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✓ General Chemistry 1 ✓

Contents:

- I. Atomic structure
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- IV. The Hydrogen atom in Quantum Mechanics
- V. The polyelectron atoms in Quantum Mechanics
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- VIII. Intermolecular forces (bonds of weak energy)

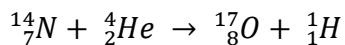
✓ Histoire (Demandée aux examens) ✓

• Les hypérons peuvent être considérés comme des états excités des protons et des neutrons (nucléons).

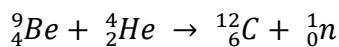
• L'existence du neutrino a été prévu par Pauli en 1927.

• Thomson a pu déterminer: $|\frac{e}{m}| = 1,759 \times 10^{-11} \text{ C/kg}$.

• L'équation de la réaction de l'expérience de Rutherford est:



• L'équation de la réaction de l'expérience de Chadwick est:



• Un proton est constitué de 2 quarks up et 1 quark down.

• Les expériences de Millikan permirent de déterminer la charge de l'électron = $-1,602 \times 10^{-19} \text{ C}$

• L'expérience de Rutherford a montré que l'atome est essentiellement constitué de l'espace vide.

• L'expérience de Rutherford a permis de détecter le noyau.

• Stoney proposa le nom d'électrons aux particules formant les rayons cathodiques.

• Le passage de l'électron d'un atome d'hydrogène fondamental à un état excité correspond au spectre d'absorption atomique de la série de Lyman.

• L'expérience des rayons cathodiques a montré que toute forme de matière contient des électrons.

• Millikan est surtout connu pour sa détermination de la charge de l'électron.

• Le principe de correspondance dit qu'une particule tend à se comporter d'une manière classique lorsque n tend vers l'infini.

• Les rayons canaux sont constitués par des charges positives découverts par Goldstein. Et en 1912 Thomson les appela protons.

- Un neutron est constitué de 2 quarks down et 1 quark up.
- Le volume essentiel de l'atome est essentiellement celui occupé par le nuage électronique.
- Dirac prévu l'existence du positon en 1932.
- En 1932, Dirac a énoncé son fameux theorem: "Pour chaque particule qui existe, il existe son anti-particule".
- L'existence du positron fut confirmée en 1933 par les travaux de Anderson, à l'aide d'une chambre de Wilson.
- En 1957, on a découvert l'anti-proton(-) et l'anti-neutrino.
- Les expériences de Thomson permirent de préciser le rapport de la masse à la charge d'un electron.
- Sommerfield améliora le modèle atomique d BOHR en remplaçant la trajectoire circulaire par une elliptique.
- Le principe qui permet d'établir le passage entre la physique classique et la physique quantique est appelé principe d correspondance.
- Chadwick et Juliet ont montré que les rayons γ frappant un metal lourd donnaient naissance à un couple négaton-positon présentant la même énergie totale.
- Rutherford put estimer que le rayon du noyau de l'atome d'or est de l'ordre du 1/10000 du rayon de l'atome.
- Lors du bombardement du beryllium par des particules α , Chadwick attribua les rayonnements observés à un nouveau type de particules neutres.
- La charge d'un quark u est égale à +2/3 e.
- La charge d'un quark d est égale à -1/3 e.
- En 1926, Heisenberg énonce son principe d'incertitude.
- D'après Bohr le module du vecteur moment cinétique de l'électron d'un atome d'hydrogène est égal à $\frac{nh}{2\pi}$.
- D'après Rutherford, l'expérience de l'énergie de l'électron d'un atome d'hydrogène est de la forme (en fonction de r) $\frac{-e^2}{8\pi\varepsilon_0 r}$.
- Les mésons peuvent être considérés comme des états excités des électrons.

- Travaux d'Anderson (1936-1938) ont permis de découvrir les mésons.

- Le principe de correspondance a été élaboré par BOHR.

→PAULI

- Né en 1900, a pu mettre en évidence les désintégrations radio-actives avec émission d'un électron β^- .

- 1925, il a défini le principe de l'exclusion.

- En 1931, il a émis une hypothèse sur l'existence du neutrino.

- En 1945, il a reçu le prix Nobel en physiques.

→THOMSON (1856-1940)

- Il a reçu le prix Nobel en 1906 en physique pour ses travaux sur la conduction de l'électricité par un gaz.

- En 1898, théorie du pain raisin.

→DIRAC (1902-1984)

- En 1928, il a énoncé la théorie relativiste pour décrire les propriétés de l'électron.

- En 1933, prix Nobel en physique. (a été partagé par Dirac et Erwin Schrödinger)

- En 1930, il a écrit un ouvrage sur les principes de la mécanique quantique.

