146}_{57}La + {}^{87}_{35}Br + 3{}^{1}_{0}n + E$$

c) Nuclear fusion reaction

Nuclear fusion is a nuclear process in which two light nuclei combine to form a heavier nucleu**s**. During the reaction, a particle such as a neutron or a proton may be emitted, and a **large amount of energy** is released.

Example:

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

VII- Mass Defect and Energy in Nuclear Reactions

Nuclear reactions can release or absorb **a lot of energy** because **mass can change** during the reaction. Einstein showed that a small mass difference corresponds to a large amount of energy:

$\mathbf{E=\Delta Mc^2}$

E: energy (J)

ΔM: mass difference (kg)

c: speed of light in vacuum (3.0×10^8 m\S)

$$\Delta M=\sum m(\text{products})-\sum m(\text{reactants})$$

- **If $\Delta M<0$** : the products have **less mass** than the reactants.

The "missing mass" is transformed into energy → the reaction **releases energy** (**exoenergetic**).

- **If $\Delta M>0$**: the products have **more mass** than the reactants.

Extra energy is needed to form them → the reaction **absorbs energy** (**endoenergetic**).

1. Energy exchanged

- The **joule (J)** is the SI unit of energy, but it is not convenient for **microscopic** (atomic and nuclear) phenomena because the values are very small or very large.
- In nuclear physics, energy is usually expressed in **electronvolts (eV)** or **mega-electronvolts (MeV)**.

Conversions: $1eV=1.602189\text{x}10^{-19}J$ **or** $1MeV=1.602189\text{x}10^{-13}J$

2. Mass defect

In many nuclear reactions, the total mass of the **products** is **slightly smaller** than the total mass of the **reactants**. The missing mass is called the **mass defect** (or **mass loss**) and is noted $|\Delta M|$.

$$|\Delta M|=\sum m(\text{products})-\sum m(\text{reactants})$$

This missing mass is converted into energy according to Einstein's relation. The energy released is:

$$E_{\text{released}}=|\Delta M|\ c2=|\sum m(\text{products})-\sum m(\text{reactants})|c^2$$

- E in **joules (J)**
- $|\Delta M|$ in **kilograms (kg)**
- c in $\mathbf{m.s^{-1}}$

Example

Let's calculate the energy released by 1 mole of (Ra-226) when it decays according to this process.

$$ {}^{226}_{88}Ra \longrightarrow {}^{222}_{86}Rn + {}^{4}_{2}\alpha + {}^{0}_{0}\gamma $$

Since

M (Ra-226) = 226.0254 a.m.u; M (Rn-222) = 222.0175 u.m. M (He-4) = 4.00388 a.m.u.

$|\Delta M| = |M_{(products)} - M_{(reactants)}|$

$|\Delta M|$ = | [M (Rn-222) + M (He-4)] - [M (Ra-226)]| = 0.0041 u.m.a

* The energy released by a nucleus: E(MeV) = ΔM (u.m.a)x931(MeV) $\Longrightarrow$ E(MeV) = 0.0041. 931= 3.82MeV.

* The energy released by 1 mole of nuclei (MeV): E(MeV) = E (released by a nucleus)* N= 23.00710^{23}MeV.

The same result can be obtained, but expressed in joules, by directly applying Einstein's relation.

*The energy released by 1 mole of nuclei (Joule): E(J) = $\Delta M .10^{3}$ (Kg) * c^{2} (c =3 10^{8} m/s)

E(J) = $0.0041.10^{3} * 3.\ 10^{8.}$ $^{=}$ E(J)=$3.69.10^{11}$Joules.

VIII-Introduction to Radiation Protection

VIII-1. Definitions

a. Exposure

Any individual subjected to ionizing radiation is considered exposed.

- External Exposure: When radiation sources are located outside the body.
- Internal Exposure: When radiation sources are inside the body.

Whole-body exposure, considered homogeneous, is referred to as global exposure, as opposed to partial exposure, which refers to a part of the body, or to one or more organs or tissues.

The sum of internal and external exposures constitutes total exposure.

b. Radioactive Contamination

Radioactive contamination is legally defined as "the undesirable presence of radioactive substances on the surface or inside any medium, including the human body."

Contamination is necessarily the result of the dissemination of a radioactive substance, due to the careless handling of unsealed sources or the accidental destruction of the containment envelope of a sealed source.

The dissemination of part of the source can create surface and/or atmospheric contamination, depending on the nature and physico-chemical form of the radioactive substance.

External contamination results in external exposure, while **internal contamination** leads to internal exposure.

External professional exposure only occurs during work hours and can be controlled (influenced by time, distance, and shielding).

External body contamination generally leads to intense exposure to the skin and underlying tissues, which continues (24 hours a day) until detected and removed.

Internal contamination results in ongoing exposure of tissues and organs, which decreases progressively due to radioactive decay and biological elimination, referred to as the "effective period." In some cases, this can be negligible in the context of a human lifetime.

Surface or body contamination that is poorly fixed can be easily decontaminated but spreads easily, while fixed contamination is harder to eliminate but less transferable.

C. Absorbed Dose

The absorbed dose is the energy transferred by radiation to a unit mass of the exposed material.

In a medium exposed to ionizing radiation, the absorbed dose (denoted as D) at a specific point is given by the relationship:

$$D = dE / dm$$

Where dE is the average energy transferred by radiation to a volume element with mass dm surrounding the point in question, i.e., the difference between the sum of the energies of the radiation that has entered the material element and the sum of the energies that have exited it.

According to this relationship, in the International System of Units (SI), absorbed dose is measured in joules per kilogram. The legal unit is the Gray (symbol: Gy), and by definition:

1 Gray (Gy) = 1 Joule per kilogram (J.kg-1)

D. Absorbed Dose Rate

The absorbed dose rate, denoted as D, is the absorbed dose per unit of time.

$$D = dD / dt$$

In the International System, the absorbed dose rate is measured in Gray per second (Gy.s-1). In practice, submultiples such as mGy.h-1 are commonly used, given the activities involved.

If the absorbed dose rate is constant over a time interval t, the relationship becomes:

$$D = D \times t$$

Example:

If the absorbed dose rate, due to ambient radiation, at a workstation is 0.3 mGy.h-1, and the operator stays there for 2 hours and 30 minutes, the total dose absorbed by their entire body is:

$$D = 0.3 \times 2.5 = 0.75 \text{ mGy}$$

IX-NATURES AND CHARACTERISTICS OF THE EFFECTS RELATED TO RADIATION EXPOSURE IN A HUMAN ORGANISM

The different effects that can result from human exposure to ionizing radiation can be classified into two categories:

- deterministic or non-stochastic effects
- the effects with random or stochastic incidences.

IX-1. Deterministic Effects

For high doses (greater than several Grays), these effects are observed in all exposed subjects. These are therefore threshold effects.

They generally manifest early, with latency periods ranging from a few days to a few months.

Their severity increases with the absorbed dose.

We are beginning to observe certain deterministic effects around 0.3 Gy for partial exposures. On the other hand, for low doses, below a threshold value primarily depending on the type of biological effect, no effect is detectable. For overall exposure, the reference value of 0.5 Gy is taken as the threshold value.

From a certain absorbed dose, for overall exposure, there is a risk of death (approximately 2 gray).

The dose lethal to 50% (DL50) is called the absorbed dose, for the entire organism (thus a global exposure), for which you have a 50% chance of dying sixty days after exposure.

This value is: DL_{50} = 4.5 Gy

Generally, deterministic effects occur in the case of a single exposure to a high dose rate.

IX-2. Stochastic Effects

They include the induction of cancer in exposed individuals and genetic mutations affecting the offspring of exposed individuals. In this case, the severity of the effect remains the same regardless of the dose; only the probability of the effect occurring is dependent on the absorbed dose. In other words, the percentage of exposed subjects in whom this type of effect is observed increases with the dose.

These effects are not specific to the action of ionizing radiation; nothing allows us to distinguish between a cancer or a radio-induced mutation. The only way to highlight these phenomena is to show that in a group of exposed individuals, the frequency of occurrence of cancers or genetic mutations is higher than in a control group composed of subjects with the same characteristics (age, sex, etc.) but not exposed.

The latency period (the time between exposure and the appearance of the effect) is on average much longer than for deterministic effects (several decades).

Finally, it is considered that even the smallest dose of radiation is likely to cause this type of effects.

X-EQUIVALENT DOSES

One should not consider, as the reading of the two paragraphs might suggest previously, only the absorbed dose is involved. In fact, the dose rate, the nature, and the energy of the ionizing radiation also comes into play, and the orders of magnitude that were given are related to short-term exposures to electromagnetic radiation of a few MeV.

For the same absorbed dose, a short-duration exposure (high dose rate) is more penalizing and alpha or neutron radiation have a notably biological "efficacy" greater than electronic or electromagnetic radiation.

In the field of low doses, still in the case of global exposure (less than 0.5 Gray environment), no influence of the dose rate could be demonstrated. We therefore created a magnitude that accounts for the biological harm of radiation in the case of stochastic effects.

The equivalent dose (H_T) in a given tissue, is the product of the average absorbed dose for the organ or the tissue T of a given radiation R ($D_{T,R}$) by the weighting factor for radiation R (wR), is the quantity directly proportional to biological detriment.

$$H_T = D_{T,R} \, . \, W_R$$

When the radiation field includes radiations of types and energies corresponding to different values of wR, the total HT equivalent dose is given by the formula:

$$H_T = \sum_R D_{T,R} \, . \, W_R$$

The unit of equivalent dose is the SIEVERT (Sv). Logically, the units that should be used are the submultiples of the Sievert: millisievert (mSv) and microsievert (µSv).

Having assigned the unit value to the weighting factor related to electronic radiation, the The following table indicates the values related to other radiations.

Nature Of Radiation	w_R
β, électrons, γ, X	1
p	10
neutrons	de 5 à 20
α	20

The biological "harm" is therefore twenty times greater, for an equal absorbed dose, for α radiation than for γ radiation.

(rem: alpha in non-fixed skin contamination have a weighting factor of 0)

The equivalent dose rate *H*° is usually expressed in millisieverts per hour (mSv.h-1) or in microsieverts per hour (μSv.h^{-1}).

XI-OBJECTIVES RELATED TO SETTING BOUNDARIES FOR INDIVIDUAL EXPOSURE

Limiting the amount of radiation exposure that any individual, particularly employees, can withstand is one of the primary goals of radiation protection. The values of these limits have been set for two main reasons:

1. to limit the occurrence of stochastic effects to a "socially acceptable" level, which is a reasonable compromise between the benefits society receives from the use of radioactivity and ionising radiation and the annoyances that result from it; and
2. to prevent any deterministic effect by keeping the dose equivalent received throughout the professional life below the dose equivalent of the lowest threshold.

The selection of a risk index was a prerequisite for carrying out the assessment associated with the second goal. The evaluation of the overall harm incurred by a group and its offspring after exposure to a radiation source served as the prior reference for the risk index. The index considered the risk of hereditary effects on the first generation of their descendants as well as the risk of cancer death for those exposed. This strategy worked well but had several drawbacks.

XI-1. The Concept of Aggregate Detriment

The notion of aggregate detriment was established in the context of stochastic effects to consider both prior impacts and further deleterious effects of radiation.

Consequently, four primary components for disadvantage have been identified:

The chance of lethal cancer in all impacted organs.

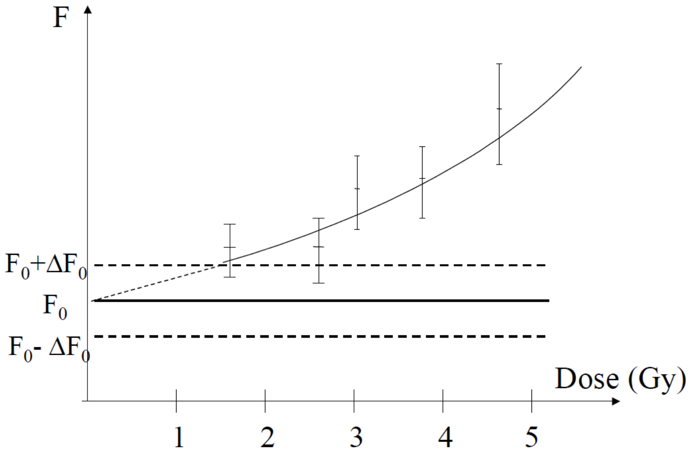
* considering the variations in latency durations that result in disparate values for life loss projections in the context of deadly tumours associated with different organs. Evaluation of morbidity resulting from the onset of non-fatal malignancies. * Assessment of the risk of serious hereditary diseases in all future generations arising from the exposed individual.

In addition to animal experimentation, which yields results that are quantitatively challenging to extrapolate to humans, the primary sources of information include survivors of the atomic bombings in Hiroshima and Nagasaki (global exposure), individuals who have received radiotherapy (partial exposure), and workers exposed through their occupations (radiologists, miners, etc.).

The International Commission on Radiological Protection (ICRP) assesses risk indicators based on data from Hiroshima and Nagasaki. She proposed the novel notion of disadvantage, aggregative, in response to the appearance of new disorders among survivors from 1977 to 1990 and subsequent dosimetric research.

The CIPR has consequently provided recommendations aimed at enhancing precautions concerning existing measures, particularly by distinguishing among different worker populations. The incidence of cancer varies between a workforce population aged 18 to 65 and the general public, which spans from 0 to 122 years old.

Regardless of the information source, only exposures with relatively high doses permit the detection of a statistically undeniable increase in risk, as graphically depicted by the Dose-Response curve below:



F: Frequency of occurrence of the effect
F0: "Natural" frequency of occurrence of the effect
2ΔF0: domain of statistical fluctuations of the natural frequency

At low doses, the statistical fluctuations in the "natural" frequency of an effect's occurrence prevent any formal conclusion. It was therefore necessary to make an assumption regarding the law of evolution in this field; among the reasonable assumptions, the one that maximizes the risk was chosen:

a linear proportionality relationship, without a threshold, between the increase in the chosen risk index and the received dose equivalent.

XI-2. The Risk Factor

The probability coefficient, often known as the "risk factor," can be used to determine the likelihood of dying from cancer assuming the equivalent dose is evenly distributed across the body.

Because the weighting factors for tissues account for non-fatal malignancies and genetic effects, the use of this total probability coefficient will be less accurate if the distribution of the equivalent dose is not uniform.

As a result, the "risk factor" is the slope of the line that shows how the risk index increases in relation to the corresponding dose.

The International Commission on Radiological Protection (ICRP) has identified the following risk factor (fatal cancers) for both workers and the general public in the event of worldwide exposure:

Frpop = 5.10-2 par Sv Frtra = 4.10-2 par Sv

The probability coefficient, which we refer to as the risk factor for convenience, is equal to the following if we consider the scenario of non-fatal malignancies and genetic effects over multiple generations:

Frpop = 7,3.10-2 par Sv Frtra = 5,6.10-2 par Sv

Examples: Attention, these are just probabilistic calculations

Assuming that one million people (population of an industrialized country) are exposed to 5 mSv, let's calculate the number of radiation-induced cancers and serious genetic disorders in their descendants:

n = 106 x 5.10-3 x 7.3.10-2 = 365

The result then breaks down as follows:

250 deaths from cancer, 48 cancers that will be non-fatal, and 67 severe genetic disorders in descendants.

The so-called "natural" frequency of cancer occurrence in an industrialized country is equal to 28%. In the same million people who were exposed, 280,000 will develop cancer during their lifetime. This explains the great difficulty in identifying a radio-induced cancer and thus the complexity of epidemiological investigations.

Assuming that 20,000 workers are exposed to 20 mSv, the result is

$$n = 2.104 \text{ x } 2.10-2 \text{ x } 5.6.10-2 = 23$$

The result then breaks down as follows: 16 cancer deaths, 4 cancers that will not be fatal, and 3 severe genetic impairments in descendants.

TUTORIAL NO. 02

Exercise 01:

a- Complete the equations for the following nuclear reactions:

1-$^{19}_{9}F + ^{1}_{1}H \longrightarrow ^{16}_{8}O + \cdots$, 2- $^{9}_{4}Be + ^{1}_{1}H \longrightarrow ^{2}_{1}H + \cdots$

3- $^{59}_{27}Co + \cdots \longrightarrow ^{60}_{27}Co + ^{1}_{1}H$, 4- ….+ $^{1}_{1}H \longrightarrow ^{13}_{7}N + ^{1}_{0}n$

5-$^{26}_{12}Mg + ^{1}_{0}n \longrightarrow ^{23}_{10}Ne + \cdots$, 6- $^{63}_{29}Cu + \cdots \longrightarrow ^{63}_{30}Zn + ^{1}_{0}n$

7- $^{27}_{13}Al + ^{4}_{2}He \longrightarrow$ ….+ $^{1}_{0}n$, 8- $^{30}_{15}P \longrightarrow$ ….+ $^{0}_{+1}\beta$

Exercise 02:

a- Write down the equations for the following nuclear reactions, identifying the element formed: reactants (products)

$^{23}{}_{11}$Na (α , p) ; $^{39}{}_{19}$K (d , p) ; $^{14}{}_{7}$N (α , p) ; $^{55}{}_{25}$Mn (d , 2n)

b- The following radioactive elements decay, emitting particles. Write down the equations and identify the element formed: reactants (products).

$^{14}{}_{6}$C (β^-) ; $^{15}{}_{8}$O (β^+) ; $^{218}{}_{84}$Po (α) ; $^{212}{}_{82}$Pb (β^-)

Exercise 03:

Le (Radon-222) se désintègre suivant la réaction :

$$^{222}_{86}Rn \qquad ^{218}_{84}Po + ^{4}_{2}He \qquad \longrightarrow$$

Data :

Core	Weight (Kg)
Radon ($^{222}_{86}$Rn)	3,685916 10^{-25}
Helium ( )α	6,644660 10^{-27}
Polonium ($^{218}_{84}$Po)	3.619369 10^{-25}
Speed of light: c= 299792458 m/s = 3 10^8 m/s	

1- What type of reaction is this?

2- Calculate the mass loss (defect) accompanying this reaction.

3- Calculate the energy produced by the decay of a nucleus of (Rn-222) in (J) and (MeV).

