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المصادقة على تقرير خبير للموافقة على مطبوعة جامعية

بعد الإطلاع على تقارير لجنة الخبراء للموافقة على المطبوعة البيداغوجية للأستاذ: : جحيش المختار - أستاذ محاضر أ، بالقاعدة المشتركة بكلية التكنولوجيا بجامعة محمد بوضياف بالمسيلة والتي كانت كلها ايجابية ، تمّ تقرير التّالي:

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Course Summaries and Corrected Exercises on the structure of matter First year ST and Renewable Energy students

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MINISTERE DE L'ENSEIGNEMENT SUPERIEUR ET DE LA RECHERCHE SCIENTIFIQUE

UNIVERSITE DE MOHAMED BOUDIAF M'SILA



FACULTE DE TECHNOLOGIE
DEPARTEMENT DE SOCLE COMMUN

Course Summaries and Corrected Exercises on the Structure of Matter

Program for first-year ST and Renewable Energy students

Handout produced by: Dr. DJEHICHE Mokhtar

Foreword

This manuscript is the culmination of five years of teaching in the Department of Technical Science at the University of Mohamed Boudiaf - M' sila . This handout, consisting mainly of exercises and course summaries, is intended for first-year ST, SM and renewable energy students. The manuscript complies with the new program of the module entitled Structure of matter developed by the educational committee of the science and technology field (CPND-ST).

The handout is presented in the form of six chapters, respectively named (as presented): Fundamental Notions, Main Constituents of Matter, Radioactivity, Electronic Structure of the Atom, Periodic Classification of Chemical Elements and Chemical Bonds.

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I. Basic concepts

1. The atom

The atom is made up of a **nucleus** (the central part of the atom) formed of nucleons (**protons** and **neutrons**), and an electronic procession formed of **electrons** .

2. Isotopes

Represents atoms that are equal in number of protons but different in number of neutrons.

Isotopic abundancex_i (%) =
$$\frac{number\ of\ atoms\ in\ a\ given\ isotope}{total\ number\ of\ atoms\ of\ all\ isotopes\ of\ this\ element} \times 100$$

 $M = \sum x_i \times M_i$ x_i denoting the natural abundance of isotope i of molar mass M_i .

3. Number of moles (n)

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

$$n = \frac{V}{V_m}$$

$$c_x = \frac{number\ of\ solute\ moles}{volume\ of\ solution} = \frac{n}{V}$$

$$V_m = \frac{V}{n}$$

$$x_i = \frac{n_i}{n_{tot}}$$

$$C_n = M*Z$$

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

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$$d = \frac{\rho_{(s \ ou \ l)}}{\rho_{H2O}}$$

$$d_{gaz} = \frac{\rho_{gaz}}{\rho_{gir}} = \frac{M_{gaz}}{29}$$

Application exercises:

Exercise 1

We weigh 5.0 g of silver, whose molar mass is equal to 107.9 g.mol⁻¹.

- 1- Calculate the amount of silver matter in these 5.0 g.
- 2- Calculate the number of silver atoms present in these 5.0 g.
- 3- Deduce the mass of a silver atom.
- 4- Calculate the mass of a silver atom knowing that the silver studied is : $^{107}_{47}Ag$. Compare this value with question 3.

Given: $m_{proton} = 1.67.10^{-27} \text{ kg}$ (mass of electrons is negligible in this exercise and mass of a neutron = mass of a proton).

Solution

1- Quantity of matter: n = m/M.

Numerical application: $n = 5/107.9 = 4.6.10^{-2}$ mol.

2-Number of silver atoms:

In 1 mole of silver atoms there is an Avogadro number (N $_{A}$ = 6.02.10 23) of silver atoms.

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In n moles of silver atoms there are N silver atoms.

So:
$$N = n*N_A/1 = 4.6.10^{-2} * 6.02.10^{23}/1 = 2.77.10^{22}$$
 silver atoms.

3-Mass of a silver atom:

We know the molar mass of silver: $M = 107.9 \text{ g.mol}^{-1}$

So: In 107.9 g of silver there are $6.02.10^{23}$ silver atoms.

In m _{atom} g of silver there is 1 atom of silver.

So:
$$m_{atom} = 107.9/6.02.10^{-23} = 1.79.10^{-22} g = 1.79.10^{-25} kg$$
.

4-Mass of a silver atom from the number of nucleons:

The number of nucleons (A) = 107 = 47 proton + 60 neutron, or m $_p = m_N$ (approximately) so $m_{atom} = A*m_p = 107*1.67.10^{-27} = 1.78.10^{-25}$ kg. The atomic masses found are the same.

Exercise 2

Calculate the molar mass of the following compounds: carbon dioxide, sucrose, ammonia, methane, hydrogen chloride, sulfur dioxide.

Solution

Carbon dioxide: CO_2 : $M = M_C + 2M_O = 12 + 32 = 44 \text{ g.mol}^{-1}$

Sucrose: $C_{12} H_{22} O_{11}$: $M = 12 M_C + 22 M_H + 11 M_O = 12.12 + 22.1 + 11.16 = 342 g.mol^{-1}$

Ammonia: NH₃: $M = M_N + 3.M_H = 14 + 3 = 17 \text{ g.mol}^{-1}$

Methane: CH₄: $M = M_C + 4 M_H = 12 + 4.1 = 16 \text{ g.mol}^{-1}$

Sulfur dioxide: SO $_2$: M = 32 + 2.16 = 64 g.mol⁻¹

Hydrogen chloride: HCl : $M = M_H + M_{Cl} = 1 + 35.5 = 36.6 \text{ g.mol}^{-1}$

Exercise 3

A cylinder weighs 37.6 g when empty; it weighs 53.2 g when filled to 7.4 mL with an unknown liquid. Calculate the density of the liquid.

Solution

The weight of the liquid is 53.2 - 37.6 g = 15.6 g.

The volume of the liquid is 7.4 ml.

The density of the liquid is m/v = 15.6/7.4 = 2.1 g/ml.

Exercise 4

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A cylindrical rod weighing 45.0 g, measures 2.00 cm in diameter and 15.0 cm in length (L). Find its density.

Solution

Mass m (rod) = 45 g

The volume V(rod) = $\pi * r^2 *L=3.14 * 1^2 * 15=47.1 \text{ cm}^3$

Density $d = m/v = 45/47.1 = 0.955 \text{ g/cm}^3$

Exercise 5

Calculate the mass required to prepare 250 ml of a solution of AgNO $_3$ at a concentration equal to 0.125 M, using solid AgNO $_3$.

Solution

From the given volume and concentration, we can calculate how many grams of AgNO $_3$ to weigh:

We have n = C*V and m = n*M

So m= $C*V*M_{AgNO3} = 0.125 * 250.10^{-3} * 169.9 = 5.903 g$

Exercise 6

What volume of 0.25 M Na2CrO4 will be needed to obtain 8.1 g of Na2CrO4?

Solution

We have m = C*V*M

This implies V = 8.1/0.25 * 162 = 0.2 L

Exercise 7

Calculate the mass required to prepare a solution of 0.0348 mole fractions of sucrose (C $_{12}$ H $_{22}$ O $_{11}$, M $_{C12H22O11}$ = 342 g/mole), using 100 g of water.

Solution

We first calculate the number of moles of H2O $_{:}$ n $_{H2O}$ = m $_{H2O}$ /M $_{H2O}$ = 100/18 = 5.55 mol.

We know that x_i (the mole fraction) = n_i/n_t

$$\Rightarrow$$
x C12H22O11 = n C12H22O11 /(n C12H22O11 + n H2O)

$$n_{C12H22O11} = (x_{C12H22O11} n_{H2O}) / (1 - x_{C12H22O11}) = (0.0348 * 5.55) / (1 - 0.0348) = 200 \text{ mol.}$$

Now we calculate the mass of sucrose:

$$m_{C12H22O11} = n_{C12H22O11}$$
. $M_{C12H22O11} = 200 * 342 = 68.4 g$

Exercise 8

Concentrated sulfuric acid is labeled as having a density of d=1840 g/l and being 96% pure by weight. Calculate the molarity of this solution

Solution

We have

$$C_{H2SO4} = n/V$$
, $n = m/M$ and $m = density * purity \rightarrow$

$$C_{H2SO4} = (density * purity / M)/V = (1840.0, 96 / 98.1)/1$$

$$=18/1=18 M$$

Exercise 9

of 18.0 M H2SO4 $_{\rm is}$ needed to prepare 2.00 liters of 3.00 $_{M\,H2SO4}\,?$

Solution

To calculate the volume required for the preparation of 2.00 liters of 3.00 M of H $_2$ SO $_4$, we apply the dilution law: C $_1$ V $_1$ =C $_2$ V $_2$

$$18 * V_1 = 3 * 2 \rightarrow V_1 = (3 * 2) / 18 = 0.33 L$$

Exercise 10

Calculate the relative atomic mass (RAM) of boron from the following data:

| Isotope | Isotopic mass (u) | Abundance (%) |
|-----------------|-------------------|---------------|
| 10 B | 10,0129 | 19,91 |
| ¹¹ B | 11.0093 | 80 .09 |

Solution

The relative atomic mass (RAM) of boron can be calculated by the following relationship:

$$MAR = (m_1 P_1 + m_2 P_2 + m_3 P_3 +)/100$$

P: Abundance (%)

m: isotopic mass

$$MAR = (10.0129 * 19.91 + 11.0093 * 80.09 = 10.81 u$$

Exercise 11

When a sample of aluminum (Al) is placed in a 25 mL graduated cylinder containing 10.5 mL of water, the water level rises to 13.5 mL. What is the mass of the aluminum? d $_{Al}$ =2.7 g/ mL

Solution

The volume of the sample is equal to the volume of water displaced in the cylinder.

Volume of aluminum = 13.5 - 10.5 = 3 ml.

We know that
$$Al = m_{Al} / V_{Al} \rightarrow m_{Al} = d_{Al} * V_{Al} = 2.7 * 3 = 8.1 g.$$

Exercise 12

What is the mass percentage of NaHCO3 $_{in}$ a solution containing 20 g of NaHCO3 $_{dissolved}$ in 600 mL of H_2O ?

Solution

That is, 1 liter of H2O is equivalent to 1 kg of H2O

→
$$m_{H2O} = 600 g$$

On the other hand NaHCO $_3$ (%) = [m $_{NaHCO3}$ /(m $_{NaHCO3}$ + m $_{H2O}$)] * 100

NaHCO₃(%) =
$$[20/(20+600)] * 100 = 3\%$$

Exercise 13

What is the volume percentage of ethanol in a solution containing 35 ml of ethanol dissolved in 155 ml of water?

Solution

We will follow the same method used in exercise 12.

$$CH_3 H_2 H (\%) = [V_{CH3CH2OH} / (V_{CH3CH2OH} + V_{H2O})] * 100$$

$$CH_3CH_2OH(\%) = [35/(35+155)] * 100 = 18\%$$

Exercise 14

What is the molality of a solution containing 16.3 g of potassium chloride dissolved in 845 g of water?

Solution

Convert the mass of solute to moles: $n_{KCl} = m_{KCl} / M_{KCl} = 16.3/74.6 = 0.218 \text{ mol}$

 $M_{H20} = 845 \text{ g} = 0.845 \text{ Kg}$ molality (b) = $n_{KCI}/m_{H2O} = 0.2018/0.845 = 0.285 \text{ mol/Kg}$

Exercise 15

A piece of magnesium burns in the presence of oxygen (O2), forming magnesium oxide (

MgO), according to the following equation:

$$2Mg(s) + O2(g) \rightarrow 2MgO(s)$$

How many moles of oxygen are needed to produce 12 moles of magnesium oxide?

Solution

$$2Mg + O_2 \rightarrow 2MgO$$

From this equation, 2 moles of Mg react with 1 mole of O2, so six moles of oxygen are needed to produce 12 moles of magnesium oxide.

Exercise 16

Balance the following equation and answer the questions below.

$$KClO_3(s) \rightarrow KCl(s) + O_2(g)$$

- a. How many moles of O2 are produced from 10 moles of KClO3?
- b. How many moles of KCl are produced using 3 moles of KClO 3?
- c. How many moles of KClO 3 are needed to produce 50 moles of O 2?

Solution

The equilibrium equation is as follows:

KClO₃(s)
$$\rightarrow$$
 KCl(s) +3/2 O₂(g)

has. 1 mole of KClO₃ produces 3/2 moles of O₂

10 moles of KClO₃ produced x moles of O₂

 \Rightarrow x= 10 * 3/2 =15 moles of O2.

b. 1 mole of KClO 3 produces 1 mole KCl

So 3 moles of KClO3 produces 3 moles of KCl

c. 1 mole of KClO $_3$ produces 3/2 moles of O $_2$

x moles of KClO $_3$ produces 50 moles of O $_2$ \Rightarrow x= 50 /(3/2) =33.33 moles of KClO $_3$.

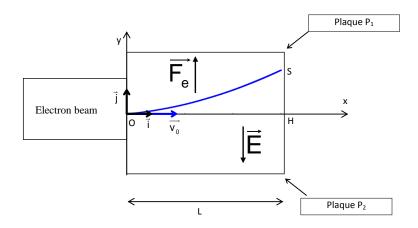


II. Main constituents of matter

II. Main constituents of matter

1. Experiments of JJ Thomson (1897)

It consists of sending electrons between two charged plates and then observing the deviation.



In this experiment he proves the existence of the electron and measures the ratio e/m:

$$\frac{e}{m_e} = \frac{2 * y * v_0^2}{E * L^2}$$

y: la déviation apparente

e : la charge de l'électron (C)

m_e : la masse de l'électron (kg)

E : la valeur du champ électrique V.m⁻¹

x: la longueur des plaques

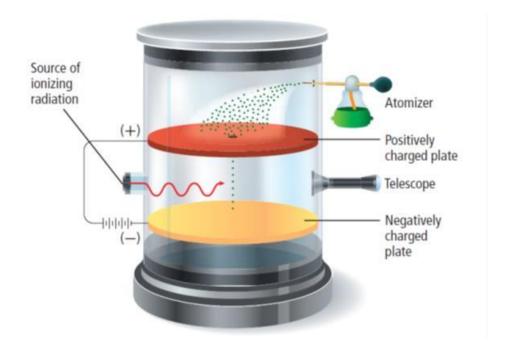
v₀ : vitesse initiale de l'électron

In the presence of a magnetic field, of which $F_m = F_e$ \rightarrow q.v.B = e.E

$$\frac{e}{m} = \frac{2*y*E}{R^2 x^2}$$

2. Millikan's experiment:

A spherical drop of oil, falling through a viscous medium such as air, will quickly reach a constant velocity. When it reaches this equilibrium state, the viscous force is balanced by other forces acting on the fall, such as gravity, buoyancy of the air, electrical forces, etc. By measuring the speed of the oil drop falling under different conditions, the amount of charge can be determined.



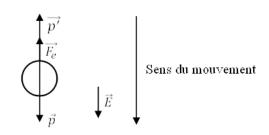
The forces acting on an oil droplet in equilibrium:

$$q = 4/3\pi r^3 g (\rho - \rho^\circ) / E$$

Force due to gravitation (\vec{p})

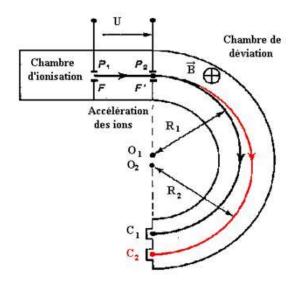
Force due to electric field $\overrightarrow{f_e}$

Stock force f (by immobilizing the drop, f=0)



3. Mass spectrometer

This technique is based on the determination of the atomic or molecular masses of the individual species present in the sample. The ions are separated in the mass spectrometer according to the ratio of mass to charge m/e of the ion



$$\implies \frac{e}{m} = \frac{v}{B * r}$$

r: the radius of the trajectory (m)

B: the value of the magnetic field (Tesla)

v: Speed of the ions to be separated

4. The main characteristics of the constituents of the atom are given in the following table:

| Particule et symbole | | Auteurs des premières mesures | Charge* | Masses (m _e , m _p , m _n)* arrondies à 4 chiffres après la virgule |
|---|----------------|---|--|---|
| Électron du grec êlektron : ambre | e ⁻ | J. J. Thomson (1897) R. A. Millikan (1911) | $-e = -1,602.10^{-19} \text{ C}$ (arrondie à $-1,6.10^{-19} \text{ C}$) | 9,1094.10 ⁻³¹ kg (arrondie à 9,11.10 ⁻³¹ kg) |
| Proton du grec prôtos : premier | p | E. Rutherford (1910) | + e = + 1,602.10 ⁻¹⁹ C (arrondie à + 1,6.10 ⁻¹⁹ C) | 1,6726.10 ⁻²⁷ kg (arrondie à 1,67.10 ⁻²⁷ kg) |
| Neutron | n | J. Chadwick (1932) | 0 | 1,6749.10 ⁻²⁷ kg (arrondie à 1,67.10 ⁻²⁷ kg) |

* The elementary charge e, and the masses me, mp, mn are fundamental constants.