→Einstein (1879-1955) a reçu un prix Nobel en 1921.

Autres

- Rutherford (1871-1937) a reçu le prix Nobel en chimie en 1908.

- Plank (1858-1947) a reçu le prix Nobel en 1919.

- Bohr (1885-1962) a reçu un prix Nobel en 1922.

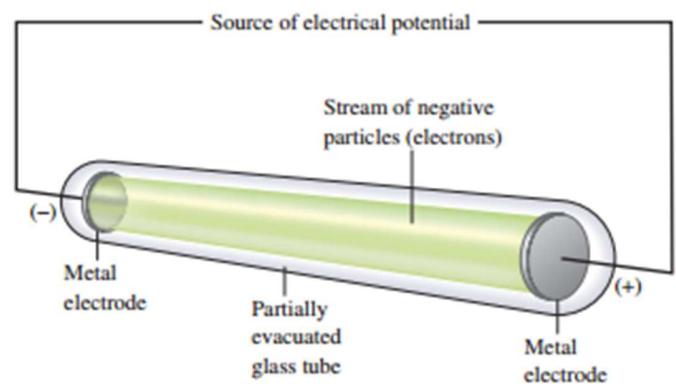
- Heisenberg (1901-1976) a reçu le prix Nobel de physique en 1932.

- Louis de Broglie a reçu le prix Nobel de physique en 1929 pour sa découverte de la nature ondulatoire des électrons en 1924.

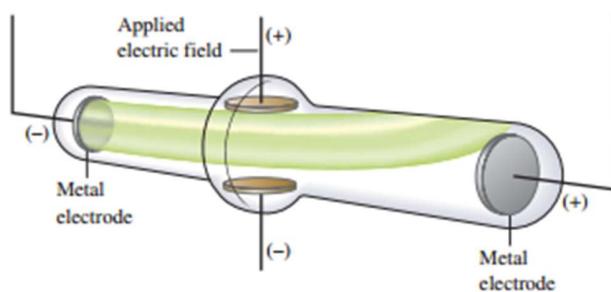
✓ Chapter I: Structure of atoms ✓

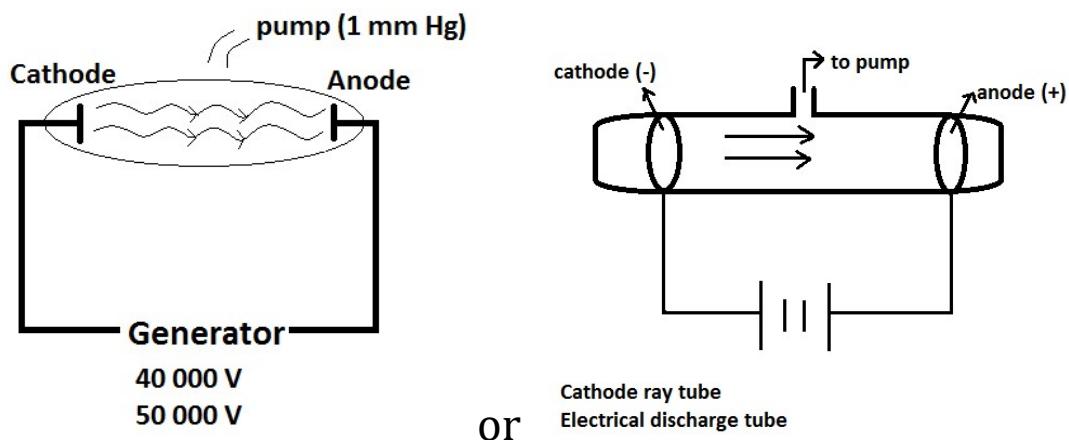
I. Discovery of the subparticles of the atom:

1. Discovery of the electrons: The cathode ray tube experiment:



Deflection of cathode rays by an applied electric field.





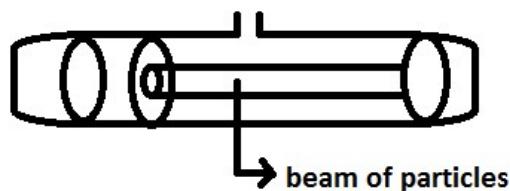
Atmospheric pressure 760 mmHg

Glass tube length = 50 cm

$p = 5-6 \text{ mmHg}$ (light inside the tube)

$p=1 \text{ mmHg}$ (Crooke's dark space) (Observation of a dark space)

$p<0.01 \text{ mmHg}$ (Interaction between the electrons and the glass)
(dark space occupies all the volume)



So the properties of these particles are independent of the nature of the cathode and anode.

