



Ministry of Higher Education and Scientific Research

Abou Bekr Belkaid University – Tlemcen –

Faculty of Technology,

Department of Hydraulic

Structure of Matter Course

Presented by: Dr. MESLI Meryem

Academic Year: 2025/2026



Syllabus

Semester: 1

Teaching Unit: IST1.4

Subject title: Structure of Matter – Chemical Element

Total Hours (VHS): 90h00 (Lectures: 1h30, Tutorials: 3h00, Practical works: 1h30)

Credits: 4 **Coefficient:** 7

Recommended Prerequisites: Basic knowledge of mathematics and general chemistry.

Course Content:

Chapter I: Fundamental Concepts

States and macroscopic characteristics of matter, phase changes of matter, concepts of atom, molecule, mole, and Avogadro's number, atomic mass unit, atomic and molecular molar mass, molar volume, Law of Conservation of Mass (Lavoisier), chemical reactions, qualitative and quantitative aspects of matter.

Chapter II: Main Components of Matter

Introduction: Faraday's experiment : relationship between matter and electricity, evidence of the constituents of matter and of the atom, some physical properties (mass and charge), Rutherford's planetary model, presentation and characteristics of the atom (symbol, atomic number Z , mass number A , number of protons, neutrons, and electrons), isotopy and relative abundance of different isotopes, isotope separation and determination of atomic mass and average atomic mass: mass spectrometry "Bainbridge spectrograph", nuclear binding and cohesion energy, nuclear stability.

Chapter III: Electronic Structure of matter

Wave-particle duality, interaction between light and matter, Bohr's atomic model (hydrogen atom), the hydrogen atom in wave mechanics, multi-electron atoms in wave mechanics.

Chapter IV: Periodic Classification of Elements

Mendeleev's periodic classification, modern periodic classification, evolution and periodicity of physico-chemical properties of elements, calculation of radii (atomic and ionic), successive ionization energies, electron affinity and electronegativity (Mulliken scale) using Slater's rules.

Chapter V: Chemical Bond

Covalent bonding in Lewis theory, polar covalent bonds, dipole moment and partial ionic character of bonds, molecular geometry: Gillespie's theory (VSEPR), chemical bonding in the quantum model.

Chapter VI: Radioactivity – Nuclear Reactions

Natural radioactivity (α , β , and γ radiation), artificial radioactivity and nuclear reactions, kinetics of radioactive decay, applications of radioactivity.

Assessment Method: Continuous assessment: 40%; Final exam: 60%.

Foreword

This course on the ‘**structure of matter**’ is intended for first year engineering students in science and technology STI and may be beneficial to other specialities such as civil engineering, electrical engineering, mechanical engineering, physics, chemistry, etc). It will also be useful for researchers in fundamental or applied research laboratories who encounter questions about the structure of matter in the course of their work.

In Chapter I, the course explores the fundamental principles of matter, focusing on key aspects such as the macroscopic characteristics of the various states of matter, phase transitions, and the atomic and molecular basis of chemical reactions. It highlights the law of conservation of mass and offers both qualitative and quantitative approaches to understanding these concepts.

Chapter II explores the fundamental components of matter, focusing on atomic structure, experimental techniques used to identify atomic particles, and the significance of isotopes. It also covers the principles of mass spectrometry and nuclear stability, offering essential insights into the atomic model and its practical applications.

Chapter III examines the electronic structure of atom, addressing concepts such as wave-particle duality, the interaction between light and matter, and the quantum mechanical model of the atom. It provides a deeper insight into atomic and molecular behavior by integrating both classical and quantum perspectives.

Chapter IV introduces the periodic classification of elements, tracing its evolution from Mendeleev’s original table to the modern quantum-based system. It explains the periodic trends in atomic properties and equips students with the knowledge to predict chemical behavior and reactivity.

Chapter V examines chemical bonding, covering covalent bonds, molecular geometry, and the quantum mechanical approach to chemical interactions. It provides a comprehensive analysis of how atoms combine to form stable molecules, a key concept for understanding complex chemical reactions.

Finally, **Chapter VI** focuses on radioactivity and nuclear reactions, addressing both natural and artificial forms. It offers a detailed study of radioactive decay kinetics and highlights their applications across multiple scientific fields, such as medicine and energy generation.

Liste of figures

Figure	Page
Figure I-1: State of matter	2
Figure I-2: Changes in the State of Matter	2
Figure I-3: Atom structure	3
Figure I-4: H ₂ SO ₄ Molecule	4
Figure I-5: Sodium ion	4
Figure I-6: Law of conservation of mass	7
Figure I-7: Classification of Matter	8
Figure I-8: Solute, Solvent and Solution	9
Figure I-9: Dilution process	9
Figure II-1: The Various Constituents of Matter	13
Figure II-2: Electrolysis of H ₂ O	13
Figure II-3: Schematic of the cathode ray tube by J.J. Thomson	15
Figure II-4: Experimental scheme of the Millikan experiment	15
Figure II-5: Rutherford experience	16
Figure II-6: Planetary Model (Rutherford) of the Atom	17
Figure II-7 : Isotopes of Hydrogen	19
Figure II-8: Principle of the Bainbridge Spectrometer	21
Figure II-9: Representation of a Mass Defect	22
Figure II-10: Aston Curve	23
Figure II-11: Diagram of stability of nuclei	24
Figure III-1: Diagram of an electromagnetic or light wave	27
Figure III-2: Effect of wavelength on wave frequency	27
Figure III-3: Electromagnetic spectrum	28
Figure III-4: Photoelectric effect	29
Figure III-5: Emission spectrum of the hydrogen atom	31
Figure III-6: Series of Lines in the Hydrogen Atom's Spectrum	32
Figure III-7: Diagram of an Electronic Transition	33
Figure III-8: The electromagnetic spectrum	33
Figure III-9: Photon absorption-emission process	35
Figure III-10: Illustration of a transition by a spectral line	35

Figure	Page
Figure III-11: Energy diagram of the hydrogen atom	36
Figure III-12: Ionisation energy E_i of the hydrogen atom	37
Figure III-13: Representation of the electron as a standing wave	39
Figure III-14: Representation of the Atom with the Principal Level (layer, shell)	41
Figure III-15: Motion of the electron on itself	43
Figure III-16: Representation of atomic orbitals	45
Figure III-17: Degenerate Atomic Orbital energy levels	45
Figure III-18: Energy Levels of Atomic Orbitals in a Poly-Electronic Atom	46
Figure III-19: Klechkowski's rule	47
Figure III-20: Hund's rule	48
Figure III-21: Pauli's exclusion principle	48
Figure IV-1: Periodic Table of D. Mendeleev in 1869	50
Figure IV-2: Modern Periodic Table	51
Figure IV-3: Different Blocks of the Periodic Table	52
Figure IV-4: Periodic Table Groups and Periods	52
Figure IV-5: Families of the periodic table	56
Figure IV-6: evolution of atomic radius	57
Figure IV-7: Ionic radius for cations and anions	58
Figure IV-8: Electronegativities of elements	59
Figure IV-9: Representation of Slater's Rule	61
Figure V-1: A comparison of metals and nonmetals.	64
Figure V-2: Metallic bond	65
Figure V-3: covalent bond	65
Figure V-4: Ionic bond	68
Figure V-5: representation of strong bonds	68
Figure V-6: Vector representation of the dipole moment of a polyatomic atom ABC	69
Figure V-7: sp^3 Hybridization	74
Figure V-8: sp^3 Hybridization of CH_4	75
Figure V-9: sp^2 Hybridization	75
Figure V-10: sp^2 Hybridization of C_2H_4	76
Figure IV-11: sp Hybridization	76
Figure V-12: sp Hybridization of C_2H_2	76
Figure VI-1: Types of radioactive decay	79

Figure	Page
Figure VI-2: Gamma rays	81
Figure VI-3: Nuclear Fission	81
Figure VI-4: Nuclear Fusio	82
Figure VI-5: Decay Kinetics	83

Table of contents

Chapter I: Fundamental Concept of Chemistry

I-Introduction	1
II-State and Macroscopic characteristics of states of matter	1
II-1-State of matter	1
II-2-Properties of matter	2
III- Notions of Atom, Molecule, Ion, Mole, and Avogadro's Number	3
III-1- Atom	3
III-2-Molecule	3
III-3- Ion	4
III-4-Mole and Avogadro's Number	4
IV-Concepts of Atomic Mass Unit, Atomic and Molecular Molar Mass, and Molar Volume	5
IV-1-Atomic Mass Unit (AMU)	5
IV-2- Atomic Molar Mass	5
IV-3- Molecular Molar Mass	5
IV-4- Molar Volume	5
V- Law of Conservation of Mass (Lavoisier) in Chemical Reactions	6
VI- Qualitative Aspect of Matter	7
VI-1- Pure Substances, Homogeneous and Heterogeneous Mixtures	7
a- Heterogeneous mixtures	8
b- Homogeneous mixtures	8
VI-2- Solutions, Solute, Solvent, Aqueous Solution and Dilution	8
VII-Quantitative aspect of matter	9
VII-1- Concentrations	9
a- Molarity (Molar Concentration)	9
b- Mass Concentration	9
VII-2-Molality	10
VII-3-Normality (N)	10
VII-4- Mass density	10
VII-5- Density	10
a- Density of Solids and Liquids Relative to Water	10
b- Density of Gases Relative to Air	11
VII-6- Mole Fraction (Xi)	11

Chapter II: Main Components of Matter

I-introduction	13
II- Discovery of the electric nature of matter: Faraday's experience, The relationship between matter and electricity	13
III- Matter constituents	14
III-1- Electron	14
III-1-1-Experience of J.J Thomson (1897): The discovery of electron	14
III-1-2-Millikan's experience (1909): measurement of the electron charge	15

IV- Planetary Atomic Model of Rutherford (1909)	16
IV-1- Discovery of the nucleus.....	16
IV-1-1- Gold foil experiment.....	16
IV-1-2-Composition of the Atomic Nucleus	17
V- Presentation and Characterization of The Atom.....	17
VI- Isotopes and Relative Abundance of Different Isotopes	19
VI-1- Non-Isotopic Atom	19
VI-2- Isotopes	19
VI-3-Relative Abundance of Different Isotopes and atomic mass	20
VI-4- Mass Spectrometer: Bainbridge Spectrograph.....	21
VII- Nuclear Binding and Cohesion Energy	22
VII-1- Mass Defect	22
VII-2-Binding Energy.....	22
VII-3- Cohesion Energy	22
VIII- Nuclear Stability	23
VIII-1- Determination of Cohesive Energy (Aston's Curve)	23
VIII-2- Stability And Number of Nucleons	24

Chapter III: electronic structure of matter

I- Introduction.....	26
II-Wave Particle Duality	26
II-1-Wave aspect of the light: electromagnetic or light wave and electromagnetic spectrum.	26
II-2- Electromagnetic Spectrum.....	27
II-3-Corpuscular nature of light.....	28
II-3-1- Photoelectric effect.....	28
III-The interaction between light and matter	30
III-1-Emission spectrum of the hydrogen atom	30
III-2-BALMER-RYDBERG empirical relationship	31
III-3- Interpretation of the Hydrogen Emission Spectrum	32
IV-Bohr's atomic model.....	34
VI-1- Absorption and Emission of Energy	35
IV-2-Ionisation energy.....	36
IV-3- Application to Hydrogen-like Ions	37
IV-4-Insufficiency of The BOHR Model	38
V-The Hydrogen Atom in Wave Mechanics	38
V-1-Wave-Corpuscle Duality and The De BROGLIE Relation.....	38
V-2-Heisenberg Uncertainty Principle	39
V-3- Concept of Probability of Presence	39
V-3-1-Schrödinger Equation.....	40
VI-Quantum Numbers and The Concept of Atomic Orbitals	41
VI-1- Quantum Numbers	41
VI-1-1- Principal Quantum Number (n)	41
VI-1-2-Secondary Quantum Number (or Azimuthal) (l)	41

VI-1-3- Magnetic Quantum Number (m)	42
VI-1-4- Spin Quantum Number (s).....	43
VII-Atomic Orbitals.....	43
VII-1-Energy of atomic orbitals	45
VIII- Electronic configuration of the atom	46
VIII-1-Klechkowski's rule (filling order).....	47
VIII-1-1 Exceptions to Klechkowski's Rule	47
VIII-2- Hund's Rule	48
VIII-3-Pauli's exclusion principle.....	48
VIII-4-Valence Shell	48

Chapter IV: periodic classification of elements

I-Introduction.....	50
II-Mendeleïev's Periodic Classification	50
III-Modern periodic classification	50
III-1-Blocks: Elements are placed in three blocks	51
III-2-Element Families.....	55
IV- Evolution And Periodicity of Physico-Chemical Properties	56
IV-1-Variation in protons number Z.....	56
IV-2-Atomic radius.....	56
IV-3-Ionic radius	57
IV-4-Ionisation energy I	58
IV-5-Electron affinity AE.....	58
IV-6-Electronegativity (χ).....	59
IV-6-1-Mulliken scale	60
IV-6-2-Slater model.....	60
IV-6-3-Calculation of the effective charge Z^*	61

Chapter V: chemical bond

I-Introduction.....	64
II-The different types of bonds	64
II-1-Strong Bonds	65
II-1-1-Metallic bond (Metal with metal).....	65
II-1-2-Covalent bond (Nonmetal with nonmetal)	65
a- Lewis structure	66
b- The octet Rule	66
II-1-3-Ionic bond (metal with nonmetal)	67
a- Concept of dipole moment μ	68
b-Partial ionic character of a bond.....	70
II-2- Weak Bonds	71
III- Geometry of molecules: GILLEPSIE or VSEPR theory (Valence Shell Electron Pair Repulsion)	71
III-1-Principle of the VSEPR method.....	71
IV-Chemical Bonding in the Quantum Model: Hybridization of Atomic Orbitals (AO).....	74
IV-1- Different Types of Hybridization.....	74

IV-1-1- SP ³ Hybridization.....	74
IV-1-2- SP ² Hybridization.....	75
IV-1-3- SP Hybridization	76
IV-2- Relation To VSEPR Theory.....	77

Chapter VI: radioactivity-nuclear reaction

I-Introduction.....	78
II- Natural Radioactivity.....	78
II-2-1-Alpha Radiation α	79
II-2-2- Beta Radiation.....	80
a- β^- Radiation	80
b- β^+ Radiation	80
II-2-3- γ Radiation	80
III- Artificial radioactivity and nuclear reactions	81
III-1- Nuclear Fission	81
III-2- Nuclear Fusion	82
III-3- Transmutation	82
IV- Kinetics of Radioactive Decay	82
IV-1-Radioactive decay law	82
IV-2- Activity of a radioactive nucleus	83
IV-3- The radioactive period or half-life	83
V- Applications of radioactivity	84
V-1- Medical field	84
V-2-Industrial field	84
V-3- Agricultural field.....	84
V-4- Energy field.....	84
V-5-Scientific and archaeological field	84

Chapter I: Fundamental Concepts

Learning Objectives :

The objectives of this chapter are

- Introduce the basic concepts necessary for understanding the subject (atom, molecule, ion).
- Describe the structure of the atom: nucleus (protons, neutrons) and electrons.
- Present the fundamental quantities used in chemistry and physics (atomic mass, charge, atomic number, amount of substance, mole, etc.).
- Explain the states of matter and their main characteristics.
- Distinguish between types of systems (open, closed, isolated), often linked to exchanges of matter and energy.
- Introduce the concepts of intensive and extensive variables.
- Establish the basic scientific vocabulary essential for the following chapters (chemical bonds, electronic structure, properties of matter).

I-Introduction

Chemistry examines matter and its possible changes. Matter is anything that has mass and takes up space.

he true impact of chemistry extends much farther than the products we use in daily life.

The most profound questions about health, climate change, even the origin of life, ultimately have chemical answers.

No matter what your reason for studying chemistry, this course will help you develop two mental skills. The first, common to all science courses, is the ability to solve problems systematically. The second is specific to chemistry, for as you comprehend its ideas, you begin to view a hidden reality filled with incredibly minute particles moving at fantastic speeds, colliding billions of times a second, and interacting in ways that determine how all the matter inside and outside of you behaves.

To study a course “the structure of matter”, it is generally necessary to have a solid grounding in physics and a knowledge of mathematics, particularly differential and integral calculus,

A good place to begin our exploration of chemistry is to define it and a few central concepts.

Chemistry, is the study of matter and its properties, the changes that matter undergoes, and the energy associated with those changes.

Matter, is the “stuff ” of the universe: air, glass, planets, students—anything that has mass and volume.

II-State and Macroscopic characteristics of states of matter

II-1-State of matter:

Matter comes in different forms called states of matter

The three fundamental states of matter are solid, liquid, and gas.

Each state of matter has its own characteristics, such as:

- ✓ Solid state keeps a constant shape and volume, cannot be compressed and cannot drain.
- ✓ Liquid state takes the shape of the container, keeps the volume constant, cannot be compressed, can flow
- ✓ Gaseous state takes the shape and volume of the container, can be compressed and can flow.

Heat and cold play essential roles in the transition of a substance from one state to another depending on the temperature (T) and pressure (P):

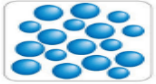
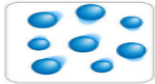
States of Matter			
Property	Solids	Liquids	Gases
Shape	Definite shape	No definite shape, takes shape of the container	No definite shape, takes shape of the container
Volume	Definite volume	Definite volume	No fixed volume
Particle Arrangement	Tightly packed  Solid	Close together but can move  Liquid	Far apart, can move  Gas
Particle Motion	Vibrating in a fixed position	Flowing and sliding past each other	Moving rapidly and freely
Example	Ice, Wood, Stone	Water, Oil, Milk	Air, Oxygen, Nitrogen

Figure I-1: State of matter

II-2-Properties of matter

We can distinguish two properties of matter:

- Physical properties: a characteristic that can be observed or measured without changing the nature of matter.

Examples: mass, temperature, color



Figure I-2: Changes in the State of Matter

The physical quantities can be expressed by the 5 basic units defined by the international system (IS).

Mesured quantity	Mesurement unit	Symbol
length	Meter,	m
mass	kilogramme	kg
temperature	kelvin	K
Time	second	s
Amount of substance	mole	mol

- Chemical properties: A chemical transformation is a process that changes the chemical composition and properties of a substance through reaction

Examples:

- + Corrosion is exemplified by the rusting of iron.
- + Combustion is demonstrated when wood burns, yielding ash and gases.
- + the reaction of zinc with hydrochloric acid gives hydrogen gas.

Chemical changes can be identified by certain indicators, such as:

- + Formation of a gas;
- + Formation of a precipitate;
- + Change in color;
- + Release of energy in the form of light and heat.

III- Notions of Atom, Molecule, Ion, Mole, and Avogadro's Number

III-1- Atom

An atom is the smallest unit of an element that can exist.

Atoms combine to form molecules.

An atom consists of a nucleus around which electrons are in motion.

The nucleus has an incredibly small diameter of approximately 10^{-14} meters.

It is composed of nucleons (protons and neutrons) and contains almost all of the atom's mass

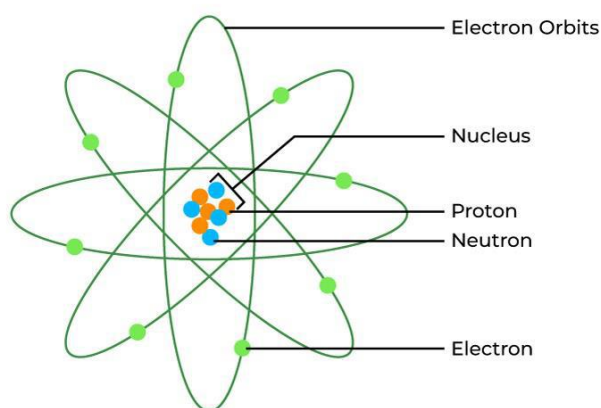


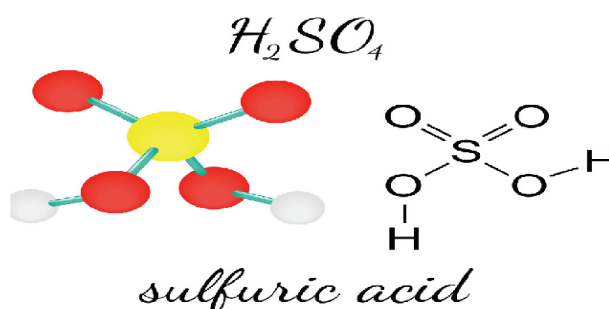
Figure I-3: Atom structure

III-2-Molecule

A molecule is the association of two or more atoms (e.g., NaCl, H₂O, O₂) bonded together by chemical bonds. It is the smallest part of a compound that retains its properties. A molecule is characterized by its molecular formula and its molecular molar mass.

Examples:

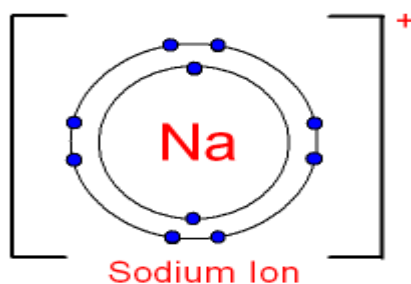
- ✚ H₂O (water);
- ✚ H₂ (hydrogen gas);
- ✚ HCl (hydrochloric acid);
- ✚ H₂SO₄ (sulfuric acid);

**Figure I-4:** H₂SO₄ Molecule**III-3- Ion**

An ion is an atom or molecule charged positively (cation) or negatively (anion)

Examples:

- ✚ cation sodium (Na⁺);
- ✚ anion chloride (Cl⁻);
- ✚ cation ammonium (NH₄⁺)

**Figure I-5:** Sodium ion**III-4-Mole and Avogadro's Number**

The mole is a unit of measurement for the amount of substance in a system containing *N* identical entities. It is defined as the ratio between the mass of the sample (*m*), expressed in grams (g), and the molar mass (*M*), expressed in grams per mole (g/mol).

$$n = m / M$$

Where:

n is the number of moles.

m is the mass of the compound in grams (g).

M is the molar mass of the compound in grams per mole (g/mol).

For example, to find the number of moles in 54 g of water:

$$n = m_{\text{water}} / M_{\text{water}} = 54 \text{ g} / 18 \text{ g/mol} = 3 \text{ moles.}$$

The number of atoms contained in a mole is called Avogadro's Number (N_A),

$$N_A = 6.023 \times 10^{23}.$$

$$1 \text{ mole (of atoms, ions, molecules, etc.)} = 6.023 \times 10^{23} \text{ (atoms, ions, molecules, etc.)}.$$

The quantity of matter, denoted as " n ," is proportional to the number of molecules, denoted as " N ," contained within a substance.

$$N = n \times N_A \quad \text{where } n = N/N_A.$$

Example:

A sample of copper oxide, CuO , has a mass $m = 1.59 \text{ g}$. How many moles and molecules of CuO , as well as atoms of Cu and O , are in this sample?

$$M_{\text{Cu}} = 63.54 \text{ g/mol}; M_{\text{O}} = 16 \text{ g/mol}.$$

Solution:

$$\text{Number of moles of CuO: } n = m / M_{\text{CuO}} = 1.59 / (63.54 + 16) = 0.01999 \text{ moles.}$$

$$\text{Number of molecules of CuO} = (m / M_{\text{CuO}}) \times N_A = 0.12 \times 10^{23} \text{ molecules.}$$

$$\text{Number of Cu atoms} = \text{Number of O atoms} = (m / M_{\text{CuO}}) \times N = 0.12 \times 10^{23} \text{ atoms.}$$

IV-Concepts of Atomic Mass Unit, Atomic and Molecular Molar Mass, and Molar Volume

IV-1-Atomic Mass Unit (AMU)

The masses of particles such as electrons, protons, neutrons, etc., are not convenient to express in kilograms (Kg) due to their very small scale. Instead, a different unit of mass called the Atomic Mass Unit (amu) or "u" is used.

One atomic mass unit, 1 u (amu) is defined as one-twelfth of the mass of a carbon-12 atom.

$$\text{So: } 1 \text{ amu} = (1/12) \cdot 12/N_A \text{ (g)} = 1/N_A \text{ (g)} = 1.66 \cdot 10^{-24} \text{ (g)} = 1.66 \cdot 10^{-27} \text{ Kg.}$$

Example:

Determine the mass of one sodium (Na) atom, knowing that its atomic molar mass is 23 g/mol.

Solution:

$$1u = 1.66 \cdot 10^{-24} \text{ g}$$

so the mass for one atom of sodium: $23 \times 1.66 \cdot 10^{-24} = 3.82 \cdot 10^{-23} \text{ g}$

IV-2- Atomic Molar Mass

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

Atomic molar mass = $N_A \times$ mass of a single atom (g/mol).

The molar mass of an element is the mass, in grams, of 6.023×10^{23} atoms of this element: It is the mass of 1 mol of this element

Examples:

Molar mass of hydrogen (H): $M(H) = 1.674 \cdot 10^{-24} \text{ g} \times N_A = 1.0079 \text{ g} \cdot \text{mol}^{-1}$;

Molar mass of oxygen (O): $M(O) = 2.657 \cdot 10^{-23} \text{ g} \times N_A = 16 \text{ g} \cdot \text{mol}^{-1}$.