Application exercises

Exercise 1

From the following terms: electron, proton, neutron, and nucleus, select the term that best matches the following expressions:

- a. Cathode ray
- b. Discovered in 1932
- c. Caused large deflections of alpha particles in Rutherford's experiment
- d. Has a charge of 1-
- e. Has no charge
- F. Contains almost all the mass of an atom
- g. In an atom, the number of these particles is equal to the number of protons.
- h. Identified by Thomson
- i. Site of the positive charge of an atom
- j. Has a positive charge and a relative mass of 1
- k. The center of an atom
- 1. Symbolized by n ⁰

Solution

- a. <u>electron</u>
- b. <u>neutron</u>
- c. <u>nucleus</u>
- d. <u>electron</u>
- e. <u>neutron</u>

| Exercise 2 |
|---|
| Give the correct answer: |
| a) In an atom, we find: |
| • Electrons and protons Protons and neutrons |
| • Electrons, protons and neutrons |
| b) |
| The nucleus of an atom contains: |
| Protons and electrons |
| Neutrons and electrons |
| Protons and neutrons |
| c) |
| In an atom the number of electrons is equal to: |
| Neutrons |
| • Protons |
| d) |
| The diameter of an atom relative to that of its nucleus is: |
| • Smaller |
| |

F.

g.

h.

i.

j.

k.

1.

nucleus

electron

electron

nucleus

proton

nucleus

neutron

- Equal
 Bigger
 The order of
- e) The order of magnitude of the diameter of an atom is:
- 10⁻⁹ m
- $10^{-10}\,\mathrm{m}$
- $10^{-8} \, \text{m}$

f)

The total electric charge of an atom is:

- Negative
- Positive
- None
- g) The mass of an atom is approximately equal to:
 - That of protons
 - That of neutrons
 - That of the core
- h) The mass of a proton is approximately equal to:
 - That of the electron
 - That of the neutron
 - That of the core

Solution

- a) In an atom, we find:
 - Electrons, protons and neutrons

b)

The nucleus of an atom contains:

Protons and neutrons

c)

In an atom the number of electrons is equal to:

Protons

d)

The diameter of an atom relative to that of its nucleus is:

- Bigger
- e) The order of magnitude of the diameter of an atom is:
- $10^{-10}\,{\rm m}$
- f) The total electric charge of an atom is:
 - None
- g) The mass of an atom is approximately equal to:
 - That of the core
- h) The mass of a proton is approximately equal to:
 - That of the neutron

Exercise 5

The following study concerns the movement of an electron of the beam which penetrates between two parallel and horizontal plates P1 and P2, in a zone where an electric field reigns \vec{E} assumed to be uniform and perpendicular to the two plates. At time t = 0 s, the electron arrives at a point O with a horizontal speed \vec{v}_0 .

The trajectory of the electron in a frame (O ,x,y) is provided in the figure below. The electron of mass m_e and charge q = -e, whose motion studied in the terrestrial frame assumed to be Galilean, is subject only to the electrostatic force $\overrightarrow{F_e}$.

1. represent without concern for scale and justifying the lines:

- the force vector $\overrightarrow{F_e}$ at a point in the electron's trajectory;

- the electric field vector \vec{E} at any point located between plates P1 and P2.

2. Using Newton's second law, determine the time equations x(t) and y(t) of the electron's

motion.

3. Check that the trajectory of the electron has the equation:

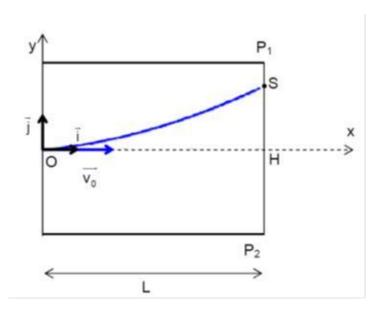
$$y = \frac{1}{2} \left(\frac{e * E}{m_e} \right) * \frac{x^2}{v_0^2}$$

4. At the exit from the zone between plates P1 and P2, the electron has undergone a vertical

deflection SH as shown in the diagram below. We measure SH = $yS = 2.0^{\circ}10^{-2}$ m.

Determine, in this experiment, the value of the e/me ratio of the electron.

Conclude.



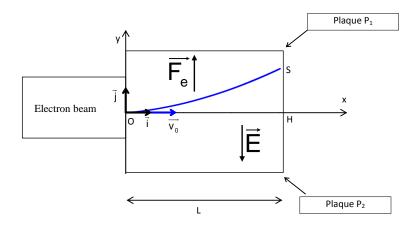
Data: Length of plates: $L = 9.0^{\circ}10^{-2} \text{ m}$

Initial speed of the electron: v $_0$ = 2.4x10 7 ms $^{\text{-1}}$

Value of the electric field: $E = 1.6x10^{4} \text{ Vm}^{-1}$

Solution

1. The trajectory of the electron is curved towards the plate P1 because of the effect of the electrostatic force $\overrightarrow{F_e}$. We deduce that this force has the direction towards the plate P1. It is indicated that the electric field \overrightarrow{E} is perpendicular to the two plates and we know that $\overrightarrow{F_e} = -e.\overrightarrow{E}$. Thus the field \overrightarrow{E} has a direction opposite to that of the force $\overrightarrow{F_e}$ and the force $\overrightarrow{F_e}$ is also vertical in direction



2. Newton's second law is applied to the electron system, in the supposed Galilean terrestrial frame of reference.

$$\overrightarrow{F_e} = m_e * \overrightarrow{a} = -e\overrightarrow{E} \implies \overrightarrow{a} = \frac{-e * \overrightarrow{E}}{m_e}$$

 \vec{a} : The acceleration vector (direction opposite to the field vector \vec{E})

By projection
$$\vec{a} \begin{cases} a_x = 0 \\ a_y = \frac{e.E}{m} \end{cases}$$
 As $\vec{a} = \frac{d\vec{v}}{dt}$, by integrating we obtain

$$\vec{v} \begin{cases} v_x = 0 + C_1 \\ v_y = \frac{e.E}{m_e}.t + C_2 \end{cases}$$

where C₁ and C₂ are constants integration that depend on the initial conditions

At
$$t = 0$$
 $\bigvee_{0} \begin{cases} v_{0x} = v_{0} \\ v_{0y} = 0 \end{cases} => C1 = v_{0} \text{ and } C2 = 0.$

SO
$$\vec{v} \begin{cases} v_x = v_0 \\ v_y = \frac{e.E}{m_e}.t \end{cases}$$

Let G be the center of inertia of the electron, $\vec{v} = \frac{d\overrightarrow{OG}}{dt}$ therefore $\overrightarrow{OG} \begin{cases} x = v_0.t + C_3 \\ y = \frac{e.E}{2.m_e}.t^2 + C_4 \end{cases}$

At t = 0, point G coincides with the origin of the reference frame $\overrightarrow{OG} \begin{cases} x = 0 \\ y = 0 \end{cases}$, we deduce that

$$C_3 = C_4 = 0.$$

So
$$\overrightarrow{OG}$$

$$\begin{cases} x = v_0.t & (1) \\ y = \frac{e.E}{2.m_e}.t^2 & (2) \end{cases}$$

1.3 • From (1), we have $t = \frac{x}{v_0}$ which we report in (2). It comes:

$$y = \frac{1}{2} \left(\frac{e * E}{m_e} \right) * \frac{x^2}{v_0^2}$$

1.4. We replace x and y by the coordinates of the point S (x_S = L; y_S), then y_S = $\frac{\text{e.E}}{2.\text{m}_{0}} \cdot \frac{\text{L}^{2}}{\text{v}_{0}^{2}}$.

We deduce that
$$\frac{e}{m} = \frac{2*y*E}{R^2 x^2}$$

$$\frac{e}{m_e} = \frac{2 \times 2,0 \times 10^{-2} \times \left(2,4 \times 10^7\right)^2}{1,6 \times 10^4 \times \left(9,0 \times 10^{-2}\right)^2} = 1.8 \times 10^{-11} \text{ C.kg}^{-1}$$

Let us calculate the value of this same ratio with the currently accepted values:

$$\frac{e}{m_o} = \frac{1,602176565 \times 10^{-19}}{9,1093826 \times 10^{-31}} = 1.7588201 \times 10^{-11} \, \text{C.kg}^{-1} \, .$$

The two values are perfectly consistent, only the number of significant digits changes.

Exercise 6

In Millikan's laboratory experiment, a droplet of mass m and negative charge q arrives between plates A and B. Archimedes' buoyancy is neglected. The droplet studied is subjected to its weight \vec{P} and to the friction force \vec{f} exerted by the air expressed by the relation $f = -6.\pi$. η .rv in which η is the viscosity of the air, r the radius of the droplet and v its speed.

- 1. Vertical fall of the droplet
- 1.1. When the droplet falls in the absence of an electric field, write the vector relationship between the friction force and the weight when the constant speed v1 is reached. Deduce the expression for v_1 as a function of η , r, m and g.
- 1.2. The previous relation can also be written: $v_1 = \frac{2}{9} \cdot \frac{\rho \cdot g \cdot r^2}{\eta}$

Or ρ is the density of the oil.

Determine the radius r of the droplet knowing that it travels, during its fall, a distance of 2.11 mm during a duration Δ t =10 s.

- 1.3. In order to facilitate measurement under the microscope, the droplet should not be too fast. Deduce whether it is preferable to select a large droplet or on the contrary a small droplet.
- 2. Rise of the droplet

A uniform electric field being established between plates A and B, the droplet undergoes an additional $\overrightarrow{F_e}$ vertical force and then rises with a constant speed v₂ reached almost instantly. It can be shown that the charge q of the droplet is given by the relation:

$$q = -\frac{6.\pi \cdot \eta \cdot r \cdot (v_1 + v_2)}{E}$$

Several measurements were made for different droplets and collected in the table below:

| Number of the | Radius r of the | Speed of | Speed of | Charge q of the |
|---------------|-----------------|-------------------------------|------------------------------|-----------------------|
| droplet | droplet | descent v ₁ | ascent v 2 | droplet |
| | (µm) | $('10^{-4} \mathrm{ms}^{-1})$ | $(10^{-4} \mathrm{ms}^{-1})$ | (10 ⁻¹⁹ C) |
| 1 | 1.2 | 1.55 | 1.59 | -6.4 |
| 2 | 1.3 | 1.82 | 1.81 | -8 |
| 3 | 1.5 | 2.42 | 1.35 | -9.6 |
| 4 | 1.6 | 2.76 | 3.13 | -1.6 |
| 5 | | 1.82 | 2.53 | -9.6 |

2.1. Droplets #2 and #5 in the table have the same descent speed v_1 but different ascent speeds v_2 .

Determine the radius of droplet no. 5 without calculation. Justify.

Why are their ascent speeds different?

- 2.2. Show, from the experimental results in the table, that the charge of these droplets is "quantized", that is to say that it only takes on values that are multiples of the same elementary charge equal to $1.6.10^{-19}$ C.
- 3. How does the protocol of the experiment carried out by Millikan differ from that carried out in the laboratory by JJ Thomson?

Data: Density of oil: $\rho = 890 \text{ kg.m}^{-3}$

Value of the gravitational field: $g = 9.8 \text{ N.kg}^{-1}$

Viscosity of air: $\eta=1.8\,\dot{}10^{-5}\,kg.m^{-1}$.s $^{-1}$

Solution

- 1. Vertical fall of the droplet
- 1.1. The droplet has a uniform rectilinear motion in the laboratory frame of reference. According to Newton's first law (principle of inertia), the forces exerted on the droplet then compensate each other $\vec{P} + \vec{f} = \vec{0}$.

$$\vec{P} = -\vec{f} = 6.\pi. \ \eta \cdot r \cdot \vec{V}_1$$
so $P = f$

$$mg = 6.\pi. \ \eta \cdot rv_1$$

$$v_1 = \frac{m.g}{6.\pi.\eta.r}$$

1.2 .
$$\mathbf{v}_1 = \frac{2}{9} \cdot \frac{\rho \cdot g \cdot r^2}{\eta} = \frac{d}{\Delta t}$$

$$r^2 = \frac{d \cdot \eta}{\rho \cdot g \cdot \Delta t} \cdot \frac{9}{2}$$

$$r = \sqrt{\frac{d \cdot \eta}{\rho \cdot g \cdot \Delta t} \cdot \frac{9}{2}}$$

$$r = \sqrt{\frac{2,11 \times 10^{-3} \times 1,8 \times 10^{-5}}{890 \times 9.8 \times 10.0}} \times \frac{9}{2} = 1.4 \times 10^{-6} \, \text{m} = 1.4 \, \mu \text{m}$$

1.3. According to the expression $v_1 = \frac{2}{9} \cdot \frac{\rho.g.r^2}{\eta}$, to decrease the speed v_1 it is necessary to decrease the radius of the droplet knowing that the other parameters ρ , g and g are considered constant.

It is best to select a small droplet.

2. Rise of the droplet

2.1 . The expression for the descent speed is $v_1 = \frac{2}{9} \cdot \frac{\rho.g.r^2}{\eta}$. It shows that two droplets which

have the same descent speed necessarily have the same radius, since ρ , g and η are constant under the conditions of the experiment.

Droplet 5 therefore has a radius $r_5 = r_2 = 1.3 \mu m$.

Using the expression for the charge q of the droplet $q = -\frac{6.\pi.\eta.r.(v_1 + v_2)}{E}$, let us express the

velocity v₂ of ascent:
$$-\frac{q.E}{6.\pi.n.r} = v_1 + v_2$$

$$v_2 = -\frac{q.E}{6.\pi.\eta.r} - v_1$$

We then notice that if the droplets do not have the same upward speed, it is because they have different electric charges q.

| Droplet number | Absolute value q of the charge q of the droplet | Report q /e |
|----------------|---|--------------|
| 1 | 6.4×10 ⁻¹⁹ | 4 |
| 2 | 8.0×10 ⁻¹⁹ | 5 |
| 3 | 9.6×10 ⁻¹⁹ | 6 |
| 4 | 1.6×10 ⁻¹⁸ | 10 |
| 5 | 9.6×10 ⁻¹⁹ | 6 |

2.2. The ratio |q|/e is always equal to an integer, |q|/e = n or |q| = ne.

The electric charge of the droplets is effectively quantified.

2.3. Millikan observed electrically charged droplets which he immobilized by varying the value of the electric field while Thomson observed the deflection of an electron beam by keeping the value of the electric field constant.

It can also be noted that Thomson's protocol neglects the effects of gravitation, which only allows the calculation of the ratio e/m; while Millikan's protocol takes them into account, which allows the calculation of the charge q.

Exercise 7: Bainbridge mass spectrography

- 1)- Natural chlorine (Cl) is a mixture of two isotopes ${}^{35}_{17}Cl$. The atomic molar mass of natural chlorine is 35.453 g/mol and that of the isotopes is 34.9688 g/mol for ${}^{35}_{17}Cl$ and 36.9659 g/mol for ${}^{37}_{17}Cl$. Give the proportions of these isotopes in natural chlorine.
- 2)- To separate these isotopes, a Bainbridge mass spectrograph is used. In the ionization chamber, Cl ^{2+ ions are formed.}
- 2.a)- What should be the speed of the ions at the exit of the speed filter, if we want to obtain a separation of their impact point of 1cm after passing through a magnetic field of intensity 0.15 Tesla.
- 2.b)- What is the intensity of the electric field in the speed filter, if the magnetic field in the speed selector has an intensity of 0.2 Tesla.

Solution

1)- The proportions of the isotopes of natural chlorine.

The atomic molar mass of natural chlorine corresponds to the average atomic mass of isotopes: $\sum M_i x_i$ with $\sum x_i = 1$ (xi: relative isotopic abundance of isotope i) in the natural mixture). We have:

$$x_{1}M_{1} + x_{2}M_{2} = \overline{M}$$

$$x_{1} + x_{2} = 1$$

$$x_{2} = \frac{\overline{M} - M_{1}}{M_{2} - M_{1}} \quad \text{either} x_{2} = \frac{35,453 - 34,9688}{36,9659 - 34,9688} = 0.2425$$

$$x_{2} = 0,2425(24.25\%) \qquad x_{1} = 0,7575(75,25)$$

2.a)- In the magnetic field, the ions follow a circular trajectory of radius r i such that:

$$r_i = \frac{m_i v}{q_B} \quad \text{And} \quad d = 2(r_2 - r_1)$$

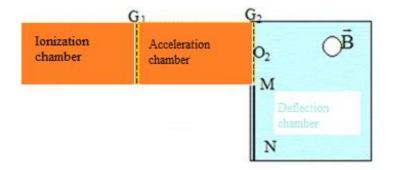
$$d = 2\left[\frac{m_2 v}{q_B} - \frac{m_1 v}{q_B}\right] = \frac{v}{NA.q.B}(M_2 - M_1)(q=2e) \Longrightarrow v = \frac{d.NA.B}{M_2 - M_1}$$

$$v = \frac{1.10^{-2}.6,02.10^{23}.1,6.10^{-19}.0.15}{(36,9659 - 34,9688).10^{-3}} = 7,24.\ 10^4 \ \text{ms}^{-1}.$$
2.b)- In the speed filter, we have
$$v = \frac{E}{R} \Longrightarrow E = v.B$$

$$E = 7,24.10^4.0,2 \implies E = 1,448.10^4 \text{V/m}$$

Exercise 8 (CAPES physics chemistry (from 2006 competition) Mass spectrograph)

A mass spectrograph consists of several parts as shown in the figure below:



- The ionization chamber in which potassium atoms $^{A1}_{19}K$ of $^{A2}_{19}K$ respective masses m $_1$ and m $_2$ brought to high temperature are ionized into K $^{+$ ions . It is considered that at the exit of this chamber, in O $_1$, the speed of these ions is almost zero.
- The acceleration chamber in which the ions are accelerated between O $_1$ and O $_2$ under the action of a potential difference established between the grids G $_1$ and G $_2$.
- The deflection chamber in which the ions are deflected by a uniform magnetic field B of direction perpendicular to the plane of the figure. A collector consisting of a photosensitive plate is placed between M and N.