Properties:

- Linear Path
- Very charged (put in electric field to test it)
- Different nature than sun rays
- Have a mass

- Traveling from the cathode to the anode
- Thomson ≈ 1890 's

$$\frac{e}{m_e} = -1.759 \times 10^{11} C \cdot kg^{-1}$$

- Millikan

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

$$m_e = 9.108 \times 10^{-3} \text{ } Kg = 0.511 \text{ } MeV/c^2$$

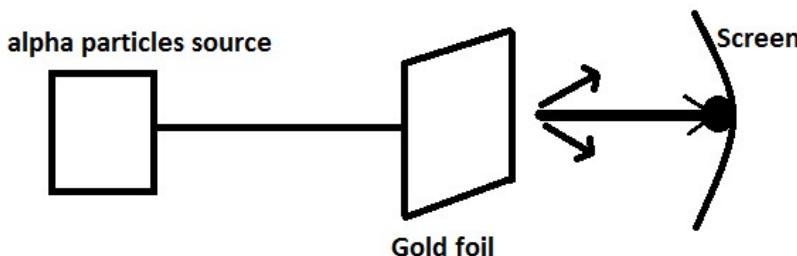
2. Discovery of canal rays: Goldstein (1886)

In addition to the already known cathode rays, recognized as electrons moving from the cathode toward the anode, there is another ray (positively charged) that travels in the opposite direction.



3. Discovery of the nucleus: Rutherford experiment (1910)

- More than 99.9 % went through without deviation
- Some were scattered
- A very small % were repelled (Something big and positively charged went through empty space)



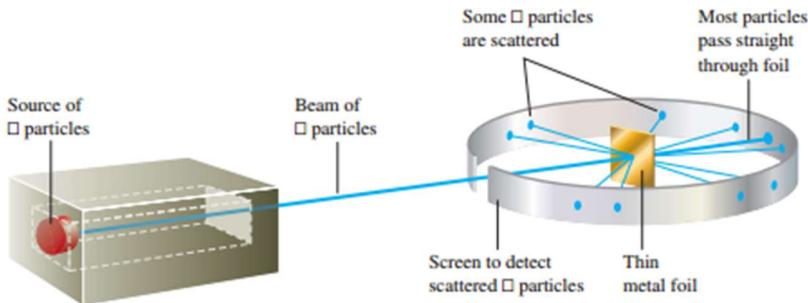


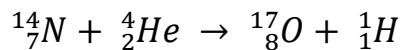
FIGURE 2.II

Rutherford's experiment on α -particle bombardment of metal foil. (Gold foil was used in the original experiments because it can be hammered into extremely thin sheets.)

$$d_{nucleus} \simeq \frac{1}{10^4} d_{atom} \text{ (important)}$$

- ✓ Nuclei have diameters of about $10^{-15} m$ whereas atomic diameters are about $10^{-10} m$.

4. Discovery of protons: Rutherford (1919)



Charge $e^+ = +1.60219 \times 10^{-19} C$

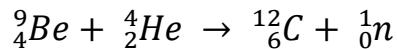
Mass $m_p = 1.67265 \times 10^{-27} Kg = 938.259 MeV/c^2$

5. Discovery of Neutrons: Chadwick (1932)

- ✓ All elements produce neutrons when they are bombarded by high energy $\alpha - particles$.
- ✓ Neutrons are non-stable because they don't have charge.

Charge: 0 C

Mass: $m_n = 1.67495 \times 10^{-27} Kg = 939.259 MeV/c^2$



II. Discovery of other particles in matter

Predicted by Dirac (1928), observed by Anderson (1932), confirmed by Joliot Curie (1933).

Neutrino ν_0 : neutral

Pauli 1927 → 1956

$$m = \frac{1}{1000} m_e$$

$$m_n = m_p = 1837 m_e$$

- ✓ Very light particle
- ✓ High penetrating power
- ✓ Harmless / chargeless

Families of:

Mesons: $206 m_e \leq m \leq 272 m_e$

Hyperons : $2181 m_e \leq m \leq 2585 m_e$

III. Matter and anti-matter

Positron → anti-particle of electron

Anti-proton: same mass , different charge

Anti-neutron: different magnetic composition

Particle + anti-particle → Energy

ex: electron + anti-electron → Energy

$$\beta^- \rightarrow \begin{array}{c} \uparrow \\ \curvearrowleft \\ \downarrow \end{array} \quad \leftarrow \beta^+ \quad \Delta E = \Delta mc^2 = (m_{\beta^-} + m_{\beta^+})c^2 = 2m_e c^2$$

IV. Quarks: 6 types called flavors

- 1) up (u) Charm (c) Top (t) (+2/3 e)
- 2) down (d) strang (s) bottom (b) (-1/3 e)

- ✓ Up and down are the smallest.
- ✓ Antiquarks exist.