Exercise 04:

In one minute, (**54 .10$^{(2)}$**) **carbon-14** disintegrations were measured in a sample from a mummy.

1- What is the activity of this sample?

2- How many disintegrations would have been measured in two minutes?

Exercise 05:

a)- Complete the nuclear reaction :

$$^{35}_{16}S \rightarrow ^{35}_{17}Cl + \cdots$$

Is the reaction natural? Give its simplified form.

b)-1- Sulphur S has a half-life of **88 days**. Given that the initial mass is **1g**, calculate the mass of sulphur remaining after **176 days**.

2- What is the activity of **1 µg** of (S-35) per day and per minute?

3- Calculate the average life of S atoms.

Exercise 06:

-Complete the following nuclear reactions and give the mass numbers and atomic numbers Of the various elements:

1- $_{92}^{235}U \xrightarrow{\alpha} Th \xrightarrow{\beta^-} P_o \xrightarrow{\beta^-} U \xrightarrow{5\alpha.} Pb \xrightarrow{2\alpha\,,4\beta^-} Pb.$

2- $_{92}^{235}U \xrightarrow{7\alpha, 4\,B^-} Pb$

b-Detail the following reactions and fill in the missing particles:

1- Ca (? , P) Sc ; **2-** N (? , γ) N ; **3-** Mg (? , P) Mg [Reactive(R,P)Product]

Exercise 07:

Na-24* (^{24}Na*) is a radioactive element that obeys 1st order kinetics. Knowing that its radioactive constant is (λ = **4.6 10^{-2} h^{-1}**).

1- Determine the expression for N_t (number of unstable nuclei at time (t) as a function of N_0, λ and t).

2- Calculate T in (hours).

3- Calculate the time after which.

a- **1%** Sodium (Na*) has disintegrated.

b- **99%** of Sodium (Na*) has disintegrated.

Solutions Exercises

Exercise 01 :

Below are the completed nuclear equations..

$$ {}^{19}_{9}\mathrm{F}+{}^{1}_{1}\mathrm{H} \rightarrow {}^{16}_{8}\mathrm{O}+{}^{4}_{2}\mathrm{He} $$

$$ {}^{9}_{4}\mathrm{Be}+{}^{1}_{1}\mathrm{H} \rightarrow {}^{2}_{1}\mathrm{H}+{}^{8}_{4}\mathrm{Be} $$

$$ {}^{59}_{27}\mathrm{Co}+{}^{1}_{1}\mathrm{H} \rightarrow {}^{60}_{27}\mathrm{Co}+\gamma $$

$$ {}^{14}_{7}\mathrm{N}+{}^{1}_{1}\mathrm{H} \rightarrow {}^{13}_{7}\mathrm{N}+{}^{2}_{1}\mathrm{H} $$

$$ {}^{26}_{12}\mathrm{Mg}+{}^{1}_{0}\mathrm{n} \rightarrow {}^{23}_{10}\mathrm{Ne}+{}^{4}_{2}\mathrm{He} $$

$$ {}^{63}_{29}\mathrm{Cu}+{}^{1}_{0}\mathrm{n} \rightarrow {}^{63}_{30}\mathrm{Zn}+{}^{0}_{-1}\beta $$

$$ {}^{27}_{13}\mathrm{Al}+{}^{4}_{2}\mathrm{He} \rightarrow {}^{30}_{15}\mathrm{P}+{}^{1}_{0}\mathrm{n} $$

$$ {}^{30}_{15}\mathrm{P} \rightarrow {}^{30}_{14}\mathrm{Si}+{}^{0}_{+1}\beta $$

Exercise 02 :

Part (a):

In nuclear reactions, particles bombard target nuclei. The notation **X(a,b)Y** means: nucleus **X** is bombarded with particle **a**, producing particle **b** and nucleus **Y**. Conservation laws for mass number (A) and atomic number (Z) must be satisfied.

1. ${}^{23}_{11}\mathrm{Na}(\alpha, p)$ **Reaction**

Equation:

$$ {}^{23}_{11}\mathrm{Na}+{}^{4}_{2}\mathrm{He} \rightarrow {}^{26}_{12}\mathrm{Mg}+{}^{1}_{1}\mathrm{H} $$

Product Element: Magnesium-26 (${}^{26}_{12}\mathrm{Mg}$)

2. ${}^{39}_{19}\mathrm{K}(d, p)$ **Reaction**

Equation:

$$ {}^{39}_{19}\mathrm{K}+{}^{2}_{1}\mathrm{H} \rightarrow {}^{40}_{20}\mathrm{Ca}+{}^{1}_{1}\mathrm{H} $$

Product Element: Calcium-40 (${}^{40}_{20}\mathrm{Ca}$)

3. ${}^{14}_{7}\mathrm{N}(\alpha, p)$ **Reaction**

Equation:

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

Product Element: Oxygen-17 (${}^{17}_{8}\mathrm{O}$)

4. ${}^{55}_{25}\mathrm{Mn}(d, 2n)$ **Reaction**

Equation:

$$ {}^{55}_{25}\mathrm{Mn}+{}^{2}_{1}\mathrm{H} \rightarrow {}^{55}_{26}\mathrm{Fe}+2\,{}^{1}_{0}\mathrm{n} $$

Product Element: Iron-55 (${}^{55}_{26}\mathrm{Fe}$)

Part (b): Radioactive Decay Equations

Radioactive elements emit particles and transform into other elements. The three decay modes shown are:

- **β^- decay:** neutron converts to proton; Z increases by 1
- **β^+ decay:** proton converts to neutron; Z decreases by 1
- **α decay:** nucleus emits helium-4; A decreases by 4, Z decreases by 2

1. $^{14}_{6}$C **Beta-Minus (β^-) Decay**

Equation:

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

Product Element: Nitrogen-14 ($^{14}_{7}$N)

2. $^{15}_{8}$O **Beta-Plus (β^+) Decay**

Equation:

$$^{15}_{8}\mathrm{O} \rightarrow ^{15}_{7}\mathrm{N} + ^{0}_{+1}\beta^+ + \nu_e$$

Product Element: Nitrogen-15 ($^{15}_{7}$N)

3. $^{218}_{84}$Po **Alpha (α) Decay**

Equation:

$$^{218}_{84}\mathrm{Po} \rightarrow ^{214}_{82}\mathrm{Pb} + ^{4}_{2}\mathrm{He}$$

Product Element: Lead-214 ($^{214}_{82}$Pb)

4. $^{212}_{82}$Pb **Beta-Minus (β^-) Decay**

Equation:

$$^{212}_{82}\mathrm{Pb} \rightarrow ^{212}_{83}\mathrm{Bi} + ^{0}_{-1}\beta^- + \bar{\nu}_e$$

Product Element: Bismuth-212 ($^{212}_{83}$Bi)

Exercise 03 :

This is an **alpha decay** reaction.

In alpha decay, an unstable nucleus spontaneously emits an alpha particle (helium-4 nucleus, $^{4}_{2}$He) and transforms into a daughter nucleus with mass number decreased by 4 and atomic number decreased by 2.

Nuclear Equation

$$^{222}_{86}\mathrm{Rn} \rightarrow ^{218}_{84}\mathrm{Po} + ^{4}_{2}\mathrm{He}$$

Question 2: Mass Defect (Δm)

Definition

The mass defect is the difference between the total mass of reactants and the total mass of products. This "missing mass" is converted to energy according to Einstein's mass-energy equivalence.

Calculation

$$\Delta m = m_{\text{initial}} - m_{\text{final}}$$

$$\Delta m = m(\text{Rn}) - [m(\text{Po}) + m(\text{He})]$$

Substituting values:

$$\Delta m = 3.685916 \times 10^{-25} - (3.619369 \times 10^{-25} + 6.644660 \times 10^{-27})\ \text{kg}$$

$$\Delta m = 3.685916 \times 10^{-25} - 3.625801 \times 10^{-25}\ \text{kg}$$

$$\Delta m = 6.011 \times 10^{-29}\ \text{kg}$$

This mass defect represents the mass converted to kinetic energy of the products and recoil energy of the polonium nucleus.

3. Energy Released by Decay

Part A: Energy in Joules

Using Einstein's mass-energy equivalence formula:

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

Substituting values:

$$E = 6.011 \times 10^{-29} \times (3 \times 10^{8})^2\ \text{J}$$

$$E = 6.011 \times 10^{-29} \times 9 \times 10^{16}\ \text{J}$$

$$E \approx 5.41 \times 10^{-12}\ \text{J}$$

More precise calculation using $c = 2.99792458 \times 10^{8}$ m/s:

$$E = 6.011 \times 10^{-29} \times (2.99792458 \times 10^{8})^2$$

$$E = 6.011 \times 10^{-29} \times 8.9875517 \times 10^{16}$$

$$E \approx 5.40 \times 10^{-12}\ \text{J}$$

Part B: Energy in MeV

To convert from joules to MeV, we use:

- $1\ \text{eV} = 1.602 \times 10^{-19}\ \text{J}$
- $1\ \text{MeV} = 10^{6}\ \text{eV} = 1.602 \times 10^{-13}\ \text{J}$

Conversion:

$$E(\text{MeV}) = \frac{E(\text{J})}{1.602 \times 10^{-13}}$$

$$E(\text{MeV}) = \frac{5.40 \times 10^{-12}}{1.602 \times 10^{-13}}$$

$$E \approx 33.7\ \text{MeV}$$

Exercise 04 :

Activity is defined as the number of nuclear disintegrations per unit time. In the SI system, the unit of activity is the **becquerel (Bq)**, where 1 Bq = 1 disintegration per second[1].

Given data:

- Number of disintegrations: $54 \times 10^2 = 5.4 \times 10^3$ disintegrations
- Time interval: 1 minute = 60 seconds

Calculation:

$$A = \frac{N}{t} = \frac{5.4 \times 10^3}{60} = 90 \text{ Bq}$$

Answer: The activity of the sample is **90 Bq** (or equivalently 5.4×10^3 disintegrations per minute).

2 .Disintegrations in Two Minutes

How many disintegrations would have been measured in two minutes?

Assuming the activity remains constant over this short time period (valid for radioactive decay over a few minutes), the number of disintegrations is directly proportional to the measurement time[2].

Given data:

- Disintegrations in 1 minute: 5.4×10^3
- Time interval: 2 minutes

Since the activity is constant, doubling the time doubles the number of disintegrations:

$$N_{2\text{ min}} = 2 \times 5.4 \times 10^3 = 1.08 \times 10^4 \text{ disintegrations}$$

Alternatively, using activity:

$$N_{2\text{ min}} = A \times t = 90 \times 120 = 1.08 \times 10^4 \text{ disintegrations}$$

In two minutes, 1.08×10^4 **disintegrations** (or 10,800 disintegrations) would be measured.

Exercise 05 :

The nuclide sulfur-35 undergoes **beta minus (β⁻) decay**:

$$^{35}_{16}\text{S} \rightarrow ^{35}_{17}\text{Cl} + ^{0}_{-1}e + \bar{\nu}_e$$

Where:

- $^{35}_{17}\text{Cl}$ is chlorine-35 (daughter nucleus)
- $^{0}_{-1}e$ is the beta particle (electron)
- $\bar{\nu}_e$ is the electron antineutrino

Is the Reaction Natural?

Yes, this is a natural radioactive decay process. Sulfur-35 is a naturally occurring radioactive isotope that spontaneously transforms into chlorine-35.

Simplified form:

$$^{35}\mathrm{S} \rightarrow ^{35}\mathrm{Cl} + \beta^-$$

In this beta decay, a neutron converts to a proton, increasing the atomic number from 16 to 17 while maintaining the mass number at 35[1].

Part b) Calculations with Sulfur-35

Given data: Half-life of S-35: $T_{1/2} = 88$ days

b1) Mass Remaining After 176 Days

Initial mass: $m_0 = 1$ g

Time elapsed: $t = 176$ days

Solution:

First, determine the number of half-lives:

$$n = \frac{t}{T_{1/2}} = \frac{176}{88} = 2 \text{ half-lives}$$

Using the decay formula:

$$m(t) = m_0 \times \left(\frac{1}{2}\right)^n = 1 \times \left(\frac{1}{2}\right)^2 = \frac{1}{4} = 0.25 \text{ g}$$

Answer: After 176 days, **0.25 g** of sulfur-35 remains.

b2) Activity of 1 µg of S-35

Given: Mass = 1 µg = 10^{-6} g

The specific activity of S-35 is related to its half-life by:

$$A_{\text{specific}} = \frac{\lambda \times N_A}{M}$$

where λ is the decay constant, N_A is Avogadro's number, and M is the molar mass.

The decay constant is:

$$\lambda = \frac{\ln 2}{T_{1/2}} = \frac{0.693}{88 \text{ days}} = \frac{0.693}{88 \times 86400 \text{ s}} = 9.10 \times 10^{-9} \text{ s}^{-1}$$

For 1 µg of S-35:

$$A = \lambda \times N = 9.10 \times 10^{-9} \times \frac{10^{-6} \times 6.022 \times 10^{23}}{35}$$

$$A \approx 1.57 \times 10^9 \text{ Bq}$$

Per day:

$$A_{\text{day}} = 1.57 \times 10^9 \text{ Bq} \times 86400 \text{ s/day} = 1.36 \times 10^{14} \text{ disintegrations/day}$$

Per minute:

$$A_{\text{min}} = 1.57 \times 10^9 \text{ Bq} \times 60 \text{ s/min} = 9.42 \times 10^{10} \text{ disintegrations/min}$$

Answer: The activity of 1 μg of S-35 is:

- 1.57×10^9 **Bq** (becquerels)
- 1.36×10^{14} **disintegrations per day**
- 9.42×10^{10} **disintegrations per minute**

b3) Average Life of S Atoms

The **mean (average) lifetime** τ of a radioactive nucleus is related to the half-life by:

$$\tau = \frac{T_{1/2}}{\ln 2} = \frac{T_{1/2}}{0.693}$$

Alternatively, $\tau = \frac{1}{\lambda}$ where λ is the decay constant.

$$\tau = \frac{88}{0.693} = 127 \text{ days}$$

Answer: The average life of S-35 atoms is **127 days**.

Exercise 06:

The uranium-235 decay series involves a sequence of alpha and beta emissions leading eventually to stable lead-207.

Reaction representation:

$${}^{235}_{92}\text{U} \xrightarrow{\alpha} {}^{231}_{90}\text{ Th} \xrightarrow{\beta^-} {}^{231}_{91}\text{ Pa} \xrightarrow{\alpha} {}^{227}_{89}\text{ Ac} \xrightarrow{\text{multiple steps}} {}^{207}_{82}\text{ Pb}$$

Complete decay chain: U-235 → (through 7 α and 4 β^- emissions) → Pb-207

Each element with mass and atomic numbers:

Nucleus	Symbol	Mass Number (A)	Atomic Number (Z)
Uranium-235	${}^{235}_{92}\text{U}$	235	92
Thorium-231	${}^{231}_{90}\text{Th}$	231	90
Protactinium-231	${}^{231}_{91}\text{Pa}$	231	91
Polonium-210 (example intermediate)	${}^{210}_{84}\text{Po}$	210	84
Lead-207 (final)	${}^{207}_{82}\text{Pb}$	207	82

Table 1: Uranium-235 decay series elements

Conservation rules:

- Alpha emission: Mass number decreases by 4, atomic number decreases by 2
- Beta minus emission: Mass number stays the same, atomic number increases by 1

Part 2: Overall decay balance

Starting nucleus: ${}^{235}_{92}\text{U}$

Final nucleus: ${}^{207}_{82}\mathrm{Pb}$

Number of alpha particles emitted: **7** (removes $7 \times 4 = 28$ from mass number)

Number of beta minus particles emitted: **4** (increases atomic number by 4)

Verification:

- Mass number: $235 - 28 = 207$ ✓
- Atomic number: $92 - 14 + 4 = 82$ ✓

Part b) Detailed Nuclear Reactions with Missing Particles

The notation Reactant(X, Y)Product represents a nuclear reaction where:

- **X** = incoming projectile (particle A)
- **Y** = emitted product (particle B)
- Reactant = target nucleus
- Product = residual nucleus

Conservation laws: Total mass number and total atomic number must be conserved.

Reaction 1: ${}^{40}_{20}\mathrm{Ca}(?\,,p){}^{40}_{19}\mathrm{K}$

Given:

- Target: Calcium-40 (Z = 20, A = 40)
- Emitted particle: proton (p = ${}^{1}_{1}\mathrm{H}$, or ${}^{1}_{1}\mathrm{p}$)
- Product: Potassium-40 (Z = 19, A = 40)

Find the missing incoming particle:

Conservation of mass number: $A_{\text{in}} + 40 = 1 + 40 \rightarrow A_{\text{in}} = 1$

Conservation of atomic number: $Z_{\text{in}} + 20 = 1 + 19 \rightarrow Z_{\text{in}} = 0$

Missing particle: neutron (n or ${}^{1}_{0}\mathrm{n}$)

Complete reaction:

$${}^{40}_{20}\mathrm{Ca}(n, p){}^{40}_{19}\mathrm{K}$$

Reaction 2: ${}^{14}_{7}\mathrm{N}(?\,,\gamma){}^{14}_{7}\mathrm{N}$

Given:

- Target: Nitrogen-14 (Z = 7, A = 14)
- Emitted particle: gamma ray (γ = photon, has Z = 0, A = 0)
- Product: Nitrogen-14 (Z = 7, A = 14)

Find the missing incoming particle:

Conservation of mass number: $A_{\text{in}} + 14 = 0 + 14 \rightarrow A_{\text{in}} = 0$

Conservation of atomic number: $Z_{\text{in}} + 7 = 0 + 7 \rightarrow Z_{\text{in}} = 0$

Missing particle: neutron (n or ${}^{1}_{0}\mathrm{n}$)

Complete reaction:

$$^{14}_{7}\mathrm{N}(n,\gamma)^{14}_{7}\mathrm{N}$$

This is a **neutron capture reaction** producing an excited nitrogen nucleus that de-excites by emitting a gamma ray.