IV-3- Molecular Molar Mass

The molecular molar mass of a molecular compound is the mass of one mole of molecules. It is equal to the sum of the molar masses of its constituent elements.

Examples:

Molar mass of CO_2 : $M(\text{CO}_2) = M(\text{C}) + 2 \cdot M(\text{O}) = 44 \text{ g/mol}$;

Molar mass of H_2O : $M(\text{H}_2\text{O}) = M(\text{O}) + 2 \cdot M(\text{H}) = 18.02 \text{ g/mol}$.

IV-4- Molar Volume

At normal temperature and pressure (NTP: 0°C and 101325 Pa or 1 atm), one mole of any gas occupies a constant volume known as the molar volume. (MV): **$MV = 22.4 \text{ mol/l}$**

Under these conditions, the number of moles can be determined using the following formula:

$$n = V/V_{\text{molar}} = V/22.4$$

Example:

Number of moles in 11.2 liters of carbon dioxide gas: $n = V_{\text{gas}}/V_{\text{molar}} = 11.2/22.4 = 0.5$ moles.

V- Law of Conservation of Mass (Lavoisier) in Chemical Reactions

the law of conservation of mass was discovered by Antoine Lavoisier in 1789 (French chemist), this law states that in chemical reactions the total mass of reagents equals the total

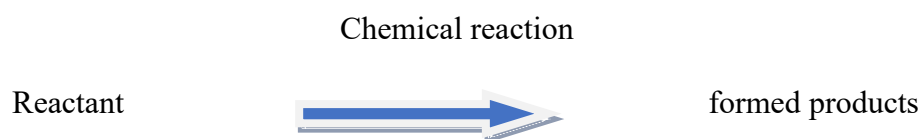
mass of products. No atoms are lost or created during chemical reactions, only rearranged, maintaining a consistent mass throughout.

This law as stated, is: "In a chemical reaction, the total mass of the reactants is equal to the total mass of the products formed," which means that nothing is lost, nothing is created; everything is transformed.

Example:

Consider one sulfur atom and two oxygen atoms arranged in a certain way to always yield one sulfur atom and two oxygen atoms, but
arranged differently: $\text{S} + \text{O}_2 \rightarrow \text{SO}_2$

You can write an equation balance of a chemical reaction:



- In a chemical reaction, the elements retain
- In a chemical reaction, the mass of the lost reagents is equal to the mass of the products formed (Lavoisier's Law)

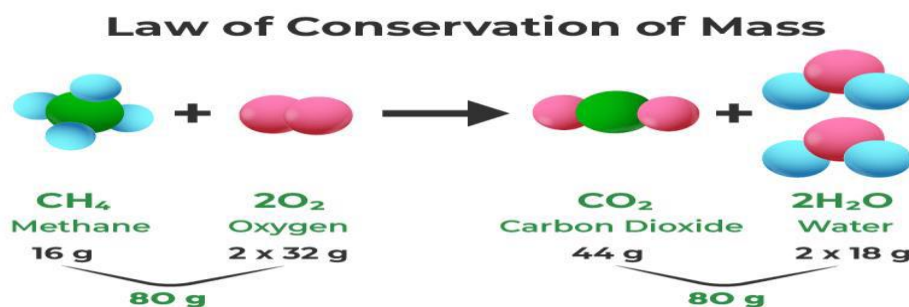


Figure I-6: Law of conservation of mass

VI- Qualitative Aspect of Matter

VI-1- Pure Substances, Homogeneous and Heterogeneous Mixtures

A pure substance contains only one kind of chemical entity, which may be an atom, ion, or molecule.

A pure substance can be either an element (simple pure substance, e.g., Cu, Fe, H₂, O₂...) or a compound (composed of multiple elements, e.g., pure water H₂O).

A mixture is a substance composed of several types of chemical entities mixed together. Mixtures can be either homogeneous (such as saltwater...) or heterogeneous (having two or more distinct phases, for example, water and oil...).

a) Heterogeneous mixtures:

It is a mixture for which we can distinguish at least 2 constituents (with the naked eye or under the microscope)

Examples: mixtures of sugar and sand, milk ...

b) Homogeneous mixtures:

it is a mixture for which one does not distinguish the different constituents with the naked eye (and even with a microscope), These are mixtures made up of a single phase

Example: sugar water, salt water, syrup, honey, air, mixture of two gases etc.

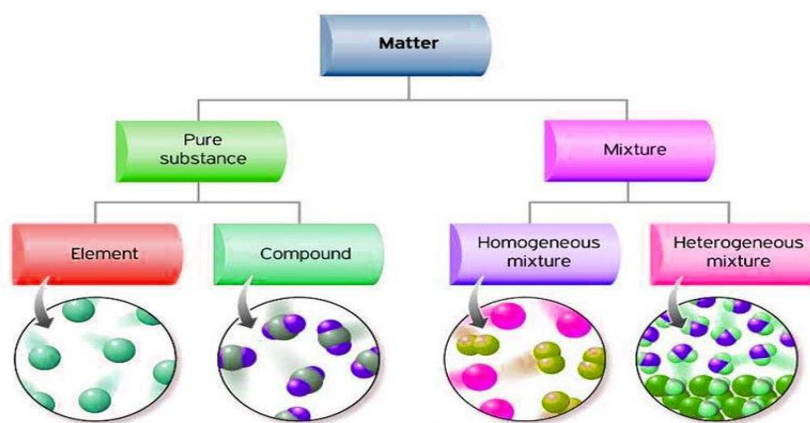


Figure I-7: Classification of Matter

VI-2- Solutions, Solute, Solvent, Aqueous Solution and Dilution

Solutions are homogeneous mixtures composed of two or more chemical components, existing in either liquid, gaseous, or solid phases.

The **solvent** is any liquid substance that has the ability to dissolve other substances.

The **solute** is a chemical species (molecular or ionic) that is dissolved in a solvent.

The solvent is always present in a much larger quantity than the solute.

This homogeneous mixture (solvent + solute) is called an aqueous solution if the solvent is **water**.

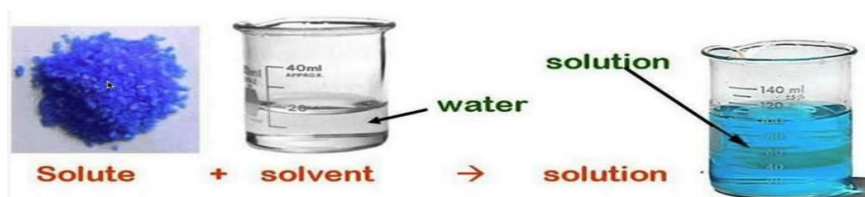


Figure I-8: Solute, Solvent and Solution

Dilution is a process that involves obtaining a final solution with a lower concentration than the initial one, either by adding a solvent or by taking a portion of the solution and then adding solvent to maintain the same volume.

Dilution is characterized by its dilution factor.

This concept assumes that the substance being diluted is soluble in the chosen solvent.

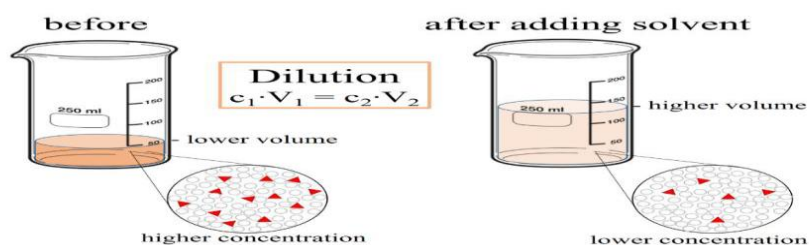


Figure I-9: Dilution process

VII-Quantitative aspect of matter

In physical chemistry, certain quantities have a quantitative aspect of matter, such as density, different types of concentrations, and mass density

VII-1- Concentrations:

Concentrations are quantities with units used to determine the proportion of solutes to that of the solvent. Depending on the chosen unit, we distinguish:

a. Molarity (Molar Concentration) (MC) It expresses the number of moles of solute per liter of solution.

$$C_n = n/V$$

b. Mass Concentration: Mass concentration, also known as content, is the mass in grams of the solute per liter of solution. Its symbol is C_m , and its unit is grams per liter ($\text{g} \cdot \text{L}^{-1}$). It can be referred to as the partial mass density of a component of the solution:

$$C_m = m/V$$

There is a relationship between molar concentration and mass concentration:

$$C_m = C_n \times M$$

VII-2-Molality

Molality expresses the amount of solute contained in 1 kg of solvent:

$$\text{molality} = \text{moles of solute} / \text{mass of solvent (kg)}$$

VII-3-Normality (N)

Normality represents the number of gram-equivalents of solute per liter of solution (geq/L).

A **gram-equivalent** corresponds to the amount of substance that contains one mole of the species involved, such as H^+ , OH^- , or electrons (e^-).

$$N = \text{geq} / V$$

Relationship between N: Normality and Cn: Molarity: $N = Cn \times \text{valence (Z)}$

Meaning of Z, Examples:

-In the case of an acid: Z is the number of H^+ protons involved.

HCl (Z=1); H_2SO_4 (Z=2); H_3PO_4 (Z=3);

-In the case of a base: Z is the number of OH^- ions involved, e.g.:

NaOH (Z=1); $Ca(OH)_2$ (Z=2);

-In the case of salts: Z is the number of metal cations multiplied by the valence of that metal. Na_2SO_4 ($Z=2 \times (+1) = 2$) ($2Na^+$; SO_4^{2-}); $Meq(Na_2SO_4) = M(Na_2SO_4)/2$;

-In the case of redox reactions: Z is the number of electrons transferred, e.g.:

$KMnO_4$: $Z=5$ $MnO_4^- (aq) + 8 H^+ (aq) + 5 e^- \rightleftharpoons Mn^{2+} (aq) + 4 H_2O(l)$.

VII-4- Mass density

Density expresses the mass of a certain volume of a solution under specific temperature and pressure conditions. It is denoted as ρ , and its unit is g/L:

$$\text{Mass density } \rho = m/v$$

Example: Determine the density of ether, knowing that half a liter of ether weighs 358 g.

Solution: Mass density $\rho = m/v = 358 \text{ g}/0.5 \text{ L} = 716 \text{ g/L}$.

VII-5- Density**a- Density of Solids and Liquids Relative to Water**

Relative density (d) is the ratio of the density of a substance to the density of a reference substance. For solids and liquids, the reference substance is pure water, which has a density of 1 kg/liter.

The density of a liquid or solid is the ratio of the density of that liquid or solid to the density of water. In mathematical terms, it is expressed as:

$$d = \rho / \rho_{\text{water}}$$

Example:

Calculate the density of iron, given that the densities of iron and water are 7.8 g/cm³ and 1 g/cm³, respectively (1 cm³ = 10⁻³ L, and 1 mL = 1 cm³).

Solution: $d = \rho / \rho_{\text{water}} = 7.8 / 1 = 7.8$.

b- Density of Gases Relative to Air

The density of a gas relative to air is equal to the ratio of the mass (m) of a volume (v) of the gas to the mass m_{air} of the same volume of air (reference substance), with both masses measured under the same conditions of temperature and pressure.

This relationship is expressed as $d = \text{mass of the gas} / \text{mass of air} = \rho \cdot V / \rho_{\text{air}} \cdot V$, which simplifies to $d = \rho / \rho_{\text{air}}$.

If the volume considered is the molar volume, then $m = M$ (molar mass), with the dry air density being equal to 1.293 g/L.

Therefore, $m_{\text{air}} = \rho_{\text{air}} \cdot V_{\text{mol}} = 1.293 \times 22.4 = 29 \text{ g}$.

Thus: $d = \text{mass of the gas} / \text{mass of air} = d = M / 29$. Density has no unit.

Example:

Calculate the molar mass of air under standard conditions ($P=1\text{atm}$; $T=25^\circ\text{C}$; $n=1\text{mol}$).

Solution:

Under standard conditions, the density of air is 1.293 g/L.

We know: 1 mol of air 22.4 L

So, the mass of air corresponding to 22.4 L is equal to the molar mass of air:

1 mol of air 22.4 L $M(\text{air})$

1 L of air 1.293 g

22.4 L of air $M(\text{air})$; $M(\text{air}) = 1.293 \times 22.4 = 29$

VII-6- Mole Fraction (X_i)

The mole fraction (X_i) indicates the ratio of the number of moles of a specific component to the total number of moles in the solution. In a solution, you have:

$\sum X_i = 1$ (The sum of the mole fractions of all components of the solution is always equal to 1).

Example:

We completely dissolve 1g of NaCl in 90 mL of water (density of 0.998 g/mL). We obtain an aqueous solution of Sodium Chloride of 90 mL.

- 1-What is the mass percentage of NaCl in this solution.
- 2-What is the NaCl mole fraction in this solution.
- 3-What is the molality of NaCl.
- 4- What is the molar concentration of NaCl. $M(\text{Na}): 23\text{g/mol}$; $M(\text{Cl}): 35.5\text{g/mol}$.

Solution:

To determine the mass percentage of NaCl in this solution:

$$\% \text{ NaCl} = m_{\text{NaCl}} / (m_{\text{NaCl}} + m_{\text{H}_2\text{O}}) \times 100$$

$$m_{\text{H}_2\text{O}} = \rho_{\text{H}_2\text{O}} \times V_{\text{H}_2\text{O}} = 0.998 \times 90 = 89.82 \text{ g}$$

$$\% \text{ NaCl} = 1 / (1 + 89.82) \times 100 = 1.1\%$$

2- What is the mole fraction of NaCl in this solution?

$$\% \text{ NaCl (molar)} = n_{\text{NaCl}} / (n_{\text{NaCl}} + n_{\text{H}_2\text{O}}) \times 100$$

$$n_{\text{NaCl}} = m_{\text{NaCl}} / M_{\text{NaCl}} = 1 / (23 + 35.5) = 0.017 \text{ mol}$$

$$n_{\text{H}_2\text{O}} = m_{\text{H}_2\text{O}} / M_{\text{H}_2\text{O}} = 89.82 / 18 = 4.99 \text{ mol}$$

$$\% \text{ NaCl (molar)} = 0.017 / (0.017 + 4.99) \times 100 = 0.34\%$$

3- What is the molality of NaCl.

$$\text{Molality} = n_{\text{NaCl}} / m_{\text{H}_2\text{O}}$$

$$\text{Molality} = 0.017 / (89.82 \times 10^{-3}) = 0.19 \text{ mol/kg.}$$

4- What is the molar concentration of NaCl?

$$MC \text{ (molar concentration)} = n_{\text{NaCl}} / V_{\text{H}_2\text{O}}$$

$$MC = 0.017 / (90 \times 10^{-3}) = 0.188 \text{ mol/l}$$

Chapter II: Main Constituents of Matter

Learning Objectives:

The objectives of this chapter are:

- Identify the fundamental constituents of matter: atoms, ions and molecules.
- Explain the internal structure of the atom (protons, neutrons, electrons) and the role of each particle.
- Introduce the concepts of chemical elements and atomic nuclei.
- Distinguish between atoms, isotopes, ions and molecules.
- Understand the formation of ions (cations and anions) through the loss or gain of electrons.

I-introduction

In the atomic theory it was considered that the atom was an indestructible entity, at the beginning of this century a large number of experiments follow one another which obliged to revise this theory.

In this chapter we will examine all the experiments that have served to affirm the theory of atomic structure

These experiments were carried out in three stages:

- 1- Discovery of the electrical nature of matter
- 2- Discovery that the atom consists of a nucleus and particles
- 3- Discovery of mechanical laws that show the behaviour of elements in the atom

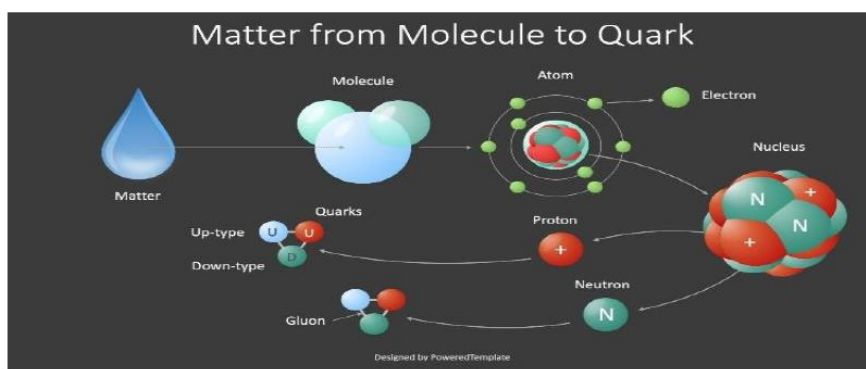


Figure II-1: The Various Constituents of Matter

II- Discovery of the electric nature of matter: Faraday's experience, The relationship between matter and electricity

The purpose of the FARADAY experiment is the conclusion of the existence of a relationship between matter and electricity.

During the electrolysis of water, hydrogen is released from the electrode (+) (anode) while oxygen is released from the electrode (-) (cathode).

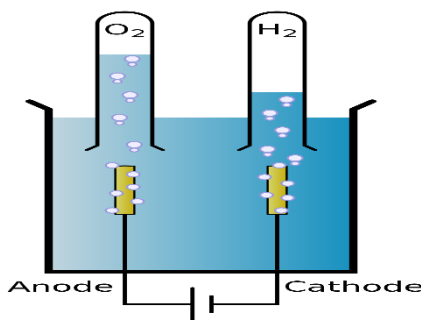
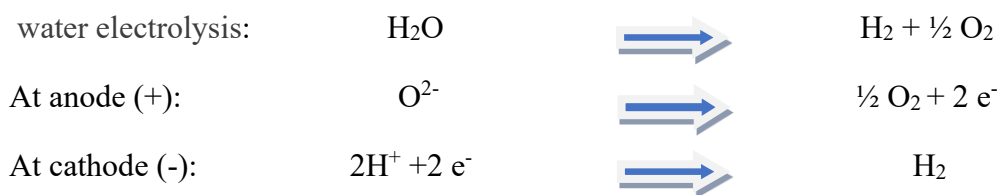


Figure II-2: Electrolysis of H_2O



H^+ captured elements to form H_2 result the transformation of O^{2-} which gave O_2 and thus we notice the appearance of an electric current thus existence of a relationship between matter and electricity.

III- Matter constituents

In 1807, John Dalton proposed a theory in which he described atoms as indivisible and stable particles. By the late 19th century, however, new experiments suggested that an atom has an internal structure: it consists of subatomic particles: the electron, the proton and the neutron.

III-1- Electron

III-1-1-Experience of J.J Thomson (1897): The discovery of electron

The aim of this experiment is the demonstration of the existence of negatively charged particles and the calculating of the mass load ratio (e/m)

- In a first part, a beam of cathodic ray is subjected to the action of an electric field (2 plates of a capacitor); it is noted that there is appearance of a luminous point C on the screen.

This explains why these rays contain negatively charged particles (attraction of charges $(-)$ towards the plate $(+)$ of the capacitor).

- In a second part of the experiment, we use a magnetic field (magnet) we notice the appearance of a luminous point A on the screen. This further proves the existence of charges $(-)$ in the cathodic ray (deviation of radiation towards the pole N which is the pole $(+)$ of the magnet).
- In a third experiment the two fields are submitted at the same time, it is noted that there is no deviation of cathode radiation (appearance of a luminous point at point B)

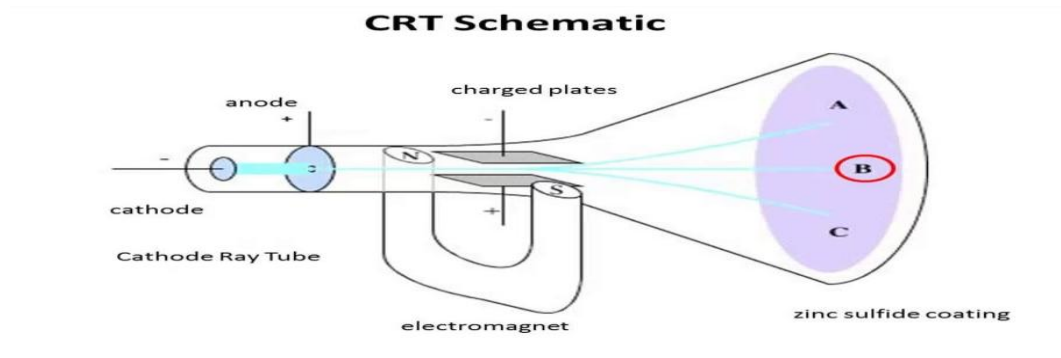


Figure II-3: Schematic of the cathode ray tube by J.J. Thomson

Conclusion

Electrons are part of the constitution of all atoms.

By combining the intensity of the electric and magnetic fields, the cathode ray beam may not deviate from its original path.

Thomson thus determined the charge-to-mass ratio of the particles:

$$e/m_e = 1.76 \times 10^{11} \text{ C/Kg}$$

III-1-2-Millikan's experience (1909): measurement of the electron charge

The purpose of this experiment is to determine the charge of the electron

- Sprayer: injects droplets of non-volatile liquid
- Microscope: used to measure droplet speed between capacitor plates

By means of X-rays these droplets are charged, when the electric field is applied the droplet rises and when the field is cut it goes down.

There are several forces that are present in each type of movement

- 1- In a climb E is different from 0
- 2- In a descent E is equal to 0

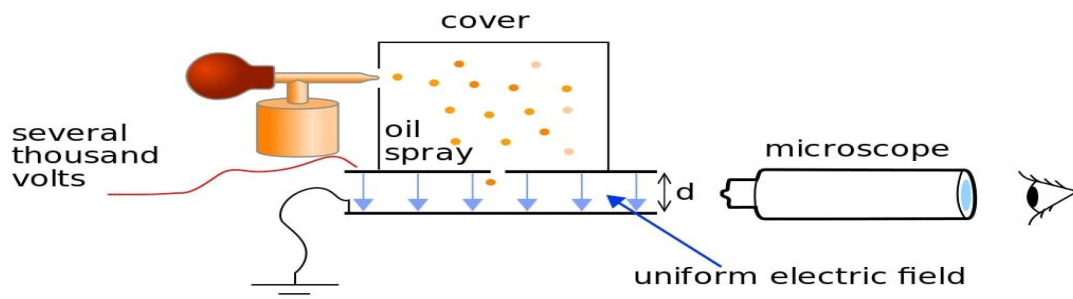


Figure II-4: Experimental scheme of the Millikan experiment

From the force of the electric field necessary to cancel the force of gravity (weight) on the droplets, Millikan was able to determine the values of the particle charges.

As each oil droplet contains several additional electrons, it assumed the smallest charge difference between two droplets

Modern value is $-e$ with $e = 1.602 \times 10^{-19} \text{ C}$

C: coulomb, the SI unit of electric charge

It is considered that $-e$ is a "unit" of negative charge, and that e , called fundamental charge, is a "unit" of positive charge.

The electron mass was determined by combining this value with the ratio $e/m_e = 1,76 \times 10^{11} \text{ C/Kg}$, calculated by Thomson we find: $m_e = 9.109 \times 10^{-31} \text{ Kg}$

IV- Planetary Atomic Model of Rutherford (1909)

IV-1- Discovery of the nucleus

IV-1-1- Gold foil experiment

A thin gold leaf is bombarded by α (charged $+$) particles emitted by a radium source. It is assumed that the mass of each atom of the gold leaf is uniformly distributed over the atom. Therefore, when particles " α " hit the leaf, they are expected to slow down and change direction only by small angles as they pass through the leaf.

However, in doing so, Rutherford and his assistants make these observations:

- ✚ Most particles pass through the gold leaf without deviation as if they had never met the gold atoms.
- ✚ Several particles α are slightly deflected during the gold leaf traverse.
- ✚ Some particles α (1 in 20.000 to 30.000) appear to be back.

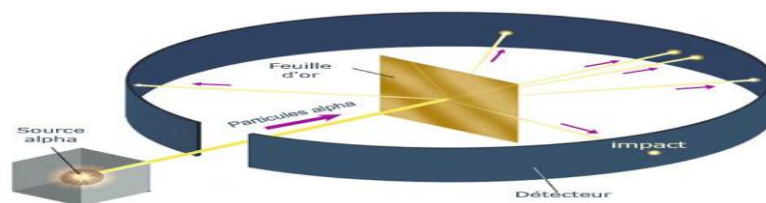


Figure II-5: Rutherford experience

Conclusion

-The particles have passed through the leaf without being deflected, most of an atom consists of empty space.

-The deflection of some positively charged α particles is caused by the enormous repulsion force. This indicates that the atom's positive charge is not uniformly distributed throughout the atom as suggested by Thomson. The positive charge must be concentrated in a very small region to deflect the positively charged α particles.

-Rutherford calculations show that the volume of the nucleus is extremely small compared to the total volume of the atom and the radius of an atom is about 10^{-10} m, while that of the nucleus is 10^{-15} m.

IV-1-2-Composition of the Atomic Nucleus

The nucleus is composed of stable elementary particles called nucleons, which exist in two forms when free: the neutron and the proton.

Protons have a positive charge: $+e = 1.602 \times 10^{-19}$ C

Proton mass: $m_p = 1.673 \times 10^{-27}$ kg

Neutrons have zero charge, and their mass is: $m_n = 1.675 \times 10^{-27}$ kg.