The chambers are under vacuum. The weight of the ions is neglected compared to the other forces and it is assumed that at the exit of the acceleration chamber, the velocity vectors of the ions are contained in the plane of the figure.

- 1. Acceleration of ions:
- a. What must be the sign of the potential difference VG $_1$ -VG $_2$ so that the ions are accelerated between O $_1$ and O $_2$.
- b. Establish the expressions for the speeds of the ions when they arrive in O2 $_{as}$ a function of m1 , m2 ,e and U $_{=\,VG1}$ -VG2 .
- 2. Ion deviation:
- a. What must be the direction of the magnetic field B, prevailing in the deflection chamber, so that the ions can reach the collector?
- b. Show that in the deflection chamber, the trajectory of the ions is flat and that the motion is uniform.
- c. Show that the trajectory of each type of ion is a circle whose radius R $_1$ (respectively R $_2$) will be given as a function of m $_1$ (respectively m $_2$), e, B and U.
- d. Assuming that the ratio of the masses of the ions is equal to the ratio of their mass numbers, express the ratio A $_2$ /A $_1$ as a function of the radii R $_1$ and R $_2$ of the trajectories.
- e. we observe on the photosensitive plate two spots T $_1$ and T $_2$ corresponding to the impact of the ions of mass m $_1$ and m $_2$ respectively and such that OT $_1$ = 103.0 cm and OT $_2$ = 105.6 cm. Determine A $_2$ knowing that A $_1$ = 39.
- f. Describe qualitatively what the trajectory of the ions would be if their speed in O2 $_{\rm was}$ no longer perpendicular to the magnetic field B.

Solution

1.

a. Sign of the potential difference VG1-VG2 so that the ions are accelerated between O $_{\rm 1}$ and O $_{\rm 2}$:

On a path, the charge will have received an equal amount of energy from the electric field called: the work of the electric force is: q (VG₁-VG₂).

If a charge is abandoned, it moves under the action of the force, it acquires speed. It receives positive work and moves in the direction of decreasing potentials. The electric field provides it with energy which it transforms into kinetic energy.

We have q=e, positive charge of the ions, so VG₁-VG₂ is positive.

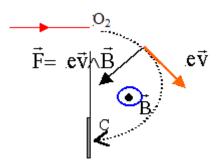
b. Expressions of the velocities of the ions when they arrive in O2 $_{as}$ a function of m1 $_{,}$ m2 $_{,}$ e and U= $_{VG1}$ - $_{VG2}$.

We know that the kinetic energy $E_c(i) = qVi$ (i for any ion) and the initial velocity is zero.

$$\begin{split} E_c(1) - 0 &= q(VG_1 - VG_2) \Rightarrow \\ \frac{1}{2}m_1v_1^2 &= qU \Rightarrow v_1 = \left[\frac{2.\,e.\,U}{m_1}\right]^{1/2} ou \\ v_2 &= \left[\frac{2.\,e.\,U}{m_2}\right]^{1/2} \end{split}$$

2. Ion deflection

a. Direction of the magnetic field B, prevailing in the deflection chamber, so that the ions can reach the collector



b. In the deflection chamber, the force F is perpendicular to the velocity vector and the magnetic field vector: the trajectory of the ions is flat and located in a plane perpendicular to B and containing the velocity vector.

The electromagnetic force is at all times perpendicular to the velocity vector . Now

$$P(watt) = \vec{f}(N).\,\vec{v}(\frac{m}{s})$$

consequently the power of the electromagnetic force is zero. This force does not work and does not modify the kinetic energy of the charged particle, the norm of the velocity vector is constant; uniform motion.

c. The charged particle is subject only to the centripetal Lorentz force. hence

$$e.v_i.B = \frac{m_i v_i^2}{R_i}$$
 soit $R_i = \frac{m_i v_i}{eB}$

$$\text{gold } v_i = \left[\frac{2.e.U}{m_i}\right]^{1/2} \Rightarrow R_i = \frac{m_i}{eB} * \left[\frac{2.e.U}{m_i}\right]^{\frac{1}{2}} = \left[\frac{2m_i.U}{e.B^2}\right]^{\frac{1}{2}}$$

R_i is constant: the trajectory is a circle.

d. Expression of the ratio A $_2$ /A $_1$ as a function of the radii R $_1$ and R $_2$ of the trajectories: Using the previous equation of Ri, the ratio R $_2$ /R $_1$ is written:

$$\frac{R_2}{R_1} = \left[\frac{m_2}{m_1}\right]^{1/2}$$

This implies that

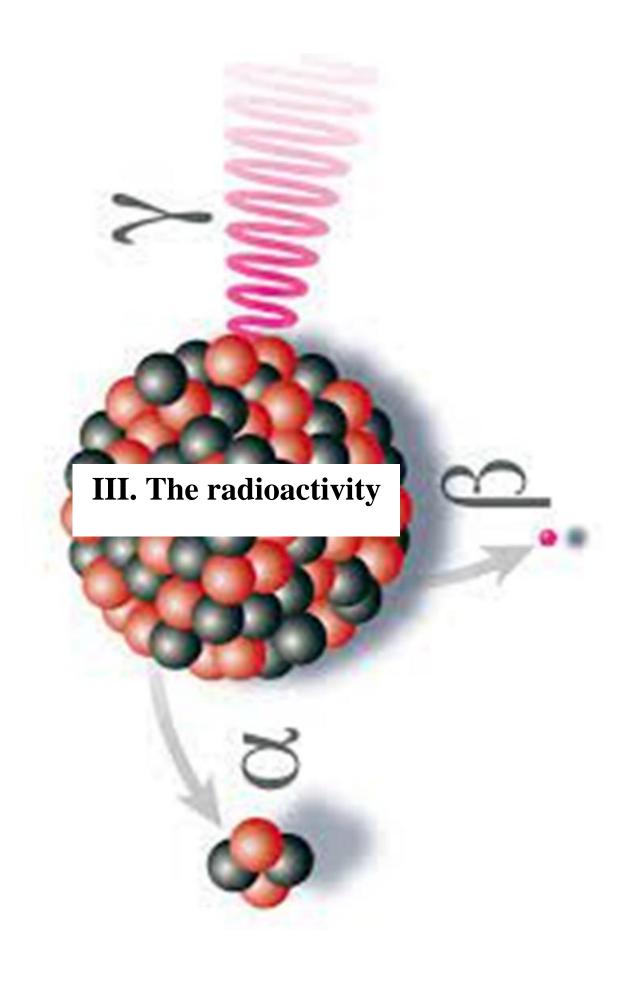
$$\frac{A_2}{A_1} = \left[\frac{m_2}{m_1}\right]^{1/2}$$

e. Two spots are observed OT $_1$ =103 cm and OT $_2$ = 105.6 cm. Knowing that A $_1$ =39

$$\frac{R_2}{R_1} = \frac{OT_2}{OT_1} = \frac{A_2}{A_1} \Rightarrow A_2 = \frac{OT_2 \cdot A_1}{OT_1} = \frac{39.105,6}{103} = 41$$

So the isotopes of potassium are $^{39}_{19}K$ And $^{41}_{19}K$

f. If the speed of the O2 ions is no longer perpendicular to the magnetic field B, the trajectory will be a helix. (the speed will have a component along B).



III. Radioactivity

1. Binding energy $\Delta E = E_L = (\Delta m)c_0^2$ Δm : mass defect, c_0 : speed of light in vacuum.

$$\Delta m = \left[Z*\left(m_p + m_e\right) + (A - Z)*m_n\right] - m({}_Z^AX)$$

m $_{\rm p}$: mass of the proton, m $_{\rm e}$: mass of the electron, m $_{\rm n}$: mass of the neutron, $m(_Z^AX)$: mass of the atom

2. Binding energy per nucleon $\frac{E_L}{A}$

3. Laws of radioactive decay $N(t) = N_0 e^{-\lambda t}, m(t) = m_0 e^{-\lambda t}$

N₀: number of nuclei at t=0, m_0 : mass of nuclei at t=0, λ : decay constant (s⁻¹),

- **4. Radioactive period** $T = t_{\frac{1}{2}} = \frac{\ln 2}{\lambda}, \quad t_{\frac{1}{2}}$: half-life time
- **5.** Activity $A_0 = \lambda * N_0$, $A(t) = A_0 * e^{-\lambda t}$

Application exercises

Exercise 1

Calculate the mass defect of lithium-7 ($^{7}_{3}Li$), let us know that its atomic mass is 7.016003 amu .

Proton mass = 1.00727 amu

Neutron mass = 1.00867 amu

Electron mass = 0.00054 amu

Solution:

$$\Delta m = \left[Z * \left(m_p + m_e\right) + (A - Z) * m_n\right] - m_{\left(\frac{A}{Z}X\right)}$$

$$\Delta m = [3 * (1,007826) + (7 - 3) * 1,00867] - 7,016003$$

 $\Delta m = 0.0421335 \ uma$

Exercise 2

Calculate the mass defect and binding energy for uranium-235. An atom of uranium-235 has a mass of 235.043924 amu .

Solution:

Step 1 : Applying the mass defect equation

we obtain $\Delta m = 1,91517$ uma

Step 2: Using the mass defect and Einstein's equation we can calculate the binding energy.

$$\Delta E = (\Delta m)c_0^2 = 1,91517 \times 1.66054 \times 10^{-27} \times (2,9979 \times 10^8)^2$$

Ce produit est constant
$$1,4923 \times 10^{-10} \text{ J} = 931254168 \text{ eV} = 931,2 \text{ MeV}$$

$$\Delta E = \Delta m(uma) \times 931,2$$

$$\Delta E = 1,91517 \times 931,2 = 1784 \text{ MeV}$$

Exercise 3

- 1. Write the decay equation for radium $^{226}_{88}Ra$
- 2. Calculate the energy released during the disintegration of a radium 226 nucleus (in MeV)

| Core | Mass (u) |
|--------|----------|
| Radium | 225,9770 |
| Radon | 221,9702 |
| Helium | 4,0015 |

$$c=2.9979\!*10^{~8}\,\text{ms}^{~\text{-}1}$$

Solution

1. Radium decay equation

$$^{226}_{88}Ra \rightarrow ^{222}_{86}Rn + \alpha$$

2. Energy released:

$$\Delta E = \Delta m^*c^2 = (225.9770 - (4.0015 + 221.9702))^*1.66054^*10^{-27} * (2.9979^*10^{-8})^2$$

$$\Delta E = 0.0053^*931.5 = 4.9369 \text{ MeV}$$

Exercise 4

- 1) Calculate the initial activity of a sample of radium 226 of mass m=1.0 g and a decay constant $\lambda=4.3.10^{-4}$ year ⁻¹
- 2) Calculate the activity of this sample 1000 years later.

Solution:

1) Mass of a radium 226 nucleus, $m = 226 u = 226 \times 1.67.10^{-27} kg$

Number of cores : N =
$$\frac{1 \times 10^{-3}}{226 \times 1,67 \times 10^{-27}}$$
 = 2,7 × 10²¹cores

$$\lambda = \frac{4.3 \times 10^{-4}}{365 \times 24 \times 3600} = 1.36 \times 10^{-11} \text{s}^{-1}$$

$$A = 1.36 \times 10^{-11} \times 2.7 \times 10^{21} = 3.6 \times 10^{10} \,\mathrm{Bq}.$$

1)
$$A(t) = A_0 * e^{-\lambda t} \implies A(1000 \text{ ans}) = 3.6 \times 10^{10} \times e^{-1.36 \times 10^{-11} \times 1000}$$

 $A = 2.3 \times 10^{10} \text{ Bg}$

Exercise 5

An ancient bone fragment contains 80 g of carbon (mainly carbon 12) and has an activity of 0.75 Bq. How old is this bone fragment?

- carbon 12 is stable;
- The period of carbon 14: $T = 5.7.10^3$ years;
- The mass of a carbon 12 nucleus: $m = 12 u = 12 \times 1.67.10^{-27} \text{ Kg}$

Solution:

We calculate the number of carbon 12 nuclei:

Number of nuclei : N (C12)=
$$\frac{80\times10^{-3}}{12\times1,67\times10^{-27}}$$
 = 4 × 10²⁴ cores

We calculate the initial number of carbon 14 nuclei N₀ (C14):

We have

$$\frac{14_C}{C_t} \implies N(C14) = 4 \times 10^{24} \times 1.3 \times 10^{-12} = 5.2 \times 10^{12} \text{ cores}$$

We calculate the current number of carbon 14 nuclei N(C14):

The activity:
$$A = \lambda N \implies N = \frac{A}{\lambda}$$

Gold
$$\lambda = \frac{ln2}{T} \Longrightarrow N = \frac{A \times T}{ln2} \Longrightarrow$$

$$N(C14) = \frac{0.75 \times 5.7 \times 10^3 \times 365 \times 24 \times 3600}{ln2} = 1.9 \times 10^{11} noyaux$$

Finally, we calculate the age of the bone fragment.

We have:

$$A = A_0 * e^{-\lambda t} \Longrightarrow N = N_0 * e^{-\lambda t}$$

$$\Rightarrow \frac{N}{N_0} = e^{-\lambda t} \Rightarrow \ln \frac{N}{N_0} = -\lambda t = -\frac{\ln 2}{T} * t$$

$$t = \frac{\ln \frac{N}{N_0}}{\ln 2} * T = \frac{\ln \left[\frac{1.9 \times 10^{11}}{5.2 \times 10^{12}} \right]}{\ln 2} \times 5.7 \times 10^3 = 2.7 \times 10^4 \text{ ans}$$

So the age of the bone fragment is 270,000 years.

Exercise 6

Complete the equations for the following nuclear reactions, indicating the nature of the particles represented by a question mark. In each case, consider the nature of the nuclear reaction.

a.
$${}^{14}_{7}N + {}^{4}_{2}He \rightarrow {}^{17}_{8}O + ?$$

b.
$${}^{7}_{4}Be \rightarrow {}^{7}_{3}Li + ?$$

c.
$${}_{3}^{6}Li+? \rightarrow 2 {}_{2}^{4}He+?$$

d.
$$^{63}_{29}Cu + ^{1}_{1}H \rightarrow ^{63}_{30}Zn + ?$$

e.
$$^{31}_{14}Si \rightarrow ^{31}_{15}P + ?$$

f.
$${}_{1}^{2}H + {}_{1}^{3}H \rightarrow {}_{0}^{1}n + ?$$

Solution

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

Decay of nitrogen by α bombardment, with emission of protons; the latter can also be written ${}^{1}_{1}P$.

b.
$${}^{7}_{4}Be \rightarrow {}^{7}_{3}Li + {}^{0}_{0}v$$

Spontaneous disintegration of beryllium 7 with positron emission. The nature of the emission indicates that ${}_{4}^{7}Be$ it is an artificial isotope.

c. ${}_{3}^{6}Li + {}_{1}^{2}H \rightarrow 2 {}_{2}^{4}He$

Fission of lithium 6 by bombardment with deuterium nuclei, also called deuterons.

d. $^{63}_{29}Cu + ^{1}_{1}H \rightarrow ^{63}_{30}Zn + ^{1}_{0}n$

Disintegration of copper 63 by bombardment with protons, and emission of neutrons.

e. ${}_{14}^{31}Si \rightarrow {}_{15}^{31}P + {}_{-1}^{0}e + {}_{0}^{1}v$

Spontaneous disintegration of silicon 31 with β – emission.

f. ${}_{1}^{2}H + {}_{1}^{3}H \rightarrow {}_{0}^{1}n + {}_{2}^{4}He$

Fusion of deuterium and tritium, the subject of experiments for the production of energy on Earth.