Proton: 3 quarks: 2 up + 1 down = +e

Neutron: 3 quarks: 2 down + 1 up = 0

V. Fundamental particles of atoms:

$$e \rightarrow -1.602 \times 10^{-1} C \rightarrow m_e = 9.11 \times 10^{-31} Kg$$

$$p \rightarrow +1.602 \times 10^{-19} C \rightarrow m_p = 1.0072 amu$$

$$n \rightarrow 0 \rightarrow m_n = 1.0086 amu$$

- ✓ Isotopes: same Z, different A (different number of neutrons)
- ✓ Z: number of protons
- ✓ A: number of protons and neutrons
- ✓ ${}_{Z}^{A_1}X \ {}_{Z}^{A_2}X \ {}_{Z}^{A_3}X$

$$\bar{A} = \frac{A_1 \cdot \% + A_2 \cdot \% + A_3 \cdot \%}{100}$$

✓ Chapter I-Summary ✓

● Mise en évidence des particules fondamentales de l'atome:

- a) Electron → expérience des rayons cathodiques
- b) Noyau → expérience de Rutherford (1910)
- c) Proton et neutron → à l'aide des rayons α

● Mise en évidence des autres particules:

- a) Neutrino
- b) Positons

● Famille de particules: (instables)

- a) Mésons (μ, π^+, π^-, π^0 et K^-)
- b) Hypérons ($A, \varepsilon^+, \varepsilon^-, \varepsilon^0, E^0$ et E^-)

● Théorie des quarks: 1) up (u) Charm (c) Top (t) (+2/3 e)

2) down (d) strang (s) bottom (b) (-1/3 e)

- Particule + anti-particule \rightarrow Energie

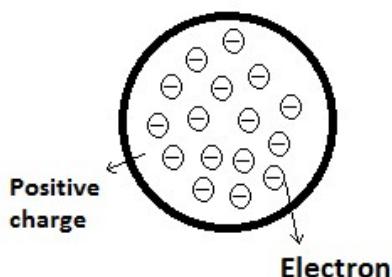
$$\begin{array}{ccc} \text{E} & \Delta m = m(\text{particule}) + m(\text{anti-particule}) \\ \uparrow \curvearrowleft & = 2m(\text{particule}) \\ \beta^- \rightarrow & \leftarrow \beta^+ & \Delta E = \Delta mc^2 = 2h\nu \\ \downarrow \curvearrowright & & (\text{Rxn nuc ou il y a perte de masse}) \\ \text{E} \end{array}$$

- Isotones: même Z, différent A
- Isotopes: même A, différent Z
- Isobares: même N, différent A et Z

✓ Chapter II: Classical models of the atom

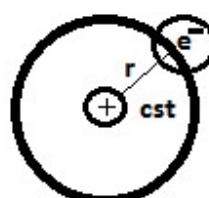
I. Thomson model and Rutherford model of the atom (1911) ✓:

- First atomic model-Thomson model: Atom was a sphere. Atoms are electrically neutrals. Atoms of different elements have different number of electrons.



- Rutherford model:

- ✓ $r=\text{constant}$
- ✓ Velocity of electron constant



- ✓ Energy of electron constant
- ✓ Constant path

He assumed that there are two forces to maintain the above. (These two forces must be equal).

He admitted that the electron is in circular motion around the nucleus.

If we consider the system [Proton-electron]:

$$\vec{F}_1 = -\vec{F}_2 \text{ where } F_1 = F_2$$

$$F_{coulomb \text{ attractive force}} = K \frac{qq'}{r^2} = \frac{1}{4\pi\epsilon_0} \frac{(e)(-e)}{r^2} = \frac{-e^2}{4\pi\epsilon_0 r^2}$$

$$F_{centrifuge} = \frac{mv^2}{r}$$

$$F_{coulomb \text{ attractive force}} = F_{centrifuge}$$

$$1) \frac{-e^2}{4\pi\epsilon_0 r^2} = \frac{mv^2}{r}$$

$$2) KE = \frac{1}{2}mv^2$$

$$1) \text{ and } 2) \text{ equations: } KE = \frac{1}{8}\frac{e^2}{\pi\epsilon_0 r}$$

$$E_T = KE + E_p \text{ where } E_p = \int F dx = -\frac{1}{4\pi\epsilon_0} \frac{e^2}{r}$$

$$E_T = KE + E_p = \frac{1}{8}\frac{e^2}{\pi\epsilon_0 r} - \frac{1}{4\pi\epsilon_0} \frac{e^2}{r} = -\frac{1}{8}\frac{e^2}{\pi\epsilon_0 r}$$

- ✓ He found out that E and r are proportional.
- ✓ e^- releases energy (law of electrodynamic)
- ✓ *Charge moving circular path.* (radiation)

Hence nucleus becomes neutral, which contradicts his experiment; so Rutherford stopped there. He used classical mechanics which is wrong.