Reaction 3: $^{26}_{12}\mathrm{Mg}(?\,,p)^{25}_{11}\mathrm{Na}$

Given:

- Target: Magnesium-26 (Z = 12, A = 26)
- Emitted particle: proton (p = $^{1}_{1}\mathrm{H}$, or $^{1}_{1}\mathrm{p}$)
- Product: Sodium-25 (Z = 11, A = 25)

Find the missing incoming particle:

Conservation of mass number: $A_{\mathrm{in}} + 26 = 1 + 25 \rightarrow A_{\mathrm{in}} = 0$

Conservation of atomic number: $Z_{\mathrm{in}} + 12 = 1 + 11 \rightarrow Z_{\mathrm{in}} = 0$

Missing particle: neutron (n or $^{1}_{0}\mathrm{n}$)

Complete reaction:

$$^{26}_{12}\mathrm{Mg}(n,p)^{25}_{11}\mathrm{Na}$$

Exercise 09:

Radioactive decay follows **first-order kinetics**, governed by the differential equation:

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

where:

- N = number of unstable nuclei at time t
- λ = decay constant (units: h^{-1})
- t = time

This differential equation has the solution:

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

where:

- N_t = number of unstable nuclei at time t
- N_0 = initial number of unstable nuclei (at $t = 0$)
- λ = decay constant
- t = time elapsed

This exponential decay law shows that:

- The number of radioactive nuclei decreases exponentially with time
- The decay is independent of external conditions (temperature, pressure, chemical state)

- After each successive half-life, the number of nuclei is halved[1]

2. Half-Life T in Hours

The half-life $T_{1/2}$ (often written as T) is the time required for half of the radioactive nuclei to decay. It is related to the decay constant by:

$$T_{1/2} = \frac{\ln\ 2}{\lambda} = \frac{0.693}{\lambda}$$

Given: $\lambda = 4.6 \times 10^{-2}$

$$T_{1/2} = \frac{0.693}{4.6 \times 10^{-2}} = \frac{0.693}{0.046} = 15.07$$

Answer: The half-life is $T \approx 15.1$ (or approximately 15 hours 4 minutes)

Verification

At $t = T_{1/2}$, we should have $N_t = 0.5N_0$:

$$N_t = N_0 e^{-\lambda T} = N_0 e^{-0.046 \times 15.07} = N_0 e^{-\ln\ 2} = N_0 \times 0.5$$

3.a. Time for 1% Disintegration

If **1% has disintegrated**, then **99% remains**:

$$N_t = 0.99N_0$$

Using the decay law $N_t = N_0 e^{-\lambda t}$:

$$0.99N_0 = N_0 e^{-\lambda t}$$

$$0.99 = e^{-\lambda t}$$

Taking the natural logarithm of both sides:

$$\ln\ (0.99) = -\lambda t$$

$$t = -\frac{\ln\ (0.99)}{\lambda}$$

$$\ln\ (0.99) = -0.01005$$

$$t = -\frac{-0.01005}{4.6 \times 10^{-2}} = \frac{0.01005}{0.046} = 0.218$$

Converting to minutes:

$$t = 0.218$$

Answer: Time for 1% disintegration = 0.218 or 13.1

3.b. Time for 99% Disintegration

If **99% has disintegrated**, then **1% remains**:

$$N_t = 0.01N_0$$

Using the decay law:

$$0.01N_0 = N_0 e^{-\lambda t}$$

$$0.01 = e^{-\lambda t}$$

Taking the natural logarithm:

$$\ln(0.01) = -\lambda t$$

$$t = -\frac{\ln(0.01)}{\lambda}$$

$$\ln(0.01) = -4.605$$

$$t = -\frac{-4.605}{4.6 \times 10^{-2}} = \frac{4.605}{0.046} = 100.1$$

Converting to days:

$$t = \frac{100.1}{24} = 4.17$$

Answer: Time for 99% disintegration = 100.1 or 4.17

Chaptre III

The Electronic Configuration of Atoms

I- Introduction

The electron configuration is a conventional notation employed to depict the electronic structure of an atom. In the orbital approximation, each electron resides in a distinct orbital, which can be characterised by a singular wave function. This method produces three quantum numbers (n, l, ml), which are congruent with those obtained from solving Schrödinger's equation for Bohr's hydrogen atom. Consequently, numerous criteria utilised to characterise an electron's position in a hydrogen atom are similarly applicable to multi-electron systems. Three fundamental principles govern the distribution of electrons among orbitals:

the Aufbau Principle, the Pauli-Exclusion Principle, and Hund's Rule.
The wave function is the solution to the Schrödinger equation. Solving this equation for a hydrogen atom yields three quantum numbers: the primary quantum number (n), the orbital angular momentum quantum number (l), and the magnetic quantum number (ml). Furthermore, there exists a fourth quantum number, the spin magnetic quantum number (ms), which is not a consequence of Schrödinger's equation. Collectively, these four quantum numbers delineate the precise position of an electron within Bohr's hydrogen atom, serving as its distinct "address" within the atom.

II-Quantic numbers

Quantum numbers are numerical values that describe the state of an electron in an atom, especially the characteristics of the orbital it occupies. There are four quantum numbers. Three come from solving the **Schrödinger equation**, while the fourth “the spin quantum number“is introduced to explain experimental observations.

II.1)- Principal quantum number (n)

The principal quantum number, noted **nnn**, determines:

- **The energy level** of the electron (n=1,2,3,…)
- **The size of the orbital** (higher n → larger orbital)

Orbitals in the same level are written: ns, np, nd, nf

II.2)- Secondary quantum number / azimuthal quantum number (*l*)

The secondary quantum number, noted **l**, is related to the electron's **angular momentum** and determines the **shape (type)** of the orbital. For a given value of n, l can take only certain integer values: l=0,1,2,…,(n−1)

Each value of lll corresponds to a subshell:

- l=0⇒ s
- l=1⇒ p
- l=2⇒d
- l=3⇒f

II.3)- Magnetic quantum number (ml)

When an atom is placed in a **magnetic field**, orbitals can adopt different **orientations in space**. The magnetic quantum number, noted **ml**, describes these orientations. For a given l, the possible values are: ml=−l,…,0,…,+l

II.4)- Spin quantum number (ms)

The electron also has an intrinsic property called spin, which can be thought of as a "rotation on itself." This concept helps explain the fine structure of atomic spectra.
The spin quantum number has only two possible values: ms=-1/2 or ms=+1/2

II.4.1) - Electron spin in an orbital

- The spin of an electron in an orbital is often represented by an **arrow** (↑\uparrow↑ or ↓\downarrow↓).
- Two electrons in the same orbital must have **opposite spins** (antiparallel).
- Therefore, **one orbital can contain a maximum of two electrons**, with spins: ↑↓

If you want, I can also make a small summary table (n, l, ml, ms + what each one represents + allowed values).

III)- Notion for orbitals

III.1) - Orbital notation and orbital shapes

Electrons in atoms occupy regions of space called **orbitals**. Each orbital is described using **quantum numbers**, and we often write orbitals with a notation like:

1s, 2s, 2p, 3d, 4f etc.

This notation contains two pieces of information:

- The **number** is the **principal quantum number** nnn: it indicates the **energy level** (shell) and also gives an idea of the **size** of the orbital. , n=1,2,3,4,…
- The letter (s,p,d,f) corresponds to the secondary (azimuthal) quantum number l: it determines the shape of the orbital.

a) Allowed values of l : For each energy level nnn, the possible values of l are: 0≤l≤n−1

So l can only take integers.

Example: level n=4 ➔ l=0,1,2,3

That means that in the fourth energy level, the atom can have **four types of subshells** (or orbital families): **4s, 4p, 4d, and 4f**.

Link between l and orbital type

Principal Quantum Number,n	Angular Momentum quntum Numbre, l l=0,1,2,3..	Subshells
1	l=0	s (1subshelle)
2	l=0 l=1	s p (2subshells)
3	l=0 l=1 l=2	s p (3subshells) d
4	l=0 l=1 l=2 l=3	s p d (4subshells) f

b) Orbital shapes

- **orbitals (l=0)**: **spherical** around the nucleus.
- **p orbitals (l=1)**: **dumbbell-shaped**, with two lobes on opposite sides of the nucleus.
- **d orbitals (l=2)**: more complex shapes, often shown as **cloverleaf** (four lobes); one dorbital has a "dumbbell with a ring."
- **f orbitals (l=3)**: even more complex shapes with more lobes.

III.2) Orbital Energy

Orbital energy is the energy an electron has when it occupies a particular orbital. This energy depends on the type of atom.

a) Hydrogen atom (one-electron atom)

For hydrogen (and other one-electron ions), the orbital energy depends **only** on the principal quantum number n.

b) Multi-electron atoms (polyelectronic atoms)

In atoms with several electrons, electron–electron repulsion and shielding make the energy depend on **both** nnn and l.

For the same n, the energy increases in this order: $s<p<d<f$

So, within a given level, an sss orbital is **lowest** in energy and an fff orbital is **highest**.

For a given principal quantum number (n), the orbitals can be classified in ascending order of energy as follows :

$$\mathbf{s < \overrightarrow{p < d < f}} \text{ (energy increases)}$$

However, it should be noted that if we compare the energy of two orbitals that do not have the same principal quantum number, for example, the energy of a (3d) orbital with that of a (5p) orbital, the latter will be the more energetic because in this case it is the orbital with the larger principal quantum number that has the greater energy.

III.3)- Wave function (Ψ)

The wave function, written Ψn,l,m,s, is a mathematical function used to describe the state of an electron in an atom—in other words, the atomic orbital it occupies. It is obtained by solving the Schrödinger equation.

To solve this equation for the different orbital types (s, p, d, f), it is more convenient to work with spherical coordinates rather than Cartesian coordinates. Therefore, we convert:

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

where:

- r is the distance from the nucleus,
- θ and φ define the direction in space.

Main properties of Ψ:

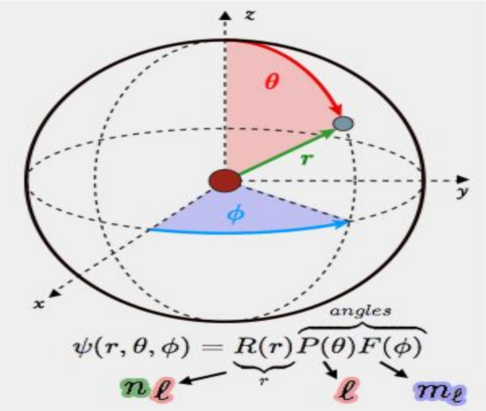
- Ψ is wave-like (oscillatory), so it can take positive values, negative values, or be zero.
- A point where $\Psi = 0$ is called a node: it is a region where the probability of finding the electron is zero.

The quantity $|\Psi|^2$ is related to the probability density of finding the electron. To represent an orbital (the electron cloud), we often draw surfaces of constant probability density defined by:

$$|\Psi|^2 = C$$

These surfaces show the regions where the electron is most likely to be found. For an s orbital (ns), the constant-probability surfaces are spheres centered on the nucleus, because the distribution is the same in all directions.

Note: The sign of Ψ (positive or negative) does not change the probability, but it is important in chemical bonding because overlapping orbitals can reinforce or cancel each other depending on their phase.



Spherical coordinates

III.4)- The Schrödinger equation

- The fundamental equation of wave mechanics **($\check{H}\Psi = E\Psi$)**.
- It is used to calculate Ψ.

III.5)- Probability density

The electron is characterized by :

Its energetic state.

- The probability of its presence at a given

location. Probability of presence.

The probability of finding the electron in a volume dV at point M(x,y,z) is written as :

$$dP = |\Psi^{`2}|\, dV$$

- The classical notion of position is replaced by the notion of ***the probability density of presence***:

- $|\Psi^{`2}|$: volume density of probability of presence or electron density.

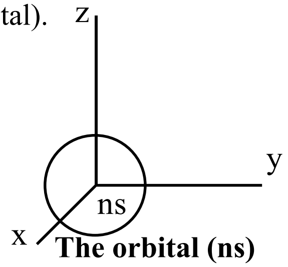
- normalisation condition :

Probability of finding an electron (1é) in all space = 1 → $\int_{(space)} dP = \int_{space} \Psi^{`2} dV = 1$.

III.6)- Graphical representation of wave function Ψ n.l.m.s

a- Description of the orbital (s)

- The condition (l=0) implies ($0 \leq l \leq n-1$) and ($m_l=0$).
- These wave functions are written as **($\Psi_{n.0.0}$)** or **(Ψ_{ns})**.
- The probability density of presence $\Psi^{(2)}$ of the electron on the surface of a sphere of radius r is the same in all directions in space, but it varies with r (the so-called spherically symmetric orbital).

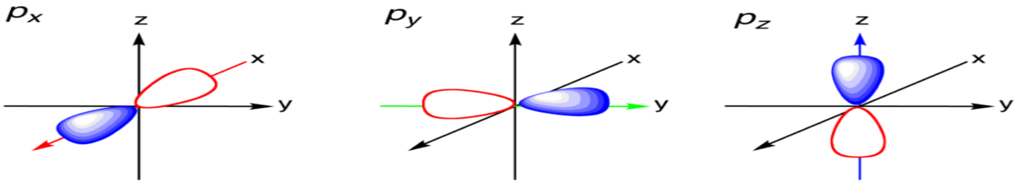


The orbital (ns)

b- Description of the (p) orbital

- The condition (l=1) implies ($0 \leq l \leq n-1$) and ($-1 \leq m \leq +1$) (m = -1, 0, +1).
- These wave functions are written as **($\Psi_{n.1.m}$)** or **($\Psi_{n(p)}$)**.
- The orbitals (np) can be represented by two approximately spherical lobes joined together, with the x, y, and z axes of symmetry of the reference trihedron.

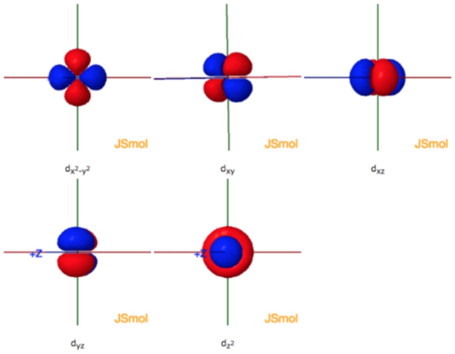
They are therefore called (np_x, np_y, np_z) depending on the value of m_l ($n \geq 2$).



The three p orbitals are aligned along perpendicular axes

c- Description of the orbital (d)

- The condition (l=2) implies ($0 \leq l \leq n-1$) and ($-2 \leq m \leq +2$) (m =-2, -1, 0, +1, +2).
- These wave functions are written as **($\Psi_{n.1.m}$)** or **($\Psi_{n(d)}$)**.



The orbital (nd)

IV - Electronic structure of poly-electron atoms (electronic configuration)

The electronic configuration of an atom is the distribution of the atom's Z electrons in A ground state on the atomic orbitals. This filling of the atomic orbitals is carried out using the four general rules.

IV.1) PAULI exclusion principle

- Two electrons in the same atom cannot have the same four quantum numbers.
- Two electrons in the same OA must differ in their spin quantum number, which can only take two values: S = (+1/2) or S= (-1/2).
- An AO can only "contain" a maximum of (2é), which in this case will have opposite spins: they are antiparallel or paired, a fully saturated quantum box (2é).
- If the orbital contains only one electron, it is said to be non-apparent or single (1e).

-An orbital is defined by the three numbers n, l, and m. Orbitals are conveniently represented using quantum bins.

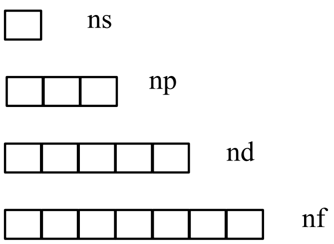
-For (n) fixed and (l) given, we have (2l+1) values of m= (2l+1) Atomic Orbitals.

l=0 → 1OAs, 2(0+1) = 2 electrons « s » (1 square)

l=1 → 3OAs, 2(2+1) = 2 electrons « s » (6 squares)

l=2 → 5OAs, 2(4+1) = 2 electrons « s » (10 squares)

l=3 → 7OAs, 2(6+1) = 2 electrons « s » (14 squares)



For a layer n, the number of squares is $n^{2,}$ and the number of electrons is $2n^2$. A quantum cell can only contain a maximum of 2 electrons with opposite spins.

IV.2) Stability principle

- The ground state of an atom is its most stable energy state, corresponding to its lowest energy.
- The electrons begin by saturating the lowest energy levels in the following order: 1s, 2s, 2p, 3s, 3p....... this is the so-called (n+l) minimum rule.
- For levels with the same (n+l): number (n) (E) . ↓ → ↓
- The first sublayer to be filled is the one with the smallest sum (n+l).

Statement of the principle: "Electrons tend to occupy the lowest energy atomic orbitals - the lowest energy levels."

Example

${}_{19}K$: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^1$ and not $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^1$

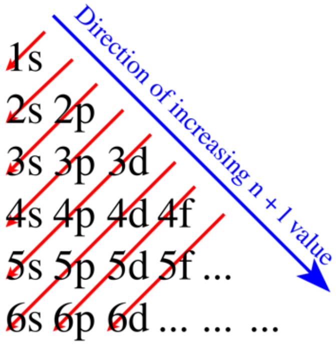
- The electrons first occupy the "4s" level before the "3d" level, and similarly between the "5s" and "4d" levels.

IV.3) HUND rule

In the fundamental state, when electrons are placed in a multiple sublayer (p, d, f), they occupy the maximum number of orbitals of the same energy with single electrons that have parallel spins (same value of s).

IV.4) KLECHKOVSKI rule

- The order of increasing energies is the order of increasing values of the sum (n + l).
- If two sublayers correspond to the same value of (n + l), the sublayer with the lowest value of n has the lowest energy.
- Orbitals in the same sublayer have the same energy



Exceptions:

- Chromium group (Z = **24**).
- Copper group (Z = **29**).

These exceptions correspond to the half-filling and full-filling of the "*3d"* layer. They can be explained by the small energy gap between the "*4s*" and "*3d*" orbitals.

Summary:

The construction of an electronic motorcade is based on :

- Pauli's principle.
- Stability principle
- Hund's rule.
- Klechkovski rule.

These rules are essential for determining the electronic structure of an atom.