Exercise 7

A naturally occurring radioactive family is a family whose parent is the naturally occurring radioactive isotope of a given element, and which is made up of isotopes of various elements derived from each other by filiation; the last constituent is a stable isotope of lead. The three natural families known on Earth today are those of uranium 238, uranium 235 and thorium 232. Radium 226 ($^{226}_{88}Ra$) is the fifth daughter element of the uranium 238 family. After a series of successive α or β – type decays, it finally gives rise to the stable lead nucleus ($^{206}_{82}Pb$)

- a) What is the number of α and β type decays that allow us to go from $^{226}_{82}Ra$ to $^{206}_{82}Pb$.
- b) The first six steps are shown below. Complete them by indicating the atomic numbers, mass numbers and type of radioactive emission:

Solution

a) If, during the transition from $^{226}_{88}Ra$ to $^{206}_{82}Pb$ there are x β emissions $^-$ and y α emissions, we can write:

$$^{226}_{88}Ra \longrightarrow x_{-1}^{0}e + y_{2}^{4}He + ^{206}_{82}Pb (+x_{0}^{0}v)$$

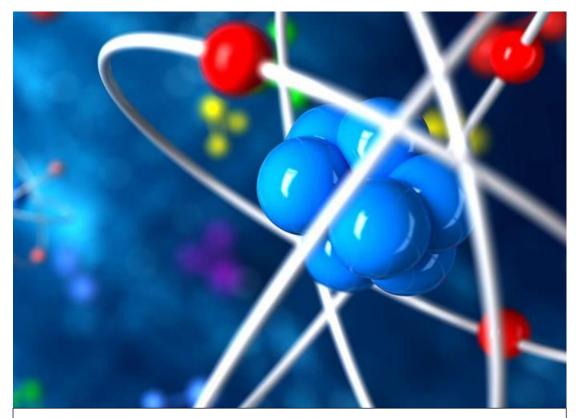
So we have:

$$226 = x \times 0 + y \times 4 + 206$$
 or $y = 5$

$$88 = x \times (-1) + y \times 2 + 82$$
 or $x = 2y - 6 = 4$

When passing from $^{226}_{88}Ra$ at $^{206}_{82}Pb$, 4 $\beta-$ emissions and 5 α emissions occur.

b) The successive steps are:



IV. Electronic structure of an atom



IV. Electronic structure of the atom

1. Photoelectric effect

In the photoelectric effect, incident light (E_{photon}) on the surface of a metal ($E_{material}$) causes the ejection of electrons. The number of electrons emitted and their kinetic energy (E_{c}) can be measured as a function of the intensity and frequency of the light.

$$E_c = E_{photon} - E_{mat\'eriau} = \frac{1}{2}mv^2$$

- g. the kinetic energy of electrons is linearly proportional to the frequency of the incident radiation.
- h. h the number of electrons is proportional to the light intensity

2. Electromagnetic radiation

It is characterized by the following equations:

$$\bar{\nu} = \frac{1}{\lambda}$$
 and $c = \lambda \times \nu$ therefore $c = \frac{\nu}{\bar{\nu}}$

 λ : wavelength (nm). ν : frequency (Hz). $\bar{\nu}$: wave number (cm $^{-1}$)

3. Emission and absorption of radiation by matter

These two phenomena occur when there is an exchange of energy through matter.

$$\Delta E = h\nu = |E_f - E_i|$$

E_f: final state

E_i: initial state

4. Radiation emission

The passage of an electron from a higher level to a lower level causes the emission of light:

i. (Balmer 1885):
$$\frac{1}{\lambda} = R_h \times \left(\frac{1}{2^2} - \frac{1}{n^2}\right)$$

n : energy level (positive integer greater than 2), R $_{\rm h}$: Rydberg constant=1.097373 10 7 m $^{-1}$

j. (Rydberg 1988)
$$\Delta E = E_f - E_i = h \times R_h \times c \times \left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

 n_f and n_i are integers such that $n_f < n_i$.

5. Bohr Model

- k. The angular momentum of the electron (\vec{L})can only take integer values n (quantization of angular momentum): $\vec{L} = mvr = \frac{nh}{2\pi}$
- 1. the distance between the nucleus and the electron $r_n = a_0 \times n^2$

n: principal quantum number, a ₀: Bohr radius

- For Total energy $E_n = -13.6 \times \frac{1}{n^2}$
- For a hydrogenoid $E_n=-\frac{13.6}{n^2}~Z^2$, $r_n=a_0\times\frac{n^2}{Z}$, $v=\mathrm{R_h}\times\mathrm{c}\times Z^2\left(\frac{1}{\mathrm{n_f^2}}-\frac{1}{\mathrm{n_i^2}}\right)$

6. Quantum numbers

- ➤ The principal quantum number n: 1, 2, 3, 4, 5, 6, 7: shell K, L, M, N, O, P, Q respectively
- \triangleright The secondary quantum number 1: between 0 and (n 1) = 0, 1, 2, 3: s, p, d, f respectively
- \triangleright The magnetic quantum number m₁= between -l and +l

Application exercises

Exercise 1

- 1. Establish for a hydrogen atom (nucleus of charge + Ze around which an electron gravitates), the formulas giving:
- a- The radius of the orbit of rank n.
- b- The energy of the nucleus-electron system corresponding to this orbit.
- c- Express the radius and the total energy of rank n for the hydrogenoid as a function of the same quantities relative to the hydrogen atom.
- 2. Calculate in eV and joules the energy of the first four levels of the hydrogenoid ion Li2+, knowing that in the ground state, the energy of the nucleus-electron system of the hydrogen atom is equal to -13.6 eV.
- 3. What energy must a Li2+ ion absorb for the electron to pass from the ground level to the first excited level?
- 4. If this energy is supplied in the form of light, what is the wavelength of the radiation capable of causing this transition?

We give: Li (Z=3) 1eV= 1.6.10-19 Joules

 $h = 6.62.10^{-34} \text{ Js c} = 3.108 \text{ ms}^{-1}$

Solution

1. Balance of forces: Two collinear forces in opposite directions are exerted on the electron, Fe (electrostatic) and Fc (centrifugal due to motion).

$$\overrightarrow{\|F_e\|} = \frac{z}{4\pi\varepsilon_0} \frac{|q_p q_e|}{r^2} \qquad \overrightarrow{\|F_c\|} = m \frac{v^2}{r}$$

For the electron to remain in an orbit of radius r, it is necessary that: $|F_e| = |F_c|$ then see the course.

2. For a hydrogenoid $E_n = -\frac{13.6}{n^2} Z^2$ This implies that the energy corresponding to the four levels of Li ²⁺: Z=3 equals

$$n= 1 E1 = -122.6 eV = -19.6.10^{-18} J$$

$$n= 2 E2 = -30.6 eV = -4.9.10^{-18} J$$

$$n= 3 E3 = -13.6 \text{ eV} = -2.18.10^{-18} \text{ J}$$

$$n=4 E4= -7.65 eV = -1.22.10^{-18} J$$

3. Let us imagine the transition between two energy levels n=1 and n=2 (absorption)

$$n = 2$$

$$n = 1$$

$$E_2$$

$$E_1$$

Absorbed energy: $\Delta E = E2 - E1 = -30.6 - (-122.4) = 91.8 \text{ eV}$

4. Conservation of energy

$$\Delta E = \left(\frac{hc}{\lambda}\right) \Longrightarrow \lambda = \left(\frac{hc}{\Delta E}\right)$$

$$\lambda = (6.62.10^{-34}\,\mathrm{x}\ 3.10^{-8}\,)/\ (91.8\ \mathrm{x}\ 1.6.10^{-19}\,) = 1.35.10^{-8}\,\mathrm{m} = 135\ \mathring{A}.$$

(Radiation in the ultraviolet range)

Exercise 2

The energy levels of the hydrogen atom have the value in eV: En = -13.6 / n2.

What is the wavelength of the radiation λ emitted during de-excitation from level E4 to level E2?

What area does this radiation belong to?

Data:
$$h = 6.626 \cdot 10^{-34} \text{ Js}$$
;

$$c = 3.00. 10^{8} \text{ ms}^{-1}$$
; $1.00 \text{ eV} = 1.60. 10^{-19} \text{ J}$.

Solution

When de-energizing from level E4 to level E2,

an energy photon $hv = |E_2 - E_4|$ is emitted.

Or
$$h \upsilon = hc / \lambda$$

The wavelength of the radiation λ associated with this photon is deduced from this:

$$\lambda = \frac{hc}{|E_2 - E_4|}$$

Or numerically:

$$\lambda = \frac{6,626 \cdot 10^{-34} \cdot 3.10^8}{1,6.10^{-19} \left| \frac{-13,6}{4} + \frac{13,6}{16} \right|}$$

$$\lambda = 4.87.10^{-7} \, m = 487 \, nm$$

The corresponding radiation belongs to visible light (400 to 800 nm). It is blue in color.

Exercise 3

The energy levels of the hydrogen atom have the value in eV: En = -13.6 / n2.

What is the wavelength of the radiation λ emitted during de-excitation from level E4 to level E2? To which domain does this radiation belong?

Data:
$$h = 6.626 \cdot 10^{-34} \text{ Js}$$
;

$$c = 3.00 \cdot 10^{-8} \text{ ms}^{-1}$$
; $1.00 \text{ eV} = 1.60 \cdot 10^{-19} \text{ J}$.

Solution

When de-energizing from level E4 to level E2,

a photon of energy $hv = |E_2 - E_4|$ is emitted. Now h $v = hc / \lambda$

The wavelength of the radiation λ associated with this photon is deduced from this:

$$\lambda = \frac{hc}{|E_2 - E_4|}$$

Or numerically:

$$\lambda = \frac{6,626 \cdot 10^{-34} \cdot 3.10^8}{1,6.10^{-19} \left| \frac{-13,6}{4} + \frac{13,6}{16} \right|}$$

$$\lambda = 4.87.10^{-7} \, m = 487 \, nm$$

The corresponding radiation belongs to visible light (400 to 800 nm). It is blue in color.

Exercise 4

Among this series of quantum numbers $\{n, \ell, m\ell, ms\}$, which are possible and which are not allowed?

- a. $\{3, 2, 1, +1/2\}$
- b. $\{2, 2, 0, -1/2\}$
- c. $\{3, -1, 0, +1/2\}$

Solution

- a. The principal quantum number n must be an integer, which it is here. The quantum number ℓ must be less than n, which it is. The quantum number $m\ell$ must be between $-\ell$ and ℓ , which it is. The spin quantum number is +1/2, which is allowed. Since this set of quantum numbers meets all the restrictions, it is possible.
- b. The quantum number n is an integer, but the quantum number ℓ must be less than n, which it is not. So it is not a permitted set of quantum numbers.
- c. The principal quantum number n is an integer, but ℓ cannot be negative, so it is not a permitted set of quantum numbers.

Exercise 5

Among this series of quantum numbers $\{n, \ell, m\ell, ms\}$, which are possible and which are not allowed?

- a. $\{4, 2, -2, 1\}$
- b. $\{3, 1, 0, -1/2\}$

Solution

- c. The spin must be either +1/2 or -1/2, so this set of quantum numbers is not allowed.
- d. Allowed

Exercise 6

- a. What are the shapes of the s, p, and d orbitals respectively?
- b. How many 1s orbitals are there in an atom? 4p orbitals? 4d orbitals?
- c. What is the maximum number of orbitals with:
 - $n = 4 \ 1 = 1$
 - $n = 2 \ 1 = 2$
 - $n = 3 \ 1 = 2$
 - n = 5 l = 1 $m_1 = -1$
- d. Which orbitals cannot exist?
- e. Write a set of quantum numbers for a 4f orbital.
- f. Describe the electrons defined by the following quantum numbers:
 - n l ml
 - 3 00
 - 2 11
 - 4 2 -1
 - 3 1 2

Solution

- a. s = spherical p = dumbbell d = clover
- b. 1s: 1 4p: 3 4d: 5
- c. M
 - 3 (4p orbitals)
 - no (1 must be < n)
 - 5 (3d orbitals)
 - 1 (3 qn . define a unique orbital)
- d. 3f and 2d
- e. n = 4 l = 3 ml = 3, 2, 1, 0, -1, -2, -3
- f. 3s
 - 2p
 - 4d

Not allowed (l must be <n)

Not allowed (ml must be between –l and +l)

Exercise 7

Are the following statements true or false? Why?

An electron for which n=4 and m=2.

- has) Must necessarily have l=2
- b) can have l=2
- c) must necessarily have a spin equal to $+\frac{1}{2}$
- d) is necessarily in a sublevel d

Solution

a)
$$n = 4 \rightarrow 1 = 0,1,2,3$$

$$1 = 0 \implies m = 0$$

$$l = 1 \rightarrow m = -1, 0, 1$$

$$1 = 2 \rightarrow m = -2, -1, 0, 1, 2$$

$$1 = 3 \implies m = -3, -2, -1, 0, 1, 2, 3$$

1 must be equal to either 3 or 2

It is therefore not obligatory that I be equal to 2: false

- b) true
- c) No, because a quantum box of given m can contain two electrons with antiparallel spins. s can therefore have indifferently the two values +1/2 or -1/2: false.
- d) false: I can have the values 2 or 3, it can be a sublevel d or f.

Exercise 8

Are the following statements true or false? Why?

- a. If l=1, the electron is in a d subshell.
- b. If n=4 the electron is in the O shell.
- c. For a d electron, m can be equal to 3.
- d. If l=2, the corresponding subshell can receive at most 6 electrons
- e. The number n of an electron in an f subshell can be equal to 3.
- f. If two "atomic structures" have the same electronic configuration, they are necessarily the same element.
- g. If two "atomic structures" have different electronic configurations, they are necessarily two different elements.

Solution

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

l = 1 with subshell p: false

b. If n = 4 the electron is in the O shell.

n = 4 at layer N: false

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

d to
$$l = 2$$
 to $m_1 = -2, -1, 0, 1, 2$: false

d. If l = 2, the corresponding subshell can receive at most 6 electrons.

l = 2 to $m_1 = -2$, -1, 0, 1, 2 to 5 quantum boxes with 10 electrons maximum: false

e. The number n of an electron in an f subshell can be equal to 3.

$$n = 3$$
 at $l = 0, 1, 2$ (s, p, d) with f steps on layer 3: false

f. If two "atomic structures" have the same electronic configuration, they are necessarily the same element. "atomic structure" = "neutral" atom or ion

An ion has the same electronic configuration as a neutral atom of another element: false.

 $\underline{Example}$: Na $^{\scriptscriptstyle +}$, Ne and O2- have the same electronic configuration.

g. If two "atomic structures" have different electronic configurations, they are necessarily two different elements.

The ion and the neutral atom of the same element necessarily have different electronic configurations: false

Exercise 9

Calculate the number of photons per m2 ^{and} per second in monochromatic radiation of wavelength $\lambda = 5000$ Å (yellow) and intensity 0.1 watt m ⁻² (intensity of a desk lamp).

Solution

A wavelength of 5000 Å gives a frequency:

$$v = \frac{c}{\lambda} = \frac{3.10^{10}}{5.10^{-5}} = 6.10^{14} \, Hz$$

The energy of a photon is:

$$E = h. \nu = 6,62.10^{-34}.6.10^{14} = 4.10^{-19} J$$

To find the intensity in number of photons per square meter, we divide the intensity of monochromatic radiation in (watt m $^{-2}$) by the energy of a photon which is h v:

N _{photon} .m ⁻² .s ⁻¹ =
$$\frac{0.1 \text{ (watt.m}^{-2})}{hv.(J.s^{-1}.s^{-1})} = \frac{0.1 \text{ (J.s}^{-1}).m^{-2}}{4.10^{-19}(J.s^{-1}.s^{-1})} = 2.5. \cdot 10^{17} \text{ photons.m}^{-2} .s ^{-1}$$
.

Exercise 10

What is the energy (in eV) of the ground state of the Be $^{3+10V}$? Can the energy be calculated of the ground state of the Be atom?

Solution

The Be $^{+3 \text{ ion}}$ is a hydrogenoid, with Z= 4. We can therefore apply Bohr's formula to it:

$$E_n = \frac{-13.6 \, Z^2}{n^2} = \frac{-13.6.4^2}{1^2} = -217.6 \, \text{eV}$$

For the beryllium atom (Be), it is not a hydrogenoid, so we cannot calculate its ground state energy.

Exercise 11

A monochromatic radiation of frequency 9.12 10 14 s $^{-1}$ is sent onto a hydrogen atom (H) already excited to the level n=2. Is the energy of the radiation sufficient to tear the electron from the H atom? Calculate the speed of the ejected electron.

Solution:

- The energy of level n=2 is written: $E_n = \frac{-13.6}{2^2} = -3.4 \text{ eV}$

The energy of monochromatic radiation is written as:

$$E = h. \nu = 6,62.10^{-34}.9,12.10^{14} = 60,43.10^{-20}J = 3,78 \text{ eV}$$

E>E 2 this means that this energy is sufficient to tear the electron from level 2 of the hydrogen atom.

- there remains a remainder of energy which is equal to the difference between the two energies:

E $_2$ - E = 3.78 – 3.4 = 0.38 eV, which must be equal to the kinetic energy (E $_c$) of the ejected electron.

$$E_c = \frac{1}{2}m_e v^2 \Rightarrow v = \sqrt{\frac{2.E_c}{m_e}} = \sqrt{\frac{2.0,38.1,6.10^{-19}}{9,1.10^{-31}}} = 3,65.10^5 \text{ m. s}^{-1}$$

Exercise 12

1. The photoelectric effect is the emission of electrons extracted from a metal by light radiation. Einstein explained it in 1905 by considering that light is made up of photons.

We have a photoelectric cell with an extraction threshold of 2.4 eV. It is illuminated by a polychromatic beam composed of two radiations of wavelengths λ_1 = 430 nm and λ_2 = 580 nm.

Does the corresponding maximum energy increase if the light intensity emitted by the lamp is increased?

- 2. In the case of a photoelectric effect, is the energy of the incident photons absorbed entirely or partially? Write the expression for this energy.
- 3. Do both radiations produce the photoelectric effect?
- 4. What is the maximum speed of electrons that are torn from the photocathode?