All the mass of the atom is concentrated in the nucleus.

V- Presentation and Characterization of The Atom

Atoms are the fundamental particles that constitute matter. At the atom's center, there is a nucleus composed of protons and neutrons. Around this nucleus are very fast moving particles, electrons. In an atom there are as many positively charged protons as negatively charged electrons, an atom is electrically neutral, characterized by a number of electrons that revolve around the nucleus and a number of nucleons that make up its nucleus

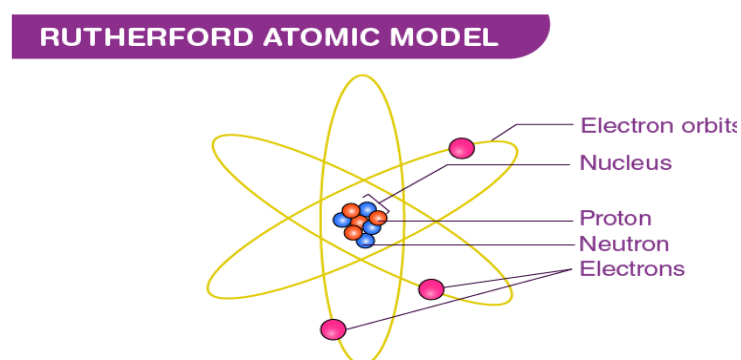
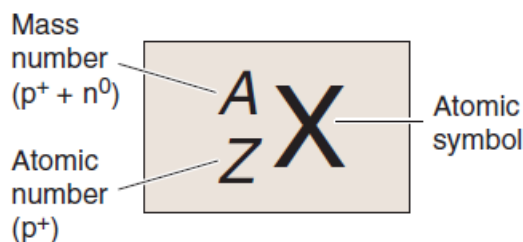


Figure II-6: Planetary Model (Rutherford) of the Atom

Matter is composed of elementary units called atoms, and there are 112 atoms or elements that have been discovered, an atom or chemical element may be presented by the following symbol:



The atom X is characterized by two numbers:

Z: The charge number or atomic number, represents the number of protons or electrons. For any element, the charge of the nucleus is $+Ze$, and the charge of the electrons is $-Ze$.

A: The mass number, represents the number of nucleons (the sum of protons Z and neutrons N) with $A = Z + N$.

A determines the number of **neutrons** N, that an atom has.

Note:

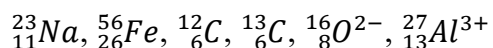
If the element is ionized (charged), the number of electrons is different from the number of protons.

If the element is an **anion** (negative charge X^{-Ze}), we must add the charge number to the number of protons. **number of electrons = $Z + Ze$**

If the element is a cation (positive charge X^{+Ze}), we must subtract the charge number from the number of protons. **number of electrons = $Z - Ze$**

Example

Give the composition of the following particles:



Solution:

The composition of the atoms:

Element	Proton (Z)	Mass Number (A)	Neutron (N)	Electrons
${}^{23}_{11}\text{Na}$	11	23	12	11
${}^{56}_{26}\text{Fe}^{2+}$	26	56	30	24
${}^{12}_6\text{C}$	6	12	6	6
${}^{13}_6\text{C}$	6	13	7	6
${}^{16}_8\text{O}^{2-}$	8	16	8	10
${}^{27}_{13}\text{Al}^{3+}$	13	27	14	10
H_2O	10	18	8	10

VI- Isotopes and Relative Abundance of Different Isotopes

There are two types of atoms: non-isotopic atoms and isotopes.

VI-1- Non-Isotopic Atom

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

$$M_{\text{atom}} = Z \times m_{e^-} + m_{\text{Nucleus}}$$

Z: Atomic number or charge number, representing the number of protons.

m_{e^-} : Mass of the electron

m_{Nucleus} : Mass of the nucleus

$$m_{\text{Nucleus}} = Z \times m_p + n \times m_n$$

m_p : Mass of the proton

n: Number of neutrons

m_n : Mass of the neutron

VI-2- Isotopes

Two atoms of the same element (same symbol) have the same atomic number or number of protons (Z) but different mass number (A), they are called isotopes.

Examples

Natural hydrogen consists of three isotopes:

^1_1H hydrogen : 1 electron + 1 proton + 0 neutron

^2_1H deuterium : 1 electron + 1 proton + 1 neutron

^3_1H tritium : 1 electron + 1 proton + 2 neutrons

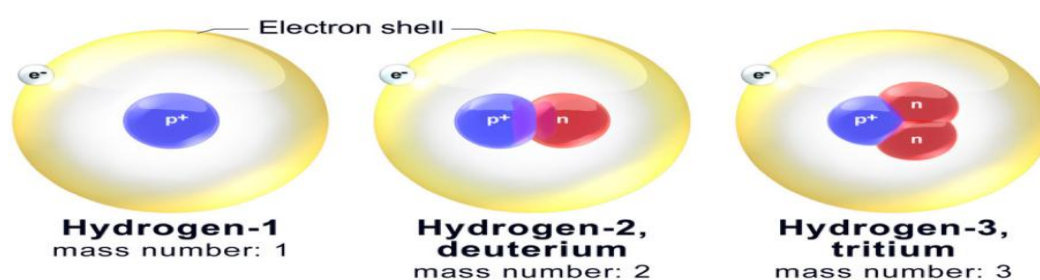


Figure II-7 : Isotopes of Hydrogen

Isotopes for carbon:

all carbon atoms ($Z = 6$) have 6 protons and 6 electrons, but only 98.89% of naturally occurring carbon atoms have 6 neutrons ($A = 12$). A small percentage (1.11%) have 7 neutrons ($A = 13$), and even fewer (less than 0.01%) have 8 ($A = 14$). These are carbon's three naturally occurring

isotopes ^{12}C , ^{13}C , and ^{14}C . A natural sample of carbon has these three isotopes in these relative proportions.

Note:

The chemical properties of two isotopes of the same element are strictly the same because they are determined by the electron configuration, which is the same for both isotopes.

VI-3-Relative Abundance of Different Isotopes and atomic mass

In the general case, an element has one or more isotopes, so the atomic mass will be the sum of the relative proportions of each isotope.

The natural abundance (x) or natural isotope content represents the percentage in number of atoms of each of the isotopes present in the natural mixture.

$m = \sum x_i m_i$ (amu) Similarly, the molar mass will be:

$$M = \sum M_i X_i \text{ (g/mol)}$$

Where: M_i : atomic mass of isotope i

X_i : natural abundance of isotope i

Example

Silver (Ag; $Z = 47$) has 46 known isotopes, but only two occur naturally, ^{107}Ag and ^{109}Ag . Given the following data, calculate the atomic mass of Ag:

isotopes	Mass(amu)	Abundance (%)
^{107}Ag	106.90509	51.84
^{109}Ag	108.90476	48.16

Solution

$$m = \sum x_i m_i \text{ (amu)}$$

Fractional abundance of $^{107}\text{Ag} = 51.84/100 = 0.5184$; similarly, $^{109}\text{Ag} = 0.4816$

$$m_a = 106.90509 \times 0.5184 + 108.90476 \times 0.4816 = 107.87 \text{ amu}$$

Example

In nature, chlorine has two stable isotopes with mass of 34.968 uma at 75.78 % and 36.965 uma at 24.22 %

Calculate the atomic mass (average) of chlorine.

VI-4- Mass Spectrometer: Bainbridge Spectrograph

to measure the mass of an atom within a mixture of isotopes, the most useful technique is to determine the q/m ratio of an ionized atom, where q denotes the ion's charge and m its mass. This is done using devices called mass spectrometers, such as the Bainbridge spectrograph. These spectrometers are able to distinguish between an element's isotopes and assess their abundances.

This Bainbridge spectrograph includes four parts:

- A source of ions,
- The speed filter,
- The analyzer
- The ion detector (photographic plate).

An electron beam emitted by a heated filament positively ionizes the atoms of a gas. It receives ions moving at different velocities.

These ions are subjected to the simultaneous action of an orthogonal electric field and a magnetic field. Therefore, the ionic beam exiting the velocity filter is monokinetic.

In this part of the apparatus, an ion with mass m is subjected to a constant magnetic field with induction B directed perpendicular to its trajectory. The ion is then deflected in a circular path. The deflected ion impacts a photographic plate. The detector collects the ions and amplifies the signal, after which a computer system transforms the received information into a mass spectrum.

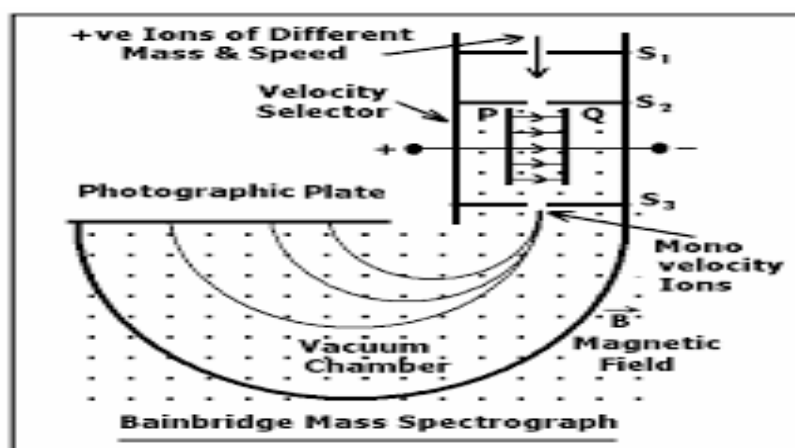


Figure II-8: Principle of the Bainbridge Spectrometer

VII- Nuclear Binding and Cohesion Energy

VII-1- Mass Defect

The formation of a nucleus from its separate nucleons is accompanied by a loss of mass Δm , also known as the mass defect. The mass defect Δm is always positive. Its expression is:

$$\Delta m = (Z \cdot m_p + (A-Z) \cdot m_n) - m_{\text{nucleus}}$$

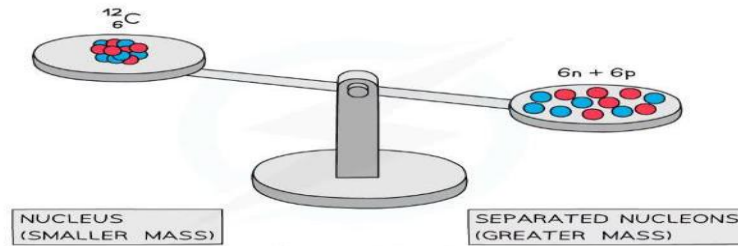


Figure II-9: Representation of a Mass Defect

VII-2-Binding Energy

According to Einstein, the mass loss is transformed into energy that allows the nucleons to remain bound within the nucleus. $\Delta E = \Delta m C^2$

Binding energy is the energy required to dissociate a nucleus into its nucleon particles.

$$E_b = \Delta m C^2$$

E_b : binding energy of the nucleus (in J, eV, or MeV)

Δm : mass defect of the nucleus (in kg)

C : speed of light (m/s)

This energy is positive because it is received by the considered system (nucleus).

An electronvolt is the energy gained by an electron under a potential difference of 1 volt.

$$1 \text{ eV} = \text{electron charge} \times \text{potential difference} = 1.6 \cdot 10^{-19} \text{ C} \cdot 1 \text{ V}$$

$$1 \text{ eV} = 1.6 \cdot 10^{-19} \text{ joules and } 1 \text{ MeV} = 10^6 \text{ eV}$$

VII-3- Cohesion Energy

Cohesion energy is the amount of energy required to destroy a nucleus into its individual neutrons and protons. This energy is typically negative, indicating that work must be done to break the nucleus apart.

It is related to the total nuclear energy (E) by the equation:

$$E_b = -E$$

Where:

E_b : represents the binding energy (the energy required to break the nucleus into free nucleons).

E : represents the total nuclear energy, which is negative due to the attractive forces that bind the nucleons together.

This negative sign reflects the fact that energy must be supplied to overcome the attractive nuclear forces. The stronger the nuclear cohesion, the more negative the energy and the higher the stability of the nucleus.

VIII- Nuclear Stability**VIII-1- Determination of Cohesive Energy (Aston's Curve)**

Aston Curve: The Aston curve illustrates how the binding energy per nucleon varies with the mass number of different nuclei. It is a crucial tool in nuclear physics for comparing nuclear stability. The binding energy per nucleon is defined as the total binding energy E_b divided by the number of nucleons (A). It is expressed in MeV/nucleon.

The curve shows that:

Light nuclei (low mass numbers) tend to increase their stability via fusion (combining to form heavier nuclei with higher binding energy per nucleon).

Heavy nuclei (high mass numbers) increase stability through fission (splitting into smaller nuclei).

The most stable nuclei are found near iron (Fe), where the binding energy per nucleon reaches a maximum, approximately 8 MeV/nucleon. This maximum indicates a highly stable configuration, explaining why fusion and fission both release energy: they lead to products with higher binding energy per nucleon.

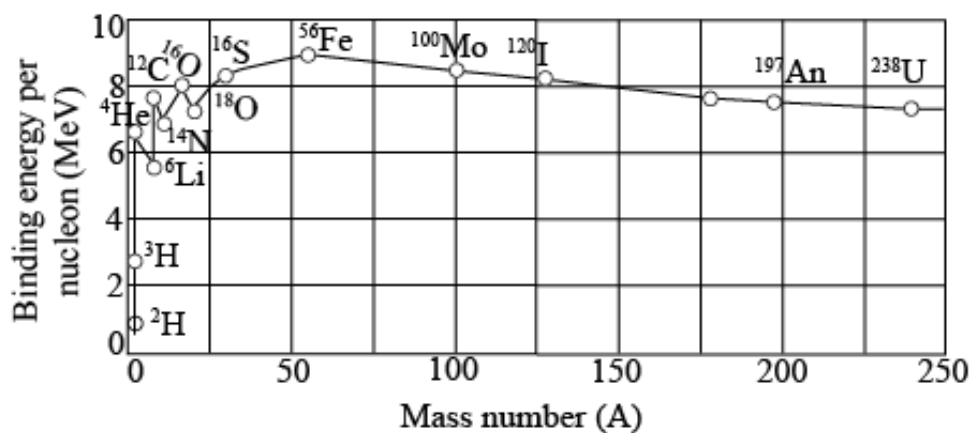


Figure II-10: Aston Curve

VIII-2- Stability And Number of Nucleons

According to Rutherford, the atom is mainly made up of vacuum and all its mass is focused in the nucleus which constitutes protons and neutrons so the stability of a nuclide will be influenced by the number of protons and neutrons. This effect is represented by a stability diagram (see figure) which shows the variation of the neutron number as a function of the atomic number Z in the nucleus.

The shape of this curve shows that stability is:

- important for all elements with $Z=N$ (shown diagonally);
- less important (not stable) between $20 \leq Z \leq 84$, $N > Z$;
- very low, the nucleus are very unstable, for $Z \geq 84$,

they are radioactive (α emission).

For the first elements with $Z < 30$, we observe that stable isotopes have a number of neutrons roughly equal to that of protons, $Z \approx N$.

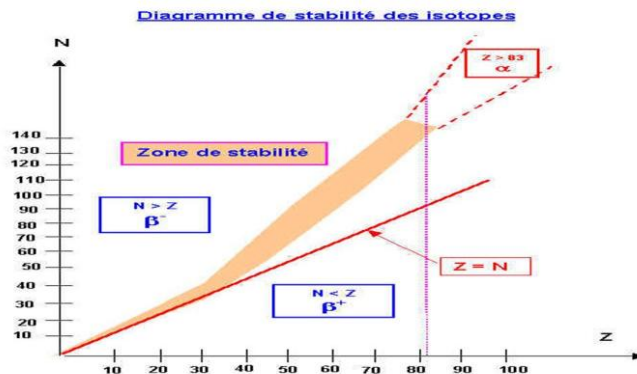


Figure II-11: Diagram of stability of nuclei

Example 1

$^{51}_{23}\text{V}$: $Z=23$ et $N=28$.

Beyond $Z=30$, stable isotopes have a higher number of neutrons than protons: $N > Z$.

Example 2

$^{75}_{33}\text{As}$: $Z=33$ and $N=42$.

Note: As the number of protons increases, the number of neutrons must also increase for the nuclide to be stable.

Example 3

1. Calculate the energy in MeV of the nucleons in the nucleus of the helium isotope ${}^6_2\text{He}$, knowing that its mass is 6.018900 amu.
2. The mass of the isotope ${}^4_2\text{He}$ is 4.001503 amu. Which isotope is more stable?

Solution

Mass defect :

$$\begin{aligned}\Delta m &= (Z \times m_p + (A - Z) \times m_n) - m_{\text{nucleus}} \\ \Delta m &= (2 \times 1.0072765 + 4 \times 1.0086649) - 6.0189 \\ &= 0.0303126 \text{ amu} \cdot 1.66 \cdot 10^{-27} \\ &= 0.0503 \cdot 10^{-27} \text{ Kg}.\end{aligned}$$

Binding energy per nucleon:

$$\begin{aligned}E &= \Delta m \cdot c^2 = 0.0503 \cdot 10^{-27} \cdot (3 \cdot 10^8)^2 = 0.4527 \cdot 10^{-11} \text{ joule} / 1.66 \cdot 10^{-19} = 0.283 \cdot 10^8 \text{ eV} \\ &= 28.3 \text{ MeV/nucleus}.\end{aligned}$$

Binding energy per nucleon for ${}^6_2\text{He}$: $E_{\text{nucleus}}/A = 28.3 / 6 = 4.716 \text{ MeV/nucleon}$.

To compare the stability of the two isotopes, we need to calculate the binding energy per nucleon for ${}^4_2\text{He}$ using the same method.

we can determine which isotope is more stable. The isotope with the higher binding energy per nucleon is more stable.

The binding energy per nucleon:

$$E_{\text{nucleus}}/A = 28.3/6 = 4.716 \text{ MeV/nucleon}.$$

The mass of the isotope ${}^4_2\text{He}$ is 4.001503 atomic mass units (amu)

To determine which isotope is more stable, we can calculate their binding energies per nucleon ($E_{\text{bond}}(\text{liaison})/A$).

$$\text{For helium } {}^4_2\text{He}: \Delta m = (2 \times 1.0072765 + 2 \times 1.0086649) - 4.001503 = 0.0303798 \text{ amu}$$

$$E_{\text{bond}} = 0.0303798 \times 933.75 = 28.34 \text{ MeV}$$

$$E_{\text{bond}}/A = 28.34/4 = 7.08 \text{ MeV/nucleon}$$

The rule states that "Nuclei with the highest binding energy per nucleon are the most stable."

According to the binding energy per nucleon curve ($E_{\text{bond}}/A = f(A)$), the most stable zone is where $7.5 < E_{\text{bond}}/A < 8.8 \text{ MeV}$.

Based on the calculated E_{bond}/A values, we can conclude that helium ${}^4_2\text{He}$ is more stable compared to helium ${}^6_2\text{He}$.

Chapter III: Electronic Structure of Atom

Learning Objectives:

At the end of this chapter, the student should be able to:

- The objectives of this chapter are:
- Understand the distribution of electrons in the atom and its importance for chemical properties.
- Introduce atomic models leading to the quantum model (Bohr $\rightarrow$ quantum model).
- Present the basic concepts of quantum mechanics as applied to atoms.
- Define quantum numbers (n, l, m, s) and their physical significance.
- Explain the concept of atomic orbitals and their representation (s, p, d, f).
- Establish the electronic configuration of atoms and ions.

I- Introduction

The theory of atomic electron structure is based on the laws describing the movement of electrons. To reconcile the dual nature of electrons, which are both particles with mass (as demonstrated by the experiments of Millikan and Thomson) and waves, various experiments have been conducted, and multiple theories have been proposed.

II-Wave Particle Duality

two concepts are distinguished: wave and corpuscle.

- Corpuscles are small (grains) of matter, located in space and with defined trajectories.

Throughout its trajectory position and velocity of corpuscle can be known.

- The waves for their part are not localized, they have a spatial extent and do not have a proper trajectory, they do not carry matter, but they can give us information, amount of movement and energy.

Regarding the light many experiments testify to a wave character: diffraction, interference.

Others prove a corpuscular behaviour and consider light as a jet of particles (photons): photoelectric effect (A.EINSTEIN 1921).

The wave and corpuscular aspect must then be considered as complementary: light sometimes manifests a wave character, sometimes a corpuscle character. We then speak of wave-particle duality.

To study atoms scientists observe them indirectly through light, which atoms emit or absorb when stimulated by heat or electric shock.

The analysis of this light made it possible to propose a model of the electronic structure of atoms and to experimentally test their model.

To do this, we need to understand the nature of light which is a form of electromagnetic radiation.

II-1-Wave aspect of the light: electromagnetic or light wave and electromagnetic spectrum

Light or electromagnetic radiation is one of the forms of energy displacement in space, it is an association of electric and magnetic fields that propagate through space with a wave motion.

It is composed of an electric field (E) and magnetic field (M).

The magnetic field is oriented perpendicular to the electric field. The two fields move at the speed of light c (equal to 3×10^8 m/s). Each of these waves is characterized by its wavelength λ or its wave number $\bar{\nu} = 1/\lambda$.

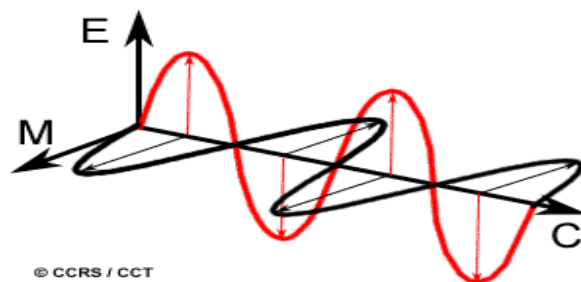


Figure III-1: Diagram of an electromagnetic or light wave

the wavelength λ (lambda) is the distance between two consecutive peaks, or two consecutive troughs. The unit is the meter (m).

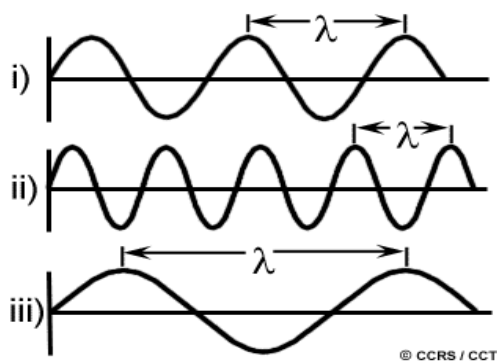


Figure III-2: Effect of wavelength on wave frequency

The frequency ν (nu) is the number of wavelengths per second. The unit is s^{-1} or hertz (Hz).

The relationship between wavelength λ and frequency ν is:

$$\lambda \nu = c$$

c : speed of light c (equal to 3×10^8 m/s).

λ : wavelength (m)

ν : frequency (s^{-1})

So Frequency and wavelength are therefore inversely proportional

II-2- Electromagnetic Spectrum

The electromagnetic spectrum consists of all electromagnetic radiation. In this set, the frequency can take all values continuously.

The visible spectrum is only a small portion of the complete electromagnetic radiation spectrum (Figure III-3). It represents the part of the full spectrum to which the human eye is sensitive. It extends from violet to red.

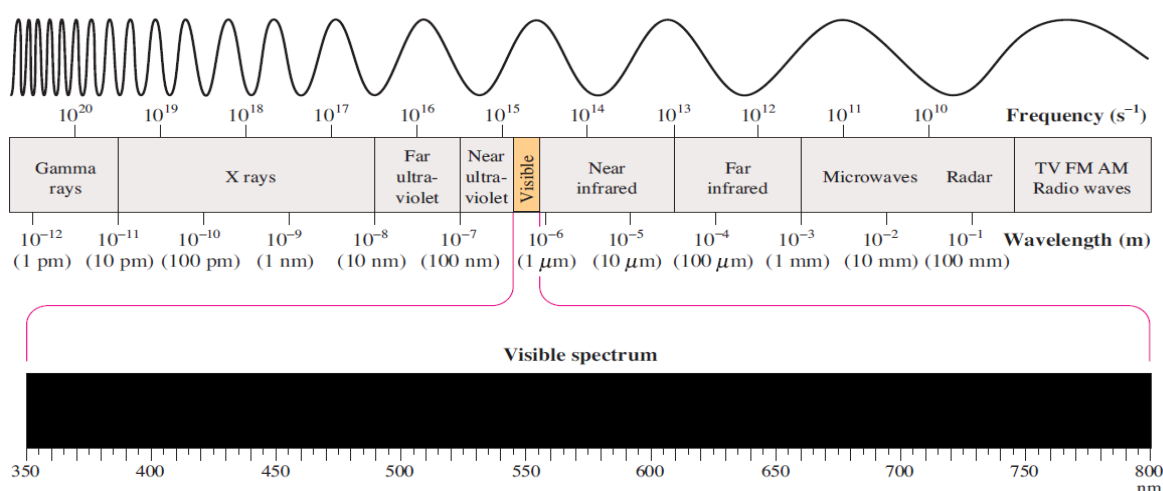


Figure III-3: Electromagnetic spectrum

II-3-Corpuscular nature of light

White light consists of multiple wavelengths emitted by the sun, it is composed of an infinity of colors: red, blue, violet, etc., and each color corresponds to an energy, a frequency and a wavelength.