II. Emission spectrum of the H atom

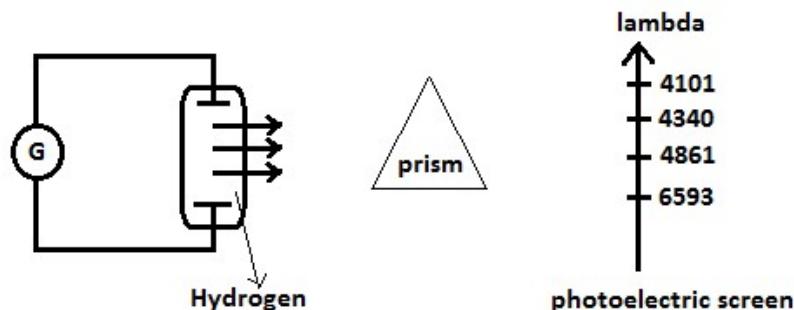
Wavelength λ

Frequency ϑ

$$c = \lambda \cdot \vartheta$$

$$1\text{Å} = 10^{-10}\text{m}$$

$$1\text{nm} = 10\text{Å}$$



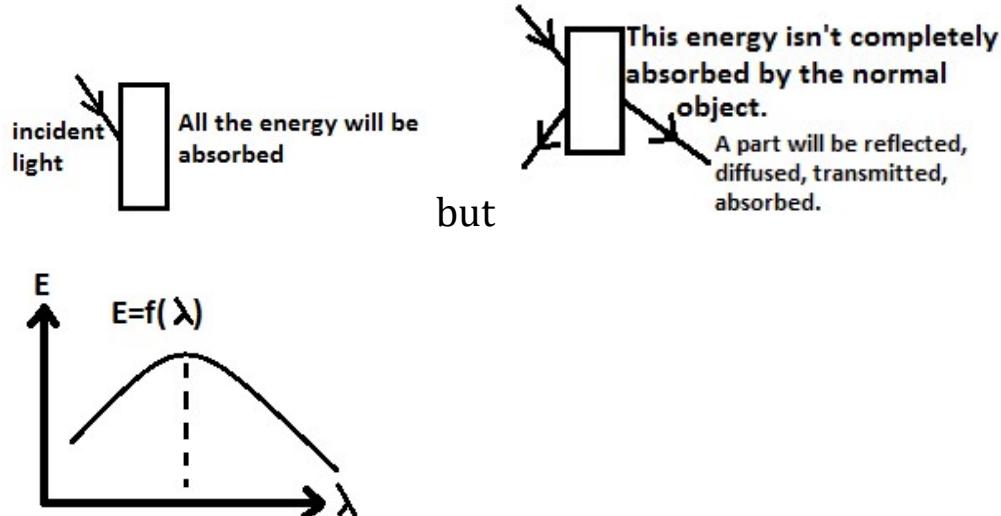
- ✓ Emission of a very poor light
- ✓ Analyze through prism
- ✓ Obtain λ on screen

1. Série de Balmer (Visible): $\frac{1}{\lambda} = R_H \left(\frac{1}{2^2} - \frac{1}{a^2} \right)$ $a > 2$
 2. Série de Lyman (UV): $\frac{1}{\lambda} = R_H \left(\frac{1}{1^2} - \frac{1}{a^2} \right)$ $a > 1$
 3. Série de Paschen (IR): $\frac{1}{\lambda} = R_H \left(\frac{1}{3^2} - \frac{1}{a^2} \right)$ $a > 3$
 4. Formule de Ritz: $\frac{1}{\lambda} = R_H \left(\frac{1}{n^2} - \frac{1}{a^2} \right)$ $a > n$
- Where $R_H = 1.0967 \times 10^7$

III. The Planck's Quantum theory

1) The blackbody radiation (1900)

Blackbody absorbs and emits energy with no loss. (ideal body)
Emitted energy and wavelength are inversely proportional.