Solution

1. Frequency calculation $V_{6\rightarrow 3}$:

$$|\Delta E| = h v_{6\rightarrow 3} \Rightarrow v_{6\rightarrow 3} = \frac{|\Delta E|}{h}$$
; moreover: $|\Delta E| = |E_3 - E_6|$

$$E_3 = \frac{-13.6}{3^2} = -1.51(eV)$$
 And $E_3 = \frac{-13.6}{6^2} = -0.38(eV) \Rightarrow |\Delta E| = 1.14(eV) = 1.18.10^{-19} J$

$$v_{6 \to 3} = 2,74.10^{14} s^{-1}$$

Wavelength of transition b:

Transitions **a** and **b** correspond to a single emission and absorption line, respectively.

Therefore $V_{6\rightarrow 3} = V_{3\rightarrow 6}$

Furthermore we have:
$$v_{(3\to6)} = \frac{c}{\lambda_{(3\to6)}} \Rightarrow \lambda_{3\to6} = \frac{c}{v_{3\to6}} = \frac{3.10^8}{2.74.10^{14}}$$

$$\lambda_{(3\to 6)} = 1095,22.10^{-9} \text{m} = 1095,22 \text{ nm}$$

2. a- Calculation of the wavelength $\lambda_{1\rightarrow 4}$:

$$\frac{1}{\lambda_{(n\to m)}} = Rh\left(\frac{1}{n^2} - \frac{1}{m^2}\right) \Longrightarrow \frac{1}{\lambda_{(1\to 4)}} = Rh\left(\frac{1}{1^2} - \frac{1}{4^2}\right) = \frac{Rh \times 15}{16}$$

$$\lambda_{l\to 4} = 96,97.10^{-9}\,\text{m}$$
 ; $\lambda_{l\to 4} \in \text{domaine UV}$

b- Calculation of the radius r_{4:}

$$r_{\rm n} = a_{\rm o}.n^2 \Longrightarrow r_{\rm 4} = a_{\rm o}.4^2 = 0.53 .16 = 8.48 (A^{\circ}) \Longrightarrow r_{\rm 4} = 8.48 .10^{-10} (m)$$

• Calculation of speed v₄:

$$v_n = \frac{2,18.10^6}{n} \Rightarrow v_n = \frac{2,18.10^6}{4}; v_n = 0,545.10^6 \text{ (m/s)}$$

• Calculation of kinetic energy Ec.

$$E_{c} = \frac{1}{2} m_{e}.v_{4}^{2} \Rightarrow E_{c} = 1.35.10^{-19} J.$$

• Calculation of potential energy Ep:

$$E_p = -\frac{Ke^2}{r_4} \Rightarrow Ep = -2.72.10^{-19} J.$$

c- calculation of the total energy E $_{\text{T:}}$

•
$$E_T = Ec + Ep$$

•
$$E_T = E_n = \frac{-13.6}{n^2}$$
 (eV) $E_T = -0.85$ (eV)

Exercise 13

1. Photoelectric threshold

A photovoltaic cell with a caesium cathode is illuminated with a wavelength of λ = 495 nm and then with radiation of wavelength λ = 720 nm. The extraction energy of a caesium electron is E $_0$ = 3.00.10 $^{-19}$ J

- a. Calculate the wavelength λ 0 which corresponds to the photoelectric threshold
- b. Check that the photoelectric emission exists only with one of the two previous radiations.
- 2. Speed of electron emission

A vacuum photoelectric cell is illuminated with monochromatic light. The extraction energy of an electron from the cathode metal is E $_0$ =3.00.10–19 J . The wavelength of the radiation is 600 nm a. What is the maximum kinetic energy Ecmax of an emitted electron?

b. What is the maximum speed Vmax of an emitted electron?

Solution

Wave model of the atom

➤ Louise De Broglie's hypothesis

all matter has a wave

$$\lambda = \frac{h}{m * v} = \frac{h}{p}$$

p: the quantity of movement, h Planck's constant.

→ Heisenberg's uncertainty principle

Not all physical quantities of the macroscopic world are simultaneously observable in the submicroscopic world.

$$\Delta x * \Delta v \ge \frac{h}{2\pi * m}$$

 Δ x: uncertainty about its position and

 Δ p: the uncertainty about its momentum p

> The psi wave function Ψ

 Ψ is a purely mathematical function, it is the wave function of the electron. :

- it has no physical meaning,
- it is a function of the coordinates of the electron,
- it is defined by the 3 quantum numbers : \mathbf{n} , l and \mathbf{m}_l : $\psi_{\mathbf{n},l,\mathbf{m}}$.

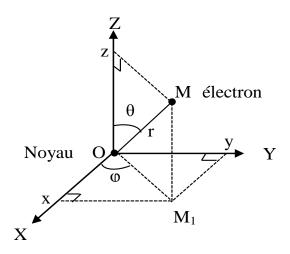
> Schrödinger equation

- Fundamental equation of wave mechanics
- It allows to calculate Ψ

Probability density

The electron is characterized by:

- its energy state,
- its probability of presence at a given location



- Probability of presence.

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

It is written:

$$dP = |\Psi|^2 \times dV$$

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

 $|\Psi|^2$: probability volume density of presence or electron density

The normalization condition :

For an infinite volume we are certain to find it there and therefore the probability equal to

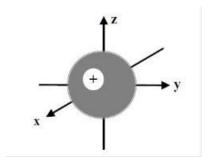
$$1 \text{ is} \int_{espace} \Psi^2 \times dV = 1$$

Solving the Schrödinger equation $\psi_{\mathrm{n,l,m}_l}(r,\theta,\varphi) = \mathrm{R}_{\mathrm{n,l}}(r)$. $\Theta_{\mathrm{1,lmll}}(\theta)$. $\Phi_{\mathrm{ml}}(\varphi)$

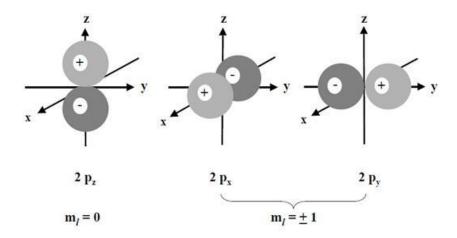
\succ Representation of Functions $\psi_{\mathbf{n},\mathbf{l},\mathbf{m}_l}$

k In the case of an ns orbital, the volume corresponding to a maximum probability of presence is spherical. The wave function ψ_{n00} , l=0, does not depend on θ or ϕ but it does depend on r. Its value

is the same in all directions. The probability of presence is also independent of the direction, the orbitals will be spherical.



The p orbitals (l = 1) can be represented by two approximately spherical lobes, joined together, having as axes of symmetry the x, y and z axes of the reference trihedron. They are therefore called "n px", "n py" and "n pz" depending on the value of $m_1(n \ge 2)$.



In the case of nd orbitals , the wave function depends on the angular quantities $\Theta(\theta)$, $\Phi(\phi)$. The probability of presence takes different values depending on the direction. The symmetry of these orbitals is no longer spherical. To represent this geometric shape, we use the square of their angular part. We then obtain a lobe-shaped envelope. $1 = 2 \Rightarrow m_1 = -2, -1, 0, 1, 2 \ (n \ge 3)$ (Figure IV.18).

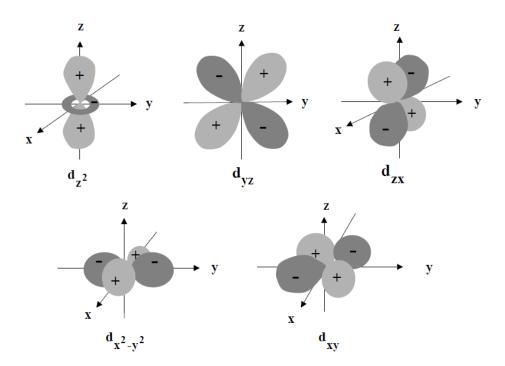


Table: Radial and angular parts of some wave functions of the hydrogen atom. These expressions involve the Bohr radius a $_0$ = 52.9 pm.

| n | l | $R_{n,\;\ell}(\mathbf{r})$ | m_{ℓ} | $Y(\theta, \varphi)$ | orbitale |
|---|---|--|------------|--|-------------------|
| 1 | 0 | $R_{1,0} = \left(\frac{1}{a_0}\right)^{3/2} \cdot 2 e^{-\frac{r}{a_0}}$ | 0 | $\frac{1}{\sqrt{4\pi}}$ | 1 s |
| 2 | 0 | $R_{2,0} = \left(\frac{1}{a_0}\right)^{3/2} \cdot \frac{1}{2\sqrt{2}} \cdot \left(2 - \frac{r}{a_0}\right) \cdot e^{-\frac{r}{2a_0}}$ | 0 | $\frac{1}{\sqrt{4 \pi}}$ | 2 s |
| 2 | 1 | $R_{2,1} = \left(\frac{1}{a_0}\right)^{3/2} \cdot \frac{1}{2\sqrt{6}} \cdot \frac{r}{a_0} \cdot e^{-\frac{r}{2a_0}}$ | 0 | $\sqrt{\frac{3}{4\pi}} \cdot \cos \theta$ | $2 p_z$ |
| 3 | 0 | $R_{3,0} = \left(\frac{1}{a_0}\right)^{3/2} \cdot \frac{1}{9\sqrt{3}} \cdot \left(6 - \frac{4r}{a_0} + \frac{4r^2}{9a_0^2}\right) \cdot e^{-\frac{r}{3}a_0}$ | 0 | $\frac{1}{\sqrt{4\pi}}$ | 3 s |
| 3 | 1 | $R_{3,1} = \left(\frac{1}{a_0}\right)^{3/2} \cdot \frac{1}{9\sqrt{6}} \cdot \frac{2r}{3a_0} \left(4 - \frac{2r}{3a_0}\right) \cdot e^{-\frac{r}{3a_0}}$ | 0 | $\sqrt{\frac{3}{4\pi}} \cdot \cos \theta$ | 3 p _z |
| 3 | 2 | $R_{3,2} = \left(\frac{1}{a_0}\right)^{3/2} \cdot \frac{1}{9\sqrt{30}} \cdot \frac{4r^2}{9a_0^2} \cdot e^{-\frac{r}{3}a_0}$ | 0 | $\sqrt{\frac{5}{16\pi}} \cdot (3\cos^2\theta - 1)$ | 3 d _{z2} |

7. Polyelectronic atoms (Screening effect: Slater approximation)

The effective charge is calculated by considering that the numerous electrostatic interactions (attractions-repulsions) in an atom can be reduced to a small number of interactions that are easy to quantify.

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

$$Z^* = Z - \sigma_I$$

With $\sigma_J = \sum \sigma_{ij}$

 σij : screening constant for each electron i that exerts a screening effect on an electron j

σj, screen constant

The energy of the jth electron is calculated by the following relation:

$$E_j = \frac{-13,6*Z^{*2}}{n^{*2}}$$

The radius between the atom and this electron equals

$$r = \frac{0.53 * n^{*2}}{Z^*}$$

n * = apparent quantum number introduced by Slater to reduce the differences between experimental and calculated values (Table IV.5).

| Electron | Electron | | | | | | |
|----------|----------|-----------|-----------|------|-----------|------|----|
| | 1s | 2s, 2p | 3s, 3p | 3d | 4s, 4p | 4d | 4f |
| 1s | 0.30 | | | | | | |
| 2s, 2p | 0.85 | 0.35 | | | | | |
| 3s, 3p | 1 | 0.85 | 0.35 | | | | |
| 3d | 1 | 1 | 1 | 0.35 | | | |
| 4s, 4p | 1 | 1 | 0.85 | 0.85 | 0.35 | | |
| 4d | 1 | 1 | 1 | 1 | 1 | 0.35 | |
| 4f | 1 (| 1 | 1 | 1 | 1 | 1 | 1 |

Table: Apparent quantum number values for each principal quantum number value n ..

| n | 1 | 2 | 3 | 4 | 5 | 6 |
|----|---|---|---|-----|---|-----|
| n* | 1 | 2 | 3 | 3.7 | 4 | 4.2 |

In the Slater approximation, the energy E of an atom is equal to the sum of the energies of the electrons of the different electron groups:

$$E = \sum n_j E_j$$

Application exercises

Exercise 1

- **1.** Using the relationships between the three quantum numbers n, l and m, determine the number of orbitals in the first three energy levels of the hydrogen atom.
- 2. Show that the maximum number of electrons that can be contained in the shell of quantum number $\bf n$ is equal to $\bf 2n^2$.
- **3.** Give the usual designation of the following orbitals: Ψ 3,0,0; Ψ 3,2,0; Ψ 2,1,-1.

Solution

1. Each orbital is designated by the term $\Psi_{\,nlm}$ as shown in the following table

| n | ı | m | orbitale |
|---|---|----|----------------------------------|
| 1 | 0 | 0 | Ψ _{1,0,0} (1s) |
| 2 | 0 | 0 | Ψ _{2,0,0} (2s) |
| | | -1 | Ψ _{2,1,-1} (2px) |
| | 1 | 0 | Ψ _{2,1,0} (2py) |
| | | 1 | $\Psi_{2,1,1}$ (2pz) |
| | 0 | 0 | Ψ _{3,0,0} (3s) |
| | 1 | -1 | Ч _{3,1,-1} (3рх) |
| | | 0 | Ч _{3,1,0} (3ру) |
| | | 1 | Ψ _{3,1,1} (3pz) |
| 3 | | -2 | Ψ _{3,2,-2} (3d) |
| | | -1 | Ψ _{3,2,-1} (3d) |
| | 2 | 0 | Ψ _{3,2,0} (3d) |
| | | 1 | Ψ _{3,2,1} (3d) |
| | | 2 | Ψ _{3,2,2} (3d) |

2. the maximum number of electrons that can be contained in the shell of quantum number n:

In the n = 1 shell we have an atomic orbital (AO) => $n^2 = 1$

In the n = 2 shell we have four atomic orbitals => $n^2 = 4$

In the n = 3 shell we have nine atomic orbitals => $n^2 = 9$

The number of OAs for each value of n (or level) is n^2 .

In each orbital we have two electrons at most. So the maximum number of electrons that the quantum number shell can hold is equal to $2n^2$. (This is no longer valid for n>4).

3. The wave function (or orbital) is determined by three quantum numbers n, l and m.

 Ψ 3 ,0,0 => Ψ n,l,m => n = 3, l = 0 (s orbital) and m = 0 => 3s orbital Ψ 3,2,0 => Ψ n,l,m => n = 3, l = 2 (d orbital) and m = 0 => 3d orbital Ψ 2 ,1 ,-1 => Ψ n,l,m => n = 2, l = 1 (p orbital) and m = -1 => 2p orbital

Exercise 2

- 1. What is the dimension of the quantity: h/mv?
- 2. What is the associated wavelength?
- to an electron whose kinetic energy is 54 eV;
- to a ball whose speed is 300 ms⁻¹ and whose mass is 2g.
- to a proton accelerated under a potential difference of 1 MV (10 ⁶ V).

Data: electron mass: me = $9.109.10^{-31}$ kg, proton mass: mp = $1.672x10^{-27}$ kg, Planck constant: h = $6.62\ 10^{-34}$ Js

3. What is the condition for an electron to generate a standing wave on a circular trajectory? Can we deduce Bohr's quantization condition from this?

Solution

1. We have h Planck constant is in kg.m 2 .s $^{-1}$, m in kg and vm.s $^{-1}$, so the relation $\frac{h}{mv}$ can be written:

$$\frac{h(kg.m^2.s^{-1})}{mv(kg.m.s^{-1})} = \frac{h}{mv}(m)$$

The quantity $\frac{h}{mv}$ has the dimension of a length

$$2.E_c = \frac{mv^2}{2}$$
 And $\lambda = \frac{h}{mv} = \frac{h}{(2m.E_c)^{1/2}}$

- The associated wavelength for an electron

$$\lambda = \frac{6,62 \cdot 10^{-34}}{2(9,1091 \cdot 10^{*31}) \cdot (541,6 \cdot 10^{-19})^{1/2}} = 0,1668 \cdot 10^{-9} = 1,67 \, \text{Å}^{\circ}$$

- The associated wavelength for a ball = $1.1.10^{-23}$ Å => For the ball, the associated wavelength λ is unobservable. There is no physical significance at the macroscopic scale. The de Broglie postulate is not applicable in this case.
- The associated wavelength for a proton = 9.10^{-5} Å => For the proton, the associated wavelength λ is of the order of the dimensions of nuclear problems.
- 3. The wave associated with the electron will be stationary if after having made one turn, the electron is in the same vibrational state. For this, the circumference of the trajectory would have to be equal to an integer times the wavelength.

$$2.\pi.r = n.\lambda = \frac{nh}{mv} \Longrightarrow m.v.r = n\frac{h}{2\pi}$$

Bohr quantization condition

Exercise 3

Apply Heisenberg's principle to the following two systems:

- 1. An electron moving in a straight line ($\Delta x = 1\text{Å}$). Calculate Δv .
- 2. A ball of mass 10g moving in a straight line ($\Delta x = 1 \mu m$). Calculate m. Δv .