TUTORIAL N° 03

Exercise 01 :

1-The wave function or (orbital) Ψ is determined by three quantum numbers n, l, m, and s (Ψn, l, m, s) and type of orbital; complete the following table:

n	l	m	s	$\Psi_{n, l, m, s}$(Type Orbitale)
1	0		+-1/2	$\Psi_{1, 0, 0, +-1/2}$(1S)
2		0	+1/2	$\Psi_{2, 0, 0, +-1/2}$( )
			+-1/2	$\Psi_{2, 1, -1, +-1/2}$( )
		0	+-1/2	
		1	+-1/2	
3			+-1/2	$\Psi_{3, 0, 0, +-1/2}$( )
		-1	+-1/2	
			+1/2	
			+-1/2	$\Psi_{3, 1, 1, +-1/2}$( )
			+-1/2	
		-1	+-1/2	$\Psi_{3, 2, -1, +-1/2}$( )
			+1/2	
			+-1/2	
		2	+1/2	

Exercise 02:

Are the following statements true or false?

a) If l = 1, the electron is in a d orbital.

b) If n = 2, m can be equal to -1.

c) If n = 4, the electron is in the O layer.

d) If l = 2, the corresponding sublayer can receive a maximum of 10 electrons.

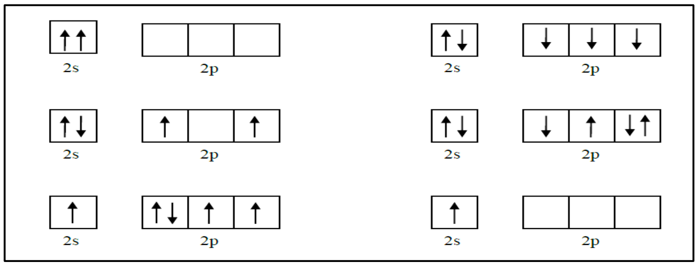
e) For a d electron, m can have the value 3.

f) The number n of an electron in a sublayer f can be equal to 3.

Exercise 03 :

1. State the rules and principles for establishing the electronic structure of an atom.

2- From the diagrams of the occupation of the quantum bins (orbitals) below, indicate those that can represent the fundamental state of an atom whose valence layer corresponds to n = 2 (the innermost layer being complete). Justify your answer briefly.



Exercise 04:

The quantum numbers of the electrons are given :

A (1,0,0,1/2) ; B (2,1,1,-1/2) ; C(3,1,-1,1/2) ; D (3,1,0,1/2) ; E (3,2,2,-1/2) ; F (4,3,-2,1/2) ; G (4,3,2,-1/2)

a) Identify the atomic orbital of each electron.

b) Represent them as quantum dots.

c) Classify the electrons in order of increasing energy.

Exercise 05 :

Consider the following electronic structures:

$1s^2 2s^2 2p^6 3s^1$

$1s^2 2s^2 2p^7 3s^2$

$1s^2 2s^2 2p^5 3s^1$

$1s^2 2s^2 2p^6 2d^{10} 3s^2$

$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 3f^6$

Which of these structures are in the ground state, which are in the excited state, and which are inaccurate?

Exercise 06:

Which of the following electronic structures do not comply with the filling rules? Please explain.

a-

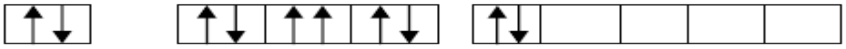
b-

c-

d-

e-

f-



g-

Exercise 07:

Are the following statements true or false? Why or why not?

a) If l=1, the electron is in a sublayer d.

b) If n=4, the electron is in the O layer.

c) For a d electron, m can be equal to 3.

d) If l=2, the corresponding sublayer can receive a maximum of 6 electrons

e) The number n of an electron in a sublayer f can be equal to 3.

f) If two "atomic buildings" have the same electronic configuration, they are necessarily the same element.

g) Iftwo "atomic edifices" have different electronic configurations; they are necessarily two different elements.

Exercises Solutions

Exercise 01:

For each set of quantum numbers, use:

- n=1→l=0n=1→l=0: s orbital
- n=2→l=0n=2→l=0: 2s, l=1l=1: 2p
- n=3→l=0n=3→l=0: 3s, l=1l=1: 3p, l=2l=2: 3d

Completed entries

- n=1,l=0,m=0,s=±1/2⇒Ψ1,0,0,±1/2 n=1, l=0, m=0, s=±1/2⇒Ψ1,0,0,±1/2: 1s orbital
- n=2,l=0,m=0,s=+1/2⇒Ψ2,0,0,+1/2n=2,l=0,m=0,s=+1/2⇒Ψ2,0,0,+1/2: 2s orbital
- n=2,l=1,m=0,s=+1/2⇒Ψ2,1,0,+1/2n=2,l=1,m=0,s=+1/2⇒Ψ2,1,0,+1/2: one of the 2p orbitals (usually 2pz)
- n=2,l=1,m=1,s=+1/2⇒Ψ2,1,1,+1/2n=2,l=1,m=1,s=+1/2⇒Ψ2,1,1,+1/2: one of the 2p orbitals (e.g. 2p+12p+1, often related to 2px2px or 2py2py)
- n=2,l=1,m=−1,s=+1/2⇒Ψ2,1,−1,+1/2n=2,l=1,m=−1,s=+1/2⇒Ψ2,1,−1,+1/2: another 2p orbital (2p−1)
- n=3,l=0,m=0,s=+1/2⇒Ψ3,0,0,+1/2n=3,l=0,m=0,s=+1/2⇒Ψ3,0,0,+1/2: 3s orbital
- n=3,l=1,m=0,s=+1/2⇒Ψ3,1,0,+1/2n=3,l=1,m=0,s=+1/2⇒Ψ3,1,0,+1/2: one of the 3p orbitals (often 3pz)
- n=3,l=1,m=1,s=+1/2⇒Ψ3,1,1,+1/2n=3,l=1,m=1,s=+1/2⇒Ψ3,1,1,+1/2: a 3p orbital (3p+1)
- n=3,l=1,m=−1,s=+1/2⇒Ψ3,1,−1,+1/2n=3,l=1,m=−1,s=+1/2⇒Ψ3,1,−1,+1/2: a 3p orbital (3p−1)
- n=3,l=2,m=−2,s=+1/2⇒Ψ3,2,−2,+1/2n=3,l=2,m=−2,s=+1/2⇒Ψ3,2,−2,+1/2: one of the 3d orbitals (3d)
- n=3,l=2,m=−1,s=+1/2⇒Ψ3,2,−1,+1/2n=3,l=2,m=−1,s=+1/2⇒Ψ3,2,−1,+1/2: one of the 3d orbitals (3d)
- n=3,l=2,m=0,s=+1/2⇒Ψ3,2,0,+1/2n=3,l=2,m=0,s=+1/2⇒Ψ3,2,0,+1/2: one of the 3d orbitals (3d)
- n=3,l=2,m=1,s=+1/2⇒Ψ3,2,1,+1/2n=3,l=2,m=1,s=+1/2⇒Ψ3,2,1,+1/2: one of the 3d orbitals (3d)
- n=3,l=2,m=2,s=+1/2⇒Ψ3,2,2,+1/2 n=3,l=2,m=2,s=+1/2⇒Ψ3,2,2,+1/2: one of the 3d orbitals (3d)

If your table needs the “type orbital” just write 1s, 2s, 2p, 3s, 3p, or 3d as indicated for each line.

Exercise 02:

a) False.

For l=1 the subshell is *p*, not *d* (which corresponds to l=2).

b) True.

For n=2, the allowed l values are 0 and 1, and for l=1 the magnetic quantum number m can be −1,0,+1, so m=−1 is possible.

c) True.

Shells are labeled K, L, M, N, O for n=1,2,3,4,5 respectively, so n=4 corresponds to the N shell and n=5 to the O shell; therefore an electron with n=4 is in the N shell, not the O shell, so the statement “electron is in the O layer” is false.

(So answer: False.)

d) True.

For a subshell with l=2 (a *d* subshell), the maximum number of electrons is $2(2l+1)=2(5)=10$.

e) False.

For a *d* electron, l=2 and thus m can only be −2,−1,0,+1,+2; m=3 is not allowed.

f) False.

An *f* subshell has l=3; since l can take values from 0 to $n-1$, n must be at least 4, so an *f* subshell cannot exist for n=3.

So the sequence of answers is:

a)False

b)True

c)False

d)True

e)False

f) False

Exercise 04:

For each electron the four quantum numbers are (n,l,ml,ms)(n,l,ml,ms).

a) Atomic orbital of each electron

Recall: l=0→sl=0→*s*, l=1→pl=1→*p*, l=2→dl=2→*d*, l=3→fl=3→*f*.

- A (1,0,0,1/2): 1*s* orbital, spin +1/2.
- B (2,1,1,−1/2): 2*p* orbital with ml=+1, spin −1/2.

- C (3,1,−1,1/2): 3*p* orbital with *ml*=−1, spin +1/2.
- D (3,1,0,1/2): 3*p* orbital with *ml*=0, spin +1/2.
- E (3,2,2,−1/2): 3*d* orbital with *ml*=+2, spin −1/2.
- F (4,3,−2,1/2): 4f4*f* orbital with *ml*=−2, spin +1/2.
- G (4,3,2,−1/2): 4*f* orbital with *ml*=+2, spin −1/2.

b) Representation as quantum dots

Quantum-dot (orbital box) notation: draw one box for each orbital specified by (*n*,*l*,*ml*), and place an up or down arrow for *ms*=+1/2 or −1/2.

- A: box labeled 1s, one upward arrow.
- B: one of the 2p boxes (the one for *ml*=+1), single downward arrow.
- C: one of the 3p boxes (for *ml*=−1), single upward arrow.
- D: middle 3p box (for *ml*=0), single upward arrow.
- E: one of the 3d boxes (for *ml*=+2), single downward arrow.
- F: one 4f box (for *ml*=−2), single upward arrow.
- G: another 4f box (for *ml*=+2), single downward arrow.

c) Order of increasing energy

For multi-electron atoms, subshell energy increases roughly with *n* and *l*; a common order is $1s<2s<2p<3s<3p<4s<3d<4p<5s<4d<5p<6s<4f\ldots$

Here the relevant subshells are 1s, 2p, 3p, 3d, 4f. Their energies increase as:

1s<2p<3p<3d<4f$1s<2p<3p<3d<4f$.

Thus the electrons in order of increasing energy are:

A (1s) < B (2p) < C and D (3p) < E (3d) < F and G (4f).

Exercise 05:

First check each configuration against the rules: allowed subshells (no 2d, 3f, etc.), correct maximum electrons per subshell (s: 2, p: 6, d: 10, f: 14), and Aufbau filling order $1s<2s<2p<3s<3p<4s<3d\ldots$

Analysis of each configuration

1. $1s^2\ 2s^2\ 2p^6\ 3s^1$
    - All subshells exist and none exceed their capacity; the filling order up to 3s is correct.
    - This is a possible ground-state configuration (it corresponds to sodium, Z = 11).
2. $1s^2\ 2s^2\ 2p^7\ 3s^2$
    - The 2p subshell can hold at most 6 electrons, so $2p^7$ is impossible.
    - This configuration is inaccurate (not allowed).

3. $1s^2\ 2s^2\ 2p^5\ 3s^1$
    - Subshells exist and capacities are not exceeded, but 3s has an electron while 2p is not full.
    - Relative energies require 2p to fill before 3s in the ground state, so this represents an excited state of an atom with Z = 10.
4. $1s^2\ 2s^2\ 2p^6\ 2d^{10}\ 3s^2$
    - A 2d subshell does not exist for n = 2 (allowed subshells are only 2s and 2p).
    - This configuration is inaccurate.
5. $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 3f^6$
    - A 3f subshell does not exist for n = 3 (allowed subshells are 3s, 3p, 3d).
    - This configuration is inaccurate.

Final classification

- Ground state: $1s^2\ 2s^2\ 2p^6\ 3s^1$
- Excited state: $1s^2\ 2s^2\ 2p^5\ 3s^1$
- Inaccurate: $1s^2\ 2s^2\ 2p^7\ 3s^2$; $1s^2\ 2s^2\ 2p^6\ 2d^{10}\ 3s^2$; $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 3f^6$

Exercise 06:

The structures that violate filling rules are: a, d, e and f only b,c and g are correct.

Use these rules: Pauli (max 2 electrons per orbital with opposite spins), Hund (for equal-energy orbitals, first put one electron with parallel spins in each, then start pairing).

Exercise 07:

a) False. If $l=1$, the electron is in a p subshell, not a d subshell.

b) False. For $n=4$, the electron is in the N shell; the O shell corresponds to $n=5$.

c) False. For a d electron, $l=2$, so the magnetic quantum number ml can only be $-2,-1,0,+1,$or $+2$, not 3.

d) False. For $l=2$, the d subshell has 5 orbitals and can therefore hold a maximum of 10 electrons.

e) False. An f subshell corresponds to $l=3$, so the principal quantum number must satisfy $n\geq4$; there is no f subshell for $n=3$.

f) False. Two atomic systems can have the same electronic configuration without being the same element (for example, different ions or different atoms/ions with the same number of electrons).

g) False. A single element can correspond to different electronic configurations (ground state and excited states, or different ionic states), so different configurations do not necessarily mean different elements.

Chapter IV

Periodic Classification of Elements

I)-Introduction

Since 1862, chemists have noted the similarity of certain properties of the elements, grouped them into families (alkalis, halogens, etc.), and tried to classify them in order of increasing molecular mass (De Chamcourtois, Lothar-Meyer, Newlands, etc.). However, it was, above all, Mendeleïev's work on the relationship between properties and atomic mass that was the most important.

Mendeleïev's idea was that there was a periodic relationship between the properties of elements and their atomic mass. On this basis, he classified the elements in existence at the time (63) by column to find the elements with similar chemical properties in each column. However, he was especially credited with predicting the properties of elements such as Gallium (Ga) and Strontium (Sr). He left empty cells in his classification, which were discovered years later. This periodic classification is still used today, except that the periodicity of the elements is linked to their external electronic structure. At present, the elements are classified by ascending atomic number (Z) by the principles and rules of filling.

The elements are combined in a table comprising seven rows or periods and 18 columns.

II) Organization of the Periodic Table (Mendeleev):

The periodic table reflects the electronic configuration of atoms. It organizes elements (by atomic number Z) so that elements with **similar outer-electron structures** show **similar chemical properties**.

- The periodic table is divided into **four blocks** according to the type of orbital being filled: **s, p, d, and f**.
- Elements arranged on the same **horizontal row** form a **period**. There are **7 periods** corresponding to the principal quantum number: n=1,2,3,4,5,6,7

- Elements in the same **vertical column** form a **group (family)** because they have the **same valence-electron configuration** (same outer layer structure), which gives them similar properties.

The periodic table contains **18 columns (groups)**. In the older classification, the first seven groups were often divided into two subgroups:

- **Subgroup A (main group elements):** outer electrons are mainly in ns and np orbitals (and for some, a completed nd^{10}.

- **Subgroup B (transition elements):** characterized by a partially filled d subshell, typically nd^1 to nd^9.

Finally, the Roman numerals **II, III, IV, V, VI, VII, VIII…** indicate the **number of electrons in the outer shell**, called **valence electrons**, which largely determine the chemical behavior of the element.

III) Main families in the periodic table:

- **Alkali metals (Group IA / 1):**

Elements with an outer electronic configuration of the type **ns1**.

- **Alkaline earth metals (Group IIA / 2):**

Elements with an outer electronic configuration of the type **ns2**.

- **Halogens (Group VIIA / 17):**

Elements with an outer electronic configuration of the type **ns2np5**.

- **Noble gases / rare gases (Group VIIIA / 18):**

Elements whose outer electronic configuration is generally **ns2np6**
(exception: helium 1s2).

- **Transition elements (d-block, Groups 3–12):**

Elements characterized by a **partially filled d subshell**.

- **Rare earth elements (f-block):**

Elements in which **f orbitals are being filled**:

- **Lanthanides:** filling the **4f** subshell
- **Actinides:** filling the **5f** subshell

IV) Study of periods

A **period** (a row in the periodic table) corresponds to the **progressive filling of electron subshells** (s,p,d,f) as the atomic number Z increases.
When you move across a period, electrons are added to orbitals until the atom reaches a **stable noble-gas configuration** at the end of the period.

each subshell can hold a maximum number of electrons:

- s: 1 orbital → **2 electrons**
- p: 3 orbitals → **6 electrons**
- d: 5 orbitals → **10 electrons**
- f: 7 orbitals → **14 electrons**

So the length of a period depends on which subshells are being filled:

- Periods 2 and 3: s+p=2+6=8 elements
- Periods 4 and 5: s+d+p=2+10+6=18 elements
- Periods 6 and 7: s+f+d+p=2+14+10+6=32 elements

Electrons do not always fill orbitals in simple order of n. They fill in order of **increasing energy**, which is often predicted by the **n+l rule** (Klechkowski rule):

- The orbital with the smaller value of n+l fills first.
- If two orbitals have the same n+l, the one with smaller n fills first.

That is why we obtain these filling sequences:

- **Period 4:** 4s→3d→4p
- **Period 5:** 5s→4d→5p
- **Period 6:** 6s→4f→5d→6p
- **Period 7:** 7s→5f→6d→7p

1st period (n=1): filling 1s

- **H (Z=1):** 1s1
- **He (Z=2):** 1s2 (noble gas)

  Only **2 elements** because the 1s subshell can hold only 2 electrons.

2nd period (n=2): filling 2s then 2p

From **Li (3)** to **Ne (10)**: Total = 2+6=8 elements.

- 2s fills (2 electrons)
- then 2p fills (6 electrons)

3rd period (n=3): filling 3s then 3p

From **Na (11)** to **Ar (18)**: Total = 8 elements.

- 3s fills (2 electrons)
- then 3p fills (6 electrons)

4th period (n=4): filling 4s, then 3d, then 4p

From **K (19)** to **Kr (36)**: Total = 2+10+6=18 elements.

- 4s fills: **K, Ca** (2 elements)
- 3d fills: **Sc to Zn** (10 elements) → **transition elements**
- 4p fills: **Ga to Kr** (6 elements)

Note (irregularities in 3d):
Some atoms are more stable when the ddd subshell is **half-filled** or **completely filled**, so an electron may shift from s to d.