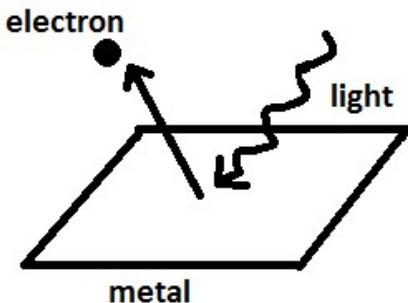
- ✓ Both parts are different.
- ✓ Energy is not cont.
- ✓ It is formed of small packets called quantum.

$$1 \text{ quantum } E=h\nu$$

$$n \text{ quanta } E=nh\nu$$

2) The photoelectric effect (Einstein 1905)

When light with sufficient frequency shines on the surface of a metal, electrons are ejected.



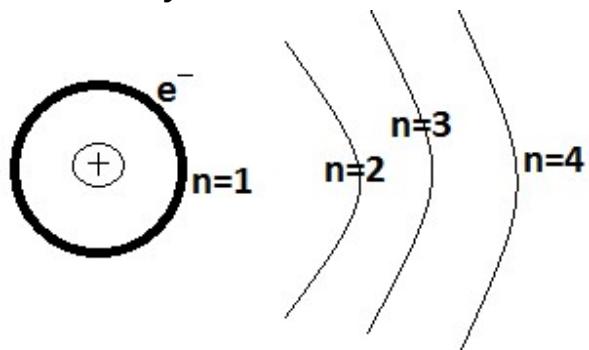
If $\vartheta \uparrow$, then $V \uparrow$

Binding energy: BE

- If $h \cdot \vartheta > BE \equiv$ Emission of electrons (goes to other side)
- If $h \cdot \vartheta < BE \equiv$ No emission of electrons (Only excitation)
- If $h \cdot \vartheta = BE \equiv$ stays in its place (electron leaves atom with no KE, excitation)
 $h \cdot \vartheta = BE + KE$ where $BE = h \cdot \vartheta_0$ (ϑ_0 is threshold frequency)

IV. Bohr Model

Stationary levels or orbits:



- Electron does not give energy (if stationary) → Violating classical physics.

- Electron absorbs energy and gets to a higher stationary level.
Electron emits energy and gets to a lower stationary level.
 - Angular momentum of the electron: mvr
It's a multiple of $\frac{h}{2\pi}$
- 3) $v = n \frac{h}{2\pi mr}$ with n integer
Rutherford: 1) $\frac{e^2}{4\pi\epsilon_0 r} = mv^2$
2) $E = \frac{-e^2}{8\pi\epsilon_0 r}$

$$3) \text{ in 1): } 4) r = \frac{n^2 h^2 \epsilon_0}{Z \pi m e^2} \quad Z > 1$$

$$4) \text{ in 2): } 5) E = \frac{-Z^2 m e^4}{n^2 8 \epsilon_0^2 h^2} \quad Z > 1$$

$$4) \text{ in 3): } 6) v = \frac{e^2 Z}{2 h \epsilon_0 n} \quad Z > 1$$

$$\text{so } E_n = \frac{-13.6}{n^2} \text{ eV}$$

Bohr's Fundamental radius: $a_0 = 0.529 \text{ \AA}^0$

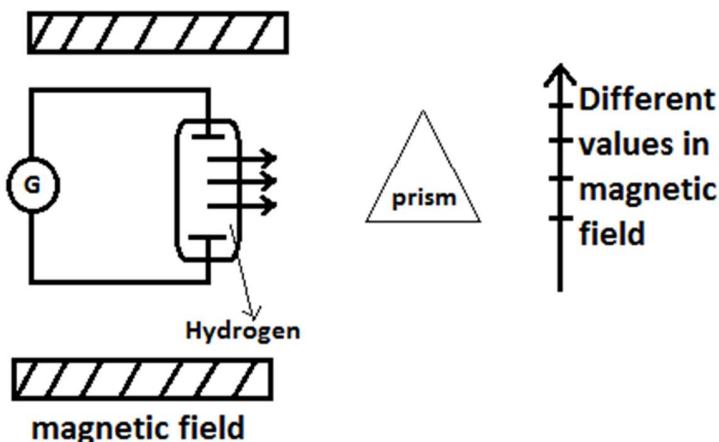
$$h\nu = \frac{-me^4}{8\epsilon_0^2 h^2 n'^2} + \frac{me^4}{n^2 8 \epsilon_0^2 h^2} \text{ where } n'^2 > n^2$$

$$\frac{hc}{\lambda} = \frac{me^4}{8\epsilon_0^2 h^2} \left(\frac{1}{n^2} - \frac{1}{n'^2} \right)$$

$$\frac{1}{\lambda} = \frac{me^4}{8\epsilon_0^2 h^3 c} \left(\frac{1}{n^2} - \frac{1}{n'^2} \right) \text{ Ritz formula}$$