Solution

According to Heisenberg's uncertainty principle, it is impossible to determine precisely both the position of the particle and its momentum (or momentum).

The uncertainty relation obeys the relation:

$$\Delta p_{x}$$
. $\Delta x \geq \frac{h}{2\pi}$

 Δ_x is the uncertainty about the position

 Δp_x Uncertainty about the quantity of movement.

Following a straight line, we have:

$$\Delta p_x$$
. $\Delta x \ge \frac{h}{2\pi} \ et \ \Delta p = m \ . \ \Delta v \Longrightarrow \Delta v \ge \frac{h}{2\pi . m . \Delta x} \ et \ \Delta x \ge \frac{h}{2\pi . m . \Delta v}$

1. For the electron: $\Delta x = 1 A^{\circ} = 10^{-10} m \ et \ m_e = 9,109. \ 10^{-31} kg$

$$\Delta v \ge \frac{6,62 \cdot 10^{-34}}{2.3,14 \cdot 9,109 \cdot 10^{-31} \cdot 10^{-10}} = 1,16 \cdot 10^6 \ m. \ s^{-1}$$

$$\Delta x \ge 1,16.10^6 \text{ m. s}^{-1}$$

At the atomic scale, the uncertainty in the speed (Δ v) is very large.

2. For the ball $\Delta x = 1 \mu \text{ m} = 10^{-6} \text{ m}$ and $\text{m} = 10 \text{g} = 10.10^{-3} \text{ kg}$)

$$\Delta v \ge 1.05.10^{-26} \, m. \, s^{-1}$$

This uncertainty is too small (not measurable). Heisenberg's principle has no physical meaning at the macroscopic scale.

Conclusion: The position and speed of an atomic particle cannot be measured simultaneously. Thus, the position of an electron, having a well-defined momentum, will only be defined with a certain uncertainty. Its presence will therefore be described in a probability domain of presence and not by its position on an orbit.

Exercise 4

The 1s orbital of the hydrogen atom is expressed as:

$$\psi = N_{1s}e^{\frac{-r}{a_0}}$$

- 1. Express the probability of the presence of the electron inside a volume between the spheres r and r+dr .
- 2. Define the radial presence probability density.
- 3. What is the radius r of the sphere on which the probability density of presence is maximum?

We give:
$$\int_0^\infty r^n e^{-\alpha r} dr = \frac{n!}{\alpha^{(n+1)}}$$
 with $\alpha >$ and n integer ≥ 0

Solution

The wave associated with an electron is a standing wave. Its amplitude at each point in space is independent of time. It is given by a mathematical function called the wave or orbital function.

 Ψ : wave function, solution of the Schrödinger equation: H Ψ =E Ψ

The wave function Y has no physical meaning. On the other hand, the value at a point of its square Ψ^2 (or of the square of its modulus Ψ^2 1, if it is a complex function) determines the probability dP of finding the electron in a volume dv around this point.

The probability of presence at a point: $1 \Psi_{s1} 1^2$.

In a volume dv: $dP =: 1 \Psi_{s1} 1^2 dv$.

The ratio dP / dv is called the probability density of the presence of the electron at the point considered (or electron density).

1. 1. The probability of presence in a space limited by two spheres of

radius r and r+dr :
$$P_{r \to r + dr} = \int_0^{\pi} sin\theta d\theta \int_0^{2\pi} d\varphi \int_r^{r + dr} r^2 \Psi_{s1} \Psi_{s1}^* dr$$
$$= 4\pi \int_r^{r + dr} r^2 \Psi_{s1} \Psi_{s1}^* dr$$

2. The probability of radial presence:

$$dPr = 1 \Psi_{s1} 1^2 dv = 4 \pi r^2 1 \Psi_{s1} 1^2 dr$$

 \Rightarrow The radial probability density is: $D_r = \frac{dP_r}{dr} = 4\pi r^2 \, 1 \, \Psi_{\rm s \, 1} \, 1^2$

Exercise 5

We have three chemical elements : $a - {}_{9}F^{-}$ $b - {}_{11}Na^{+}$ $c - {}_{10}Ne$.

- 1- Write the electronic structures of the following ions and atom:
- 2- Determine the effective charge to which an electron in the outer shell is subjected

| j | j ls | | 3s3p |
|------|------|------|------|
| i | | | |
| 1s | 0,31 | | |
| 2s2p | 0,85 | 0,35 | |
| 3s3p | 1 | 0,85 | 0,35 |

- 3- Calculate the energy of an electron $E(\bar{e})$ of the external shell of each of these chemical species: 4- Compare the stability S of these electrons.
- 5- For these three species, compare without doing any calculation:
 - a- the rays (r).
 - b- first ionization energies (EI).

Data: EH = -13.6 eV. Table of values of screening constants (j is the electron that screens electron i).

Solution:

1) a -
$$1s^2 2s^2 2p^6$$

b-
$$1s^2 2s^2 2p^6$$

c- 1s
2
 2s 2 2p 6

The three species are isoelectronic with different + Ze charges of the 3 nuclei.

2) For an electron in the outer shell, the electrons which screen it are 7 e from the 2s2p shell and 2 e from the 1s shell, i.e.:

a- For
$$_9$$
 F $^-$, Z * (F $^-$) = Z - 7 σ $_{2s2p/2s2p}$ - 2 σ $_{1s/2s2p}$ = 9 - 7*0.35 - 2*0.85 = 4.85

b- For
$$_{11}$$
 Na $^+$, Z * (Na $^+$) = Z - 7 σ $_{2s2p/2s2p}$ - 2 σ $_{1s/2s2p}$ = 11 - 7*0.35 - 2*0.85 = 6.85

c- For
$$_{10}$$
 Ne, Z * (Ne) = Z - 7 σ $_{2s2p/2s2p}$ - 2 σ $_{1s/2s2p}$ = $10 - 7*0.35 - 2*0.85 = 5.85$

3) a - For
$$_9$$
 F $^-$ E(\bar{e}) = E $_H$ (Z $_{2s2p}$ *) 2 /n 2 = -13.6* (4.85)/2 2 = -79.97 eV

b- For ¹¹ Na ⁺ E(
$$\bar{e}$$
) = E _H (Z _{2s2p} *) ²/n ² = -13.6* (6.85) ²/2 ² = -159.54 eV

c- For
$$_{10}$$
 Ne, E(\bar{e}) = E $_{H}$ (Z $_{2s2p}$ *) 2 /n 2 = -13.6* (5.85) 2 /2 2 = -116.36 eV

4) For the same number of electrons, Na $^+$ has the highest nuclear charge and attracts the electron the most, The highest energy value to tear off a 2s2p electron is that of Na $^+$ equal to +159, 54 eV

The electron of Na + is then the most stable, i.e.:

$$S(Na^+) > S(Ne) > S(F^-)$$

5)

- **a- The nucleus external** electron attraction force being the highest for Na $^+$ and as this force varies in 1/r 2 then r(Na $^+$) < r(Ne) < r(F $^-$).
- b For the same reason as 4) EI(Na $^+$) > EI(Ne) > EI(F $^-$).

7. Electronic configuration

> Pauli exclusion principle.

Two electrons in the same atom cannot have all four numbers.

identical quantum.

- Two electrons in the same atomic orbital must differ in their spin quantum number, which can only take two values m $_s$ =1/2 (\downarrow) or -1/2 (\uparrow)
- An atomic orbital can only "contain" a maximum of 2 electrons which in this case will have opposite spins: they are antiparallel or paired ↑↓



- If the orbital contains only one electron, it is said to be **unpaired or single** .
- An empty orbital constitutes an electron vacancy.

> Stability principle

- In the ground state, an atom is in its most stable energy state corresponding to the lowest energy.
- The electrons start by saturating the lowest energy levels, in the order: "1s", "2s", "2p", "3s", "3p"... this is the so-called "(n + 1) minimal" rule.

The first sublayer to be filled is the one with the smallest sum (n + 1).

Klechkowski rule:

The electronic configuration of any chemical element is of the following form:

Exceptions to Klechkowski's Rule

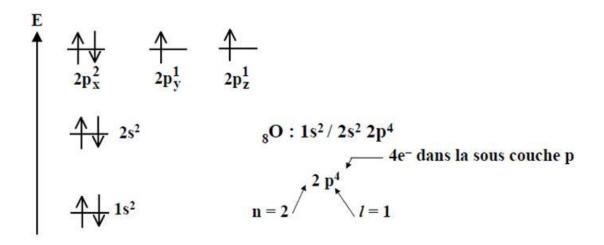
(n - 1)d 4 ns 2 replaced by (n - 1)d 5 ns 1 (example $_{24}$ Cr : [Ar]4s 2 3d 4 becomes $_{24}$ Cr : [Ar]4s 1 3d 5)

(n - 1)d 9 ns 2 replaced by (n - 1)d 10 ns 1 (example $_{29}$ Cu : [Ar]4s 2 3d 9 becomes $_{29}$ Cu : [Ar]4s 1 3d 10)

(n-1)f 2 nd 0 replaced by (n-1)f 1 nd 1 (example Ce: [Xe] 6s 2 4f 2 4d 0 becomes This: [Xe] 6s 2 5d 1 4f 1 .

> Hund 's Rule

For a given subshell, the lowest energy electronic configuration is obtained by placing a maximum of electrons of the same spin (same ms value) in different orbitals, before pairing electrons of opposite spins (opposite ms values).



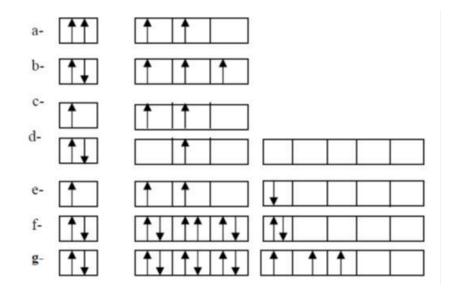
- Use of quantum boxes each symbolizing an atomic orbital.

Application exercises

Exercises 1

Among the following electronic structures, which ones do not respect the filling rules?

Explain



Solution

- a) Inexact state: the two spins must be opposite (Pauli rule).
- b) Ground state
- c) Excited state
- d) Ground state
- e) Excited state

Hund 's rule and Pauli principle are not

g) Ground state

Exercise 2

Let the following electronic structures be

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

Solution

$$1s^2 2s^2 2p^6 3s^1 \text{ Ground state}$$

$$1s^2 2s^2 2p^7 3s^2 \text{ Inexact state (6 electrons maximum on p)}$$

$$1s^2 2s^2 2p^5 3s^1 \text{ State excited}$$

$$1s^2 2s^2 2p^6 2d^{10} 3s^2 \text{ Inexact state (no d orbital for n=2)}$$

$$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 3f^6 \text{ Inexact state (no f orbital for n=3)}$$

Exercise 3

What is the number of valence electrons in vanadium V (Z=23) and gallium Ga (Z=31)? Give the four quantum numbers of these valence electrons.

Solution

For transition elements, valence electrons occupy the last shell and the subshell **being** filled.

- For vanadium, there are five valence electrons (s-type and d-type)

V (Z=23) 1s
2
 2s 2 2p 6 3s 2 3p 6 4s 2 3d 3 (according to Klechkowski's rule)

3d corresponds to
$$n = 3$$
, $l = 2$ $m = -2, -1$, 0 , $1, 2$ $ms = +1/2$

4s corresponds to
$$n = 4$$
 $l = 0$ $m = 0$ $ms = \pm 1/2$

- For gallium, there are three valence electrons (s-type and p-type)

Ga (Z = 31) 1s
2
 2s 2 2p 6 3s 2 3p 6 3d 10 4s 2 4p 1

4s corresponds to n = 4, l = 0 m = 0 $ms = \pm 1/2$

4p corresponds to n = 4, l = 1 m = -1, 0, 1 ms = +1/2

Exercise 4

Find the electronic configuration of the following elements and give the possible ions they can form:

- 1. Of an alkali with atomic number Z greater than 12.
- 2. Of an alkaline earth with atomic number equal to 12.
- 3. Of a halogen with atomic number less than 18.
- 4. From a rare gas of the same period as chlorine (Z = 17).
- 5. Of the third halogen.
- 6. From the second transition metal.
- 7. Of the fourth alkali.

Solution

- ${f 1}$. K (19): [Ar] 4s 1 only one possible ion K $^+$. K tends to have the stable structure of the inert gas argon.
- **2.** Mg (12): [Ne]3s 2 two possible ions Mg $^{2+}$ and Mg $^+$
- 3. Cl (17): [Ne]3s 2 3p 5 only one possible ion Cl- (structure of argon: inert gas
- **4.** Ar (18): [Ne]3s ² 3p ⁶ there is no possible ionization because its state is stable; it is an inert gas
- **5.** Br (35): [Ar]3d 10 4s 2 4p 5 only one possible ion Br $^{-}$ (structure of the inert gas krypton)
- **6.** Ti (22): [Ar]3d ² 4s ² four possible ions Ti ⁴⁺, Ti ³⁺, Ti ²⁺ and Ti ⁺.(Ti ⁴⁺, Ti ³⁺ are the most stable)
- **7.** Rb (37): [Kr]5s 1 only one possible ion Rb $^{+}$

Exercise 5

Molybdenum (Mo) belongs to the chromium family Cr (Z=24) and to the fifth period. Give its

electronic configuration and atomic number.

Solution

The electronic structure of chromium Cr: [Ar] 3d ⁵ 4s ¹. It belongs to the family of transition

metals with an electronic structure of the valence layer of type (n-1)d 5 ns 1

Molybdenum Mo belongs to the same family as chromium and to the 5th period, therefore the

structure of its valence layer is of type (n-1)d5ns1 with n=5:

Mo: $[Kr]4d^5 5s^1 => Z = 42$

Exercise 6

We consider two elements of the fourth period whose external electronic structure has three

single electrons.

1. Write the complete electronic structures of each of these elements and determine their

atomic number.

2. Justifying your answer, determine the atomic number and give the electronic configuration

of the element located in the same period as iron (Z = 26) and belonging to the same family as

carbon (Z = 6).

Solution

1. The two elements are vanadium and arsenic.

Vanadium V: 1s 2 2s 2 2p 6 3s 2 3p 6 4s 2 3d 3

According to Klechkowski's rule

According to the spatial arrangement The atomic number is : Z = 23

Note: By not respecting Klechkowski's rule, the structure would be as follows:

$$1s^2 2s^2 2p^6 3s^2 3p^6 3d^5$$
 This structure is inaccurate.

It will therefore be necessary to respect the Klechkowski rule to have the existing electronic structure.

This can be explained that before filling, the level of the 4s orbital is slightly lower than that of the 3d atomic orbitals, and that after filling, this 4s level becomes higher than the 3d level.

Electronic structure of arsenic

Ace: 1s 2 2s2 2p 6 3s 2 3p 6 4s 2 3d 10 4p 3 according to Klechkowski's rule

$$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^3$$
 according to the spatial arrangement

The atomic number is Z = 33

2- Electronic structure of iron Fe (Z=26):

[Ar] $3d^6 4s^2$; Iron belongs to the 4th period n= 4

Electronic structure of carbon C (Z=6) 1s ² 2s ² ² p ²

So the electronic structure of germanium is: Ge [Ar] 3d 10 4s 2 4p 2

Exercise 7

How many electrons can the third shell hold at most?

How many elements are in the third period of the periodic table?

For what value of Z (number of protons) will the third layer be completely filled?

Solution

² np ² valence shell electronic structure family .

The third layer can contain a maximum of 2n2 electrons, i.e. 18 electrons.

The third period has 8 elements (s block and p block)

The two values of Z, for which the 3rd layer would be filled are:

$$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} Z = 30$$
 (Zinc Zn)

$$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^{10} Z = 29$$
 (exception) (Copper Cu)

Exercise 8

Give the symbols and name the main elements (their valence shell is of type nsx npy where l

 \leq x \leq 2.and $0 \leq$ y \leq 6.) having an outer shell with 8 electrons.

What is the name of their group?

Do they have varied chemical properties?

What are their physical characteristics?

Do they have any uses in industry?

Solution

The main elements with an eight-electron outer shell are the noble gases:

The six noble gases are inert.

They are not harmful to us, which is why they have several uses.

We give some examples of their applications.

Helium:

- In deep-sea diving tanks
- In cryogenics because of its low temperature in the liquid state.

Argon and neon:

- In illuminated signs and in lasers.

Radon:

- In industries, it is used to initiate and influence chemical reactions.
- In devices used to prevent earthquakes.
- In medicine, for anti-cancer treatments.

Xenon:

- In high intensity lamp manufacturing industries
- In ultraviolet lasers.
- In medicine, especially for anesthesia.