- **Cr (Z=24):** expected [Ar] $4s^2 3d^4$ → actual [Ar]$4s^1 3d^5$ (half-filled d)

- **Cu (Z=29):** expected [Ar] $4s^2 3d^9$ → actual [Ar]$4s^1 3d^{10}$ (filled d)

5th period (n=5): filling 5s, 4d, 5p

From **Rb (37)** to **Xe (54)**: Total = 18 elements.

- 5s: 2 elements
- 4d: 10 elements (transition series)
- 5p: 6 elements

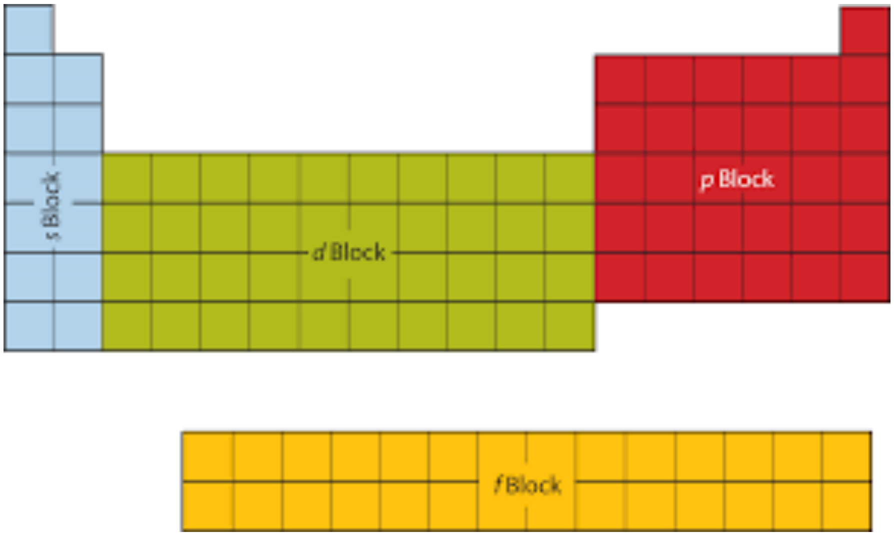
Similar stability exceptions exist (e.g., **Mo**, **Ag**).

6th period (n=6): filling 6s, 4f, 5d, 6p

From **Cs (55)** to **Rn (86)**: Total = 32 elements

- 6s: 2 elements
- 4f: 14 elements → **lanthanides**
- 5d: 10 elements
- 6p: 6 elements.

The other elements are filled in according to the established rules.



V)- Physical properties of elements

a) Three main categories

- *Metals*: Metals are *materials* widely used in many fields. A metal is, therefore, defined as a material whose atoms are held together by a *metallic bond*: all the atoms in the object share one or more electrons.

- *Non-metals:* The non-metals form a *chemical series of* the *periodic table* that groups together *elements* that are neither *Metals*, *Metalloids*, *Halogens,* nor *Rare Gases*. This series includes *Hydrogen*, *Carbon*, *Nitrogen*, *Oxygen*, *Phosphorus*, *Sulphur,* and *Selenium*.

- *Semi-metals*: From the earliest days of chemistry until 1965, **metalloid** was used to designate a chemical body, then a *chemical element* that was not a *metal.* Today, the concept of **metalloid** refers to a *chemical element* that cannot be classified either as a *metal* or as a *non-metal.*

b- Valence electrons :

Are electrons located on the outer layer of the atom's electronic configuration, giving the element's chemical group or family?

c- The stability of the nd underlay :

The nd undercoat is stable in two cases

- √ If it is saturated with 10 electrons (nd10).
- √ If it is half-saturated, it is filled with 5 electrons (nd5).

VI)- Periodicity of ownership

VI .1- Atomic radius ra

The atomic radius can be defined as half the distance between the centers of the two atoms linked by a single bond.

- √ Over a period: if **Z** increases, then **ra** decreases.
- √ On a column: if **Z** increases, then **the rate** increases.

VI .2- Ionic radius ri :

Generally speaking :

- √ Cations are smaller than their parent atoms: **ri (cation) < ra**
- √ Anions are larger than their parent atoms: **ri (anion) > ra**
- √ For ions with the same electronic configuration (S2-, Cl-, K+ , Ca2+, Ti4+, etc.):

If **Z** increases, $\mathbf{r_i}$ decreases.

For equal charges, the ionic radius varies in the same direction as the atomic radius :
If **Z** increases, then **ri** decreases.

VI .3- Ionisation energy (EI)

This is the energy required to extract an electron from an atom (or ion) in the ground and gaseous states.

- Over the same period, if **Z** increases, then **E. I** increase.
- In the same group, if Z increases, then **E. I** decrease.

VI .4- Electronic affinity (A.$_E$)

This is the opposite of ionization. The electron affinity of an atom **X** is the energy released when this atom captures an electron.

VI .5-Electronegativity (E.N)

This is the power of an element to attract an electron. An element that easily loses one or more electrons is said to be electropositive. The electronegativity χ an element X.

- Over the same period: if **Z** increases, then **E.$_N$** increases
- In the same group, if **Z** increases, then **E.$_N$** decreases

VI .6-Valencia

This is the capacity of each atom to form a bond. Its value is equal to the number of unpaired (single) electrons. <u>Example:</u>

1) Hydrogen: 1s1; v= 1

2) Oxygen: 2s2 2p4; v= 2

3) Potassium: 4s1, v = 1

VII .7-Magnetic properties

- Diamagnetism: Atoms (or molecules) with no single electrons are said to be diamagnetic.

- Paramagnetism: Atoms (or molecules) with single electrons are said to be paramagnetic.

TUTORIAL N° 04

Exercise 01:

1-Determine the configuration, electronic brokerage, period, and group for each element:

2- Determine the number of core electrons and the number of valence electrons.

P(15), Cu(29), Fe(26), Ce(58), Hg(80), Br(35)

Exercise 02 :

What is the number of valence electrons in vanadium V (Z=23) and gallium Ga (Z=31)? Give the four quantum numbers of these valence electrons.

Exercise 03:

Let us consider the following elements: A, B, C, and D in their fundamental state.

- Element (A) is located in the same period as Cl (17) and group Va.
- The element (B) of the stable anion (B-2) takes on the same electronic configuration as the element (Rn=86).
- The element (C) has the same Ag group (47) and the same Ce period (58).
- Element (D) has a single electron in the sub-layer (n=4, l=3) according to the electronic configuration. Determine the atomic radius (Z) for each element (A, B, C, D) and compare the three elements (B, C, D) in terms of atomic radius (ra) and (C, A) in terms of ionization energy (Ei).

Exercise 04 :

Let be the following elements :

Al(13), Cr(24), Rb(37), Ta(73).

1- Give the electronic configuration of these elements.

2- Place them in the periodic table (period and group).

3- What are the values of the four quantum numbers for the valence electrons of Cr(24)?

4-What are the ions obtained with Al and Cr?

5- What is the atomic number (Z) of the elements with the same period as Al (13)?

Exercise 05:

The tin atom (Sn) has two electrons in its ground state on the 5p sublayer.

1. Give its electronic structure, its atomic number, and the number of valence electrons.
2. Is it a transition metal? Why or why not?

Exercise 06 :

Let the two chemical elements, A and B, have atomic numbers Z and Z'.

A [18 Ar] 4S2 3d3 and B [36 Kr] 5S2 4d5

1- Determine Z and Z'.

2- Determine (group and period) (A and B).

3- Give the electronic configuration of A' and B' (A' = (Z+5); B' = (Z'+3)).

4- Determine (group and period) (A' and B').

Exercise 07 :

1- An element has less than 18 electrons and has two single electrons. What are the possible electron configurations for this element? What is this element, knowing that it belongs to the lithium period(3) and the tin group(50)?

2- The element in question belongs to one of the first three lines of the classification. The quantum box representation shows that only the p2 and p4 configurations have "exactly" two single electrons. The s2p3 configuration can also be considered suitable since it has three single electrons. The element in question can, therefore, only be C, Si, O, S, N, or P.

Exercise 08:

An element belongs to the fourth period and has two and only two "single" electrons (the only ones in a quantum cell).

1- How many possibilities are there? Specify the column and row numbers for each.

2- We also know that this element is not a transition element. How many possibilities are there? Specify the column and row numbers for each.

3- We also know that this element belongs to the chalcogen family. How many possibilities are there? Specify the column and row numbers for each.

Exercises Solutions

Exercise 01:

Phosphorus P (Z = 15)

- Electron configuration: $1s^2 2s^2 2p^6 3s^2 3p^3$.
- Period: 3.
- Group: 15 (VA).
- Valence electrons: 5 ($3s^2 3p^3$).
- Core electrons: 10.

Copper Cu (Z = 29)

- Electron configuration: $[Ar]3d^{10}4s^1$.
- Period: 4.
- Group: 11.
- Valence electrons: often taken as 1 ($4s^1$) in simple chemistry; in transition-metal context, 11 ($3d^{10}4s^1$).
- Core electrons: 28 or 18, respectively (depending on whether 3d is counted as core or valence in course).

Iron Fe (Z = 26)

- Electron configuration: $[Ar]3d^6 4s^2$.
- Period: 4.
- Group: 8.
- Valence electrons: usually 8 ($3d^6 4s^2$).
- Core electrons: 18.

Cerium Ce (Z = 58)

- Electron configuration (ground state): $[Xe]4f^1 5d^1 6s^2$.
- Period: 6.
- Group: lanthanide (often written group 3 block).
- Valence electrons: typically 4 ($4f^1 5d^1 6s^2$).
- Core electrons: 54.

Mercury Hg (Z = 80)

- Electron configuration: $[Xe]4f^{14} 5d^{10} 6s^2$.
- Period: 6.
- Group: 12.
- Valence electrons: 2 ($6s^2$).
- Core electrons: 78.

Bromine Br (Z = 35)

- Electron configuration: $[Ar]3d^{10}4s^24p^5$.
- Period: 4.
- Group: 17 (halogen).
- Valence electrons: 7 ($4s^24p^5$).
- Core electrons: 28.

Exercise 02:

Vanadium has 5 valence electrons, and gallium has 3 valence electrons.

Vanadium (Z = 23)

The ground-state electron configuration of vanadium is $[Ar]3d^34s^2$, so the valence electrons are the two 4*s* and three 3*d* electrons, for a total of 5.

Typical sets of quantum numbers (*n*,*l*,*ml*,*ms*) for these valence electrons (one possible assignment) are:

- 4*s* electron 1: $n=4, l=0, ml=0, ms=+1/2$
- 4*s* electron 2: $n=4, l=0, ml=0, ms=-1/2$
- 3*d* electron 1: $n=3, l=2, ml=-2, ms=+1/2$
- 3*d* electron 2: $n=3, l=2, ml=-1, ms=+1/2$
- 3*d* electron 3: $n=3, l=2, ml=0, ms=+1/2$

(Any choice of distinct *ml* values for the three 3*d* electrons with parallel spins is acceptable, by Hund's rule.)

Gallium (Z = 31)

The ground-state electron configuration of gallium is $[Ar]3d^{10}4s^24p^1$; the valence shell $n=4$ has $4s^24p^1$, so there are 3 valence electrons.

One possible set of quantum numbers for these three valence electrons is:

- 4*s* electron 1: $n=4, l=0, ml=0, ms=+1/2$
- 4*s* electron 2: $n=4, l=0, ml=0, ms=-1/2$
- 4*p* electron: $n=4, l=1, ml=+1, ms=+1/2$

(For the 4*p* electron, any of $ml=-1,0,+1$ with either spin is acceptable, as they are degenerate orbitals.)

Exercise 03:

Identify each element (Z)

- A: Same period as Cl (period 3) and group Va (group 15), so it is phosphorus, Z = 15.
- B: The stable anion B^{-2} is isoelectronic with Rn (Z = 86), so neutral B has Z = 84, which is polonium.

- C: Same group as Ag (group 11) and same period as Ce (period 6), so C is the group-11 element in period 6, gold with Z = 79.
- D: One electron in the subshell with n=4,l=3, i.e. a 4f1 configuration. The first element with 4f1 is lanthanum-like but, in the standard lanthanide series, a single 4f electron in the ground state occurs for gadolinium when written as $4f^7 5d^1 6s^2$, so D is taken as Gd, Z = 64, in this exercise framework.

Atomic radius comparison (B, C, D)

Going down a group or into the 6th period increases atomic radius, while moving across a period to higher Z generally decreases it.

Approximate metallic atomic radii place Au (C, period-6 transition metal) smaller than Gd (D, period-6 lanthanide), and both smaller than Po (B, heavy p-block element), giving:

- Smallest: C (Au, Z = 79)
- Intermediate: D (Gd, Z = 64)
- Largest: B (Po, Z = 84)

Ionization energy comparison (C vs A)

Phosphorus (A, Z = 15, period 3 nonmetal) has a significantly lower first ionization energy than gold (C, Z = 79, period 6 transition metal), despite relativistic effects that increase Au's effective nuclear charge.

Therefore $Ei(C)>Ei(A)$ (gold requires more energy to remove an electron than phosphorus).

Exercise 04:

1. Electronic configurations

- Al (Z = 13): $1s^2 2s^2 2p^6 3s^2 3p^1$ or $[Ne]3s^2 3p^1$.
- Cr (Z =24): $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^5$ or $[Ar]3d^5 4s^1$.
- Rb (Z = 37): $[Kr]5s^1$.
- Ta (Z = 73): $[Xe]4f^{14} 5d^3 6s^2$.

Position in periodic table

- Al: period 3, group 13 (IIIA).
- Cr: period 4, group 6 (VIB), d-block transition metal.
- Rb: period 5, group 1 (IA), alkali metal.
- Ta: period 6, group 5 (VB), d-block transition metal.

Period and group summary

Element	Period	Group
Al	3	13
Cr	4	6
Rb	5	1
Ta	6	5

Quantum numbers for valence Cr

For ground-state Cr, valence electrons are 4s14s1 and 3d53d5.

- For the 4s4s electron: n=4, l=0, ml=0, ms=+1/2.
- For a 3d electron (any one of the five equivalent 3d electrons): n=3, l=2, ml=−2,−1,0,+1 or +2 (one value), ms=+1/2.

Ions of Al and Cr

- Aluminium commonly forms Al^{+3} by losing its three valence electrons.
- Chromium most commonly forms Cr^{+2} and Cr^{+3} by losing the 4s electron and one or two 3d electrons.

Atomic numbers in Al's period

Elements in period 3 have atomic numbers from 11 to 18 (Na, Mg, Al, Si, P, S, Cl, Ar).
So the atomic numbers of elements in the same period as Al are Z=11,12,13,14,15,16,17, and 18.

Exercise 05 :

Tin (Sn) has the ground-state configuration $[Kr]4d^{10}5s^{2}5p^{2}$, atomic number 50, and 4 valence electrons in the 5s and 5p subshells.

It is not a transition metal because it is a p-block element in group 14, not a d-block element with partially filled d orbitals in its common oxidation states.

1. Electronic structure, Z, valence electrons

- Full electronic structure: $1s^{2}2s^{2}2p^{6}3s^{2}3p^{6}3d^{10}4s^{2}4p^{6}4d^{10}5s^{2}5p^{2}$.
- Atomic number: Z=50.
- Valence electrons: 4 (the $5s^{2}5p^{2}$ electrons).

2. Transition-metal character

Transition metals are defined as d-block elements (groups 3–12) that form at least one ion with a partially filled d subshell.

Tin lies in group 14 of the p-block and its stable ions Sn^{2+} and Sn^{4+} have filled 4d subshells, so it is classified as a post-transition metal, not a transition metal.

Exercise 06 :

1. Determine Z and Z′

- A has configuration $[Ar]4s^2 3d^3$. Counting electrons: Ar has 18, plus 2+3=5 gives 23, so Z=23, which is vanadium (V).
- B has configuration $[Kr]5s^2 4d^5$. Kr has 36, plus 2+5=7 gives 43, so Z'=43, which is technetium (Tc).

2. Group and period of A and B

- A (V, Z = 23): highest principal quantum number n=4 → period 4; outer pattern $4s^2 3d^3$ → 5 outer (s + d) electrons → group 5, d-block transition metal.
- B (Tc, Z′ = 43): highest n=5 → period 5; $5s^2 4d^5$ → 7 outer electrons → group 7, d-block transition metal.

Period and group (A, B)

Element	Z	Config (abbrev.)	Period	Group
A (V)	23	$[Ar]\ 4s^2\ 3d^3$	4	5
B (Tc)	43	$[Kr]\ 5s^2\ 4d^5$	5	7

3. Configurations of A′ and B′

- A′ has atomic number Z+5=23+5=28, which is nickel (Ni). Abbreviated configuration: $[Ar]4s^2 3d^8$.
- B′ has atomic number Z'+3=43+3=46, which is palladium (Pd). Ground-state configuration: $[Kr]4d^{10}$ (5s subshell is empty).

4. Group and period of A′ and B′

- A′ (Ni, Z = 28): highest n=4 → period 4; $4s^2 3d^8$ → 10 outer (s + d) electrons → group 10, d-block.
- B′ (Pd, Z = 46): electrons occupy up to 4d with pattern $[Kr]4d^{10}$, placing it in period 5, group 10, d-block.

Exercise 07 :

The element is silicon (Si), with electron configuration $[Ne]3s^2 3p^2$ and atomic number 14.

It fits the conditions “less than 18 electrons”, “two single electrons”, “lithium period (3)” and “tin group (group 14, ns^2np^2 configuration)”.

1. Possible configurations and identification

- For atoms with p electrons, having exactly two unpaired (single) electrons corresponds to a p2*p*2 or p4*p*4 valence configuration; an s^2p^3 configuration gives three unpaired electrons.
- In period 3, group 14 (same group as tin), the element has valence $3s^23p^2$, so the full configuration is $1s^22s^22p^63s^23p^2$; this is silicon, with $Z=14$ (< 18 electrons).

2. Check with the candidate list (C, Si, O, S, N, P)

- Among C, Si, O, S, N, and P, only Si is both in period 3 and group 14 (tin's group); C is period 2, while O, S, N, and P belong to groups 15 or 16, not group 14.
- Therefore the only element satisfying all given constraints (two single electrons, first three periods, lithium period 3, tin group 14) is silicon.