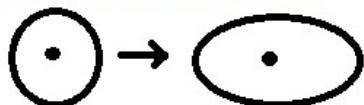
V. Defects of Bohr's model:

Zeeman effects (factor)



- Bohr's defect: Using chemical mechanics and quantum mechanics together.
- Sommerfield (Bohr's student) tried to save The Bohr model by proposing that the electron move in an elliptical orbit not circular. But was only valid for 1H , not for others.
- Bohr's model was accepted 1913 → 1927 till quantum mechanics gave a satisfying model used until today.

Sommerfeld proposition



✓ Chapter II-Summary ✓

1. Série de Balmer (Visible): $\frac{1}{\lambda} = R_H \left(\frac{1}{2^2} - \frac{1}{a^2} \right)$ $a > 2$
2. Série de Lyman (UV): $\frac{1}{\lambda} = R_H \left(\frac{1}{1^2} - \frac{1}{a^2} \right)$ $a > 1$
3. Série de Paschen (IR): $\frac{1}{\lambda} = R_H \left(\frac{1}{3^2} - \frac{1}{a^2} \right)$ $a > 3$
4. Formule de Ritz: $\frac{1}{\lambda} = R_H \left(\frac{1}{n^2} - \frac{1}{a^2} \right)$ $a > n$

- Théorie des quantas: $E = h\nu$ pour un quantum

$$E = nh\nu \text{ pour } n \text{ quantas}$$

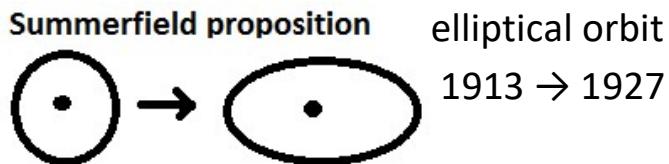
• Effet photoélectrique: $E = W_e + E_c$ avec $W_e = h\nu_e$

- a) Si $E < W_e$, électron excité mais ne quitte pas l'atome
- b) Si $E > W_e$, électron quitte l'atome avec une E_c
- c) Si $E = W_e$, l'électron quitte l'atome sans E_c

• $E_c = eV$ (c'est le potential d'arrêt)

• Formules de Bohr:

$$\heartsuit \quad E = -\frac{me^4}{8h^2\varepsilon_0^2} \times \frac{Z^2}{n^2} \quad 2. \nu = \frac{e^2}{2h\varepsilon_0} \times \frac{Z}{n} \quad 3. r = r^2 \frac{h^2\varepsilon_0}{Z \pi m e^2}$$



✓ Chapter III-Introduction to Quantum Mechanics ✓

I-Introduction

Bohr theory is the first atomic model that could explain and reproduce experimental results. Then we had a new quantum theory.

<i>Macroscopic scale</i>	<i>Microscopic scale</i>
Can-ball-rocket	Electrons-atoms
Classical mechanics: ϑ, E	Quantum mechanics, different rules, laws
$\vec{F} = m\vec{a}$	$H(\varphi) = E \cdot \varphi$

We cannot use classical mechanics in the microscopic scale. That's why BOHR failed.

✓ Einstein(1905)

$$E = h \cdot \vartheta \text{ (wave)}$$

$$E = m \cdot c^2 \text{ (matter) (m is fictive mass of a photon)}$$

⇒ Double nature of light

- He said mass could be transformed to Energy and vice versa.
- For him, E and m are the same entity.
- Accumulation of E ⇒ mass

II-Wave nature of particles

Photon has a dual character: wave and corpuscle.

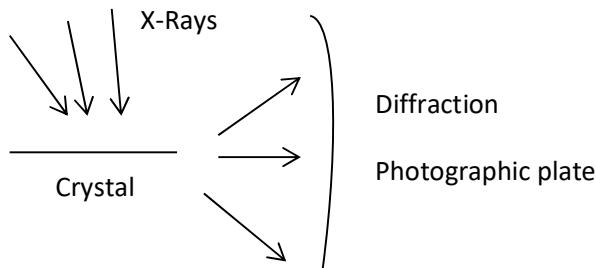
In 1924, a French physicist Louis de Broglie presented a new hypothesis concerning the nature of matter.