Planck's studies the corpuscular aspect of a luminous radiation, he says that led can be considered as a collection of particles each carrying a quantum (quanta) of energy known as a photon. Whose value is proportional to the associated frequency and carrying an energy ΔE :

$$E = h\nu = h \frac{c}{\lambda}$$

h : Planck's constant ($h = 6.626 \times 10^{-34}$ J.s)

E : Energy of the light carried by the radiation in Joule

ν : frequency of the radiation in s^{-1} (Hz)

c : speed of light in a vacuum in (m/s)

λ : wavelength in vacuum in (m)

II-3-1- Photoelectric effect

The photoelectric effect is the ejection of electrons from the surface of a metal or from another material when light shines on it. Electrons are ejected, however, only when the frequency of light exceeds a certain threshold ν_0 value characteristic of the particular metal.

To explain this dependence of the photoelectric effect on the frequency, Einstein assumed that an electron is ejected from a metal when it is struck by a single photon. Therefore, this photon must have at least enough energy to remove the electron from the attractive forces of the metal.

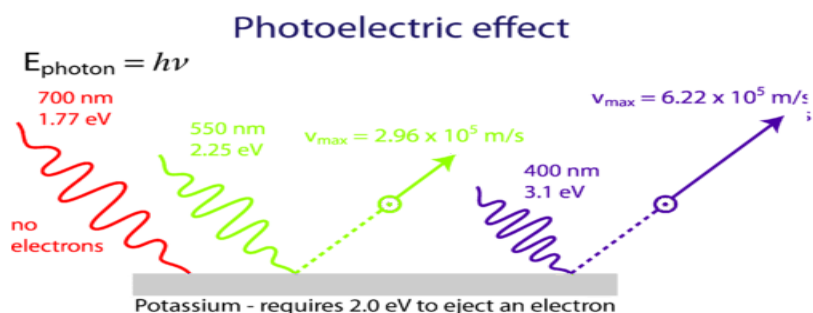


Figure III-4: Photoelectric effect

Explanations given by Einstein

Albert Einstein, who proposed that light sometimes acts as a collection of particles of electromagnetic energy known today as **photons**.

The energy of a photon is defined by the Planck-Einstein relation Each photon is a packet of energy E

If ν_0 is the frequency threshold of the emitted light, the minimum energy required to eject an electron is $h\nu_0$, so the excess energy over $h\nu_0$ is given by:

$$E_c = E - E_0 = h\nu - h\nu_0$$

E_c represents the kinetic energy of the ejected electrons.

The photoelectric effect occurs only if the energy of the incident photon $E = h\nu$ is greater than the work of extraction $E_0 = h\nu_0$ of an electron from the metal, the energy of extraction depending only on the nature of the metal and the threshold frequency ($\nu_0 = c/\lambda_0$, λ_0 threshold wavelength).

$E < E_0 \Rightarrow \nu < \nu_0 \Rightarrow \lambda > \lambda_0 \Rightarrow$ the electron is not injected from the metal,

$E > E_0 \Rightarrow \nu > \nu_0 \Rightarrow \lambda < \lambda_0 \Rightarrow$ the electron leaves the metal with a Speed

$$E_c = E - E_0 = h(\nu - \nu_0)$$

If a photon with energy ($E = h\nu$) $\geq$ ($E_0 = h\nu_0$) is absorbed, the emitted electron will reach a maximum kinetic energy:

$$E_c = \frac{1}{2} m v^2 = h(\nu - \nu_0) = hc \left(\frac{1}{\lambda} - \frac{1}{\lambda_0} \right)$$

Conclusion

Light not only has wave-like properties, it also has corpuscular characteristics. We therefore speak of the dual nature of light

Exercise of application

A polychromatic light consisting of 3 radiations ($\lambda_1 = 450\text{nm}$; $\lambda_2 = 610\text{nm}$; $\lambda_3 = 750\text{nm}$) irradiates a sample of potassium contained in a bulb. The ionization energy is 2.14 eV (the energy required to remove an electron from a potassium atom).

1-Establish the relationship $E \text{ (eV)} = 1241/\lambda \text{ (nm)}$.

2-Which radiations lead to the photoelectric effect?

3-What is the speed of the electrons expelled from the metal? Electron mass $9.1 \times 10^{-31} \text{ kg}$.

Solution

Photon energy $E = h\nu = hc/\lambda$, $E(\text{J}) = 6.62 \times 10^{-34} \times 3 \times 10^8 / \lambda$.

$1 \text{ eV} = 1.6 \times 10^{-19} \text{ J}$, and $1 \text{ nm} = 10^{-9} \text{ m}$. $E \text{ (eV)} = 1241/\lambda \text{ (nm)}$.

Use the above relationship to calculate the energy for each photon:

$E_1 = 1241/450 = 2.76 \text{ eV}$;

$E_2 = 2.03 \text{ eV}$;

$E_3 = 1.65 \text{ eV}$. Only the radiation λ_1 is sufficiently energetic.

The electron removed from the atom carries away $2.76 - 2.14 = 0.62 \text{ eV}$ as kinetic energy.

$\frac{1}{2} mv^2 = 0.62 \times 1.6 \times 10^{-19} = 10^{-19} \text{ J}$; $v^2 = 10^{-19} / (0.5 \times 9.1 \times 10^{-31})$.

Therefore, $v \approx 4.7 \times 10^5 \text{ m/s}$.

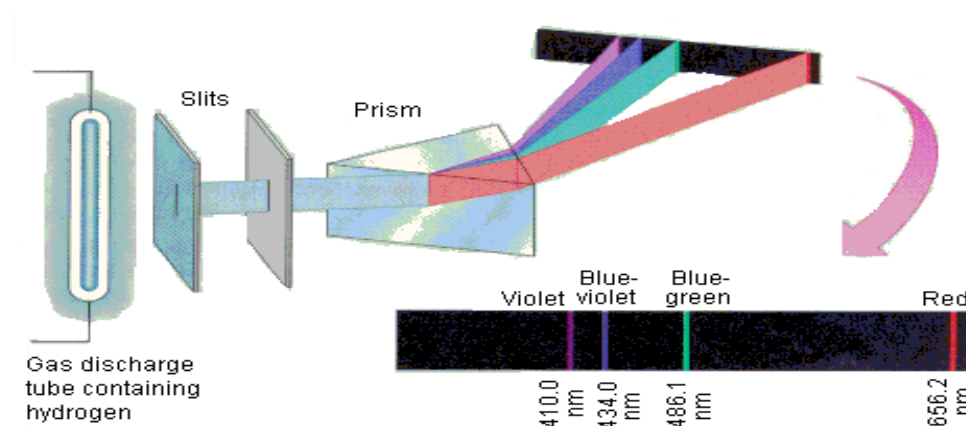
III-The interaction between light and matter

When a source of energy strikes an object, it will send back radiation at a certain wavelength and will therefore appear in a specific color, depending on the mechanisms of emission, reflection, absorption and transmission.

III-1-Emission spectrum of the hydrogen atom

The emission spectrum of the hydrogen atom consists of the electromagnetic waves emitted by an excited hydrogen atom that has absorbed excess energy. This is obtained experimentally (figure III-1) in a discharge tube containing dihydrogen and fitted with two metal electrodes. The tube contains dihydrogen under low pressure, and a discharge is produced that partially ionises the dihydrogen H_2 .

The ions generated are accelerated by the potential difference between the two electrodes and collide at high speed with the dihydrogen molecules, causing the hydrogen atoms to dissociate and the atoms formed to become excited. The atoms do not retain this excess energy for very long: they release it in the form of light, we say they de-excite. The emitted radiation consists of a series of lines with different wavelengths, representing the spectrum of the hydrogen atom.



FigureIII-5: Emission spectrum of the hydrogen atom

- certain types of radiation, with very specific energies, are emitted by the hydrogen atom. The spectrum takes the form of a series of lines. The emission spectrum of the hydrogen atom is known as a line spectrum (discontinuous spectrum).
- Radiation appears in groups: the spectrum is made up of several series of lines. The first series was observed by BALMER (a series in the visible range). LYMAN discovered a series in the ultra-violet, then PASHEN located a new series in the infra-red range.

III-2-BALMER-RYDBERG empirical relationship

Balmer proposed an empirical formula in 1885 to calculate the wavelengths (λ) of the visible hydrogen lines (Balmer series). His formula was later generalized by Rydberg, who expressed it in terms of wavenumber ($\bar{\nu}$).

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

Where:

λ : wavelength.

R_H : Rydberg constant for hydrogen, found experimentally ($1.09677 \times 10^7 \text{ m}^{-1}$)

n_1 and n_2 : integers taking the following values for each series:

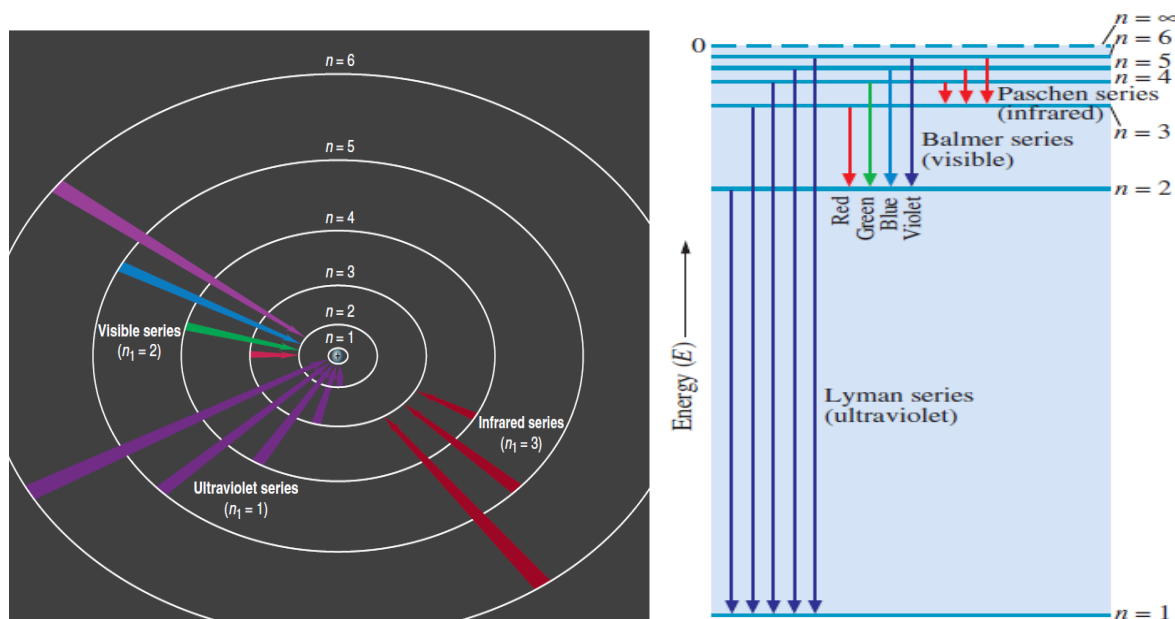


Figure III-6: Series of Lines in the Hydrogen Atom's Spectrum

the first series, known as the **Lyman** series, corresponds to the electron returning from an excited state to the ground state ($n_1=1$ and $n' > n$)

The hydrogen atom's emission spectrum is composed of monochromatic radiations with well-defined wavelengths.

Experimental observations have shown that the hydrogen atom's emission spectrum contains numerous lines in the ultraviolet, visible, and infrared regions. The first lines studied are found in the visible range and belong to the "**Balmer series**".

n_1	n_2	series	Range
1	2, 3, 4, etc ...	Lyman	UV
2	3, 4, 5, etc...	Balmer	Visible
3	4, 5, 6, etc...	Paschen	IR

III-3- Interpretation of the Hydrogen Emission Spectrum

Due to the high voltage, the electron in H_2 is excited, absorbing energy and moving away from the nucleus, making it unstable. To regain stability, it prefers to return near the nucleus, emitting energy in the form of visible light radiation (photons with frequency ν).

Absorption of Light: When the hydrogen atom is not excited, the electron is in a low-energy orbit, which is called the ground state. When this atom is subjected to a potential, it absorbs energy, resulting in an electronic transition from the ground state to a higher energy level (excited state).

Emission of Light: The excited electron in the atom is in an unstable state and returns to its most stable energy level, the ground state, emitting radiation. The hydrogen emission spectrum shows that only certain energy levels are allowed.

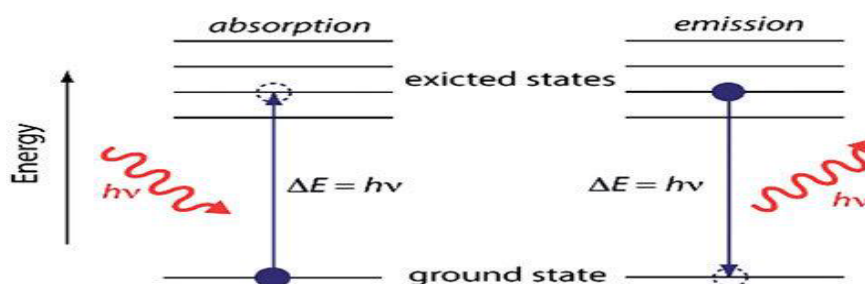


Figure III-7: Diagram of an Electronic Transition

Exercise of application

The element Strontium is known for producing a bright red color in flames. This color is due to the presence of two visible lines in its spectrum, at 605 nm and 461 nm. One of these lines appears yellow-orange, and the other is blue.

1. Assign the color to each of these lines.
2. Calculate the energy and frequency of the corresponding photons.

Solution

The visible spectrum extends approximately from 400 nm to 800 nm. The order of colors is well-known as ROYGBIV: Red - Orange - Yellow - Green - Blue - Indigo - Violet.

Violet corresponds to high energy, high frequency, and short wavelengths.

Conversely, red corresponds to low energy, low frequency, and long wavelengths. It is easy to assign a color to each line based on this information.

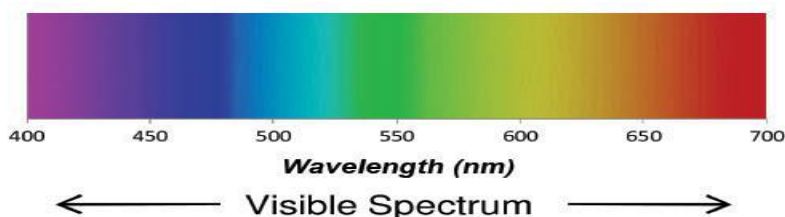


Figure III-8: The electromagnetic spectrum

$$\nu = c / \lambda$$

$$E = h\nu = hc / \lambda$$

Line 1 : $\lambda_1 = 605 \text{ nm}$

$$\nu_1 = 3 \cdot 10^8 / 605 \cdot 10^{-9} = 4,96 \cdot 10^{14} \text{ Hz}$$

$$E_1 = 6,62 \cdot 10^{-34} \times 4,96 \cdot 10^{14} = 3,28 \cdot 10^{-19} \text{ J}$$

Color: Yellow-orange (long wavelength, low frequency, and low energy)

Line 2 : $\lambda_2 = 461 \text{ nm}$

$$\nu_2 = 3 \cdot 10^8 / 461 \cdot 10^{-9} = 6,51 \cdot 10^{14} \text{ Hz}$$

$$E_2 = 6,62 \cdot 10^{-34} \times 6,51 \cdot 10^{14} = 4,31 \cdot 10^{-19} \text{ J}$$

Color: Blue (short wavelength, high frequency, and high energy)

IV-Bohr's atomic model

A new model of the atom based on the quantification of energy was presented in 1913 by Niels Bohr. This model explained the structure of the hydrogen atom and its spectrum; it also provided a theoretical basis for the Rydberg equation. The characteristics of this model are summarised in three postulates:

- 1st postulate/mechanical postulate:

The atom does not radiate when the electron is in motion on well-defined orbits or stationary orbits.

- 2nd postulate/postulate of kinetic moment:

the angular momentum of the electron, which is the product of the mass times the velocity times the radius of the orbit, is :

$$mvr = \frac{nh}{2\pi}$$

h: Planck's constant, n: quantum number

- 3rd postulate/optical postulate:

when the electron moves from one stationary orbit to another, the atom's energy undergoes a sudden change

$$\Delta E = E_{n2} - E_{n1} = h\nu = \frac{hc}{\lambda}$$

This relationship is known as the Bohr frequency condition

h: Planck's constant = $6.623 \cdot 10^{-34} \text{ J.s}$

ν : frequency of radiation

The most important equation stemming from Bohr's model expresses the energy levels of the electron in the hydrogen atom:

$$E_n = -2,178.10^{-18}(Z^2/n^2) \text{ (J)}$$

$$E_n = -13,6 (Z^2/n^2) \text{ (eV)}$$

VI-1- Absorption and Emission of Energy

An electron can only absorb or emit energy, radiate, when transitioning from one level (orbit) to another. The amount of energy absorbed or emitted is equal to the difference in energy between the two levels $\Delta E = E_2 - E_1$

Where:

E_2 : Energy of the final state.

E_1 : Energy of the initial state.

During an **emission** process, the electron jumps from the orbit of rank n_2 to the orbit of rank n_1 , such that the atom passes from an energy level E_{n_2} to a lower level E_{n_1} , it then releases its excess energy in the form of light. The radiation emitted will be $E_1 - E_2 < 0$

During an **absorption** process, the electron jumps from an orbit of rank n_1 to an orbit of rank n_2 , such that the atom passes from an energy level E_{n_1} to a higher level E_{n_2} , so the radiation absorbed will be $E_2 - E_1 > 0$.

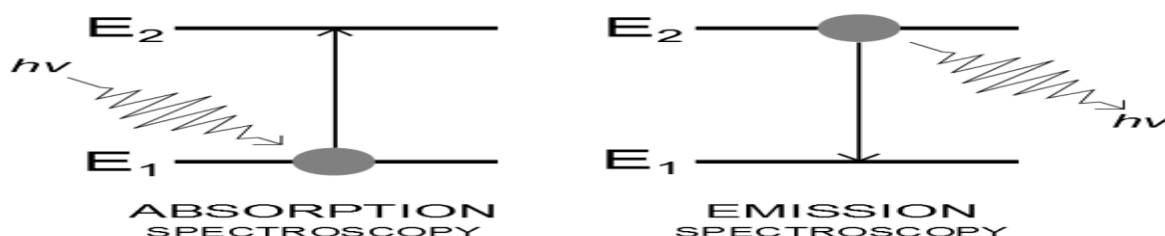


Figure III-9: Photon absorption-emission process

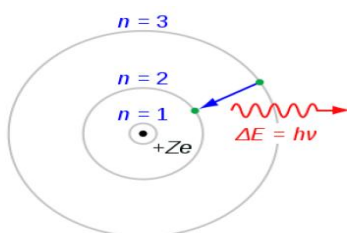


Figure III-10: Illustration of a transition by a spectral line

The lowest energy stationary state ($n=1$) is called the **ground** state, and the higher energy permitted states are called **excited** states.

The negative sign simply means that the electron's energy is lower close to the nucleus than at an infinite distance ($n=\infty$), where, in the absence of any interaction, the energy is zero.

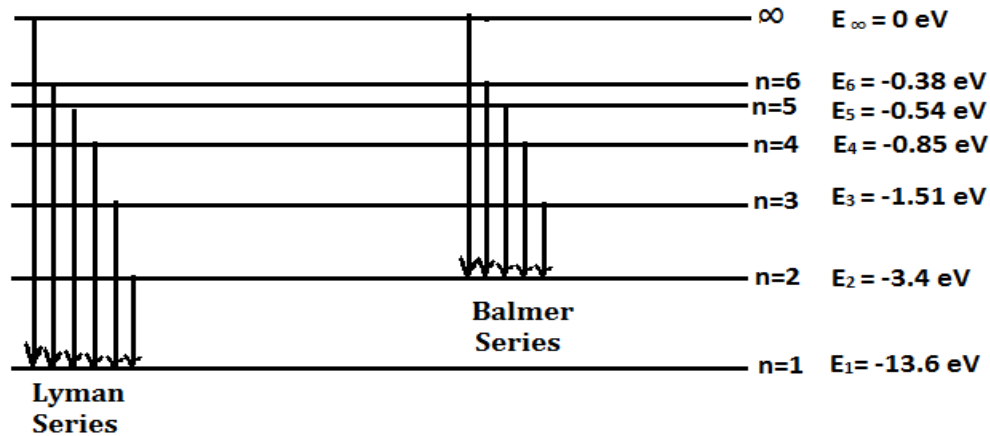


Figure III-11: Energy diagram of the hydrogen atom

Example

What is the wavelength emitted when an electron transitions from the initial level $n_i = 3$ to the final level $n_f = 2$?

Solution

$$E_n = -13.6 (Z^2 / n^2)$$

$$E_2 = -3.40 \text{ eV and } E_3 = -1.51 \text{ eV}$$

$$\Delta E = E_2 - E_3$$

$$\Delta E = -1.89 \text{ eV}$$

$$\text{Conversion to Joules : } \Delta E = -3.02 \times 10^{-19} \text{ J}$$

$\Delta E < 0$; it is an emission of energy.

$$\text{According to Planck-Einstein : } \Delta E = h.c / \lambda \text{ so } \lambda = h.c / \Delta E$$

$$\lambda = 657 \text{ nm}$$

IV-2-Ionisation energy

The ionisation energy E_i is the energy required to move the electron from the ground state to infinite distance. This phenomenon corresponds to the tearing of the electron from the atom, i.e. sending the electron to the energy level $E = 0$.

Example

The ionisation energy E_i of the hydrogen atom is:

$E_i = E_\infty - E_1 = 13,6 \text{ eV}$, for the hydrogen atom. With $E_\infty = 0$

Note:

The excitation energy of the hydrogen atom is the energy needed to move the electron from the n_1 to n_2 orbit ($n_1 < n_2$).

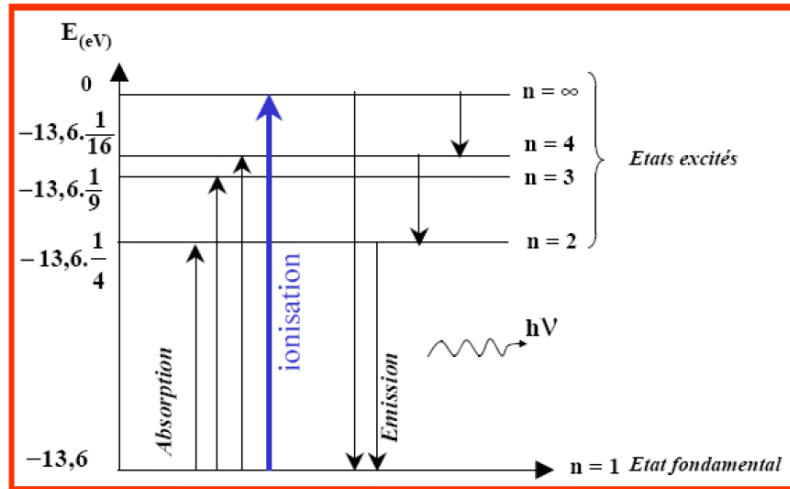


Figure III-12: Ionisation energy E_i of the hydrogen atom

IV-3- Application to Hydrogen-like Ions

These are atoms that have lost all their electrons except one, making them similar to hydrogen in terms of the number of electrons. Therefore, Bohr's theory can be applied to these hydrogen-like ions

Example: ${}_2\text{He}^+$; ${}_3\text{Li}^{+2}$; ${}_4\text{Be}^{+3}\dots$

Calculating the energy of the electron of a hydrogen-like ion in an orbit n gives the following expressions:

$$E_n = - 2,178 \cdot 10^{-18} \left(\frac{Z^2}{n^2} \right) \text{ J} = -13,6 \left(\frac{Z^2}{n^2} \right) \text{ eV}$$

These expressions can be determined by replacing the charge on the nucleus ($+e$) with $(+Ze)$ in the expressions for the hydrogen atom.

The wave numbers $1/\lambda$ (Rydberg formula) of the series observed in the spectrum of hydrogen ions are given by:

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

With R_H : Rydberg constant

IV-4-Insufficiency of The BOHR Model

Bohr's model is based on his ability to explain the experimental results for the hydrogen atom. This modelling revealed a number of inconsistencies and several shortcomings quickly became apparent in Bohr's model

The model is valid only for chemical species with a single electron, i.e. the hydrogen atom and the He^+ , Li^{2+} , Be^{3+} , ect.

He was unable to explain the presence of additional lines in more refined spectroscopes.

It was an important step towards quantum mechanics, which describes the behaviour of electrons more precisely.