Exercise 08 :

The key idea is that "two single electrons" means the valence subshell has either a *p*2 or *p*4 pattern (two unpaired electrons in Hund's rule boxes), while any suitable d-block case would also give two unpaired electrons such as *d*2, *d*4, or *d*7 etc..

Period 4 runs from K (Z = 19) to Kr (Z = 36), with Ca as the last s-block, Sc–Zn as the d-block (transition metals), and Ga–Kr as the p-block.

1. All possibilities in period 4

In period 4, the p-block elements are Ga ($4p^1$), Ge ($4p^2$), As ($4p^3$), Se ($4p^4$), Br ($4p^5$), Kr ($4p^6$); only Ge ($4p^2$) and Se ($4p^4$) have exactly two unpaired electrons in the p subshell.

There are also d-block cases with two unpaired d electrons; examples are Ti ($3d^24s^2$) and Ni ($3d^84s^2$), each having two unpaired electrons in the 3d subshell.

So, counting all (p plus d) possibilities in period 4 that have exactly two unpaired electrons, typical answers are:

- Ti (group 4, period 4)
- Ge (group 14, period 4)
- Se (group 16, period 4)
- Ni (group 10, period 4)

(Your teacher may accept only p-block answers if the course has not yet treated d-block unpaired-electron counting.)

2. Restricting to non-transition elements

"Not a transition element" excludes the d-block (Sc–Zn), so only the s- and p-block in period 4 remain: K, Ca, Ga, Ge, As, Se, Br, Kr.

Among these, only Ge (group 14, 4th period) and Se (group 16, 4th period) have exactly two unpaired electrons ($4p^2$ or $4p^4$).

So there are 2 possibilities:

- Ge: period 4, group 14
- Se: period 4, group 16

3. Restricting further to chalcogens

Chalcogens are group 16 elements (oxygen family).

In period 4, the only chalcogen is selenium (Se), period 4, group 16, with valence configuration $4s^2 4p^4$ and exactly two unpaired p electrons.

So:

- There is only 1 possibility: Se, column (group) 16, row (period) 4.

Chapter V

Chemical bonding

I- Introduction

Matter, in its various states, is generally formed by molecules and sometimes by ionic assemblies. Apart from the elements in column VIIIA, which are monatomic rare gases stable in the standard state, all the other atoms exist in a combined state, in the form of simple or complex molecules. The formation of these edifices (molecules) follows the general law of thermodynamics, according to which any system evolves spontaneously towards the state in which it is simplest.

From a structural point of view, it is important to understand the reasons why the assembly of atoms (electrons and nuclei) in a molecule or crystal is more stable than an edifice made up of isolated atoms in the fundamental state; study (as with atoms) the distribution of electrons in a molecule and find the cause(s) of the stability of the edifices formed: this is the purpose of chemical bonding.

a) Octet rule:

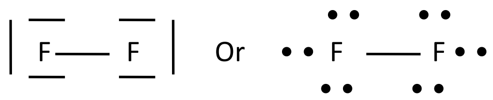
Within a molecule, each atom taking part in a reaction tends to stabilize by acquiring the most stable outer-shell configuration (that of the noble gases: $ns^2\ np^6$).

b) Lewis structure:

A Lewis structure is a simplified representation of a molecule. In this model, only the electrons that effectively participate in bonding are considered. A covalent bond is shown by a line, and non-bonding electron pairs are shown by dots (or sometimes short lines).

Example: F_2

F_2 :



If the doublet initially belongs to a single donor, the covalent bond is called a ***dative bond.***

II. Different types of chemical bonds

II.1. Localized bonds

a) Covalent bond

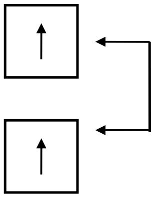
Any bond obtained by sharing electrons is called a covalent bond.

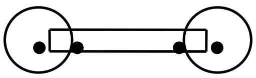
1a) Single covalent bond (SCB)

One pair of electrons is shared; each atom contributes one electron.

Examples: Ex : - molécule H_2 :

$_1H : 1s^1$





$_1H : 1s^1$

- H_2 molecule: each H $(1s^1)$ shares one electron to form one shared pair.
- Cl_2 molecule: each Cl $(\ldots 3s^2\ 3p^5)$ shares one electron to form a single bond; each Cl keeps three lone pairs.

1b) Multiple covalent bond (MCB)

Two or three pairs of electrons are shared (double or triple bond).

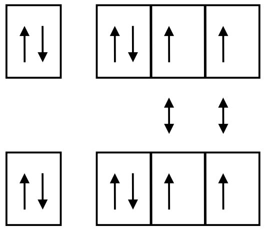
Examples:

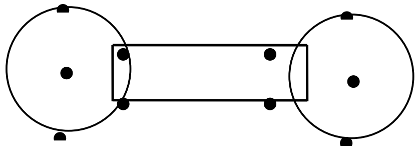
- O_2: double bond (two shared pairs) between the oxygen atoms.
- N_2: triple bond (three shared pairs) between the nitrogen atoms.

\- molécule O_2 :

$_8O : 1s^2\ (2s^2\ 2p^4)$

$_8O : 1s^2\ (2s^2\ 2p^4)$

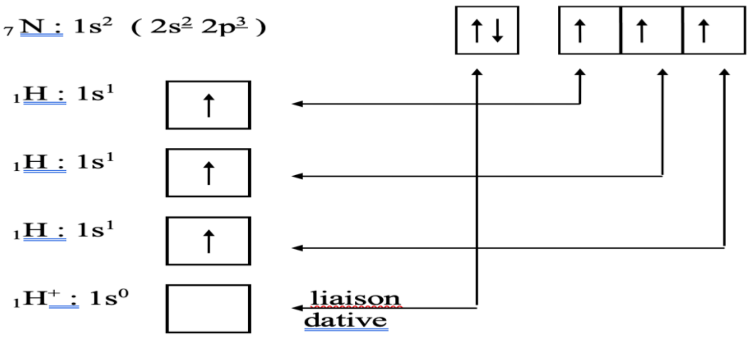




b) Dative (coordinate) bond

A dative (coordinate) bond is a bond in which a donor atom provides the bonding electron pair to an acceptor atom that has an electron vacancy (an empty orbital). Once formed, a coordinate bond is not distinguished from an ordinary covalent bond.

Example: NH_4^+ formation by donation of a lone pair from N to H^+.



c) Polar covalent bond

A covalent bond between two atoms with different electronegativities is called a polar covalent bond. The shared electron pair is shifted toward the more electronegative atom, which acquires a partial negative charge (δ−). The other atom acquires a partial positive charge (δ+). A dipole appears, with dipole moment:

$\mu = \delta \cdot d$

where d is the internuclear distance (bond length) and δ is the partial charge ($\delta < e$). The unit of dipole moment is the Debye (D), with 1 D = 0.33×10^{-29} C·m.

Remarks:

1) The dipole-moment vector is oriented from the negative pole (δ−) toward the positive pole (δ+).

Example: HCl — H is less electronegative than Cl, so $\mathrm{H}\delta+$—$\mathrm{Cl}\delta-$.

2) The larger the electronegativity difference, the more polar the bond.

3) One also speaks of an angular (resultant) dipole moment for bent molecules.

Example: water. If the two O–H bond dipoles are μ_1 and μ_2 and the H–O–H angle is α, then:

$$\mu = \mu_1 + \mu_2 = 2\ \mu_1 \cos(\alpha/2).$$

d) Ionic bonding

Electrons are exchanged between the atoms that make up the molecule to form stable ions (this transfer of electrons is possible when there is a large difference in electronegativity ($\Delta\chi>2$).

Example:

NaCl (Na = 0.93; Cl = 3.16) → $\Delta\chi = 3.16 - 0.93 = 2.23 > 2$.

Na → Na+ + 1é: 1s2/ **2s22p6** (structure of a rare gas, Neon: ^{10}Ne).

Cl + 1é → Cl-: 1s2 2s22p6/**3s23p6** (structure of a rare gas, Argon: ^{18}Ar). Na^+ and Cl^- are stable ions. The nature of the bond is purely electrostatic.

Ex : NaCl $\quad Na \longrightarrow Na^+ + 1é\ ;\ Cl + 1é \longrightarrow Cl^-$

$$Na^+ + Cl^- \longrightarrow NaCl$$

NaCl= r (Na^+) + r (Cl^-)→ $\mu = ed$ (ionic bond→ polar molecule)

The partial ionic character of a bond **(% C.I)** is also defined by :

% C.I = $\boldsymbol{\mu_{real} * 100/\mu_{ionic}}$

II.2 Delocalized bonds

So far, the bonds in the molecules considered were localized between two atoms. However, many molecules exhibit delocalized bonding.

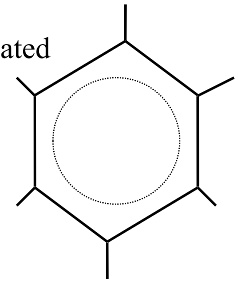
a) Conjugated molecules

1a) Cyclic case: benzene (C_6H_6)

The C–C bond in benzene is neither a pure single bond nor a pure double bond. Its length is intermediate and closer to that of a double bond, as shown by bond lengths:

Single C–C: 1.54 Å ; Benzene C–C: 1.40 Å ; Double C=C: 1.34 Å

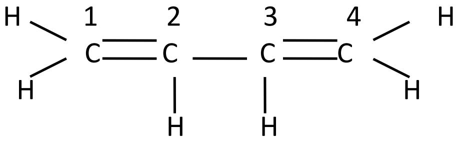
The three “double bonds” are delocalized around the ring; they are also called conjugated bonds.



	Simple Bond C — C	Bond in benzene C — C	Double Bond C = C
Bond lenght (A°)	1,54	1,40	1,34

1b) Acyclic systems: butadiene (C_4H_6)

Conjugation of double bonds is also found in many open-chain molecules such as butadiene. A simple Lewis diagram does not fully account for conjugation. In fact, the p_z orbitals of carbons 2 and 3 overlap and the electron cloud extends over the four carbon atoms.



e)- Metallic bonding

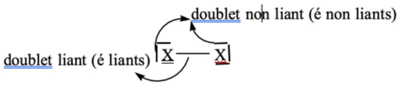
A metallic bond is weaker than a covalent bond between two atoms. It is not fundamentally different from a covalent bond; it is a delocalized bond extending over the entire crystal.

Example: in solid lithium, each atom is surrounded by several others; it is not possible to localize orbitals between pairs of atoms, so one considers delocalized molecular orbitals extending over the whole crystal.

III- Lewis notation

III.1)- Binding and non-binding doublet

In a molecule, all the peripheral electrons of the atoms are grouped in pairs called "electron doublets". A distinction is made between binding and non-binding doublets.



A bonding pair is made up of two electrons shared in a covalent bond. It belongs to two atoms. Other doublets are called non-bonding doublets. They belong to a single atom.

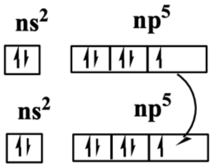
III.2)- Lewis representation of a molecule

The Lewis representation of a molecule is a representation of the atoms and all the binding and non-binding doublets in this molecule. By convention, a binding doublet between two atoms is represented by a line between the symbols of these atoms; a non-binding doublet of an atom is represented by a line next to the symbol of the atom.

Example

$_{17}$Cl [$_{10}$Ne] **$\underline{3s^2 3p^5}$** $|\overline{\underline{Cl}}—\overline{\underline{Cl}}|$

$_9$F [$_2$He] **$\underline{2s^2 2p^5}$** $|\overline{\underline{F}}—\overline{\underline{F}}|$



IV- The covalent bond and the theory of molecular orbitals

The inadequacies of Lewis's theory necessitated the introduction of wave mechanics. An electron in an atom is described by a wave function ΦΨ = OA

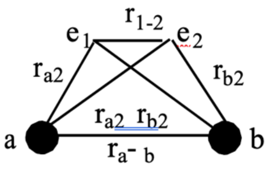
An electron in a molecule will be described by a wave function Φ = OM

Atomic bonding occurs when there is a single electron on an oxygen atom which can bond with another single electron belonging to another oxygen atom of the same or similar energy to form an oxygen atom whose energy level is lower than that of the two oxygen atoms.

Let Ha and Hb be two hydrogen atoms.

Ha → Ψ(a) (Ha isolated) For there to be a bond between Ha and Hb to form the H2 molecule

Hb → Ψ(b) (Hb isolated), the two atoms would have to approach a distance r1-2



One of the calculation methods used is the L.C.A.O. method (Linear Combination of Atomic. Orbitals).

If the two atoms bond to each other, we will have a linear combination of the OA Ψ(a) and Ψ(b) => $\Psi = a\Psi_a + b\Psi_b$.

The calculations give a/b = +1 and a/b = -1

$\Psi^+ = \Psi_a + \Psi_b$ $\quad \Psi \longrightarrow$ O.M (Binding)

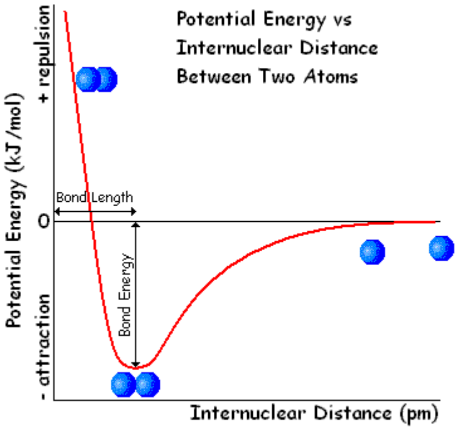
Ψ

$\Psi^- = \Psi_a + \Psi_b$ $\quad \Psi^* \longrightarrow$ O.M (anti-Binding)

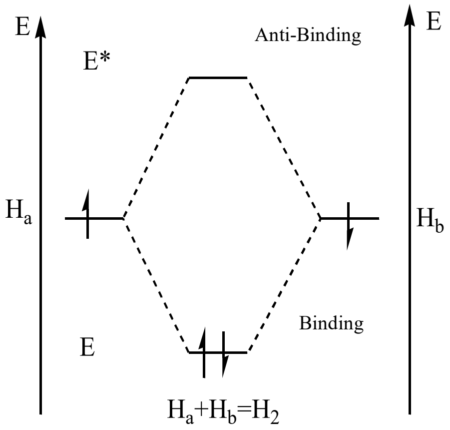
Ψ and Ψ (*), which are, in fact, linear combinations of the OA Ψ (a) and Ψ (b), are called molecular orbitals or OM

à $\Psi+ \longrightarrow E_+$ Binding energy (E).

to $\Psi- \longrightarrow E+$ Anti-binding energy (E*).

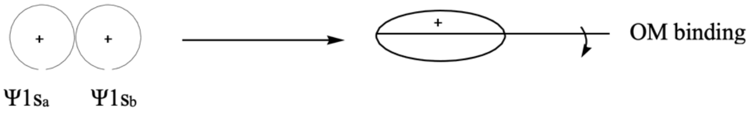


The two electrons in the H2 molecule will have opposite spins and will move to the lowest energy (most stable) level, the bonding OM Ψ.



Extrapolating: 1OA or 1OM will contain a maximum of 2é

2 OA combine to give 2 OM (Ψ, Ψ*)

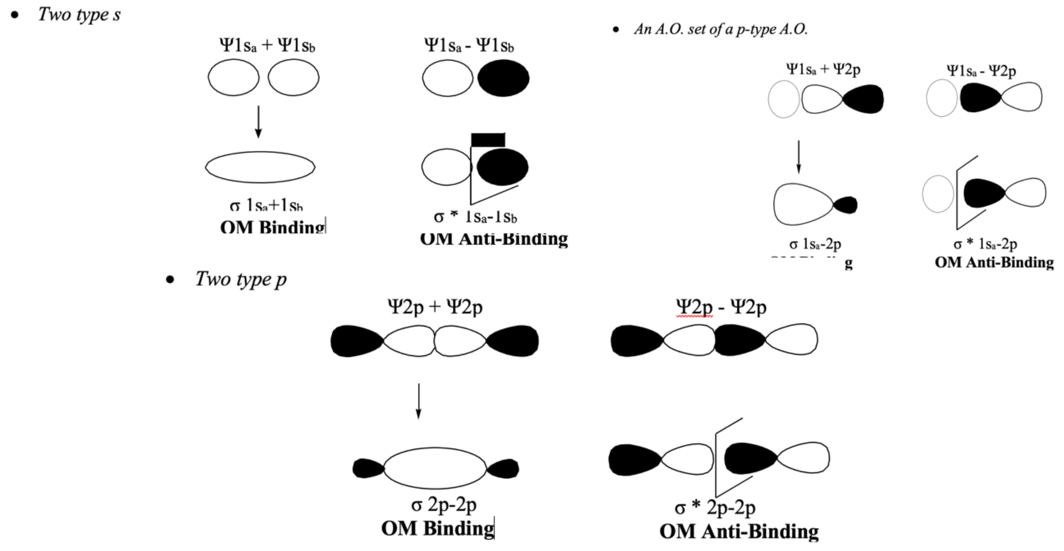


representation of the σ $_{1s\text{-}1s}$ bond in the H_2 molecule

Overlapping types of A.O.s form a covalent bond. We have a charge distribution with cylindrical symmetry of revolution; the overlap is axial (occurs along the axes joining the two nuclei), and the M.O formed will be of type σ.

IV.1)- The sigma(σ) bond

A bond (σ) is formed by axial overlap of 2 OA, the molecular orbital exhibiting rotational cylindrical symmetry about the internuclear axis. A bond (σ) can be formed from :



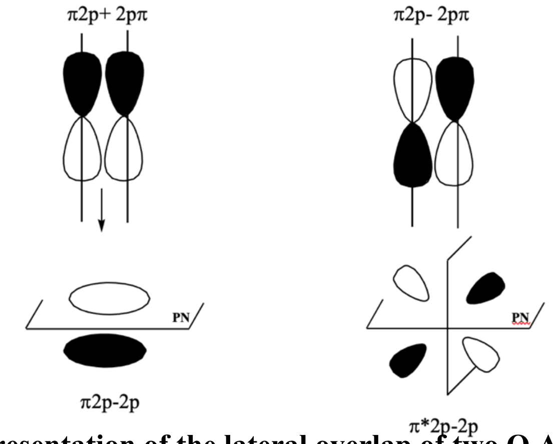
Representation of the axial overlap of two O.A.(ss)(sp)(pp)

The (σ)-bond (σ-bonding OM) induces free rotation about the axis of revolution (axis of the molecule).