Krypton:

- In some incandescent and fluorescent light bulbs
- In lasers and holography
- 1. Sn:

$$1s\ ^2 2s\ ^2 2p\ ^6 3s\ ^2 3p\ ^6 4s\ ^2 3d\ ^{10} 4p\ ^6 5s\ ^2 4d\ ^{10} 5p\ ^2$$

According to Klechkowski's rule

$$1s\ ^2 2s\ ^2 2p\ ^6 3s\ ^2 3p\ ^6 4s\ ^2 3d\ ^{10} 4p\ ^6 4d\ ^{10} 5s\ ^2 5p\ ^2$$

According to the spatial arrangement

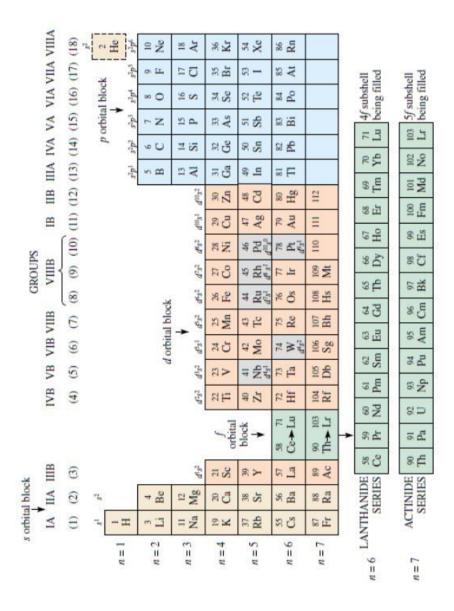
The tin atom has four valence electrons and its atomic number is 50.

2. No, it is not part of the transition metals because the 4d subshell is filled.

Denderneha. $F_1 = 50$ $Z_2 = 90$? = 180 V = 51 N6 = 94 $F_4 = 182$ $C_2 = 52$ $N_0 = 96$ W = 186 $M_1 = 55$ $R_1 = 1044$ $P_2 = 197, 4$ $F_2 = 56$ $R_0 = 1044$ $F_2 = 198$ V. Periodic classification of the elements Be=9.4. Mg=24 Zn=65,2 Co=112 Ma=183? B=11 Al=274 9=68 Mn=116 Na=183? ERNO ANYECTO

V. Periodic table of elements

- 1. In the periodic table, the elements are arranged from left to right in order of increasing atomic number Z.
- 2. A new period is used each time the electronic configuration of the atom corresponding to the element considered involves a new value of the principal quantum number n.
- 3. The atoms of chemical elements in the same column have the same valence electronic configuration; these elements constitute a chemical family and have similar chemical properties.



- 4. The physical and chemical properties of the elements are periodic functions of their atomic numbers :
- 5. Atomic radius: In a column of the periodic table, when the period number (n) increases, the atomic radius increases. In a period, n is constant, Z increases. The screening effect varies little, the electrons tend to be more attracted by the nucleus and consequently the radius decreases.
- 6. Ionization energy: This is the energy required to provide an atom in its ground state (first ionization) or an ion (second or third ionization) to remove an electron from it. It decreases when the atomic radius increases and it increases when the radius decreases.
- 7. Electron affinity: this is the energy released (released in many cases) when an electron is captured by an atom to form an anion.
- 8. Electronegativity: This is the tendency of an atom to attract the electrons of the bond. It varies in the same direction as the ionization energy.

Application exercises

Exercise 1

Let the following atoms be:

- 1. Give the electronic configurations of the atoms. Present the valence electrons for each atom. Deduce the number of valence electrons.
- 2. Place these atoms in the periodic table and group them if possible by family or by period.
- 3. Cesium (Cs) belongs to the same family as potassium (K) and to the same period as gold (Au). Give its electronic configuration and atomic number.

Solution

1. We will write for each element its electronic structure according to the Klechkowski rule and according to the spatial arrangement, and give the number of valence electrons:

Representation of the valence shell using quantum boxes:

| la règle de Klechkowski la d N (7): 1s ² 2s ² 2p ³ | isposition spatiale [He]2s² 2p³ | Nombre d'électrons 5 |
|---|--|-----------------------------------|
| K (19): 1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ¹ | [Ar]4s1 | 1 |
| Sc (21) 1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ² 3d ¹ | [Ar] 3d1 4s2 | 3 |
| Cr (24) 1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ¹ 3d | ⁵ [Ar] 3d ⁵ 4s ¹ | 6 |
| Mn (25)1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ² 3d | ⁵ [Ar]3d ⁵ 4s ² | 7 |
| Fe (26) 1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ² 3d ⁶ | [Ar]3d ⁶ 4s ² | 8 |
| Cu (29) 1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ¹ 3d | ¹⁰ [Ar]3d ¹⁰ 4s ¹ | 11 |
| Zn (30) 1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ² 3d ¹ | ⁰ [Ar]3d ¹⁰ 4s ² | 2 |
| Ag (47) 1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 3d ¹⁰ 4s | s ² 4p ⁶ 5s ¹ 4d ¹⁰ [Kr]4d ¹⁰ 5s ¹ | 11 |
| Au (79) 1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ² 3d | ¹⁰ 4p ⁶ 5s ² 4d ¹⁰ 5p ⁶ 6s ¹ [Xe]5d ¹⁰ 6s ¹ | 4f ¹⁴ 5d ¹⁰ |

Noticed:

In the case of chromium Cr (Z=24), the structure of the valence shell must be according to the Klechkowski rule: 4s 2 3d 4 . This structure is unstable. The most stable structure is therefore 4s1 3d5. The electronic structure of the 3d subshell is half filled.

In the case of copper Cu (Z=29), the structure of the valence layer must be according to the Klechkowski rule: 4s 2 3d 9 , this structure is unstable. The most stable structure is therefore 4s 1 3d 10 . The electronic structure of the 3d sublayer is completely filled. "Half-filled or completely filled d orbitals are more stable"

- 2. 2. Only one element belongs to the period n=2: N (Z=7) (group VA)
- The elements that belong to period n=4 are: K (group IA), Sc (group IIIB), Cr (group VIB), Mn (group VIIB), Fe (group VIIIB), Cu (group IB), Zn (group IIB)
- The elements that belong to the IB family are: Cu (4th period) Ag (5th period), Au (6th period)
- Elements that belong to the transition metal family (their valence shell is of type (n-1) dy nsx where $1 \le x \le 2$ and $1 \le y \le 10$) are: Sc (group IIIB), Cr (group VIB), Mn (group VIIB), Fe (group VIIIB), Cu (group IB), Zn (group IIB).
- 3. Cs: 1s 2 2s 2 2p 6 3s 2 3p 6 4s 2 3d 10 4p 6 5s 2 4d 10 5p 6 6s 1 4f 14 According to Klechkowski 's rule

 $1s2\ 2s2\ 2p6\ 3s\ ^2\ 3p\ ^6\ 3d\ ^{10}\ 4s\ ^2\ 4p\ ^6\ 4d\ ^{10}\ 4f\ ^{14}$. $5s\ ^2$. $5p\ ^6\ 6s\ ^1$ According to the spatial arrangement

The electronic structure of the cesium atom is:

[Xe] 6s ¹ and its atomic number is equal to 55 (Z=55).

Exercise 2

There are currently 6 known elements belonging to the alkaline earth family which are (classified in ascending order of their atomic number): Beryllium – Magnesium - Calcium – Strontium – Barium and Radium.

- 1) Which column of the periodic table does the alkaline earth family occupy?
- 2) Give each one its atomic number and electronic configuration.
- 3) Another element should normally belong in this family but has been excluded. Which one and for what reason?
- 4) If one day we succeed in obtaining a seventh alkaline earth, what will its atomic number and electronic configuration be?
- 5) Using Sanderson 's rule show that these elements are metals.
- 6) What type of ion do alkaline earth metals give?
- 7) What are the formulas of the alkaline earth oxides knowing that they are ionic compounds?
- 8) Are these oxides acidic or basic?

Solution

- 1) Column 2
- 2) It is enough to know that an alkaline earth is equivalent to "a rare gas to which 2 electrons have been added"

| | | Z | Electronic configuration |
|-----------|------|----|--|
| Beryllium | Be | 4 | $1s^2 2s^2 = (He) 2s^2$ |
| Magnesium | Mg | 12 | (He) $2s^2 2p^6 3 s^2 = (Ne) 3s^2$ |
| Calcium | That | 20 | (Ne) $3s^2 3p^6 4s^2 = (Ar) 4s^2$ |
| Strontium | Mr. | 38 | $(Ar) 3 d^{10} 4s^2 4p^6 5s^2 = (Kr) 5s^2$ |
| Barium | Well | 56 | (Kr) 4d 10 5s 2 5p 6 6s 2 = (Xe) 6s 2 |
| Radium | Ra | 88 | $(Xe)4f^{14}5d^{10}6s^{2}6p^{6}7s^{2} = (Rn)7s^{2}$ |

3) Helium He: Z = 2 or 1s 2 2s 2 but it belongs to the family of rare gases (chemically almost inert) and is therefore placed in column 18.

4)
$$Z = 120$$

(Rn)
$$7s^2 5f^{14} 6d^{10} 7p^6 8s^2$$

Sanderson 's rule states that elements whose number of electrons in the outer shell is less than their period are metals; otherwise, they are non-metals.

- 6) They lose their two ns2 electrons to resemble the previous noble gas: X^{2+} .
- 7) O takes 2 electrons to look like Ne or O ²⁻

$$M^{2+} + O^{2-} \rightarrow MB$$

8) With only 2 electrons in their valence shell, alkaline earths are all metals and their oxides are therefore basic. (Sanderson 's rule).

Exercise 3

An element has less than 18 electrons and has 2 unpaired electrons. What are the possible electronic configurations for this element? What is this element knowing that it belongs to the lithium period(3) and the tin group(50).

Solution

The element in question belongs to one of the first three lines of the classification.

The quantum box representation shows that only the p 2 and p 4 configurations have "exactly" two single electrons. We can also consider that the s 2 p 3 configuration can be suitable since it has 3 single electrons. The element in question can therefore only be: C, Si, O, S, N or P.

We know that it belongs to the lithium period, so Si, S and P are eliminated.

Let's look for the configuration of tin (Z = 50)

$$50 = 36 + 14$$
 to (Kr) 4d 10 5s 2 5p 2

The element sought belonging to the same group as tin is therefore Carbon C.

Exercise 2

What are the elements that are different? Explain.

- a. Lithium and potassium
- b. Carbon and Neon
- c. Sulfur and oxygen
- d. Aluminum and thallium

Solution

b. Carbon and neon, because they belong to different groups. Neon is a noble gas with 8 valence electrons. Carbon is a nonmetal with only 4 valence electrons.

Exercise 3

Determine which atom is larger in each pair of elements.

- a. Na or Mg
- b. Ga or Al
- c. As or Cs
- d. Br or Fe

Solution

a) Na or Mg:

If we look at the periodic table on the far left, you will find both sodium and magnesium. If you look in the first row, you will find sodium and to the right of it, you will find magnesium. Looking at our rules, from left to right the atomic radius decreases, so sodium has a larger atomic radius! Na is larger than Mg.

B) Ga or Al

When you locate the two elements on the periodic table, you will notice that both of them are in the same column.

From our rules, we know that the lower the element is in the periodic table, the larger the radius! So, of the two elements, gallium is the larger of the two in terms of atomic radius!

Ga is larger than Al.

C) As or Cs

With Cesium on the first row, and almost at the bottom of the table of elements, we assume from our rules that Cesium carries a large atomic radius. We locate the Ace which is two rows below and to the far right of the table.

The rules state that from left to right, atoms decrease, and going down the slope of the table, they increase. So for both cases of these rules, cesium has a larger radius, making it the larger atom.

Cs is greater than As.

D) Br or Fe

Located on the same row, we see that Iron is located further to the left of the periodic table than Bromine. The rules once again state that as the elements move from left to right, the atomic radius decreases, making Bromine the smallest atom.

because of its location in the periodic table relative to iron. Iron in this case is the largest atom.

Fe is greater than Br.

Exercise 4

List these elements in descending order of their first ionization energy: In, F, Se, Br.

Solution

- a. Determine the location of the elements on the periodic table
- b. Recall the increasing trend of ionization energy in KJ/mol (exception in the case of boron) from left to right on the periodic table
- c. Remember the decreasing trend of ionization energies (Kj /mol) from top to bottom (Cs is the exception in the first group).

So in descending order of first ionization energy:

F > Br > Se > In

Exercise 5

To which second period element do these ionization values belong?

Solution

To understand and solve this problem, you must first understand the definition of ionization energy. You must also know which elements belong to which period.

From left to right, the ionization energy increases, which makes sense because metals (left side) lose electrons easily, while nonmetals (right side) do not. That being said, every ionization energy of an element means we have lost an electron.

The question gives you 4 values, which means that this particular element can lose 4 electrons. This eliminates lithium since it only has 3 all together. Also, when there is a big

jump from one value to another, it means that you have gone from valence electrons to core electrons. This is because core electrons are harder to remove. Notice that between the second and third values, there is a significant jump in energy. This means that after removing two valence electrons, we have entered core electron territory. The only element that has 2 valence

electrons in the second period is beryllium.

Exercise 6

According to the given ionization energies, how many valence electrons does the following

atom have?

IE = 1,402.3 kJ/mol

IE = 2,856.0 kJ/mol

IE = 4,578.1 kJ/mol

IE = 7,475.0 kJ/mol

IE = 9,444.9 kJ/mol

IE = 53,266.6 kJ/mol

IE = 64,360.0 kJ/mol

Solution

We know that the ionization energy is much larger for the inner orbitals than for the outer orbitals. So, looking at the given ionization energies, we can see that the 6 ionization energy is

much larger than the 5.

This means that electron 5 is the last electron in the outer shell, which means that this atom

has 5 valence electrons.

Exercise 7:

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1) Determine the Pauling electronegativities of the F and Cl atoms. We will take k=2.2 for H.

We know that HF and HCl are acids that dissociate into X^- and H^+ , so F and Cl are more electronegative than H.

Solution

Pauling electronegativity can be calculated using either the arithmetic mean or the geometric mean.

Arithmetic mean: DX 2 = { E_{AB} - 1/2 (E_{AA} +E_{BB}) } / k

If we use energies in kJ.mol-1: k = N e / 1000 = F / 1000 = 96.5

$$(X_F - X_H)^2 = \{ E_{HF} - 1/2 (E_{HH} + E_{FF}) \} / k$$

$$X_F -$$

$$(X_F - X_H) = 1.676$$

$$X_F = 2.2 + 1.676 = 3.88$$

$$(X_{Cl}-X_{H})^2 = \{E_{HCl}-1/2(E_{HH}+E_{ClCl})\}/k$$

$$(X_{Cl} - X_{H})^2 = \{431 - 1/2 (435 + 242)\} / 96.5 = 0.958$$

$$(X_{Cl} - X_H) = 0.979$$

$$X_{Cl} = 2.2 + 0.979 = 3.18$$

$$\underline{Geometric\ mean}$$
 : DX 2 = { E $_{AB}$ - (E $_{AA}$ *E $_{BB}$) $^{1/2}$ } / k

If we use energies in kJ.mol-1: $k=N\ e\ /\ 1000=F\ /\ 1000=96.5$

(X
$$_{F}-$$
 X $_{H}$) $^{2}=$ { E $_{HF}$ - (E $_{HH}$ +E $_{FF})$ } $^{1/2}$ / k

$$X_F$$

$$(X_F - X_H) = 1.78$$

$$X_F = 2.2 + 1.78 = 3.98$$

(
$$X_{Cl} - X_{H}$$
) $^2 = \{ E_{HCl} - (E_{HH} * E_{ClCl})^{1/2} \} / k$

$$(X_{Cl} - X_H) = 1.05$$

$$X_{Cl} = 2.2 + 1.05 = 3.25$$

Exercise 8

Let the elements of the periodic table be: 11 Na, 13 Al, 17 Cl, 22 Ti, 26 Fe, 29 Cu, 35 Br, 37 Rb, 40 Zr.

 1° / Give the electronic configuration in the ground state of each of the elements in simple form and in abbreviated form (core structure) .

2°/ Place the different elements in the periodic table by giving the period, group, subgroup, column, block and family.

3°/ Which ions will they give preferentially? Justify the answer.

4°/ Classify the elements 17 Cl, 22 Ti, 26 Fe, 29 Cu, 35 Br, 37 Rb, 40 Zr in decreasing order of atomic radius and ionization energy.