V-The Hydrogen Atom in Wave Mechanics

V-1-Wave-Corpuscle Duality and The De BROGLIE Relation

In 1924 LOUIS DE BROGLIE put forward the hypothesis that wave-corpuscle duality is a general property of physics. He stated that any particle in motion is associated with an associated wave of wavelength λ :

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

λ : DE BROGLIE wavelength

h : PLANCK's constant (6.626×10^{-34} j.s)

p : Momentum

m : Particle mass

v : Particle velocity

BROGLIE's law can be used to find the quantification condition used by BOHR if we consider the electron as a wave, the electron can only move in orbits for which it has been designed.

$$mvr = nh/2\pi.$$

In fact, by isolating the number mv from this equation and the BROGLIE equation, we can demonstrate that $2\pi r$, which is the circumference of the orbit, corresponds to an integer wavelength λ .

$$mvr = \frac{nh}{2\pi} \Rightarrow mv = \frac{nh}{2\pi r} ; \quad \lambda = \frac{h}{mv} \Rightarrow mv = \frac{h}{\lambda} \text{ et } \frac{nh}{2\pi r} = \frac{h}{\lambda} \Rightarrow 2\pi r = n\lambda$$

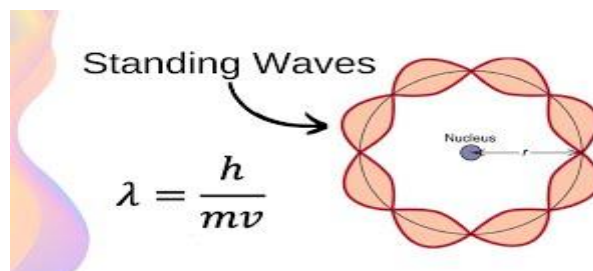


Figure III-13: Representation of the electron as a standing wave

V-2-Heisenberg Uncertainty Principle

If we describe the electron using the wave model and the particle model "It is impossible to know the position and velocity of a moving particle precisely at the same time".

$$\Delta x \cdot \Delta(mv) \geq \frac{h}{4\pi}$$

Δx : uncertainty relative to the position of the electron

$\Delta(mv)$ or Δp : uncertainty relative to the quantity of movement (i.e. speed/velocity)

h : Planck's constant

According to this principle, we cannot therefore know the precise trajectory of the electron around the nucleus. Consequently, we cannot assume that the electron describes a well-defined orbit, as Bohr's model does.

Application Exercise

An electron is moving in a straight line. Given that its position can be known within 1 Ångström, what is the uncertainty in its velocity?

Solution:

$$\Delta x = 1 \text{ Å} = 10^{-10} \text{ m}, m_e = 9.11 \times 10^{-31} \text{ kg},$$

$$\Delta v \geq h / 4\pi m \Delta x$$

$$\text{So, } \Delta V \geq 6.625 \cdot 10^{-34} / 4\pi \cdot 9,11 \cdot 10^{-31} 10^{-10} \Leftrightarrow \Delta v \geq \mathbf{5.79 \cdot 10^5 \text{ m/s}}$$

The uncertainty in the velocity of the electron is significant.

This means that if we measure the position of the electron within 1 Ångström (which is a high level of precision), we will introduce a significant error in the measurement of its velocity, and vice versa.

V-3- Concept of Probability of Presence

In classical mechanics (Bohr's conception), studying the motion of an electron involves precisely determining its trajectory. However, in quantum mechanics, we discuss the probability of finding the electron at a certain point in space.

This spatial distribution is described by a function of the electron's coordinates called the wave function Ψ .

V-3-1-Schrödinger Equation

Schrödinger's method: replace the electron orbit (Bohr's model) with a mathematical function called the wave function Ψ (psi). the value of Ψ depends on the x,y,z coordinates of the point in the space.

This wave function must be a solution of the Schrödinger equation.

Atomic orbitals are the wave functions of atomic electrons. In 1926, Schrödinger demonstrated that the wave function and the energy E are solutions to a second-order partial differential equation. The Schrödinger equation is written as:

$$H\Psi = E\Psi$$

This is the fundamental principle of quantum mechanics. Where:

E : Total energy of the electron, called the eigenvalue

Ψ : Wave function, called the eigenfunction

H is called the Hamiltonian operator of the hydrogen atom, and it is expressed as:

$H = (-\hbar^2 / 8\pi^2m) \Delta + V$; this is called the Hamiltonian operator of the hydrogen atom.

$\Delta = \partial^2 / \partial x^2 + \partial^2 / \partial y^2 + \partial^2 / \partial z^2$; this is the Laplacian operator.

m : mass of the electron

V : potential energy operator

This equation is the fundamental principle of quantum mechanics. Solving this equation leads to different values of E and Ψ :

$$E_n = - \frac{2mZ^2K^2\Pi^2e^4}{n^2\hbar^2}$$

It is the same expression as that found by the Bohr model. With quantum mechanics, we can also explain the quantization of energy.

In other words, $\Psi^2 \cdot dV$ is the probability of finding the electron in a volume dV surrounding the point(x,y,z) $\Longrightarrow$ The position of the electron cannot be determined precisely, but we can give a probability that the electron is in a particular region of space.

The volume in which this probability of the electron's presence has a fixed value (99%, for example) is called an atomic orbital.

VI-Quantum Numbers and The Concept of Atomic Orbitals

VI-1- Quantum Numbers

Atomic orbitals depend on four numbers called quantum numbers: principal, azimuthal, magnetic and spin.

VI-1-1- Principal Quantum Number (n)

It characterizes the energy level occupied by the electron or the shell it occupies. It is sometimes designated by an uppercase letter.

 $n = 1, 2, 3, \dots$ Each value of n corresponds to a layer (level)

Example: orbitals with $n = 1$ are the orbitals of the first layer.

This defines **the size** of the orbital and **the energy** associated with it.

$n=1$ layer K

$n=2$ layer L

$n=3$ layer M

$n=4$ layer N

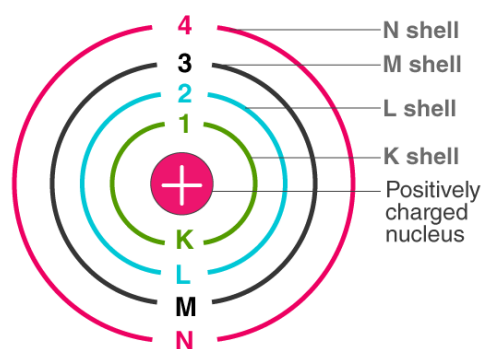


Figure III-14: Representation of the Atom with the Principal Level (layer, shell)

VI-1-2-Secondary Quantum Number (or Azimuthal) (l)

It defines **the shape** of the orbital; it characterizes the sublayer (subshell) occupied by the electron.

 The azimuthal number can take the values: $0 \leq l \leq n-1$ ($l = 0, 1, 2, \dots, n-1$)

$l=0$ Subshell s

$l=1$ Subshell p

$l=2$ Subshell d

$l=3$ Subshell f

Example: $n = 3$ $l = 0, 1, 2$

$l = 0$ 1 sublayer s

$l = 1$ 1 sublayer p

$l = 2$ 1 sublayer d

✚ Orbitals are designated by first writing the value of n (1,2,3,...) followed by the letter indicating the value of l (s, p, d, f...)

Example: orbital 2p: $n = 2$ and $l = 1$

Exercise of application

Which of the following orbitals do not exist?

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

VI-1-3- Magnetic Quantum Number (m)

It characterizes the quantum box occupied by the electron and determines its **orientation** in a magnetic field. Its value depends on the value of the secondary quantum number (l).

There are $2l+1$ different values for m .

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

✚ The magnetic number can take the values: $-l \leq m_l \leq +l$ or $m_l = -l, \dots, 0, \dots, +l$

A different orbital corresponds to each value of m_l , for given values of n and l

Example:

Permitted values of l and m for n from 1 to 3

n	l	m_l	orbital number	orbital's
1	0	0	1s	1
2	0	0	2s	1
	1	-1, 0, +1	2p	3
3	0	0	3s	1
	1	-1, 0, +1	3p	3
	2	-2, -1, 0, +1, +2	3d	5

These three quantum numbers define a quantum box, and this box can contain two electrons.

To distinguish between the two electrons, a fourth quantum number, spin (s), is introduced.

VI-1-4- Spin Quantum Number (s)

It characterizes the intrinsic angular momentum of the electron and can only take two different values: $\pm \frac{1}{2}$

By convention: $s = +\frac{1}{2} \uparrow$ and $s = -\frac{1}{2} \downarrow$

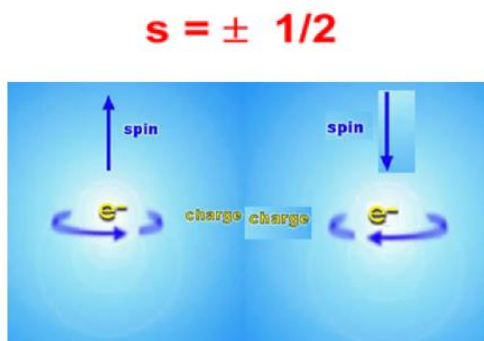


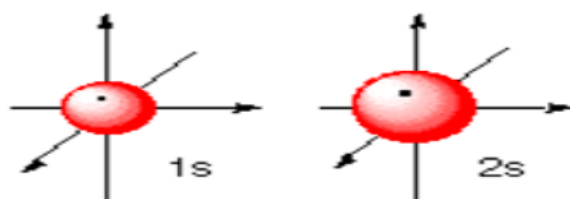
Figure III-15: Motion of the electron on itself

Exercise:

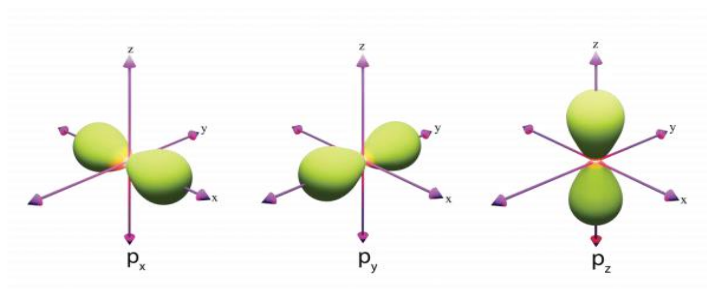
What are the possible combinations of the four quantum numbers for an electron occupying the $n=2$ layer in an atom?

VII-Atomic Orbitals

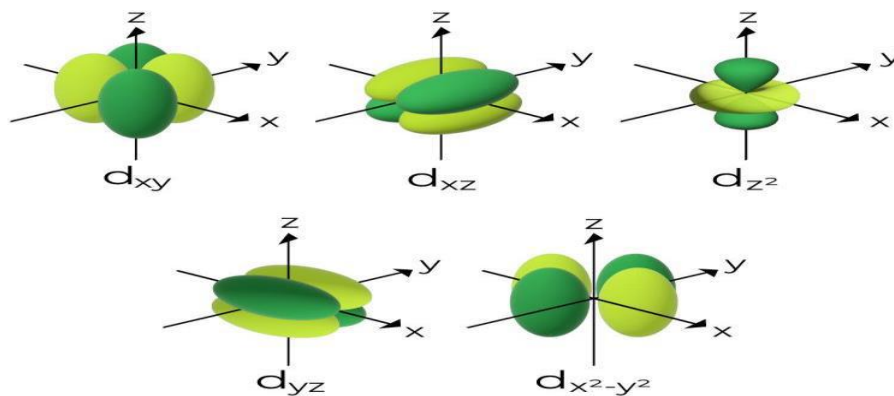
s orbitals: These are spheres whose volume increases with the value of n



p orbitals: these are made up of two lobes separated by a zone of zero probability called a node. They are identified according to the axis of the coordinate system (x, y, z) along which the orbital is oriented.

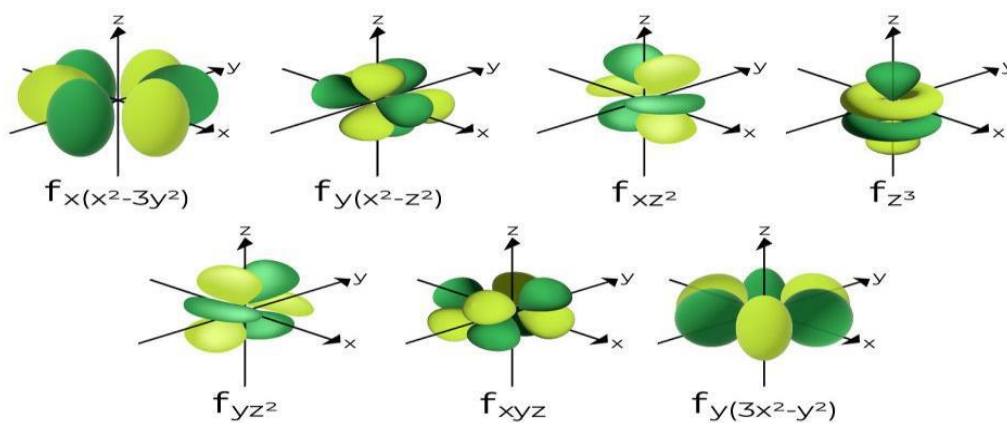


✚ **d orbitals:** these orbitals are found from $n = 3$ ($l = 2$). There are 5 forms of 3d orbitals



Shape of d-orbital

✚ **f orbitals:** If $l = 3$, m can take the values: $m = (-3, -2, -1, 0, +1, +2, +3)$, resulting in seven f orbitals.



Shape of f-orbital

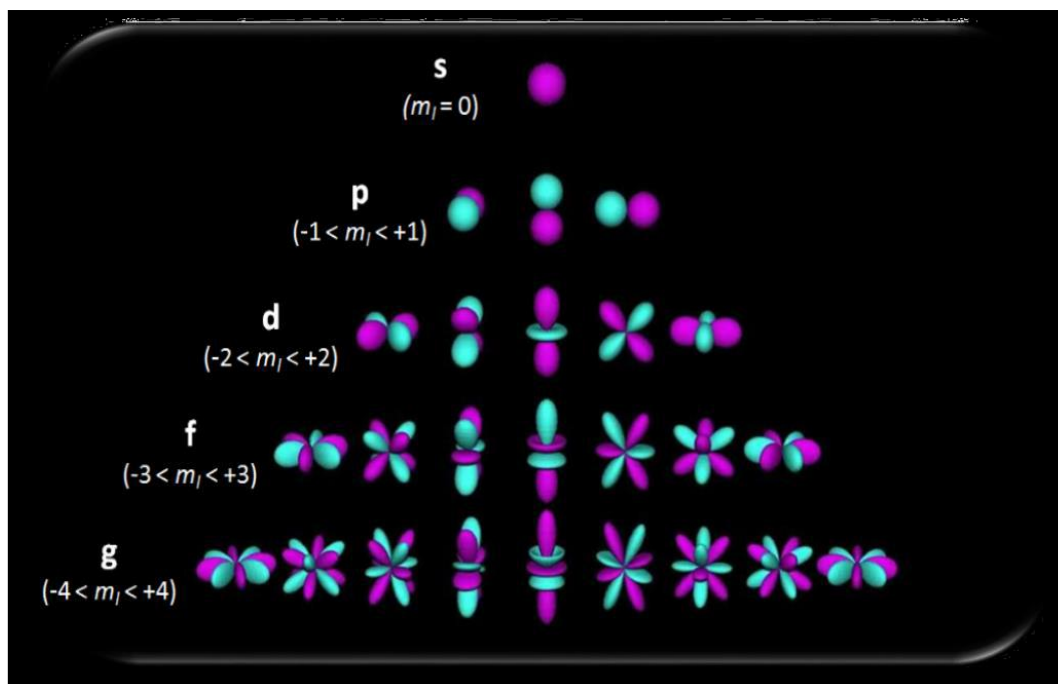


Figure III-16: Representation of atomic orbitals

VII-1- Energy of Atomic Orbitals

In the atom, the energy of a given orbital is a function of its n value (obtained by solving Schrödinger's equation)

$$E_n = -13.6 (Z^2/n^2)(\text{eV})$$

This is the same energy expression as that obtained by Bohr.

Therefore, all orbitals with the same value of n have the same energy: they are said to be degenerate orbitals.

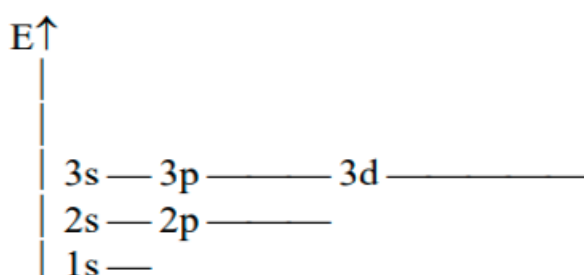


Figure III-17: Degenerate Atomic Orbital energy levels

In polyelectronic atoms,

Each electron is subject to the attraction of the nucleus but also, to repulsive forces from the other electrons in the atom. the electrons occupy orbitals similar to that of hydrogen. But the energies of these orbitals are not the same as those of hydrogen.

✚ There are two opposing effects:

- electron-core attraction
- electron-electron repulsion

✚ In polyelectronic atoms, because of inter-electronic repulsions, the energy of the orbitals varies according to the order :

$$E_{ns} < E_{np} < E_{nd} < E_{nf}$$

For example, for the $n = 3$ shell: $E_{3s} < E_{3p} < E_{3d}$

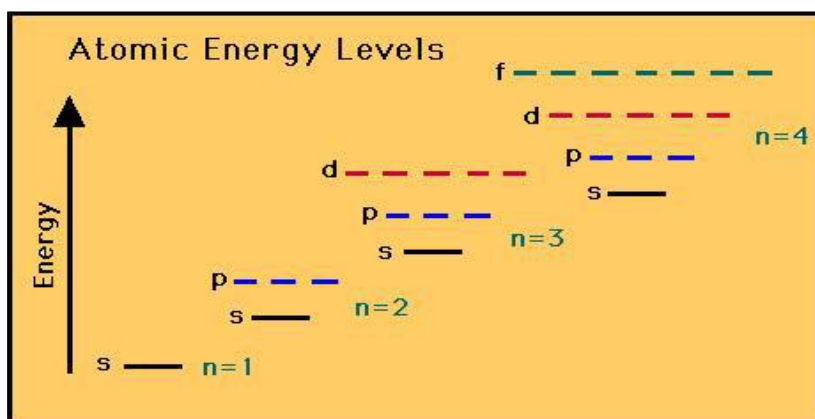


Figure III-18: Energy Levels of Atomic Orbitals in a Poly-Electronic Atom

VIII- Electronic configuration of the atom

We try to place Z electrons (neutral atom) on the different levels, this is called: Writing the electronic configuration.

The electronic configuration of an atom is the distribution of Z electrons of the atom in a ground state over the atomic orbitals.

Step 1: place the electrons, one after the other, in the orbitals according to Klechkowski's rule. Never put more than two electrons in the same orbital (Pauli's principle).

Step 2: If there is more than one orbital in a sublayer, place the electrons, with parallel spins, in different orbitals instead of pairing two electrons in one of them (Hund's rule).

- The electrons in the outermost layer (the largest value of n) are called valence electrons (or peripheral electrons).

□ In general, only valence electrons can be given up during chemical reactions, because the core electrons are too tightly bound.

The atomic orbitals are filled using the following three rules:

- ❖ KLECHKOWSKY rule.
- ❖ PAULI rule.
- ❖ HUND rule.

VIII-1-Klechkowski's rule (filling order)

"With a few exceptions, the energy of the electronic orbitals or layers follows the order of $(n + l)$ increasing."

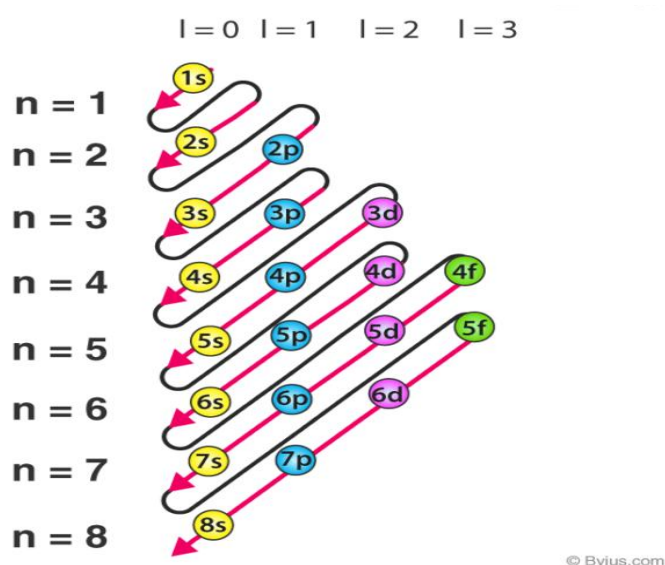


Figure III-19: Klechkowski's rule

VIII-1-1 Exceptions to Klechkowski's Rule

Starting from the $n = 4$ level, the filling of atomic orbitals does not strictly adhere to Klechkowski's rule.

Example:

Copper (^{29}Cu): The most stable configuration is $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^{10}$

Chromium (^{24}Cr): The most stable configuration is $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^5$

These exceptions correspond to half-filling and full-filling of the 3d sublayer.

They are explained by the small energy gap between the 4s and 3d orbitals.

VIII-2- Hund's Rule

When electrons fill the orbitals of a given energy level, they successively occupy the maximum number of orbitals with parallel spins. When a subshell is not complete, electrons occupy the maximum number of orbitals with the same spin.

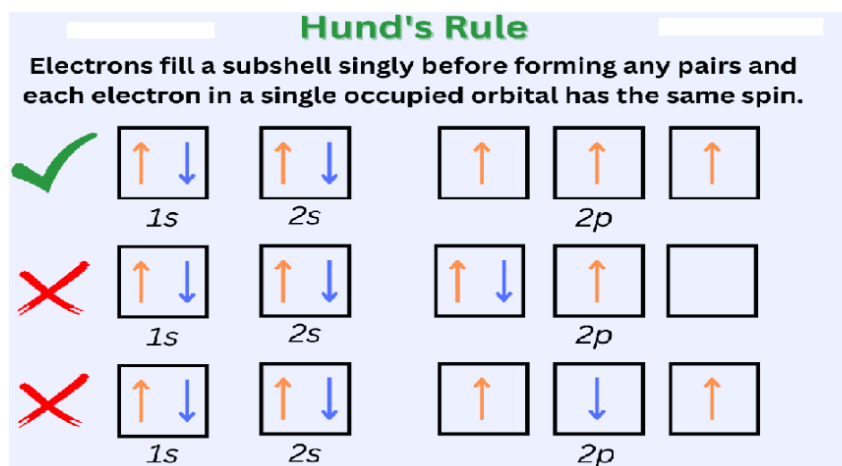


Figure III-20: Hund's rule

VIII-3-Pauli's exclusion principle

"Two electrons of the same atom cannot have their four quantum numbers n , l , m_l and m_s equal". if electrons in the same orbital have the same values of n , l and m , they must necessarily have different values of spin. However, we know that spin has only two values, so an orbital can have at most two electrons, which must be of opposite spin.



Figure III-21: Pauli's exclusion principle

VIII-4-Valence Shell

The electrons in the shell (layer) with the highest value of the principal quantum number (n) play a significant role in chemical reactions, especially in the formation of chemical bonds between atoms. This shell is called the outermost valence shell.

Example:

Lithium (${}_3\text{Li}$): $1s^2 2s^1$, the valence shell is ($n = 2$), and the number of valence electrons is (1).

Carbon (${}_6\text{C}$): $1s^2 2s^2 2p^2$, the valence shell is ($n = 2$), and the number of valence electrons is (4).

Examples of Applications:**Exercise:**

Determine the complete electronic configurations of the following atomic species:

Na ($Z=11$), O ($Z=8$), Mg ($Z=12$), K^+ ($Z=19$), N^+ ($Z=7$), F^- ($Z=9$)

Solution:

Na ($Z=11$): $1s^2 2s^2 2p^6 3s^1$

O ($Z=8$): $1s^2 2s^2 2p^4$

Mg ($Z=12$): $1s^2 2s^2 2p^6 3s^2$

K^+ ($Z=19$): $1s^2 2s^2 2p^6 3s^2 3p^6$

N^+ ($Z=7$): $1s^2 2s^2 2p^2$

F^- ($Z=9$): $1s^2 2s^2 2p^6$

Chapter IV: Periodic classification of elements

Learning Objectives:

At the end of this chapter, the student should be able to:

- Understand the principle of the periodic classification of chemical elements.
- Identify the organisation of the periodic table: periods, groups, blocks (s, p, d, f).
- Link the position of an element in the table to its electronic configuration.
- Distinguish between the major chemical families.
- Analyse the evolution of periodic properties

MODERN PERIODIC TABLE

Legend:

- Alkali Metals
- Alkaline Earth Metals
- Transition Metals
- Post-transition Metals
- Metalloids
- Reactive Nonmetals
- Noble Gases
- Alkali Metals
- Actinides
- Unknown Properties

Example element: **La** (Lanthanum), Atomic Number 57, Atomic Mass 138.906, Name Lanthanum, Average Atomic Mass 138.906.

Figure IV-2: Modern Periodic Table

The periodic table is described as follows:

III-1-Blocks: Elements are placed in three blocks:

Block (S): Corresponds to the filling of the subshell (ns). The s-block consists of elements found in columns 1 (alkali metals) and 2 (alkaline earth metals) of the periodic table, as well as hydrogen and helium. They are called so because their highest (in energy) occupied orbital is of type s.

Block (P): Corresponds to the filling of the subshell (np). The p-block consists of elements found in columns 13 to 18 of the periodic table. They are called so because their highest (in energy) occupied orbital is of type p. This block includes the icosagens (column 13), the crystallogens (column 14), the pnictogens (column 15), the chalcogens (column 16), the halogens (column 17), and the noble gases (column 18), excluding helium.