IV.2)- The pi bond (π)

The bond (π) can only be formed from two OA p. and only if a bond of type (σ) already exists. An M.O. (π) is formed by lateral overlap (no cylindrical symmetry of revolution). This overlap requires the axes of the A.O.s to be parallel, whereas, for the (σ) connection, the axes are merged.

Lateral symmetry leads to the presence of two nodal planes perpendicular to each other and the axis joining the nuclei (remember that a nodal plane is an area of space where the probability of finding the electron is zero $\Psi(2) = 0$). The presence of a bond (π) blocks free rotation (fixed geometry).



Representation of the lateral overlap of two O.A.p

IV.3)- Energy diagram of a molecule

As with atoms, an energy diagram (representation of energy levels) will be defined for molecules. *The M.Os are filled in according to the rules established for atoms (stability principle, Pauli's principle and Hand's rule). There is maximum overlap (bonding) between A.O.s of the same or similar energy.*

We also define the Bond order (or index or number)

BO or i = (n-n*)/2

n: number of bonding electrons (located on a bonding M.O.).

n*: number of antibonding electrons (located on an antibonding M.O.)

IV.3.1)- Homonuclear molecules (A2)

The (O2) molecule:$1s^2 2s^2 2p^4$

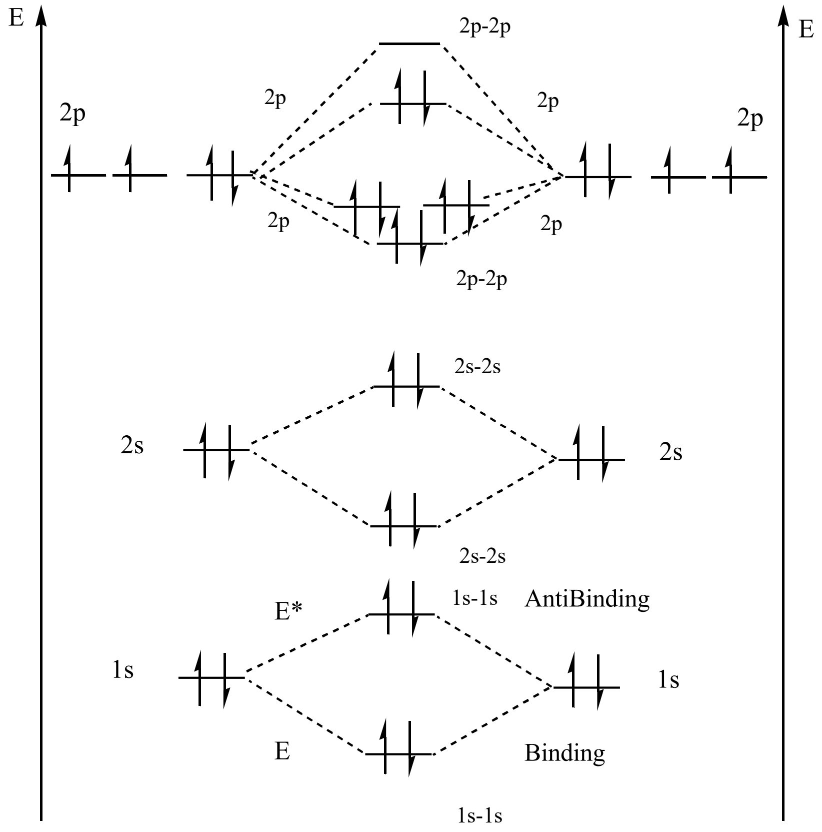


Diagram of the OMs of the homoatomic molecule of type (A2)

The electronic structure of the molecule: $(\sigma_1s\text{-}_1s)^2$ $(\sigma^*_1s\text{-}_1s)^2$ $(\sigma_2s\text{-}_2s)^2$ $(\sigma^*_2s\text{-}_2s)^2$ $(\sigma_2p\text{-}_2p)^2$ $(\sigma^*_2p\text{-}_2p)^2$ $(\pi_2p)^2$ $(\pi_2p)^2$ $(\pi^*_2p)^2$ $(\pi^*_2p)^2$.

We calculate:

B. O. (i) = ½(n-n*) = ½ (10-6)=2 B.O (i) = 2

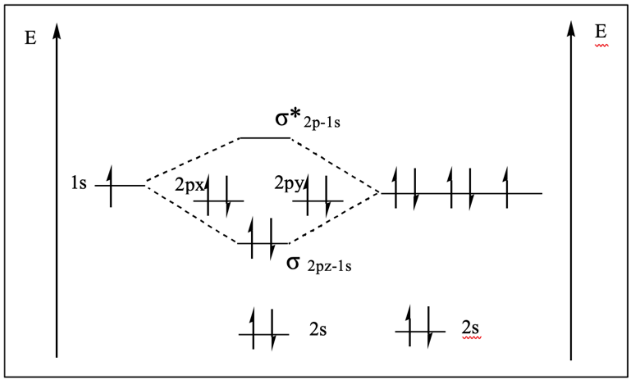
There is a double bond between the two Oxygen atoms (in the *Lewis* notion O=O), but this is not a true reflection of reality, as we can see from the diagram that there are two single electrons located in the two antibonding orbitals (*Hand's rule*), which gives this molecule paramagnetic properties. The explanation of this paramagnetic phenomenon in oxygen was a notable success for the theory of molecular orbitals.

IV.3.2)- Heteronuclear molecules (AB)

The molecule (HF) / H: 1s1 / F: $1s^2 2s^2 2p^5$

As the fluorine atom is more electronegative than hydrogen, its OA will be more stable. (lower energy than that of the hydrogen atom).

The A.O.s that will combine will be those with the closest energies (the 1s A.O. of H and one of the 2p A.O.s of F).



OMs diagram of the heteroatomic molecule of type (AB)

-The linear combination of the 1s A.O. of H and the 2pz A.O. gives rise to two M.O.s: a binding (σ) M.O. of lower energy than the two A.O.s and an antibonding (σ*) M.O. of raised energy.

- The unused 2s, 2px and 2p(y) A.O.s will give M.O.s of the same energy as these A.O.s. These are non-bonding M.O.s located around the Fluorine atom. A bond (σ2p-1s) is formed between F and H.

Calculation:

B.O (i) = ½(n-n*) = ½ (2-0)=1 B.O (i) = 1

Tutorial N° 05

Exercise 01:

Give the type of bond that exists in each of the following compounds: F_2, HCl, BF^{4-}, $AlCl_3$, BF_3, NH^{4+}, NaCl.

Exercise 02:

Let's react sulphur and oxygen:

1- Recall the electronic structure of sulphur and oxygen.

2- Which compound should be obtained using the simple theory of covalency?

3- Does this compound actually exist?

4- What are the formulae of the sulphur and oxygen compounds you know?

5- Based on the fact that a dative bond is involved, propose the symbolic formula for SO2 and SO3.

Exercise 03:

Show the least charged mesomer in Lewis form for the following acyclic molecules. The central atom is shown in bold in case of ambiguity.

1) H_2O, Hydroxide ion OH^- , Hydronium ion H_3O^+ , Hydrogen peroxide H_2O_2, Proton H^+

2) Ammonia NH_3, ammonium NH^{4+} , amide $NH(2)^-$.

3) Some gases: Dihydrogen, Methane CH_4, Difluor F_2, Chlorine Cl_2, Dioxygen O_2, Diazote N_2, Carbon Monoxide CO, Carbon Dioxide CO_2, Ozone O_3.

4) Some compounds (NO): nitric oxide NO, Nitronium ion NO_2^+, Nitrite ion NO_2^-, Nitrate ion NO_3^- then some dimers NNO, O_2N-NO, O_2N-NO_2, ON-NO.

Exercise 05:

The following inter halogenated compounds are given: CIF, CIF3 BrF, BrF3 BrF5 IF IF_3 IF_5 IF_7

1- Give the Lewis structure of CIF, CIF_3, BrF_5, IF_7

2- Knowing that the electronic transitions allowed to the electron must satisfy the rule Δ I= ± 1 (s ↔ p, p ↔ d...) and based on the knowledge acquired, explain why:

- Fluorine has a covalency of 1.
- Chlorine has a covalency equal to 1 and 3.
- Bromine has a covalency equal to 1, 3 and 5.
- Iodine has covalences equal to 1, 3, 5 and 7.

Exercise 06:

The partial ionic character (%C.I) of the H-Cl molecule is 17%.

1- Calculate the partial charge carried by H and Cl.

2- Calculate in Debye the dipole moment of this molecule, knowing that due to the intermolecular distance dH-Cl = 1.28

Data: 1D= $10^{-29}/3$ C.m; e = 1.610^{-19} C; 1Å = 10^{-10} m

Exercise 07:

The angle of the S-O bonds in the SO2 molecule is 119°. Its measured dipole moment is 1.65D.

1- What is the ionicity of the bonds?

2- What is the value of the charges located on S and the two O?

Data: 1D = 3.33 10^{-30} SI; e = 1.6 10^{-19} C; $d_{S\text{-}O}$ = 0.145 10^{-9} m

Exercise 08:

Assign the appropriate dipole moment and ionic percentage to each of the following diatomic molecules and explain why: HB, HCl, LiF, and HI.

D (Debyes)	6.30	0.38	1.03	0.79
CI (%)	11	84.6	6.8	16.9

Data: $_{1}H$; $_{3}Li$; $_{9}F$; $_{17}Cl$; $_{35}Br$; $_{53}I$

Exercises Solutions

Exercise 01:

- H (Z = 1): 1*s*1.
- B (Z = 5): $1s^2 2s^2 2p^1$ or $[He]2s^2 2p^1$.
- N (Z = 7): $1s^2 2s^2 2p^3$ or $[He]2s^2 2p^3$.
- F (Z = 9): $1s^2 2s^2 2p^5$ or $[He]2s^2 2p^5$.
- Cl (Z = 17): $1s^2 2s^2 2p^6 3s^2 3p^5$ or $[Ne]3s^2 3p^5$.
- Al (Z = 13): $1s^2 2s^2 2p^6 3s^2 3p^1$ or $[Ne]3s^2 3p^1$.
- Na (Z = 11): $1s^2 2s^2 2p^6 3s^1$ or $[Ne]3s^1$.

- F_2: Non-polar covalent bond (same non-metal atoms sharing electrons equally).
- HCl: Polar covalent bond (covalent, but electrons shifted toward the more electronegative Cl).
- BF_4^-: Covalent B–F bonds inside the BF_4^- ion (often described as covalent/partly coordinate within the polyatomic ion).
- $AlCl_3$: Predominantly covalent Al–Cl bonds in the molecular form $AlCl_3$.
- BF_3: Covalent B–F bonds (molecular covalent compound).
- NH_4^+: N–H bonds are covalent, with one of them formed as a coordinate (dative) covalent bond from N to H^+.
- NaCl: Ionic bond between Na^+ and Cl^- ions (metal–nonmetal, electron transfer).

Exercice 02:

Sulphur and oxygen each have six valence electrons, so simple covalency would predict a 1:1 compound (SO), but in reality stable bulk compounds are mainly SO_2 and SO_3, whose bonding is better described using double and dative S–O bonds. The symbolic (Lewis-type) formulas of SO_2 and SO_3 usually show one S=O double bond and one or two S–O dative (coordinate) bonds that are equivalent by resonance.

1. Electronic structures

- Oxygen (Z = 8): full configuration $1s^2 2s^2 2p^4$, often written by shells as 2,6; it has 6 valence electrons in the 2s and 2p orbitals.
- Sulphur (Z = 16): full configuration $1s^2 2s^2 2p^6 3s^2 3p^4$, written by shells as 2,8,6; it also has 6 valence electrons in the 3s and 3p orbitals.

2. Compound from simple covalency

Using a very simple covalency model, both S and O have valency 2, so each would form two single bonds. Combining one S and one O with two single bonds leads to a hypothetical sulphur monoxide, SO, where each atom completes an octet with two S–O bonds (formally S=O).

3. Does SO exist?

Neutral SO does exist as a diatomic molecule, but it is observed mainly in the gas phase (e.g., as a transient species in flames, the atmosphere, and interstellar space) rather than as a stable, isolable macroscopic compound like SO_2. Under ordinary conditions the thermodynamically stable oxides of sulphur are SO_2 and SO_3, not SO.

4. Known sulphur–oxygen compounds

Common sulphur–oxygen compounds include:

- Sulphur dioxide: SO_2 (major product from burning sulphur or sulphur-containing fuels).
- Sulphur trioxide: SO_3 (formed from oxidation of SO_2; precursor to sulfuric acid).
- Sulfuric acid and related oxyanions: H_2SO_4, sulphate SO_4^{2-}, bisulfate HSO_4^-.
- Other less common species: sulphurous acid H_2SO_3 (in aqueous SO_2), thiosulfate $S_2O_3^{2-}$, etc.

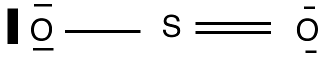
Main sulphur–oxygen species

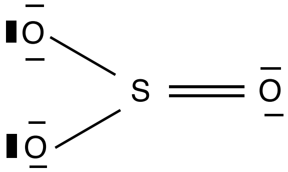
Species type	Formula examples
Neutral oxides	SO_2, SO_3, transient SO
Oxyacids	H_2SO_4, H_2SO_3
Oxyanions	SO_4^{2-}, HSO_4^-, $S_2O_3^{2-}$

5. Symbolic formulas with dative bonds

- SO_2: draw S in the center, one S=O double bond, and one S→O dative bond (from an O lone pair to an empty S orbital); resonance makes the two S–O bonds equivalent overall.

- SO_3: draw S in the center, one S=O double bond and two S→O dative bonds (each O donating a lone pair to S); again, resonance among the three equivalent S–O bonds is implied.





Chapter VI

Hybridization And Molecule Geometries

I- Introduction

The hybrid orbital model is used to simulate orbital deformation. It involves expressing the deformed atomic orbitals as linear combinations of valence atomic orbitals belonging to different sublayers (for the same atom). The new orbitals are, therefore, called hybrid orbitals. By mixing orbitals with different symmetries that belong to the same electronic layer, the orientation of the new orbitals can be modified to give a better qualitative description of the bonds between atoms. A hybrid orbital is written as :

$$\varphi = \sum_{p=1}^{N} C_P \, \chi_p$$

Where φ is the hybrid orbital, Cp is the coefficient of the linear combination, giving the influence of each atomic orbital χ_p in the hybrid. There are three types of hybrid orbital: sp^3, sp^2 and sp.

II- Theory of hybridization of atomic orbitals:

Using pure atomic orbitals (s,p,d,f) does not always lead to the correct molecular geometry. These orbitals combine (mix) to form new orbitals that differ in shape and orientation. They are called **hybrid orbitals**.

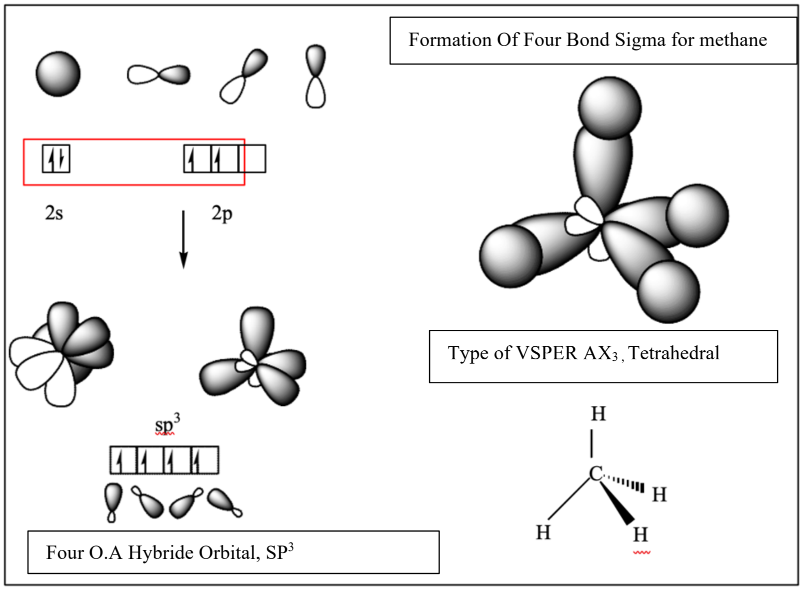
- Each type of hybridization corresponds to a specific geometry.
- Combining n pure atomic orbitals produces n hybrid orbitals.
- x (s AO) + y (p AO) → (x+y) $s^x p^y$.

II.1)-Diagonal hybridization (sp3)

It results from the linear combination of an s orbital with 3 p orbitals of the same atom. To describe a tetrahedral molecule such as CH_4, a pyramidal molecule with one non-bonding pair such as NH_3 or an angular molecule with two non-bonding pairs such as H_2O.