Solution

1°/ Electronic configuration in the ground state

- **Simple form**: distribution of electrons in subshells.
- **Short form**: use of rare gases as "core structure".

| Element | Simple form | Short form |
|------------------|---|--------------------------------------|
| ₁₁ Na | 1s ² 2s ² 2p ⁶ 3s ¹ | [Ne] 3s ¹ |
| ₁₃ Al | 1s ² 2s ² 2p ⁶ 3s ² 3p ¹ | [Ne] 3s ² 3p ¹ |
| ₁₇ Cl | 1s ² 2s ² 2p ⁶ 3s ² 3p ⁵ | [Ne] 3s ² 3p ⁵ |
| 22 Ti | 1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ² 3d ² | [Ar] 4s ² 3d ² |
| ₂₆ Fe | 1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ² 3d ⁶ | [Ar] 4s ² 3d ⁶ |

| ₂₉ Cu | 1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ¹ 3d ¹ ⁰ | [Ar] 4s ¹ 3d ¹ |
|------------------|--|---|
| 35 Br | 1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ² 3d ¹ ⁰ 4p ⁵ | [Ar] 4s ² 3d ¹ ⁰ 4p ⁵ |
| 37 Rb | 1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ² 3d ¹ ⁰ 4p ⁶ 5s ¹ | [Kr] 5s ¹ |
| 40 Zr | 1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ² 3d ¹ ⁰ 4p ⁶ 5s ² 4d ² | [Kr] 5s ² 4d ² |

$2^{\circ}\!/\,Location$ in the periodic table

| Element | Period | Band | Subgroup | Column | Block | Family |
|------------------|--------|------|-----------------|--------|---------------|-------------------|
| ₁₁ Na | 3 | I | Main 1 s Alkali | | Alkali metals | |
| ₁₃ Al | 3 | III | Main | 13 | p | Poor metals |
| ₁₇ Cl | 3 | VII | Main | 17 | p | Halogens |
| 22 Ti | 4 | IV | Secondary | 4 | d | Transition metals |
| ₂₆ Fe | 4 | VIII | Secondary | 8 | d | Transition metals |
| 29 Cu | 4 | I | Secondary | 11 | d | Transition metals |
| 35 Br | 4 | VII | Main | 17 | p | Halogens |
| 37 Rb | 5 | I | Main | 1 | S | Alkali metals |
| 40 Zr | 5 | IV | Secondary | 4 | d | Transition metals |

$3^{\circ}\!/\,Preferential$ ions and justification

| Element | Preferential ions | Justification |
|------------------|---------------------------------------|---|
| ₁₁ Na | Na ⁺ | Loss of 1 electron to reach [Ne]. |
| 13 Al | Al ^{3 +} | Loss of 3 electrons to reach [Ne]. |
| ₁₇ Cl | Cl - | Gain 1 electron to reach [Ar]. |
| ₂₂ Ti | Ti ^{3 +} , Ti ⁴⁺ | Loss of 3 or 4 electrons to reach a stable configuration ([Ar]). |
| ₂₆ Fe | Fe ^{2 +} , Fe ^{3 +} | Loss of 2 or 3 electrons for a d subshell and a stable rare gas. |
| ₂₉ Cu | Cu + , Cu 2 + | Loss of 1 or 2 electrons, stabilization by the complete d subshell. |

| 35 Br | Br - | Gain 1 electron to reach [Kr]. |
|-------|------------------|------------------------------------|
| 37 Rb | Rb + | Loss of 1 electron to reach [Kr]. |
| 40 Zr | Zr ⁴⁺ | Loss of 4 electrons to reach [Kr]. |

4°/ Sorting in descending order

Criteria:

- **Atomic radius**: Increases when descending in a group and decreases when advancing in a period. - **Ionization energy**: Decreases when descending in a group and increases when advancing in a period. **a) Atomic radius (decreasing order)* *:

$$37Rb > 40Zr > 35Br > 29Cu > 26Fe > 22Ti > 17Cl$$

**b) Ionization energy (decreasing order)* *:

$$17Cl > 35Br > 29Cu > 26Fe > 22Ti > 40Zr > 37Rb$$

Exercise 9

Let the elements of the periodic table be: A, B, C, D, E, F and G

| Elément | A | В | C | D | E | F | G |
|---------|--------|--------|--------|---------|-------|---------|-------|
| Groupe | II_A | II_A | II_B | V_{B} | I_A | VII_A | VIIIA |
| Période | 4 | 5 | 4 | 4 | 5 | 4 | 4 |

- 1° / Establish the electronic configurations and deduce the atomic number Z of each element. Indicate the family to which each element belongs.
- 2° / Give the valence shell. Indicate the number of core electrons and the number of valence electrons.
- **3**°/ Give the most stable ion likely to form for each element.
- **4**°/ Assign to each element its atomic radius and its electronegativity among the following values:

| Rayons (Å) | 2.48 | 1.74 | 1.17 | 1.25 | 1.91 | 1.22 |
|-------------------|------|------|------|------|------|------|
| Electronégativité | 1.66 | 1.04 | 2.74 | 0.99 | 1.45 | 0.89 |

Solution

$1^{\circ}\!/\,Electronic$ configuration and atomic number

| Element | Electronic configuration | Z | Family |
|---------|---|----|-----------------------|
| HAS | [Ar] 4s ² | 20 | Metals alkaline earth |
| В | [Kr] 5s ² | 38 | Metals alkaline earth |
| С | [Ar] 4s ² 3d ¹ | 30 | Transition metals |
| D | [Ar] 4s ² 3d ³ | 23 | Transition metals |
| Е | [Kr] 5s ¹ | 37 | Metals alkaline |
| F | [Ar] 4s ² 3d ¹ ⁰ 4p ⁵ | 35 | Halogens |
| G | [Ar] 4s ² 3d ¹ ⁰ 4p ⁶ | 36 | Noble gases |

2°/ Valence layer and electrons

| Element | Valence layer | Heart Electrons | Valence electrons |
|---------|--|-----------------|-------------------|
| HAS | 4s ² | 18 | 2 |
| В | 5s ² | 36 | 2 |
| С | 4s² 3d¹ 0 | 18 | 12 |
| D | 4s² 3d³ | 18 | 5 |
| Е | 5s ¹ | 36 | 1 |
| F | 4s ² 3d ¹ 0 4p 5 | 18 | 7 |
| G | 4s ² 3d ¹ ⁰ 4p ⁶ | 18 | 8 |

3°/ Most stable ions

| Element | Stable ion | Justification |
|---------|------------------|------------------------------------|
| HAS | A ^{2 +} | Loss of 2 electrons to reach [Ar]. |

| В | B ^{2 +} | Loss of 2 electrons to reach [Kr]. |
|---|------------------|--|
| С | C ^{2 +} | Loss of 2 electrons for stabilization. |
| D | D ₃ + | Loss of 3 electrons to reach a stable configuration. |
| Е | E + | Loss of 1 electron to reach [Kr]. |
| F | F - | Gain 1 electron to reach [Ar]. |
| G | G | Noble gas, does not form ions. |

4°/ Atomic radius And electronegativity

| Element | Atomic radius (Å) | Electronegativity |
|---------|-------------------|-------------------|
| HAS | 1.74 | 1.66 |
| В | 2.48 | 1.04 |
| С | 1.22 | 1.45 |
| D | 1.25 | 1.89 |
| Е | 2.48 | 0.99 |
| F | 1.17 | 2.74 |
| G | 1.22 | 0.89 |

Exercise 10

Find the electronic configuration of the following elements and determine the stable ions they can form:

- a. The 6th transition element.
- b. An alkali metal from the 3rd period.
- c. An alkaline earth metal from the 4th period.
- d. A halogen from the 5th period.
- e. A noble gas in the same period as ^{34}Se .
- f. An element in the same period as ^{20}Ca and the same group as ^{43}Tc .
- g. An element in the same period as ^{23}V and the same group as ^{16}S .

Solutions

a. The 6th transition element

- ullet Element: Cr (Chromium)
- Electronic Configuration: $[Ar]3d^54s^1$
- Stable Ion: Cr^{3+}

b. An alkali metal from the 3rd period

- Element: Na (Sodium)
- Electronic Configuration: $[Ne]3s^1$
- Stable Ion: Na^+

c. An alkaline earth metal from the 4th period

- Element: Ca (Calcium)
- Electronic Configuration: $[Ar]4s^2$
- Stable Ion: Ca^{2+}

d. A halogen from the 5th period

- Element: I (lodine)
- ullet Electronic Configuration: $[Kr]4d^{10}5s^25p^5$
- ullet Stable Ion: I^-

e. A noble gas in the same period as ^{34}Se

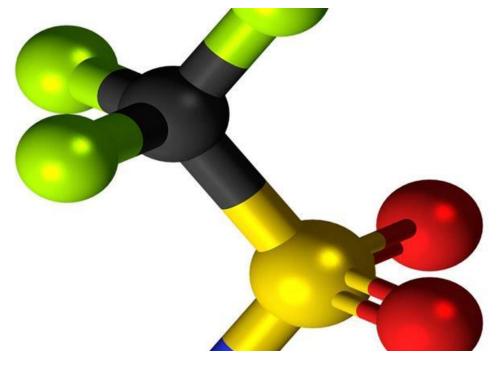
- Element: Kr (Krypton)
- Electronic Configuration: $[Ar]3d^{10}4s^24p^6$
- Stable Ion: None, noble gases are chemically inert.

f. An element in the same period as ^{20}Ca and the same group as ^{43}Tc

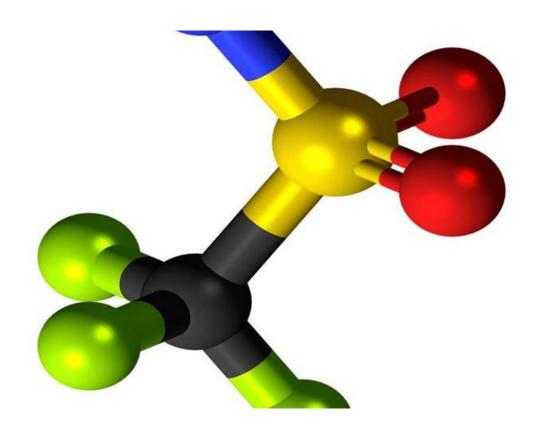
- Element: Mn (Manganese)
- Electronic Configuration: $[Ar]3d^54s^2$
- ullet Stable Ion: Mn^{2+} , Mn^{4+}

g. An element in the same period as ^{23}V and the same group as ^{16}S

- Element: P (Phosphorus)
- Electronic Configuration: $[Ne]3s^23p^3$
- Stable Ion: P^{3-}



The chemical bond



VI. Chemical bond

1. Valence electrons: The last electron shell partially or completely filled

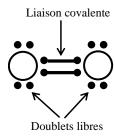
If:
$$1s^2 2s^2 2p^6$$
 $3s^2 3p^2$

Centrals Valence

[Ne]
$$3s^2 3p^2$$

$$=>$$
 If: [Ne] 3s 2 3p 2

2. Covalent bond: is a chemical bond in which two atoms share two electrons from one of their outer shells in order to form an electron doublet linking the two atoms.



3. Dative bond (coordination bond): Is a description of the covalent bond between two atoms for which the two electrons shared in the bond come from the same atom.

$$A \square + B \longrightarrow A - B$$

4. Ionic bond: Can be formed by a pair of atoms having a large difference in electronegativity

$$Na \circ + \circ Cl \circ \longrightarrow Na^+ + Cl^- \longrightarrow NaCl$$

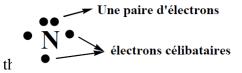
5. The Lewis Molecular Diagram

In the Lewis Molecular diagram, we present the molecule by showing how the atoms are linked together. We show not only the chemical bonds between atoms (X doublets) but also the electrons that do not participate in the bonds (E doublets).

A B

Lewis notation represents valence e

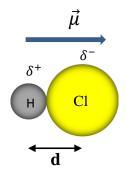
e Doublets de liaison (X) nding the element symbol.



6. Dipole moment: Equal to th

of each of its bonds:

$$\|\vec{\mu}\| = \mu = \delta * d$$
 μ = vector quantity having a direction, a sense and a module $q = \text{coulomb charge} > 0$
 $d = \text{distance between charges in meters}$



7. Geometry of molecules: Gillespie theory or VSEPR

| m + n | Basic Geometries |
|-------|-------------------------|
| 2 | linear |
| 3 | triangular plane |
| 4 | tetrahedral |
| 5 | trigonal bipyramid |
| 6 | octahedral |



AX2E0: l'édifice est linéaire; BeH2, CO2, HCN,...

m + n = 3: doublets d'électrons pointant vers les sommets d'un triangle



AX₃E₀: Γédifice triangulaire; AICl₃, NO₃, SO₃,...



 AX_2E_1 : édifice coudé ; SnCl₂, O₃, SO₂,...

m + n = 4: doublets d'électrons pointant vers les sommets d'un tétraèdre



AX₄E₀: édifice tétraédrique; CH₄, SO₄², OPCl₃,...



AX₃E₁: édifice pyramidal à base triangulaire; NH₃, OSCl₂,...



 AX_2E_2 : édifice coudé; H_2O , SCl_2 , $ClO_{\overline{2}}$,...

m + n = 5: doublets d'électrons pointant vers les sommets d'une bipyramide à base triangulaire



AX₅E₀: édifice bipyramidal à base triangulaire PCl₅, SOF₄,...



AX₄E₁: édifice tétraédrique irrégulier en papillon SF₄, XeF₂O₂,...



 AX_3E_2 : édifice en T; $CIF_3,...$



AX₂E₃: édifice linéaire; 13,...

m + n = 6: doublets d'électrons pointant vers les sommets d'un octaèdre



 AX_6E_0 : édifice octaédrique; SF₆, $PCl_{\overline{6}}$, IF_5O ,...



AX₅E₁: édifice pyramidal à base carrée, BrF₅, XeF₄O,...



AX₄E₂: édifice carré; BrF₄, XeF₄....

Exercise 1

Draw the best Lewis dot structure for each of the following species.

a) BeF
$$_2$$
 , b) BCl $_3$, c) CCl $_4$, d) PBr $_5$, e) SI $_6$

Solution

| Species Name | Lewis Dot Structure | Electronic Arrangement | Molecular Geometry |
|-------------------------------|----------------------------|------------------------|----------------------|
| BeF ₂ | : <u>F</u> —Be— <u>F</u> : | linear | linear |
| BCl ₃ | :Či Či: | trigonal planar | trigonal planar |
| CCI ₄ | :ä:c-:ä: | tetrahedral | tetrahedral |
| PBr ₅ | :Br: Br: Br: Br: Br: | trigonal bipyramidal | trigonal bipyramidal |
| SI ₆ | | octahedral | octahedral |
| $\mathrm{BH_2}^-$ | н — Ё — н | trigonal planar | bent |
| NI ₃ | ii. ii. —∷i: | tetrahedral | trigonal pyramidal |
| CIF ₄ ⁺ | | trigonal bipyramidal | see saw |
| SF ₅ ⁻ | :F:F: | octahedral | square pyramidal |

Exercise 2

Are these compounds ionic or covalent?

CH₄

FeO₃

KNO₃

 I_2 C_4

 H_2O

BeCl₂

Solution

From left to right: Covalent, Ionic, Ionic, Covalent, Covalent, Covalent, Ionic.

Exercise 3

Draw the Lewis structures of the following molecules and, if necessary, assign charges, and identify the polar covalent bonds with δ + and - δ on the atoms based on their electronegativity.

- a. BrF
- b. ClCN
- c. SOCl 2
- d. CH ₃ CH ₂ NH ₂
- e. CH 3 CH 2 OCH 2 CH 3
- f. (CH₃)₂NNH₂
- g. CH 3 NCNCH 3
- h. CH 3 COOH
- i. N₂O₄

Solution

Lewis structures of molecules

Polar covalent bonds

Exercise 4

Draw the Lewis structures of the following species and, if necessary, assign charges. a. H $_3$ O $^+$

- b. NH ₄ +
- c. CH₃CH₂⁺
- d. CH $_3$ CH $_2$ $^+$
- e. CH₃CH₂
- f. CH₃CH
- g. H ⁺
- h. CH₃COO⁻

Solution

Exercise 5

Let us find the formal charges in Cl₃ AlNH₃.

Solution

- The aluminum atom (Z = 13), with the electronic configuration in its state
- fundamental 1s2 2s2 2p6 3s2 3p1, has three valence electrons, Nv (Al) = 3.
- the chlorine atom (Z = 17), with the electronic configuration in its ground state 1s2 2s2 2p6 3s2 3p5, has seven, Nv (Cl) = 7,
- the nitrogen atom has five and the hydrogen atom has one.

Hence the number of valence electrons in the molecule to be taken into account:

$$Ne = 3 \times 7 + 3 + 5 + 3 \times 1 = 32$$

Let there be sixteen doublets to place ($D = \frac{32}{2} = 16$).

Knowing the sequence of atoms, we first obtain:

$$|\overline{CI}| \quad H$$

$$|\overline{CI} - AI - N - H$$

$$|\underline{CI}| \quad H$$

In this structure, the aluminum atom has four bonding pairs, so we can assign it four valence electrons and a formal charge number z $_f = N_v - N_a = 3 - 4 = -1$.

the nitrogen atom also has four doublets, i.e.

$$N_a = 4$$
 and $z_f = N_v - N_a = 5 - 4 = +1$.

Chlorine atoms have three lone pairs and one bonding pair, i.e.

$$N_v = N_a$$
 and $z_f = 0$.

Hydrogen atoms have a bonding pair, i.e.

$$N_v = N_a$$
 and $z_f = 0$.

Lewis's representation of this building is deduced from this:

$$\begin{array}{c|c} |CI| & H \\ |\underline{CI} - AI - N - H \\ |\underline{CI}| & H \end{array}$$

Exercise 6

Add charges to the following Lewis structures, if they are neutral, add no charges.

Solution

Exercise 7

Predict the geometry for each atom highlighted in red and give the hybridization of this center.

Solution

a. dichloroethane: The carbon center highlighted is tetrahedral with sp hybridization; it is linked to four other groups.

sp hybridization; it is bonded to three groups and has no lone pairs.

c. propene: The carbon center is trigonal planar with sp hybridization; it is bonded to three groups and has no lone pairs.

sp hybridization; it is bonded to two groups without lone pairs.

e. triethylamine: The nitrogen center is tetrahedral with sp hybridization; it is linked to three groups with a lone pair.

triethylammonium ion : The nitrogen center is tetrahedral with sp hybridization ; it is linked to four groups without

pairs . All are sigma bonds.

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