Block (d): Corresponds to the filling of the subshell ((n-1) d). The d-block consists of elements found in columns 3 to 12 of the periodic table. They are called so because the highest (in energy) occupied orbital is of type d.

Block (f): Corresponds to the filling of the subshell ((n-2) f). The f-block consists of internal transition elements of the periodic table: the lanthanides and actinides. They are called so because the highest (in energy) occupied orbital of these atoms is of type f.

The diagram illustrates the periodic table with color-coded blocks and orbital labels:

- s-block (Green):** Includes groups 1A and 2A, and the 18th group (8A). Orbitals shown are 1s, 2s, 3s, 4s, 5s, 6s, and 7s.
- p-block (Orange):** Includes groups 13A through 17A. Orbitals shown are 2p, 3p, 4p, 5p, 6p, and 7p.
- d-block (Light Blue):** Includes groups 3B through 10B. Orbitals shown are 3d, 4d, 5d, and 6d.
- f-block (Pink):** Includes groups 3B and 4B. Orbitals shown are 4f and 5f.

Figure IV-3: Different Blocks of the Periodic Table

Periods (Rows): A period corresponds to an electron shell identified by its principal quantum number denoted as (n). There are seven electron shells known in the ground state, hence seven periods.

Groups (Columns): There are eighteen columns, including Eight in subgroup A ten in subgroup B Elements of the same family have the same number of valence electrons; the family number corresponds to the number of valence electrons. Each subgroup consists of 8 groups, as shown in Figure. The group is symbolized by Roman numerals (I-VIII). By definition, the group represents the valence electrons

Elements belonging to the same period have an identical core electron configuration.

Elements belonging to the same column have an identical valence electron configuration.

These two classifications, which are not very different from each other, are presented in the form of a table containing 7 rows (period) and, depending on their external structure, these elements are classified in 18 columns.

IA		IIA										13		14		15		16		17		18	
												IIIA	IVA	VA	VIA	VIIA	VIIIA						
	1s ²																						
2s ¹		3	4	5	6	7	8	9	10	11	12	2p ¹	2p ²	2p ³	2p ⁴	2p ⁵	2p ⁶						
	3s ²	IIIB	IVB	VB	VIB	VIB	VIBB	VIBB	VIBB	IB	IIIB	3p ¹	3p ²	3p ³	3p ⁴	3p ⁵	3p ⁶						
4s ¹	4s ²	3d ¹	3d ²	3d ³	3d ⁴	3d ⁵	3d ⁶	3d ⁷	3d ⁸	3d ⁹	3d ¹⁰	4p ¹	4p ²	4p ³	4p ⁴	4p ⁵	4p ⁶						
5s ¹	5s ²	4d ¹	4d ²	4d ³	4d ⁴	4d ⁵	4d ⁶	4d ⁷	4d ⁸	4d ⁹	4d ¹⁰	5p ¹	5p ²	5p ³	5p ⁴	5p ⁵	5p ⁶						
6s ¹	6s ²	5d ¹	5d ²	5d ³	5d ⁴	5d ⁵	5d ⁶	5d ⁷	5d ⁸	5d ⁹	5d ¹⁰	6p ¹	6p ²	6p ³	6p ⁴	6p ⁵	6p ⁶						
7s ¹		6d ¹	6d ²	6d ³	6d ⁴	6d ⁵	6d ⁶	6d ⁷	6d ⁸	6d ⁹	6d ¹⁰	7p ¹	7p ²	7p ³	7p ⁴	7p ⁵	7p ⁶						
		4f ¹	4f ²	4f ³	4f ⁴	4f ⁵	4f ⁶	4f ⁷	4f ⁸	4f ⁹	4f ¹⁰	4f ¹¹	4f ¹²	4f ¹³	4f ¹⁴								
		5f ¹	5f ²	5f ³	5f ⁴	5f ⁵	5f ⁶	5f ⁷	5f ⁸	5f ⁹	5f ¹⁰	5f ¹¹	5f ¹²	5f ¹³	5f ¹⁴								

Figure IV-4: Periodic Table Groups and Periods

The 18 columns of the periodic table are divided into groups. The group contain 2 subgroups:

An element belongs to subgroup A if the valence electrons are distributed in the subshell (ns^x), ($ns^x np^y$), or $ns^x (n-1)d^{10} np^y$, with x and y different from 0.

An element belongs to subgroup B if its valence electrons are distributed in the shell $ns^2(n-1)d^x np^0$, with x ranging from 1 to 10, or $ns (n-2) f (n-1) d np^0$. (the f subshell appears from $n=6$ onwards).

Subgroup A

Group I: ns^1
 Group II: ns^2
 Group III: $ns^2 np^1$
 Group IV: $ns^2 np^2$
 Group V: $ns^2 np^3$
 Group VI: $ns^2 np^4$
 Group VII: $ns^2 np^5$
 Group VIII: (noble gas): $ns^2 np^6$

Subgroup B

Group I: $(n-1)d^{10} ns^1$
 Group II: $(n-1)d^{10} ns^2$
 Group III: $(n-1)d^1 ns^2$
 Group VI: $(n-1)d^2 ns^2$
 Group V: $(n-1)d^3 ns^2$
 Group VI: $(n-1)d^4 ns^2$
 Group VII: $(n-1)d^5 ns^2$
 Group VIII(Triade): $(n-1)d^x ns^2$

Example for Elements of Subgroup A (Main Group Elements):

column	group	Electron Configuration
1	IA	ns^1
2	IIA	ns^2
13	IIIA	$ns^2 np^1$
14	IVA	$ns^2 np^2$
15	VA	$ns^2 np^3$
16	VIA	$ns^2 np^4$
17	VIIA	$ns^2 np^5$
18	VIIIA	$ns^2 np^6$

Example for Elements of Subgroup B (Transition Elements):

column	group	Electron Configuration
3	IIIB	[Ar]4s ² 3d ¹
4	IVB	[Ar]4s ² 3d ²
5	VB	[Ar]4s ² 3d ³
6	VIB	[Ar]4s ¹ 3d ⁵ (Cr exception)
7	VIIB	[Ar]4s ² 3d ⁵
8	VIIIB	[Ar]4s ² 3d ⁶
9	IXB	[Ar]4s ² 3d ⁷
10	XB	[Ar]4s ² 3d ⁸
11	IB	[Ar]4s ¹ 3d ¹⁰ (Cu exception)
12	IIB	[Ar]4s ² 3d ¹⁰

General Notes on Exceptions :

These exceptions occur because a **half-filled (d⁵)** or **fully filled (d¹⁰)** subshell is more stable than expected from strict application of the Aufbau principle.

They mostly appear in **transition metals** and **lanthanides/actinides** where the energy difference between subshells is minimal.

Key Exceptions in Electron Configurations:

 **Chromium (Cr, Z=24) Expected:** [Ar] 4s² 3d⁴

Actual: [Ar] 4s¹ 3d⁵

Reason: Stability of a half-filled 3d subshell.

 **Copper (Cu, Z=29) Expected:** [Ar] 4s² 3d⁹

Actual: [Ar] 4s¹ 3d¹⁰

Reason: Stability of a fully filled 3d subshell.

 **Molybdenum (Mo, Z=42) Expected:** [Kr] 5s² 4d⁴

Actual: [Kr] 5s¹ 4d⁵

Reason: Stability of a half-filled 4d subshell.

 **Palladium (Pd, Z=46) Expected:** [Kr] 5s² 4d⁸

Actual: [Kr] 4d¹⁰

Reason: Completely filled d-orbitals compensate for empty 5s orbital.

 **Silver (Ag, Z=47) Expected:** [Kr] 5s² 4d⁹

Actual: [Kr] 5s¹ 4d¹⁰

Reason: Stability of a fully filled 4d subshell.

 **Gold (Au, Z=79) Expected:** [Xe] 6s² 4f¹⁴ 5d⁹

Actual: [Xe] 6s¹ 4f¹⁴ 5d¹⁰

Reason: Stability of a fully filled 5d subshell.

Example: determine the group, subgroup for the following elements

Element	Electronic configuration	Valence Electrons	Period	Group/Subgroup
¹¹ Na	1S ² 2S ² 2p ⁶ <u>3S¹</u>	1	3	I _A
¹⁸ Ar	1S ² 2S ² 2p ⁶ <u>3S²3p⁶</u>	8	3	VIII _A
²² Ti	1S ² 2S ² 2p ⁶ 3S ² 3p ⁶ <u>4S²3d²</u>	4	4	IV _B
²⁵ Mn	1S ² 2S ² 2p ⁶ 3S ² 3p ⁶ <u>4S²3d⁵</u>	7	4	VII _B
²⁶ Fe	1S ² 2S ² 2p ⁶ 3S ² 3p ⁶ <u>4S²3d⁶</u>	8	4	VIII _B Triades
³⁰ Zn	1S ² 2S ² 2p ⁶ 3S ² 3p ⁶ <u>4S²3d¹⁰</u>	2	4	II _B
³⁵ Br	1S ² 2S ² 2p ⁶ 3S ² 3p ⁶ <u>4S²3d¹⁰4p⁵</u>	7	4	VII _A
⁴² Mo	1S ² 2S ² 2p ⁶ 3S ² 3p ⁶ 3d ¹⁰ <u>4S²3d¹⁰5s¹4d⁵</u>	6	5	VI _B
⁴⁷ Ag	1S ² 2S ² 2p ⁶ 3S ² 3p ⁶ 4S ² 3d ¹⁰ <u>4p⁶5s¹4d¹⁰</u>	1	5	I _B

III-2-Element Families

The periodic table is divided into several families, each consisting of elements whose atoms share the same valence shell configuration. The principal families of the periodic table include:

Alkali Metals Family (Column 1): Group IA, with an electron configuration of the type ns¹.

Alkaline Earth Metals Family (Column 2): Group IIA, with an electron configuration of ns².

Halogens Family (Column 17): Group VIIA, with an electron configuration of ns²np⁵.

Noble Gases Family (Column 18): Group VIIIA, with an electron configuration of ns²np⁶.

Metalloids (Semiconductors) Family: These elements form a boundary that separates metals and non-metals. It includes all elements from the 13th column to the 18th column. These elements share properties with non-metals but conduct electric current to varying degrees. Examples include Si, Ge, As, and Sb.

Transition Elements Family (Columns 3 to 12): These elements have incompletely filled (d) orbitals.

Rare Earth Elements Family: Involves f-orbital elements, with two types in this family: Lanthanides, corresponding to elements in the 6th period with $57 \leq Z \leq 71$, and Actinides, concerning atoms in the 7th period with $89 \leq Z \leq 103$.

Figur IV-5: Families of the periodic table

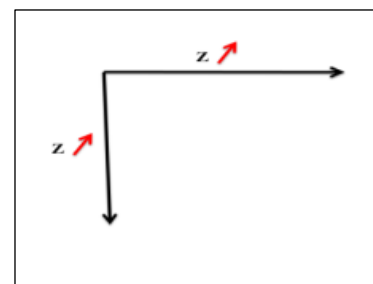
IV- Evolution And Periodicity of Physico-Chemical Properties

IV-1-Variation in protons number Z

On a row of the classification, number of proton

Z increases regularly from left to right.

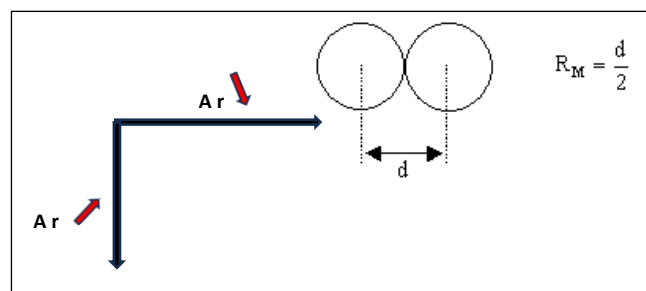
In the same column, Z increases from top to bottom.



IV-2-Atomic radius

The atomic radius corresponds the covalent radius,

It is defined as the half-distance between the nuclei of two adjacent atoms.



When the atomic number Z increases over a period, the atomic radius decreases.

In a group: when the atomic number Z increases, the atomic radius increases.

And as the quantum number n main orbitals valence increases, the size of the orbitals increases

Explanation:

The nuclear charge increases from left to right within a period, leading to an increase in nuclear attraction. Consequently, the atomic radius of elements decreases within a period from left to right.

When descending a column, the nuclear charge increases, causing an increase in nuclear attraction. However, the atomic radius do not decrease as expected because the outermost electrons are accommodated in new shells, generating an effect that outweighs nuclear attraction. Therefore, the atomic radii of elements increase within a column from top to bottom.

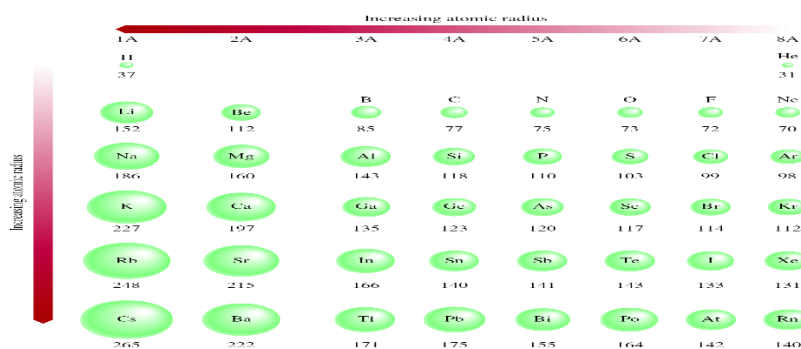


Figure IV-6: evolution of atomic radius

IV-3-Ionic radius

The ionic radius represents the spatial extent of the electron cloud. In ions, the number of electrons differs from that of the neutral atom, leading to opposite effects. In the case of cations, the loss of electrons causes a contraction of the electron cloud, so the ionic radius is smaller than the atomic radius of the corresponding neutral atom.

Conversely, anions carry a negative charge and possess a greater number of electrons, which leads to an expansion of the electron cloud. As a result, their ionic radius is larger than the atomic radius, and it increases with increasing negative charge.

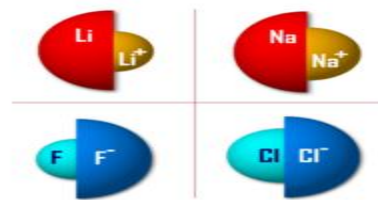
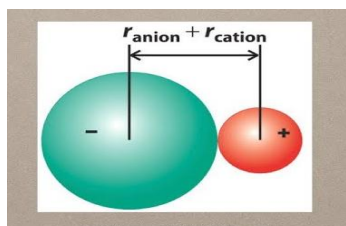


Figure IV-7: Ionic radius for cations and anions

IV-4-Ionisation energy I

This is the energy required to remove an electron from an atom or ion in the gaseous state:



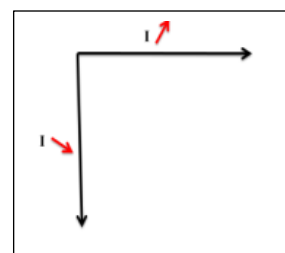
In one period:

the peripheral electrons are harder to pull off
as Z increases, because the attractive force
of the nucleus increases, so if Z increases, EI increases.



In a group:

Ionisation energy EI decreases as Z increases, as we move from the n layer to the $(n+1)$ layer, so the peripheral electrons are further away from the nucleus.

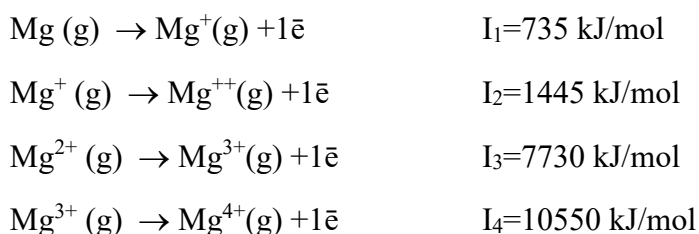


Explanation:

When moving from left to right across a period, the number of outermost electrons increases. Consequently, the nuclear attraction toward these electrons also increases. The higher this attraction, the more difficult it is to remove one of these electrons. Therefore, the first ionization energy increases within a period from left to right.

When descending a column, the electron to be removed is increasingly farther from the nucleus of the atom. Consequently, the nuclear attraction toward this electron decreases. The weaker this attraction, the easier it is to remove the electron. Therefore, the first ionization energy decreases within a column from top to bottom.

Examples



I_1 : first ionisation energy

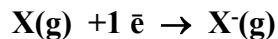
I_2 : second ionisation energy

I_3 : third ionisation energy

I_4 : fourth ionisation energy

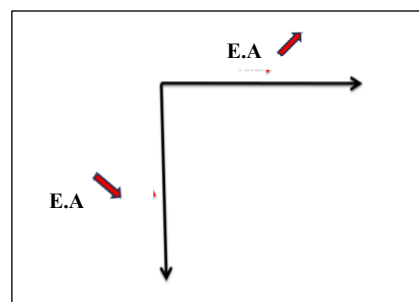
IV-5-Electron affinity AE

The electron affinity **AE** is the amount of energy associated when an atom in the gas phase captures an electron



In a period, when Z increases, A increases (in absolute value). There are several exceptions to this rule. The variation in A as a function of Z can be explained by a variation in inter-electron repulsion depending on the electronic configuration.

In a group, AE generally decreases (in absolute value) as Z increases because the added electron has to occupy an orbital further and further away from the nucleus.



IV-6-Electronegativity (χ)

Electronegativity is the ability of an element to attract an electron.

In a period: χ increases as you move to the right,

In a group: χ decreases as you move downwards.

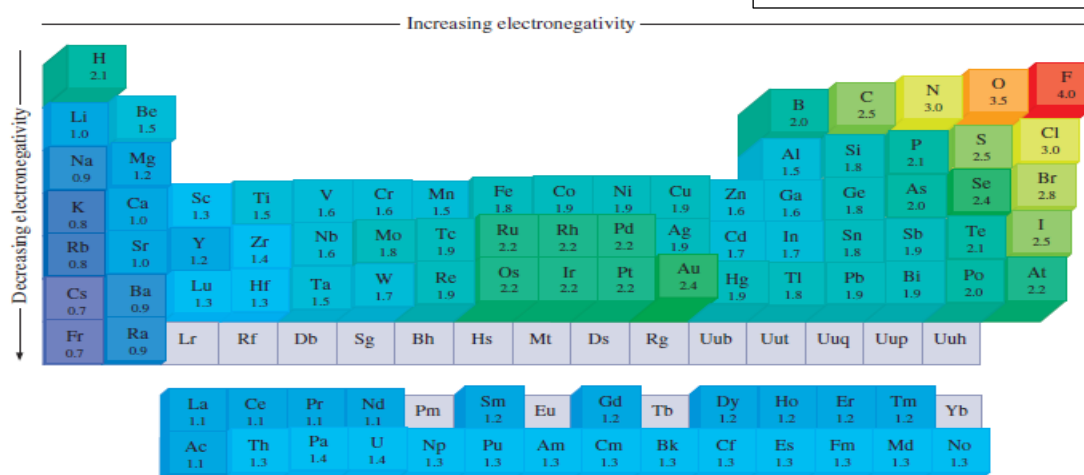
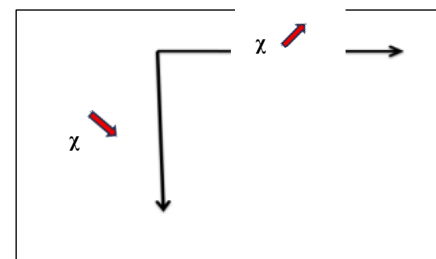


Figure IV-8: Electronegativities of elements

Electronegativity varies inversely with atomic radius, similar to ionization energy. When an atom has a high electron affinity, it releases a large amount of energy upon capturing an

electron, which stabilizes the resulting species. If the electron affinity is negative, the atom must absorb energy to gain an electron.

There are three different scales to measure electronegativity:

Mulliken Scale

Pauling Scale

Allred and Rochow Scale

IV-6-1-Mulliken scale

Mulliken originally defined electronegativity as the average of an element's first ionization energy and its electron affinity. A highly electronegative element tends to attract electrons strongly, meaning it requires a large amount of energy to remove an electron (high ionization energy) but readily gains one.

The electronegativity of an atom of a chemical element involved in a chemical bond is given by the relationship:

$$\chi = 0,5 (I_1 + A) \text{ (eV. atome}^{-1}\text{)}$$

Where:

I_1 : Energy of the first ionisation of the atom,

A: Electron affinity.

IV-6-2-Slater model

Slater's model is a simple model which allows us to calculate average charges, actually perceived by the electrons (taking into account the charge of the nucleus and those of the other electrons, the latter eclipsing the nucleus).

From these effective charges, we can calculate the energy levels of the atomic orbitals and the electronic energies of atoms in their ground state.

Consider an atom whose nucleus has a charge Z . Consider the attraction between the Z protons in the nucleus and any electron E in the atom.

The attraction is disturbed by the electrons located between the nucleus and electron E .

These electrons form a **screen**. We then define a screen constant that depends on the position of the atom's electrons relative to electron E

 The charge Z of the nucleus of the atom then becomes an effective charge $Z^* < Z$ relative to the electron E :

$$Z^* = Z - \sigma = Z - \sum \sigma_i$$

where σ is called the screen constant.

Note!

The effective charge Z^* depends on the electron for which the calculations are being made.

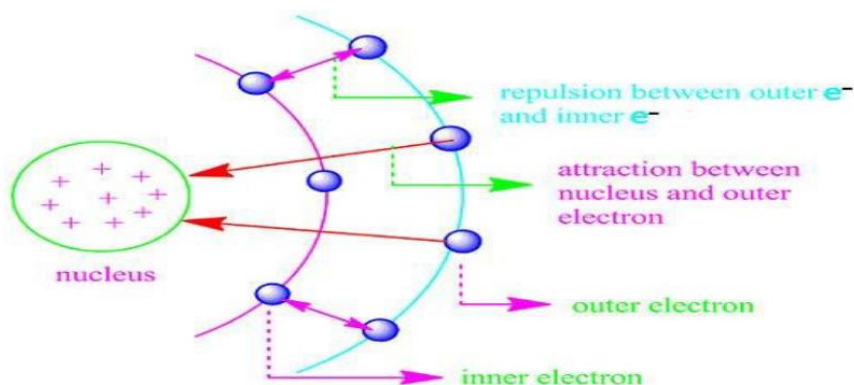


Figure IV-9: Representation of Slater's Rule

IV-6-3-Calculation of the effective charge Z^*

1- Write down the electronic configuration of the element and order it according to: (1s) (2s,2p) (3s, 3p) (3d) (4s, 4p) (4d) (4f) (5s, 5p)...

2- Choose the electron for which we are looking for the effective charge. All the other electrons will make a partial contribution σ_i to the total screen constant σ .

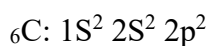
This contribution depends on:

- the type of orbital (s, p), (d) or (f) of the electron,
- the electron's electronic layer n.

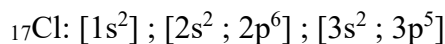
3- The value of σ_i is summarised in the following table:

		e_j							
		1s	2s,2p	3s,3p	3d	4s,4p	4d	4f	5s,5p
e_i	1s	0.31	0	0	0	0	0	0	0
	2s,2p	0.85	0.35	0	0	0	0	0	0
	3s,3p	1	0.85	0.35	0	0	0	0	0
	3d	1	1	1	0.35	0	0	0	0
	4s,4p	1	1	0.85	0.85	0.35	0	0	0
	4d	1	1	1	1	1	0.35	0	0
	4f	1	1	1	1	1	1	0.35	0
	5s,5p	1	1	1	1	0.85	0.85	0.85	0.35

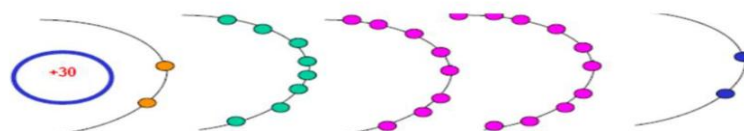
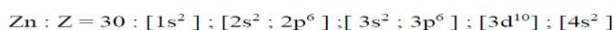
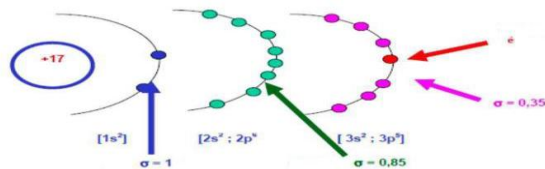
Examples: Calculate the effective atomic number of: ${}_6\text{C}$ and ${}_{17}\text{Cl}$



$$Z_{\text{eff}} = 6 - (3 \times 0,35 + 2 \times 0,85) \Rightarrow z_{\text{eff}} = 3,25$$



$$Z_{\text{eff}} = 17 - (6 \times 0.35) - (8 \times 0.85) - (2 \times 1) = 6.1$$



$$Z^* 4s = 30 - (1 \times 0.35) - (18 \times 0.85) - (8 \times 1) - (2 \times 1) = 4.35$$

$$Z^* 3d = 30 - (9 \times 0.35) - (8 \times 1) - (8 \times 1) - (2 \times 1) = 8.85$$

$$Z^* 3s 3p = 30 - (7 \times 0.35) - (8 \times 0.85) - (2 \times 1) = 18.75$$

Exercise of application:

Consider the following atoms: C(6), P(15), V(23), Cr(24), Co(27), Zn(30) and Ge (32),

1- Provide the location of these elements in the periodic table (indicate the group and period), specify the core electrons and valence electrons, as well as the number of lone electrons.