Example: CH_4/

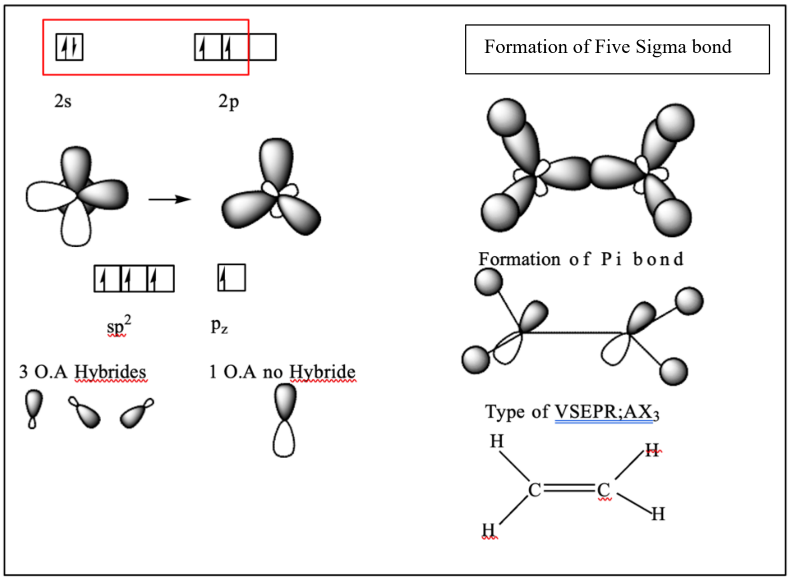
$_6C$: $1s^2$ $\underline{2s^2 2p^2}$



II.2)-Trigonal hybridization (sp^2)

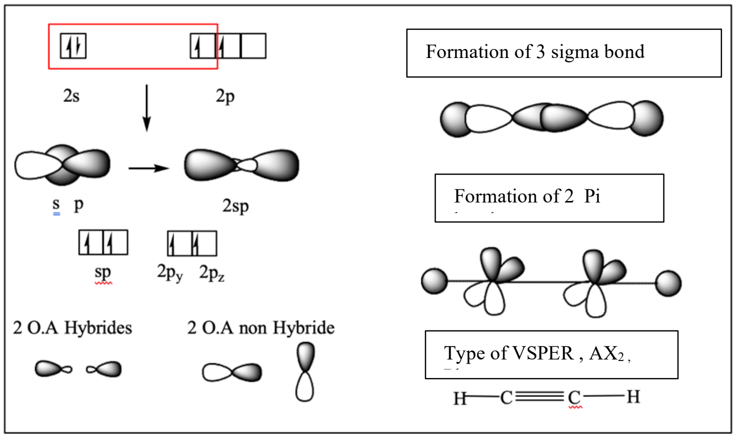
It results from the linear combination of an s orbital with 2 p orbitals of the same atom. To describe a trigonal molecule such as BH3, the other p orbital is unchanged and will be at the origin of the π bond in ethylene.

Example C_2H_2



II.3)-Triangular hybridization (sp)

It results from the linear combination of an s orbital with a p orbital of the same atom. To describe a linear molecule such as BeF_2, the other two p orbitals are unchanged and will be origin, for example, of the two π bonds in acetylene.



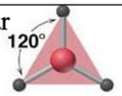
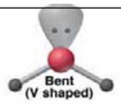
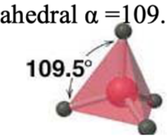
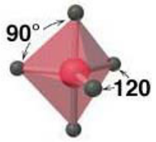
III- Principle of the Gillespie rules

The principle is that the various electron pairs in the valence layer of a central atom **A** repel each other: the geometry of the structure will be that for which the repulsions are minimal, i.e. that which generates maximum distances between the doublets.

Molecules with central atoms **A** are noted **AX_mE_n**

- where m is the number of atoms **X** bonded to **A**
- n: the number of non-bonding doublets E in the valence shell of the central atom **A**.

A double or triple bond is counted as a single bond in this theory: it is, therefore, the number of bond directions predicted by Lewis that determines the value of m. It is assumed that the binding and non-binding doublets of the outer layer move at the same distance from the nucleus of the central atom **A**; they, therefore, move on the surface of a sphere whose centre is atom **A** (comparison with the globe). The doublets repel each other and are located in positions that minimize repulsion, i.e. as far away from each other as possible.

<table>
<tr><th colspan="7">Structure of molecules and ions according to the V.S.E.P.R molecule
AX_mE_n</th></tr>
<tr><th>m+n</th><th>m</th><th>n</th><th>Type</th><th>Hyb.</th><th>Geometries</th><th>Examples</th></tr>
<tr><td>2</td><td>2</td><td>0</td><td>AX_2</td><td>sp</td><td>Linear α =180°
 </td><td>BeH_2, HCN, CO_2</td></tr>
<tr><td rowspan="2">3</td><td>3</td><td>0</td><td>AX_3</td><td rowspan="2">sp^2</td><td>Triangular α =120
 </td><td>BCl_3, BF_3, NO_3^-
CO_3^-, SO_3, AlCl2</td></tr>
<tr><td>2</td><td>1</td><td>AX_2E_1</td><td>Angled α≅ 120
 </td><td>SO_2, $SnCl_2$, O_3,
NOCl</td></tr>
<tr><td rowspan="2">4</td><td>4</td><td>0</td><td>AX_4</td><td rowspan="2">Sp^3</td><td>Tetrahedral α =109.5°
 </td><td rowspan="2">CH_4, $CHCL_3$
NH_3, NH_4^+
H_2O, $POCl_3$</td></tr>
<tr><td>3</td><td>1</td><td>AX_3E_1</td><td>Pyramid with triangular base
 </td></tr>
</table>

Note :

There are two types of electron doublets in the valence layer:

- Bonding pairs, which make up chemical bonds.
- Non-bonding pairs, which are in the outer layer but do not form chemical bonds

IV. Intermolecular interactions

IV.1) Molecular crystals

These crystals consist of an assembly of molecules. Intermolecular forces ensure cohesion. We distinguish Van der Waals interactions and hydrogen bonds.

a) Hydrogen bonding

This very important interaction associates molecules containing bonds such as F–H, O–H, or N–H with molecules that possess an electronegative atom bearing a lone pair (O, N, or F). It is therefore mainly electrostatic in nature.
Example: O–H···O hydrogen bonding in water (or alcohols).

b**) Van der Waals interactions**

Interactions between neutral molecules generally fall within an energy range of about 1 to 10 $kJ\cdot mol^{-1}$. These forces, grouped under the generic term Van der Waals forces, can be explained as follows:

- **Polar molecules:**

Permanent dipoles interact like ordinary electric charges, but paired and of opposite sign, leading to an intermolecular interaction such as $X^{\delta+}–Y^{\delta-} \ldots X^{\delta+}–Y^{\delta-}$.

- **Non-polar molecules:**

Although neutral, non-polar molecules can be distorted (polarized) by the electric field of nearby dipoles. The field shifts positive and negative charges in opposite directions depending on the polarizability of the molecule, creating an induced dipole that can then interact with permanent (or other induced) dipoles.

IV.2) Covalent crystals

In covalent crystals, the particles in the lattice are atoms and the bonds are true covalent bonds. Three types are commonly distinguished:

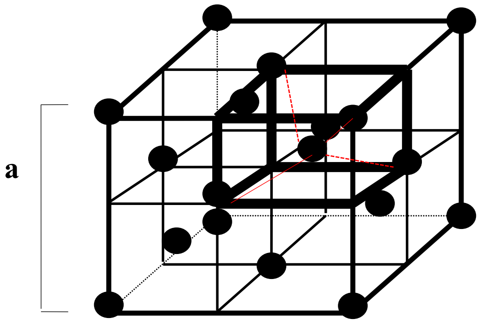
- Three-dimensional networks (macromolecules extending in three directions).
- Layered (sheet) structures, where atoms can be grouped into planes.
- Linear structures (not discussed here).

a) Three-dimensional structure: diamond

- Carbon is sp^3 hybridized (each atom is tetrahedrally surrounded by four others).
- All atoms are covalently bonded and all C–C bonds are identical.
- By repeating an infinite number of structural motifs, one obtains the three-dimensional crystal lattice of diamond.

In this motif, carbon atoms occupy the corners and face centers of a cube of edge a, as well as alternating centers of smaller cubes of edge a/2.

Typical values: ∠C–C–C = 109°28′ ; d(C–C) = 1.54 Å ; a = 3.55 Å.



CCC = 109°28'

d_{C-C} = 1.54 A°

a = 3,55 A°

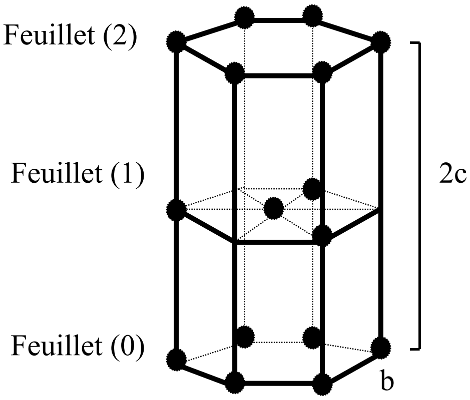
Diamant structure

b) Two-dimensional structure: graphite

- Carbon atoms are sp^2 hybridized and arranged in parallel planes. In each plane the atoms form a lattice of fused regular hexagons.

The structural motif is a right prism with a hexagonal base (side b) and height 2c. The orthogonal projection of sheet (1) onto sheet (0) shows the two lattices are shifted by b.

Typical values: c = 3.35 Å ; b = 1.41 Å.



c = 3,35 A°
b = 1,41 A°

Graphite Structure

c) Ionic crystals

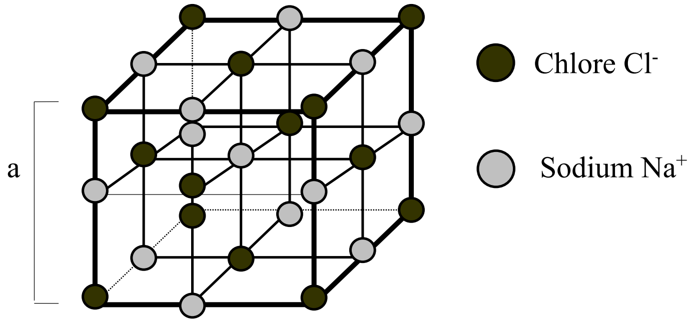
In an ionic crystal, lattice sites are occupied by positive ions (cations) and negative ions (anions).

Example: sodium chloride crystal (NaCl).

The ions occupy the corners of a cube of edge a, the midpoints of the edges, the cube center, and the face centers. This is called a face-centered cubic (FCC) structure.

For NaCl: a = 5.58 Å.

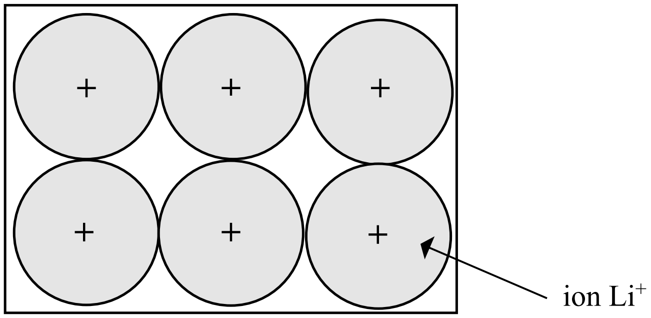
Note : along any line, Na^+ and Cl^- alternate.



NaCl Structure

d) Metallic crystals: lithium crystal

A metal can be viewed as a set of positive ions (Li^+) immersed in an electron cloud that is delocalized throughout the crystal.



lithium crystal Structure

TUTORIAL NO. 06

Exercise 1

1- What is the geometry of the phosphorus pentafluoride PF_5? Indicate the angle values**.**

2- In the solid state, phosphorus pentachloride has an ionic structure involving the species

PCl_4^+ and PCl_6^- . Determine the geometry of these two ions.

3- Suggest three possible geometries for the PCl_3F_2 compound.

Exercise 2

In the V.S.E.P.R. model, the arrangement of bonds around a central atom depends on both the number of pairs of valence electrons and the characteristics of the occupied orbitals.

1- In the species $AB_m= AX_m\ E_0$, the geometry of the molecule is that of the geometric coordination figure formed by the$m$ atoms B= X around the central atom .A

a- Write down the nature and represent this figure in the case of a geometry: (1) linear; (2) triangular; (3) tetrahedral; (4) triangular bipyramidal; (5) octahedral.

b- Deduce the coordination number Ic of the central atom .A

c- Indicate the value(s) of the valency angles α for each of the geometries (1) to (5).

2- The geometry of the electronic system involves the doublets of the central atom.

a- Rank the interaction forces between electron pairs in descending order.

b- Correlate the electronegativities of the ligand or the central atom with the volume occupied by a pair of bonding electrons.

Exercise 3

According to Gillespie's rules, give the type of hybridization of the atoms and the geometry of the following molecules, respecting the values of the valence angles (these molecules will be represented schematically by: non-bonding doublet– (NL); bonding doublet (L);↑↑ bond π

(1)- BCl_3; PCl_3; $POCl_3$; BeCl3. (2)- $CH_2—CH_2$; C_2H_2; $NH_2—NH_2$; CH2— C= C— CH_2

Exercise 4

The geometry of molecules is linked to the number of non-bonding electron doublets and the electronegativity of the different atoms that make up the molecule.

1- Give the type of hybridization, the geometry and the variation in the valence angle (according to increasing) for each of the following two series: NH_3; PH_3; AsH_3; SbH_3 and $AsCl_3$; $AsBr_3$; AsI_3.

2- What can we conclude?

Exercise 5

Consider the hydrazine molecule N_2H_4.

1- Give its Lewis structure.

2- What is the hybridization of the nitrogen atoms? Is it the same as that of the nitrogen atom in :

a)- NH_3 ; b)- NH_4^+ ; c)- RCH= NR .$^+$

3- Is the hybridization acidic or basic? Justify your answer.

Exercise 6

Aluminium chloride has the formula $AlCl_3$.

1- Give its Lewis formula and specify, with justification, its geometry.

2-In solution in benzene, the aluminium chloride molecule combines with the chloride ion to form a Tetra-chloroaluminate 3 complex ion. Why does this happen? What geometry does this structure have?

3- We also observe that Aluminium chloride tends, under other conditions, to give rise to a molecule of formula Al_2Cl_6 in which all the atoms satisfy the octet rule. Propose a Lewis formula for this molecule.

Exercise Solutions

Exercise 01:

1) Geometry of phosphorus pentafluoride (PF_5):

PF_5 adopts a trigonal bipyramidal geometry (VSEPR: AX_5).

- Equatorial–equatorial angles: 120°
- Axial–equatorial angles: 90°
- Axial–axial angle: 180°

  The three equatorial F atoms lie in one plane, while the two axial F atoms are perpendicular to that plane.

2) Solid-state structure of phosphorus pentachloride (PCl_5):

In the solid state, PCl_5 is ionic, consisting of:

- PCl_4^+ (tetrahedral cation)
- PCl_6^- (octahedral anion)

So, solid PCl_5 can be represented as $[PCl_4^+][PCl_6^-]$.

Exercise 03:

Molecule	Central atom(s)	Hybridization	Geometry	Valence angles
BCl_3	B	sp^2	Trigonal planar	120°
PCl_3	P	sp^3	Trigonal pyramidal	~100–103°
$POCl_3$	P	sp^3	Tetrahedral	109.5°
$BeCl_3$	Be	sp^2	Trigonal planar	120°
$CH_2–CH_2$	C	sp^2	Trigonal planar	120°
C_2H_2	C	sp	Linear	180°
$NH_2–NH_2$	N	sp^3	Bent	~104–107°
$CH_2–C=C–CH_2$	C	sp^2	Trigonal planar	120°

Exercice 4:

The geometry of these molecules is analyzed using the VSEPR (Gillespie) model, taking into account lone pairs and electronegativity effects.

1) Series: NH_3; PH_3; AsH_3; SbH_3

Hybridization and geometry

All these molecules belong to group 15 hydrides:

- Central atom: N, P, As, Sb
- Electron pairs: 3 bonding + 1 lone pair → AX_3E
- Hybridization: sp^3 (formal VSEPR description)

- Geometry: trigonal pyramidal

Variation of the valence angle (increasing order)

As we go down the group:

- The central atom becomes larger.
- Orbital hybridization becomes less effective (bonding uses more p-character).
- Lone pair–bond pair repulsion decreases.

Bond angles decrease down the group.

$$SbH_3 < AsH_3 < PH_3 < NH_3$$

Typical angles:

- $NH_3 \approx 107°$
- $PH_3 \approx 93.5°$
- $AsH_3 \approx 92°$
- $SbH_3 \approx 91°$

2) Series: $AsCl_3$; $AsBr_3$; AsI_3

Hybridization and geometry

- Central atom: As
- Electron pairs: 3 bonding + 1 lone pair → AX_3E
- Hybridization: sp^3
- Geometry: trigonal pyramidal

Variation of the valence angle (increasing order)

From Cl → Br → I:

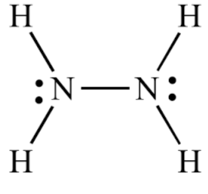
- Electronegativity of the ligand decreases.
- Bonding electron pairs are less attracted away from As.
- Bonding pairs occupy a larger volume near the central atom.
- Lone pair–bond pair repulsion increases → larger bond angles.

Bond angles increase from $AsCl_3$ to AsI_3.

$$AsCl_3 < AsBr_3 < AsI_3$$

Exercise 05:

1) Lewis structure of hydrazine



Each nitrogen has **5 valence electrons**.

Each nitrogen:

- 3 σ bonds (N–H, N–H, N–N)
- 1 lone pair

2) Hybridization of the nitrogen atoms

In hydrazine N2H4

- Electron pairs around each N:

  3 bonding pairs + 1 lone pair → AX_3E
- **Hybridization: sp^3**
- Geometry around each N: **trigonal pyramidal**

Comparison with other nitrogen species

a) NH_3

- Electron pairs: 3 bonds + 1 lone pair
- **Hybridization:** sp^3
- **Same hybridization as in hydrazine**

b) NH_4^+

- Electron pairs: 4 bonds, 0 lone pairs
- **Hybridization:** sp^3
- Geometry: tetrahedral
- Same hybridization, but **no lone pair**

c) $RCH = NR^+$ (iminium ion)

- Nitrogen:
  - One double bond (C=N)
  - Two σ bonds
  - No lone pair (positive charge)
- Electron pairs: 3 bonding regions
- **Hybridization: sp^2**
- Geometry: trigonal planar
- **Different from hydrazine**

3) Is the hybridization acidic or basic?

Hydrazine N2H4

- Each nitrogen has a **lone pair**.
- Lone pairs are available to **accept protons (H^+)**.

- Therefore, hydrazine behaves as a **Lewis base** and a **Brønsted base**.

Relation to hybridization

- **sp³ nitrogen**:
    - Lone pair is localized
    - High electron density
    - → **Basic character**
- **sp² or sp nitrogen**:
    - Lone pair is more delocalized or involved in π systems
    - → **Weaker basicity**

Species	Hybridization of N	Lone pair	Acidic / Basic
N_2H_4	sp³	Yes	Basic
NH_3	sp³	Yes	Basic
NH_4^+	sp³	No	Not basic
$RCH{=}NR^+$	sp²	No	Not basic

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