2- Classify these elements in ascending order for elements belonging to the same period, and then within the same group with respect to their:

Ionization energy, Atomic radius, Electronegativity

Solution

Element	Atomic Number	Electronic Configuration	Period	Group	Core Electrons	Valence Electrons	Lone Electrons
${}_6\text{C}$	6	$1s^2 2s^2 2p^2$	2	IV _A	2	4	2
${}_{15}\text{P}$	15	$1s^2 2s^2 2p^6 3s^2 3p^3$	3	V _A	10	5	3
${}_{23}\text{V}$	23	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^3$	3	V _B	18	5	3
${}_{24}\text{Cr}$	24	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^5$	4	VI _B	18	6	6
${}_{27}\text{Co}$	27	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^7$	4	VIII _B	18	9	3
${}_{30}\text{Zn}$	30	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10}$	4	II _B	18	2	0
${}_{32}\text{Ge}$	32	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^2$	4	IV _A	28	4	2

Ranking:

In a column: (from top to bottom) As Z increases: atomic radius (ra) increases Ionization energy and electronegativity decrease,

In a period: (from left to right) As Z increases: atomic radius (ra) decreases; Ionization energy (EI) and electronegativity increase;

✚ Ionization energy:

$IE(V) < IE(Cr) < IE(Co) < IE(Zn) < IE(Ge)$ (in the same period)

$IE(Ge) < IE(C)$ (in the same column)

✚ Atomic radius:

$ar(Ge) < ar(Zn) < ar(Co) < ar(Cr) < ar(V)$ (in the same period)

$ar(C) < ar(Ge)$ (in the same column)

✚ Electronegativity:

$\chi V < \chi Cr < \chi Co < \chi Zn < \chi Ge$ (in the same period)

$\chi Ge < \chi C$ (in the same column).

Chapter V : Chemical Bond

Learning Objectives:

At the end of this chapter, the student should be able to:

- understand the nature of chemical bonding in the formation of matter.
- distinguish between the main types of chemical bonds:
- introduce Lewis structures and the concept of the octet (and duet) rule.
- understand bond polarity and electronegativity differences.
- relate chemical bonding to the geometry and properties of molecules.

I-Introduction

Before we examine the types of chemical bonding, we should start with the most fundamental question: why do atoms bond at all? In general, bonding lowers the potential energy between positive and negative particles, whether they are oppositely charged ions or nuclei and electron pairs. Just as the strength of attractions and repulsions among nucleus and electrons determines the properties of an atom, the type and strength of chemical bonds determine the properties of a substance.

Atoms do not exist in a free state. They join together to form chemical structure.

The cohesion of the particles in the chemical structure is due to interactions between the different atoms or ions involved, which lead to the formation of the most stable structure.

These interactions are called *chemical bonds*.

A chemical bond is formed if the energy of the resulting arrangement of atoms is less than that of the separate atoms.

The purpose of studying chemical bonds is to explain how two atoms in a chemical structure are linked together.

II-The different types of bonds

There are two types of bonds: strong bonds and weak bonds

1A (1)		2A (2)												3A (13)				4A (14)		5A (15)		6A (16)		7A (17)		8A (18)	
Li	Be											B	C	N	O	F	Ne										
Na	Mg	3B (3)	4B (4)	5B (5)	6B (6)	7B (7)	8B (8) (9) (10)		1B (11)	2B (12)	Al	Si	P	S	Cl	Ar											
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr										
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe										
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn										
Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	113	114	115	116	118											

Key:

- Metals
- Nonmetals
- Metalloids

Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

A

Figure V-1: A comparison of metals and nonmetals.

A, Location within the periodic table.

B. Relative magnitudes of some atomic properties across a period

All chemical bonds involve the valence states of atoms, but the latter are involved in different ways, giving rise to several types of bonds.

II-1-Strong Bonds

There are three types of strong bond:

- 1- Metallic bond (metal with metal)
- 2- The covalent bond (Nonmetal with nonmetal)
- 3- Ionic bond

II-1-1-Metallic bond (Metal with metal)

A metallic bond involves a very large number of atoms (several million). These atoms share one or more electrons, known as ‘free electrons’

Metallic bonds are formed between atoms with low electronegativities and few electrons on their outer layer, but they can only form if there is a sufficiently large number of such atoms. This is why it is rarely observed except in certain solids or liquids.

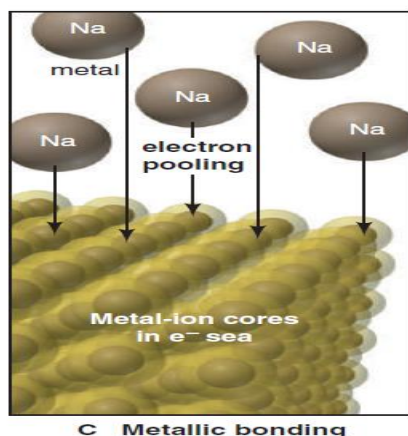


Figure V-2: Metallic bond

II-1-2-Covalent bond (Nonmetal with nonmetal)

a covalent bond is a chemical bond in which each of the bonded atoms shares an electron from one of its valence layers to form a doublet of electrons linking the two atoms.

Only an atom's valence electrons, i.e. electrons in excess of the configuration of the rare gas that precedes the element, can be involved in bond formation.

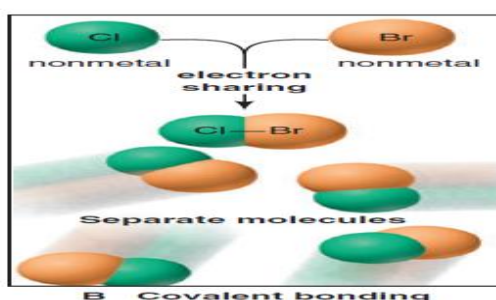


Figure V-3: covalent bond

a- Lewis structure

The Lewis structure consists of the allocation of electrons on or between the atoms of the molecule. Only valence electrons are considered.

The Lewis representation illustrates the valence electron configuration of an atom, also known as the valence layer.

Paired electrons are represented by dashes —

Single electrons are represented by dots .

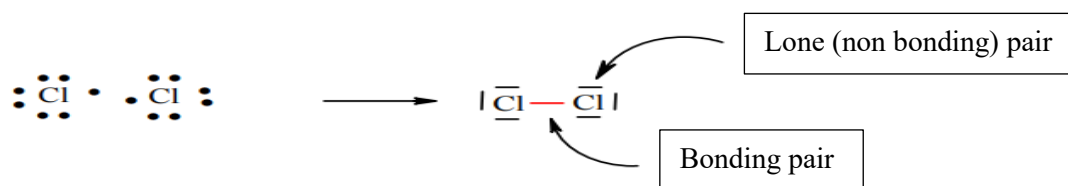
The number of single electrons gives the valency of the atom

Example: $_{17}\text{Cl} : 1s^2 2s^2 2p^6 3s^2 3p^5$: valence layer: $3s^2 3p^5$ $\cdot \overline{\text{Cl}}$

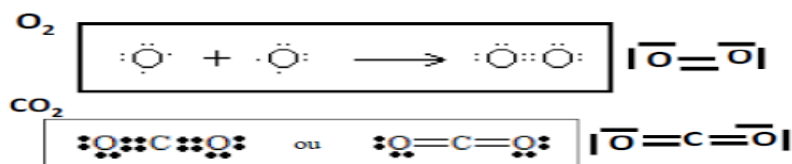
$_{7}\text{N} : 1s^2 2s^2 2p^3$: valence layer: $2s^2 2p^3$ $\cdot \overline{\text{N}} \cdot$

A distinction is made between "bonding doublets (or pairs)" and "non-bonding doublets (or pairs)", also known as "free" doublets.

Example: Formation of the covalent bond of chlorine



Example of double bonds: O_2 and CO_2 :



Example of triple bonds: N_2 and HCN :

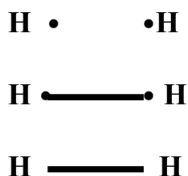
**b- The octet Rule**

In a molecule, each atom tends to surround itself with eight electrons, except for the hydrogen molecule, to have the configuration of the noble gases $\Rightarrow$ This is what is known as the Octet rule

There are three types of covalent bond:

- ❖ **Apolar or non-polar covalent bond:** If the difference in electronegativity between these two atoms is zero or less than 0.4, the bond is said to be apolar.

Example: According to the Lewis Representation, H_2 is represented as:



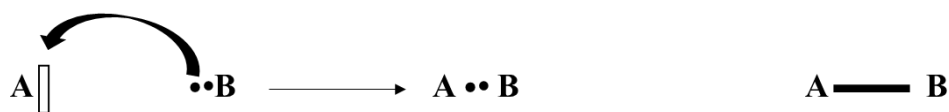
- ❖ **Polar covalent bond:** A covalent bond is polar if the difference in the electronegativities of the two atoms forming the bond is not zero. The most electronegative atom in a polar bond attracts the electrons in the covalent bond towards itself.

Example:



- ❖ **Dative covalent bond:** It forms between two atoms where one of the atoms (atom B) (the donor) provides a lone pair from its outer shell, and the other atom (atom A) (the acceptor), which has an electron deficiency (empty box) in its valence shell (rectangle), receives this lone pair.

Example:



II-1-3-Ionic bond (*metal with nonmetal*)

Ionic bonds are formed between ions of opposite charge. These bonds involve the classic electrostatic force. An ionic bond is the result of one or more ions being transferred from one atom to another. The atoms thus become ions; the one that gives up the electron is the cation and the one that receives the electron is the anion. The transfer is made from the least electronegative atom to the most electronegative atom.

This bond forms between two atoms, A and B, with a significant difference in electronegativity.

As a result of this difference, electrons move from the less electronegative atom to the more electronegative atom, producing a cation and an anion.

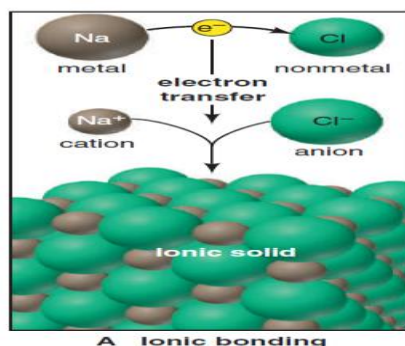
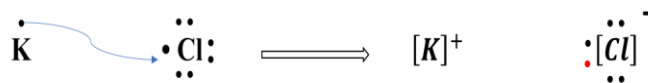


Figure V-4: Ionic bond

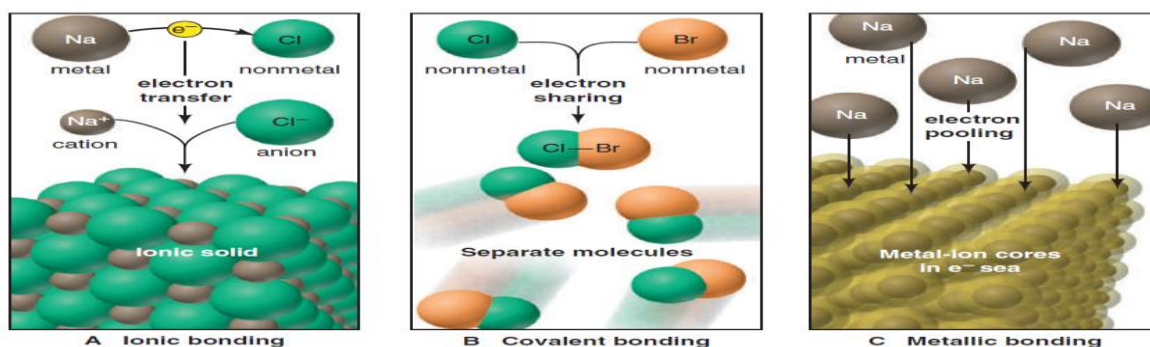


Figure V-5: representation of strong bonds

a- Concept of dipole moment μ

A dipole is a system formed by two equal but opposite charges separated by a distance d .

It is considered an electric dipole if the difference in electronegativity between the two atoms creates polarization, it results in a negatively charged pole rich in electrons and a positively charged pole lacking electrons at a distance (d) from each other



This dipole is characterized by its dipole moment, also known as the electric moment (μ_{AB}). This quantity (μ_{AB}) is represented by a vector oriented from the negative charge (more electronegative element) to the positive charge (less electronegative element).

The notations $+\delta$ and $-\delta$ represent partial charges, the more electronegative atom that carries the partial negative charge.

A dipole is characterised by its electric dipole moment μ such that:

$$|\vec{\mu}| = q \cdot d = \mu$$

Where:

d is the length of the A-B bond, δ is the partial charge.

The effective partial charges are: $+q = +\delta \cdot e$ and $-q = -\delta \cdot e$,

where:

δ is the partial charge,

e is the elementary charge.

$$\mu = |\delta| \cdot e \cdot d$$

μ is expressed in Coulomb. Metre (C.m). This quantity is also often expressed in Debye:

$$1 \text{ Debye} = 1 \text{ D} = 3.33 \cdot 10^{-30} \text{ C.m}$$

For the case of a 100% ionic molecule: $\mu = e \cdot d$

With e representing the charge of an electron ($1.6 \times 10^{-19} \text{ C}$), for the case of a polarized polyatomic molecule, the overall dipole moment of the molecule is the geometric sum of the dipole moments of the individual bonds in the molecule.

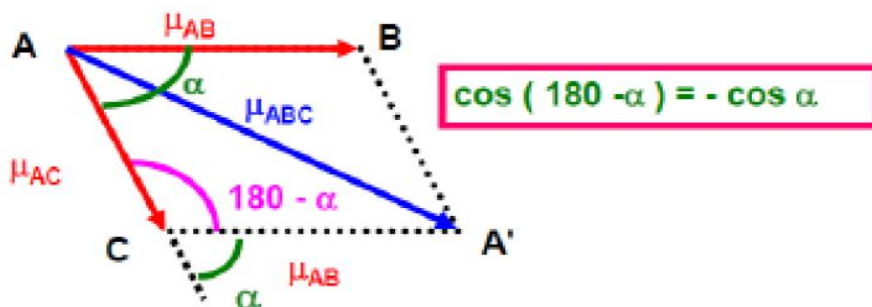


Figure V-6: Vector representation of the dipole moment of a polyatomic atom ABC

By convention, we can know the nature of the bond by simply calculating the difference in electronegativity of the atoms forming the bond.

$$\Delta\chi : \text{difference in electronegativity} \quad \Delta\chi = |\chi_2 - \chi_1|$$

- $\Delta\chi \leq 0.4$ $\Rightarrow$ non polar covalente bond non polar
- $0.4 < \Delta\chi < 1.7$ $\Rightarrow$ polar covalente bond
- $\Delta\chi \geq 1.7$ $\Rightarrow$ ionique bond

b-Partial ionic character of a bond

the percentage of ionic character of the bond is calculated from the following formula:

$$\% \text{ ionique} = \frac{\mu_{exp}}{\mu_{theo}} \cdot 100 = \frac{\delta \cdot d}{e \cdot d} \cdot 100$$

Where:

d: length of the bond

e: electron charge

δ : partial charge

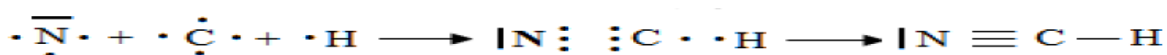
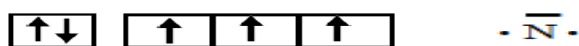
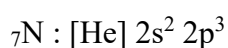
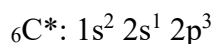
Exercise of application

Represent using Lewis diagrams for the following molecules and molecular ions: HCN, HClO₄.

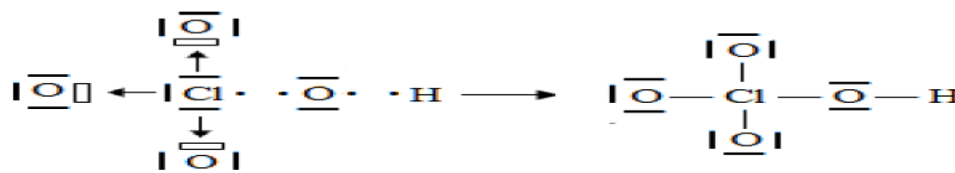
The HF molecule has a dipole moment (μ) of 1.83 Debye and a bond length (d) of 0.92 Å. Calculate the ionic percentage of this bond.

Solution

• HCN



• HClO₄



Ionic Character Percentage:

$$\text{ionic \%} = \frac{\mu_{exp}}{\mu_{theo}} \cdot 100 = \frac{\delta \cdot d}{e \cdot d} \cdot 100$$

$$\Rightarrow \text{ionic \%} = \frac{\mu_{exp}}{e.d} \cdot 100$$

$$= \frac{1.83 \times 3.33 \times 10^{-30}}{1.6 \times 10^{-19} \times 0.82 \times 10^{-10}} \cdot 100$$

$$\Rightarrow \text{ionic \%} = 41.35\%$$

II-2- Weak Bonds

Weak bonds have dissociation energies ranging from about 1 to 40 kJ·mol⁻¹, in any case, less than 50 kJ·mol⁻¹. These bonds result from cohesive forces between atoms incapable of forming valence bonds or between molecules where the possibilities of strong bonds are already saturated. There are two types of weak bonds: Hydrogen bond and van der Waals bonds.

III- Geometry of molecules: GILLEPSIE or VSEPR theory (Valence Shell Electron Pair Repulsion)

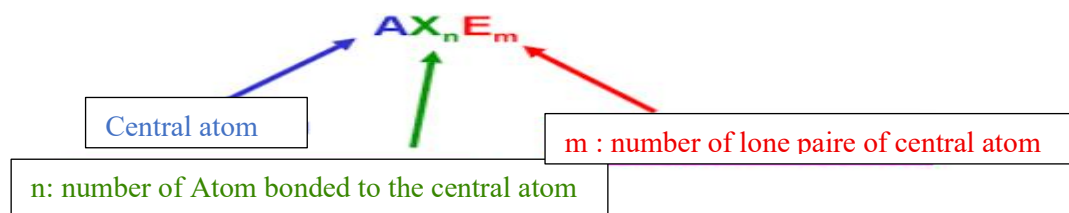
Gillespie's theory or the VSEPR method is a fairly recent method (1960). The aim of this theory is to predict the geometry of molecules.

The geometry of a polyatomic molecule is the arrangement of its atoms in space.

The doublets of the outer electrons (binding or non-binding) of a single atom repel each other: the geometry adapted by a molecule is one in which the electron doublets of each atom are as far apart from each other as possible.

The **VSEPR** method can be used to predict the geometry of simple molecules or ions. It applies to molecules or ions of type : **AX_nE_m**

A: designates the central atom which is bonded to n atoms X and has m pairs of free electrons E (or m non-bonding doublets E)



III-1-Principle of the VSEPR method

The VSEPR method is based on a number of assumptions, particularly concerning the nature of the bonds between atoms:

- Atoms in a molecule are linked by pairs of electrons.
- Two atoms can be linked by more than one pair of electrons. These are known as multiple bonds.

- Some atoms may also have pairs of electrons that are not involved in a bond. These are known as non-bonding doublets.
- The electrons making up these bonding or non-bonding doublets exert repulsive electrical forces on each other. The doublets are therefore arranged around each atom in such a way as to minimise the values of these forces.
- Non-bonding doublets take up more space than bonding doublets.
- Multiple bonds take up more space than single bonds.

The sum $(n+m)$, called the total number of electrons pairs, provides information about the basic geometry of the molecule

In table below we present different Possible Shapes Using the VSEPR Theory

Table V-1: Different Possible Shapes Using the VSEPR Theory

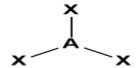
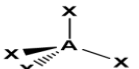
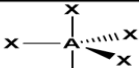
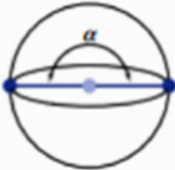
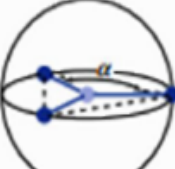
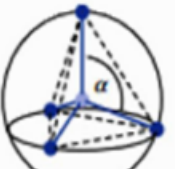
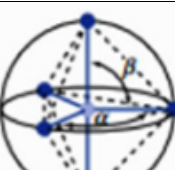
AXE Formula	Molecular Geometry	Bond Angle	Molecule Shape
AX_2E_0	Linear	180°	
AX_3E_0	Trigonal planar	120°	
AX_2E_1	Bent	119°	
AX_4E_0	Tetrahedral	109.5°	
AX_3E_1	Trigonal pyramidal	107.3°	
AX_2E_2	Bent	104.5°	
AX_5E_0	Trigonal bipyramidal	$90^\circ, 120^\circ, 190^\circ$	
AX_4E_1	See-saw	$86.5^\circ, 102^\circ, 187^\circ$	
AX_3E_2	T-shape	$87.5^\circ, 185^\circ$	
AX_2E_3	Linear	180°	
AX_6E_0	Octahedral	90°	
AX_5E_1	Square pyramidal	$84.8^\circ, 180^\circ$	

Table V-2: Examples for different Possible Shapes Using the VSEPR Theory

Repulsion	AX _n E _m	n+m	n	Geometry	Example
 $\alpha=180^\circ$	AX ₂	2	2	linear	BeCl ₂ , CO ₂ , HCN
 $\alpha=120^\circ$	AX ₃	3	3	Trigonal plan	BF ₃ , AlCl ₃ , NO ₃ ⁻
	AX ₂ E ₁	2	2	in V	SO ₂ , SnCl ₂ ,
 $\alpha=109,47^\circ$	AX ₄	4	4	Tetraedric	CH ₄ , SiCl ₄ , NH ₄ ⁺
	AX ₃ E ₁	4	3	Pyramid	NH ₃ , H ₃ O ⁺ , PCl ₃
	AX ₂ E ₂	2	2	in V	H ₂ O, H ₂ S
 $\alpha=120^\circ, \beta=90^\circ$	AX ₅	5	5	Bipyramide	PCl ₅
	AX ₄ E ₁	4	4	Bipyramide	TeCl ₄
	AX ₃ E ₂	3	3	in T	ICl ₃
	AX ₂ E ₃	2	2	linear	XeF ₂
 $\alpha=90^\circ$	AX ₆	6	6	Octaedric	SF ₆
	AX ₅ E ₁	6	5	Pyramid	BrF ₅
	AX ₄ E ₂	4	4	scare	XeF ₄

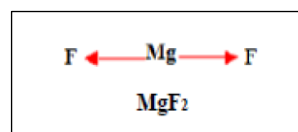
Examples for applications

give the geometry of the following molecules:

- **MgF₂**

Mg (Z = 12): 1s²2s²2p⁶ 3s² (2 valence electrons).

Type: AX₂ (2 bonds, no lone pairs).



Geometry: Linear, angle = 180° .

- AlCl_3

Al ($Z = 13$) : (3 valence electrons).

Type: AX_3 (3 bonds, no lone pairs).

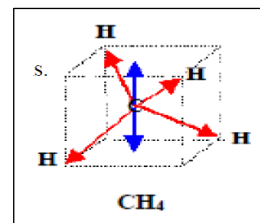
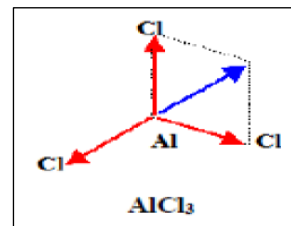
Geometry: Planar triangular, angle = 120° .

- CH_4

C ($Z = 6$) : (4 valence electrons).

Type: AX_4 (4 bonds, no lone pairs).

Geometry: Tetrahedral, angle = 109.5° .



IV-Chemical Bonding in the Quantum Model: Hybridization of Atomic Orbitals (AO)

In chemistry, the use of normal atomic orbitals cannot explain the different geometric shapes of molecules involving identical atomic orbitals.

To do this, we use the concept of atomic orbital hybridization, it is the formation of equivalent hybrid orbitals through the linear combination of atomic orbitals (s and p) or (s, p and d) of the same atom. This phenomenon can occur after electron excitation.

It consists of mixing the orbitals of an atom to form new hybrid orbitals that provide a better qualitative description of the bonds between atoms.

The resulting hybrid orbitals are very useful for explaining the shape of molecular orbitals in molecules. Hybridization theory can be used to explain the geometry of certain molecules. It also gives the values of the angles between the directions of the bonds in a polyatomic molecule.

IV-1- Different Types of Hybridization

IV-1-1- SP^3 Hybridization

The theory of hybridisation explains the CH_4 molecule. The carbon atom is the centre of the CH_4 molecule. The carbon atom has four valence orbitals (2s, 2p_x, 2p_y and 2p_z). Before forming bonds with hydrogen atoms, the carbon atom hybridises its valence orbitals.

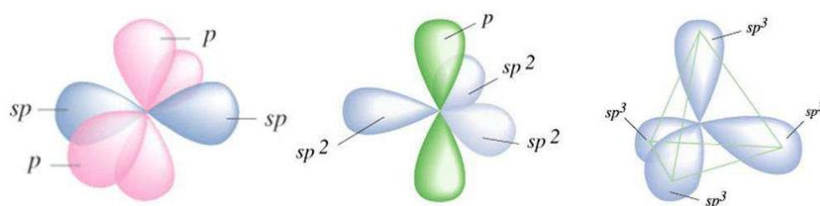


Figure V-7: SP^3 Hybridization

If we conceptually combine the valence orbitals of carbon (the 2s and the three 2p orbitals: 2p_x, 2p_y, and 2p_z), we obtain a set of four equivalent hybrid orbitals. Through the process of **sp³ hybridization**, the 2s orbital mixes with the three 2p orbitals to form four new orbitals of identical energy and geometry. These sp³ hybrid orbitals are oriented in a tetrahedral arrangement, optimizing electron repulsion and providing the characteristic bonding framework observed in tetrahedral carbon compounds such as methane (CH₄).

Example:

the methane molecule CH₄

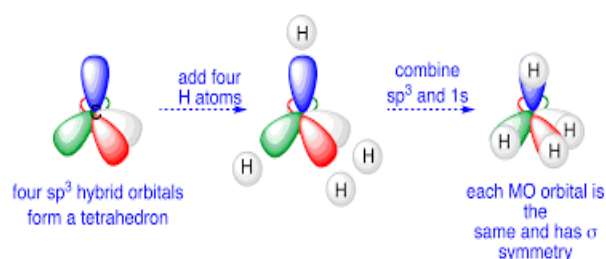


Figure V-8: SP³ Hybridization of CH₄

IV-1-2- SP² Hybridization

The exponent 2 here indicates that only two p orbitals will be combined with the s orbital to obtain this type of hybrid orbitals.

Thus, there will be one remaining p orbital on each carbon atom: $1s + 3p \rightarrow 3sp^2 + 1p$.

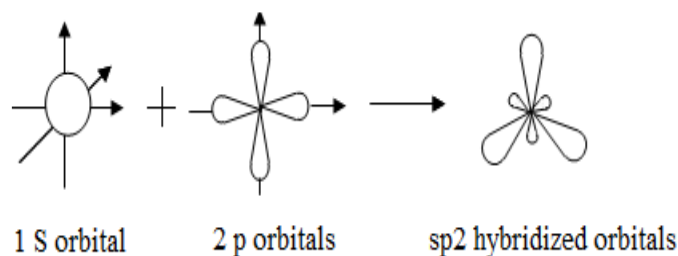
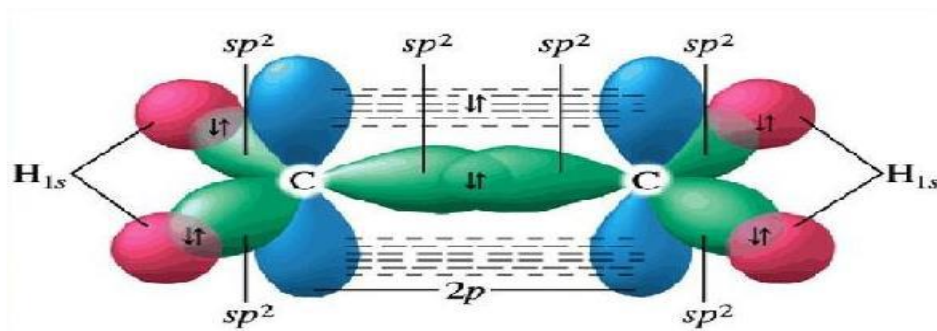


Figure V-9: SP² Hybridization

These sp² hybrid orbitals will point in the directions of an equilateral triangle centered on the carbon atom.

The sp² hybridization explains the spatial configuration of molecules such as C₂H₄ with the following diagram:

Figure V-10: sp^2 Hybridization of C_2H_4

IV-1-3- SP Hybridization

To describe the C_2H_2 molecule, we will use hybrid atomic orbitals obtained by a linear combination of the $2s$ atomic orbital and only one of the $2p$ atomic orbitals. This results in 2 sp hybrid atomic orbitals and 2 remaining pure $2p$ atomic orbitals.

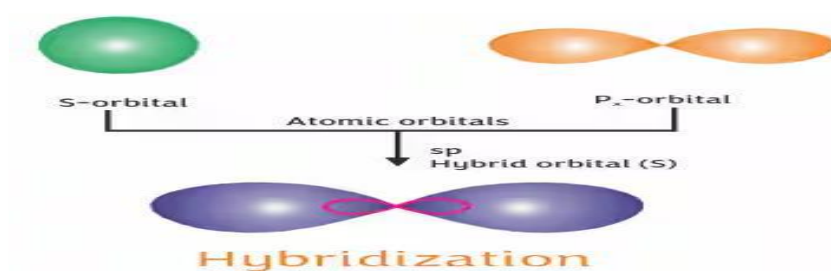
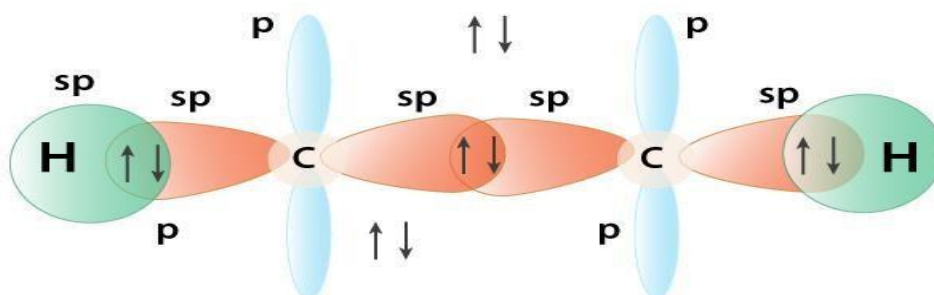


Figure IV-11: SP Hybridization

These hybrid orbitals are denoted as sp and point 180° away from each other. SP hybridization explains the spatial configuration of molecules like acetylene (C_2H_2), which is a linear molecule with two carbons triply bonded, as shown in the following diagram:

Figure V-12: SP Hybridization of C_2H_2

IV-2- Relation To VSEPR Theory

The table below shows the relation between the different forms of hybrid orbitals and VSEPR theory.

Table V-3: Relation between hybridisation and VSEPR

Hybridization	AX _n E _m	Geometry	Bond type	Bond
sp³	4	Tetrahedral	Simple	σ
sp²	3	Trigonal planar	Doble	$\sigma + \pi$
sp	2	linear	Triple	$\sigma + \pi + \pi$

Application:

The molecule CCl₄ is nonpolar. What can be deduced about its geometric shape?

What is the hybridization state of the carbon atom in this compound?

Solution:

Since CCl₄ is nonpolar, the chlorine atoms are arranged symmetrically around the central atom (the central atom occupies the centroid of the geometric figure), minimizing the interactions between the chlorine atoms.

The hybridization state of carbon is sp³; four sp³ hybridized atomic orbitals form four single bonds with four chlorine atoms, resulting in a tetrahedral shape for CCl₄.

Chapter VI: Radioactivity-Nuclear Reaction

Learning Objectives:

At the end of this chapter, the student should be able to:

- Understand the structure of the atomic nucleus and the origin of nuclear stability.
- Distinguish between the different types of radioactive decay
- Write and interpret nuclear equations and balance nuclear reactions.
- Define key concepts such as half-life, decay constant, and activity.
- Understand nuclear reactions (fission and fusion) and their energy release.
- Explain the mass–energy relationship
- Discuss applications of radioactivity in science, medicine, and industry.

I-Introduction

The discovery of the radioactivity was in 1896 by French physicist Antoine Becquerel and has become increasingly important during the twentieth and twenty-first centuries, providing the basis for various technologies related to energy, medicine, geology, and many other areas.

The stability of a nucleus mainly depends on the ratio between the number of protons and neutrons $\frac{N}{Z}$ it contains.

Protons all have a positive charge and therefore repel each other. Neutrons, which have no electrical charge, help stabilize the nucleus by reducing this repulsion between protons.

When the number of protons becomes too large ($Z > 84$), the repulsive forces are too strong, and neutrons can no longer balance them — the nucleus becomes unstable. In general, if the ratio $(A - Z)/Z$ is greater than 1.5, the element is radioactive.

During a nuclear reaction, both the atomic number (Z) and the mass number (A) remain conserved.

Radioactivity is a spontaneous transformation of an atomic nucleus that changes its composition and, as a result, the nature of the atom. This transformation of one nucleus into another is called **radioactive transmutation**.

There are two types of transmutations:

- **Spontaneous transmutation:** Natural radioactive decay (radioactivity exhibited by natural nuclides);
- **Artificial transmutation:** radioactivity produced by human intervention, such as in experiments or reactors.

II- Natural Radioactivity

Natural radioactivity results from the instability of the nuclei of certain natural elements.

It is the property of an unstable atomic nucleus to spontaneously transform into nuclei of another chemical species, emitting radiation and particles.

Protons and neutrons are held together by a cohesive force called ‘nuclear interaction’, which is generally sufficient to keep them together. The nucleus is then said to be ‘stable’.

Some nuclei contain too many particles or too much energy, so that the cohesive force is no longer sufficient to hold the neutrons and protons together. They spontaneously transform, emitting particles without any external intervention. These nuclei are said to be ‘unstable’. Unstable nuclides are called ‘radioactive’.

This imbalance of internal forces within the nucleus causes the emission of ionising radiation.

E. Rutherford identified three types of radiation: α , β and γ .

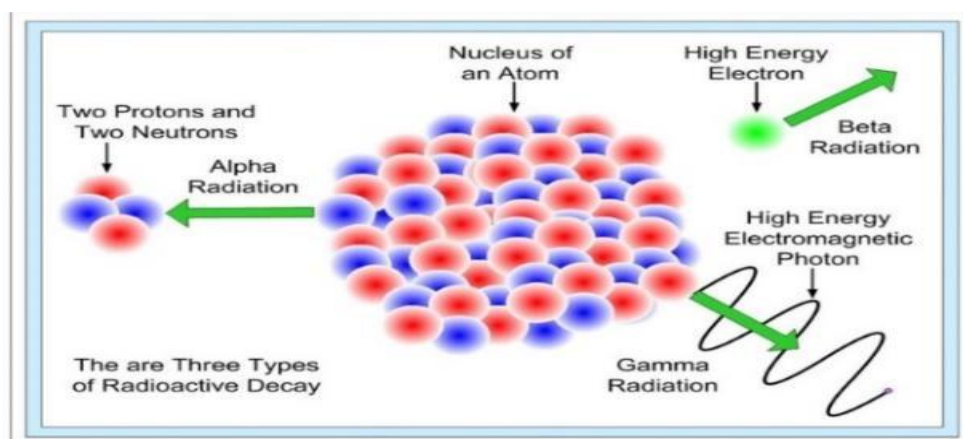
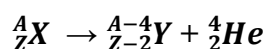


Figure VI-1: Types of radioactive decay

II-2-1-Alpha Radiation α : ${}^4_2\text{He}$

These are helium nuclei or helium ${}^4_2\text{He}^{2+}$ (notation ${}^4_2\alpha$ or α) emitted mainly by heavy nuclei ($Z > 83$) during their transformation into smaller nuclei.

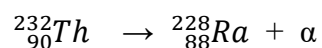
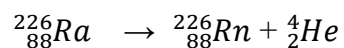
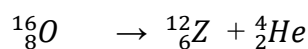
The general nuclear equation is as follows:



To correctly write a radioactive decay reaction, one must verify Soddy and Fajans' law, which states the conservation of:

-  Mass number (A of both sides must be equal);
-  Atomic number (Z of both sides must be equal).

Examples:



The nucleus of helium is also called alpha radiation in common usage;

This radiation is not very dangerous because a few millimeters of paper are sufficient to stop it.

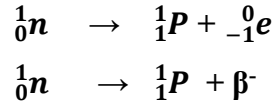
This radioactivity only concerns heavy nuclei, usually with atomic numbers greater than 74 (tungsten). The heaviest nucleus affected by this radioactivity is uranium-238.

II-2-2- Beta Radiation

There are two types of beta radiation: β^- (electron) and β^+ (positron).

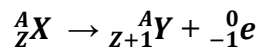
a- β^- Radiation

When the N/Z ratio is too high, a neutron tends to transform into a proton, giving rise to a particle with the same characteristics as an electron called β^- : negaton.



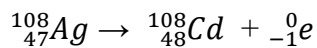
The electron cannot exist inside a nucleus and is therefore emitted (ejected).

The nuclear equation is:



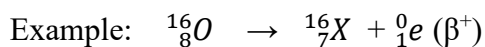
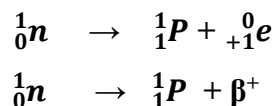
They are more penetrating but less ionising than α particles. They penetrate the skin to a depth of a few millimetres. They are dangerous to the skin.

Example:



b- β^+ Radiation

Nuclei with too many protons (or too few neutrons, i.e. located to the right of the stability curve) emit a positron, which comes from the decay of a proton into a positron, a neutron and an electron neutrino. This is characteristic radiation from light elements.



A positron is an antimatter particle that has the same properties as an electron but with a positive electric charge (+).

When an electron encounters a positron, they annihilate each other and emit high-energy radiation.

II-2-3- γ Radiation

Electromagnetic radiation of very high energy of the same nature as light (i.e. photons). With this type of radioactivity, there is no emission of particles or disintegration. In general, when a nucleus is formed during α or β decay, it does not immediately reach its ground state, but remains in an excited state. The transition from the excited state to the ground state releases a γ photon.

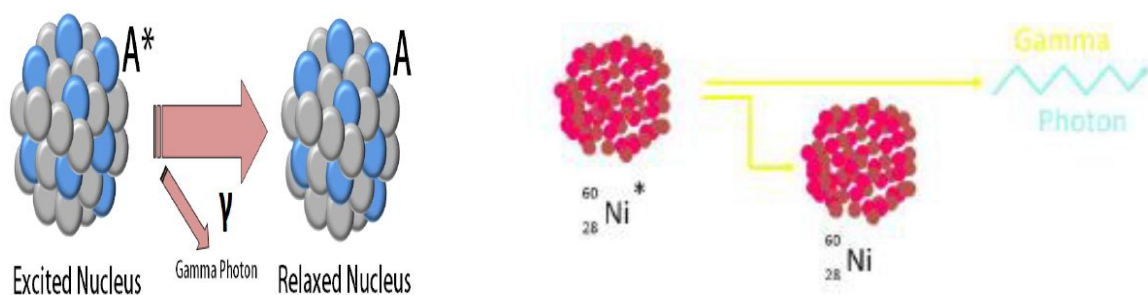


Figure VI-2: Gamma rays

III- Artificial radioactivity and nuclear reactions

This refers to radioactivity caused in certain nuclei as a result of human intervention.

There are three types:

- a- Nuclear fission
- b- Nuclear fusion
- c- Transmutations

III-1- Nuclear Fission

Atoms with very high mass numbers (A), when bombarded with neutrons, can undergo a break, resulting in lighter atoms and the regeneration of neutrons

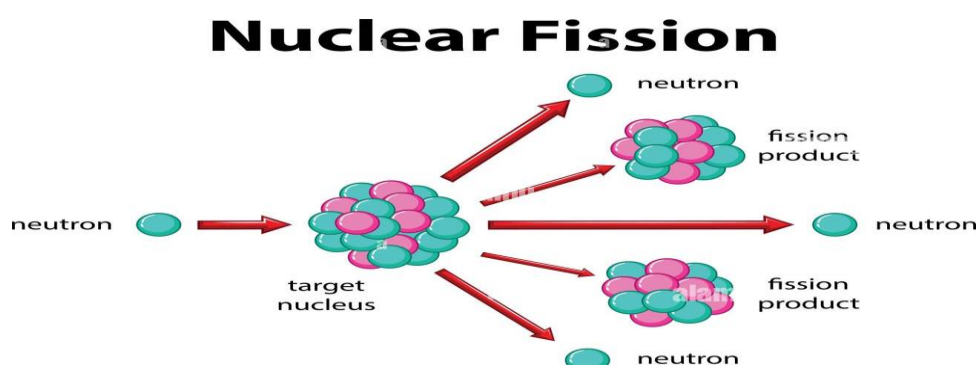
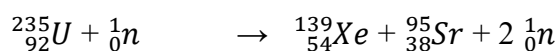
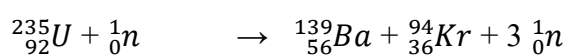


Figure VI-3: Nuclear Fission

Examples:



III-2- Nuclear Fusion

It is the combination of two light nuclei into a heavier nucleus with the release of a considerable amount of energy.

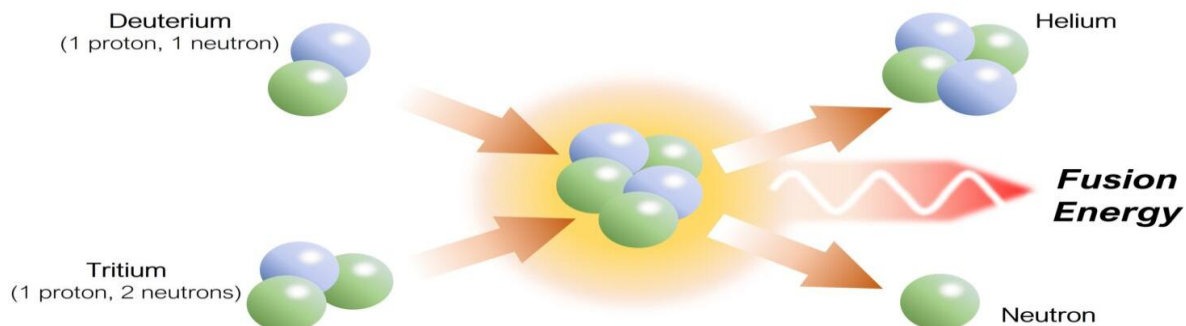
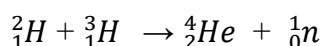
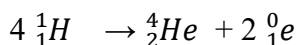


Figure VI-4: Nuclear Fusion

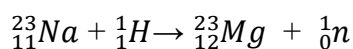
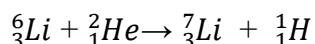
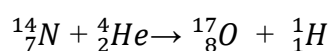
Examples:



III-3- Transmutation

The resulting nuclides have mass numbers equal or nearly equal to the target nuclide. The formed nuclides can be stable or radioactive

Examples:



IV- Kinetics of Radioactive Decay

IV-1-Radioactive decay law

The decay of a radioactive element can be very quick, taking a few milliseconds, or extremely long, taking several thousand years. This decay is defined by the law of first-order reaction rate.

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

where:

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

λ : radioactive constant of the element in question, can be expressed in s^{-1} , min^{-1} , h^{-1} , day^{-1} , etc.

The units of radioactivity are: disintegration per second (d.p.s), Curie (C) or Becquerel (Bq) ;

Knowing that:

$$1 \text{ Cu} = 3.7 \times 10^{10} \text{ d.p.s}$$

$$1 \text{ Bq} = 1 \text{ dps}$$

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

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

Where:

N_0 represent the initial concentration of the radioactive spice at time t.

IV-2- Activity of a radioactive nucleus

Activity is represented by the number of decays that occur per second.

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

Where: A_0 : represents the initial activity, with $A_0 = \lambda \times N_0$

IV-3- The radioactive period or half-life

It is defined as the time required for half of the nuclei present at time t to undergo decay:

$$N_t = N_0 / 2$$

As shown in the Figure 4-3, the period (T), also known as the half-life ($t_{1/2}$), is given by the following expression:

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

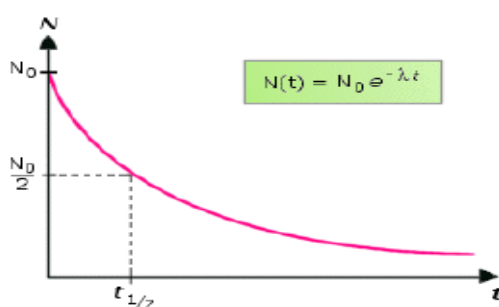


Figure VI-5: Decay Kinetics

V- Applications of radioactivity

V-1- Medical field

- ✚ Radiotherapy: used to treat cancer by applying radiation (such as cobalt-60 or cesium-137) that destroys cancer cells.
- ✚ Medical diagnostics (nuclear medicine): radioactive isotopes (technetium-99m, iodine-131, etc.) are used to visualize organ function (scintigraphy).
- ✚ Sterilization of medical equipment: gamma rays kill bacteria and microorganisms on surgical tools and materials.

V-2-Industrial field

- ✚ Quality control: checking the thickness or density of materials (e.g., in metal or plastic sheets).
- ✚ Industrial radiography: inspecting the interior of metal parts to detect cracks or defects without dismantling them.
- ✚ Level and flow measurement: radioactive sources are used to measure the level of a liquid or the density of a fluid.

V-3- Agricultural field

- ✚ Seed improvement: controlled mutations induced by radiation produce new, more resistant plant varieties.
- ✚ Study of fertilizers and irrigation: radioactive tracers are used to follow nutrients in soil and plants.
- ✚ Pest control: irradiation is used to sterilize insects and prevent their reproduction.

V-4- Energy field

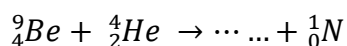
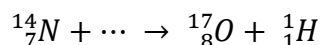
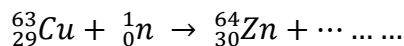
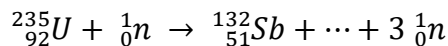
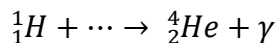
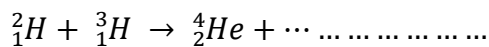
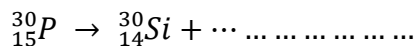
- ✚ Nuclear power generation: fission reactions in nuclear reactors produce large amounts of electrical energy.
- ✚ Power sources for space probes: radioisotope thermoelectric generators (RTGs) use the heat released by radioactive decay.

V-5-Scientific and archaeological field

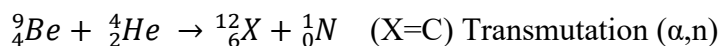
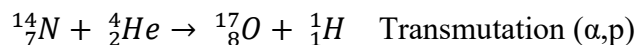
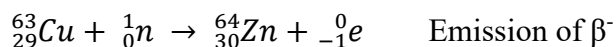
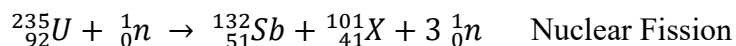
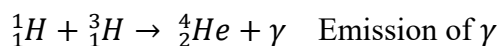
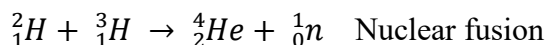
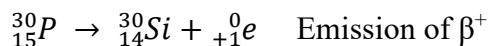
- ✚ Dating of ancient objects: carbon-14 dating determines the age of organic remains.
- ✚ Research in chemistry and biology: radioactive isotopes serve as tracers to study reaction mechanisms.

Exercise

1-Complete the following radioactive equations by specifying the type of each reaction:

**Correction**

1-Complete the following radioactive equations by specifying the type of each reaction:



References

References

- [1] Atomic Structure And Periodicity, third edition
- [2] Atomic structure and periodicity
- [3] Chemistry, OpenStax College ISBN-10 1938168399
- [4] General chemistry ninth edition. Ebing gammon
- [5] Principals of general chemistry, Silberberg Third Edition
- [6] A. Gedeon, A. Kozak, *General Chemistry Course, Chemical Bonding*, University Pierre and Marie Curie, 2007.
- [7] B. Baharmast, *Understanding and Deepening Chemistry: Volume 2 Atomistics and Structure of Matter*, Dunod, 1997.
- [8] F.Z Benhachem, A. Miraoui, *Structure of matter, Course and Solved Exercises*, University of Tlemcen, 2024/2025.
- [9] B. Meroufel, *Structure of Matter: Course and Solved Exercises*, University of Tlemcen, 2023.
- [10] F. Cherkaoui El-Moursli, A. Rhalib Kniazeva, K. Nabih, *Corrected Exercises of Structure of Matter and Chemical Bonds*, ISESCO, 2016.
- [11] F. Barka-Bouaifel, *Structure of Matter*, Handout, University Abderrahmane Mira Béjaïa, 2015.
- [12] C. Meyer, *Structure and Chemical Bonds*, Ellipses, Paris, 1986.
- [13] D.A. McQuarrie, *General Chemistry*, 3rd Edition, 2012.
- [14] E. Bardez, *General Chemistry*, Dunod, 2009.
- [15] E. Flamand, J.J. Allard, *General Chemistry*, Modulo, 2004.
- [16] F. Addouni, *Constitution of the Atom - Chemical Bonds*, O.P.U Editions, 2016.
- [17] Chemistry principals and reactions Masterton | Hurley
- [18] MEYER C., *Structure et liaisons chimiques*, Ellipses, Paris, 1986.
- [20] PAULING L. ETWILSON E.B., *Introduction to quantum mechanics*, McGraw-Hill, New York, 1935.
- [19] M. Guymont, *Structure of Matter: Atoms, Chemical Bonds, and Crystallography*, Belin, 2003.
- [20] P.W. Atkins, *Elements of Physical Chemistry*, De Boeck, 1993.
- [21] R. Chang, *General Chemistry*, 3rd Edition, 2009.
- [22] R. Kotz, P. Treichel, *General Chemistry*, De Boeck, 2006.
- [23] R. Lissillour, *Theoretical Chemistry*, Dunod, Paris, 2001