Hypothesis: To any microscopic particle in motion is associated a wave having a wavelength.

$$E = h\nu = h\frac{c}{\lambda} \quad \text{and} \quad E = mc^2$$

So, $\lambda = \frac{h}{mv}$ (sub-atomic particles)

- ✓ In 1927, Davisson and Germer shows that electrons are diffracted by crystals (same behavior as the X-rays)



- They used their experience but instead of X-Rays, they used electrons.
- They got the same result as X-Rays (waves).
- Electrons behaved as waves.
- Hence scientists accepted the idea of the double nature of particles.

III-Heisenberg's uncertainty principle (1927)

$$|\Delta x| \cdot |\Delta p| \geq \frac{h}{4\pi} = \frac{h}{2}$$

Position \rightarrow ↑ Momentum, quantité de mouvement

$$\rho = m \cdot v$$

- One cannot be certain about the position and velocity at the same time.
- For example, when we know the position we can predict the velocity.
- As Δx decrease, uncertainty of v increase.
- Bottom and line, both cannot be determined at the same time.
- With advanced technology, nowadays, we still cannot determine them exactly.

Its effect is also hidden at our scale

Example 1 A base-ball

mass=200 g

speed=30 m/s

$$\rho = m \cdot v = 6 \cdot 10^5 \text{ g cm/s} = 6 \text{ kg m/s}$$

$$\Delta \rho = 6 \cdot 10^{-12} \text{ kg m/s}$$

$$\Delta x \geq 8,8 \cdot 10^{-24} \text{ m} = \frac{h}{4\pi \Delta \rho}$$

Example 2 An electron

mass= $10^{-27} g$

speed= 30 m/s

$$\rho = m \cdot v = 3 \cdot 10^{-29} \text{ kg m/s}$$

$$\Delta\rho = 3 \cdot 10^{-41} \text{ kg m/s}$$

$$\Delta x \geq 1,8 \cdot 10^6 \text{ m} = \frac{h}{4\pi \Delta\rho}$$

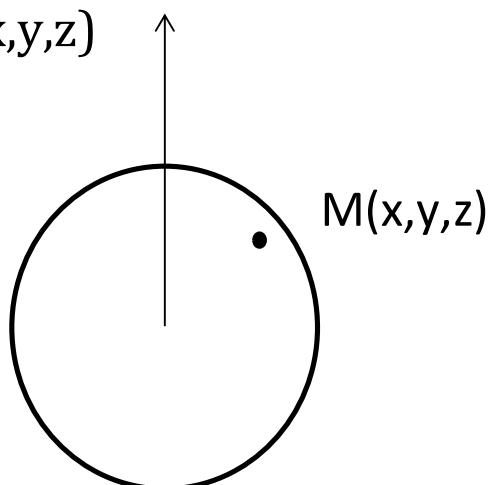
♥ $2\pi r = n\lambda$

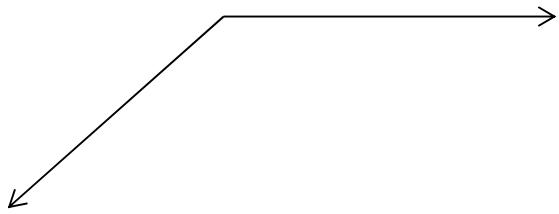
♥ $mvr = \frac{n \cdot h}{2\pi}$

IV-The Shrodinger wave equation (1927)

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

- m: mass of the particle
- E: total energy of the particle
- U: Potential energy of the particle
- h: Plank's constant
- Ψ : Amplitude (wave function) associated to the e^-
- $\Psi = \Psi(x, y, z)$





$$\Psi^2 = \text{Probability}$$

$$\text{Probability} = \int \Psi^2(M)$$

$$\sum P = 1$$

$$dv = dx dy dz$$

$$P = \int_x \int_y \int_z \Psi^2 \cdot dv$$

$$P = \iiint \Psi^2 \cdot dx \cdot dy \cdot dz = 1$$

Other forms of the schrodinger equation

There exist two forms of operators

1) Laplacian operator:

$$\begin{aligned}\Delta &= \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \\ \Delta \Psi &= \frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2}\end{aligned}$$

$$\text{Schrodinger equation: } \Delta \Psi + \frac{8\pi^2}{h^2} m(E - U) \Psi = 0$$

2) Hamiltonian operator:

$$\hat{H} = -\frac{\hbar^2}{8\pi^2 m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + U$$

$$\hat{H}\Psi = -\frac{\hbar^2}{8\pi^2 m} \left(\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2} \right) + U\Psi$$

NB: The wave associated to the electron is a standing wave.

$$\Phi(x,y,z,t) = \Psi(x,y,z)\sin(2\pi\vartheta t)$$

The product of two terms, the first one depends on the position, the second one depends on time t.

We will consider the simplest case, when the wave function is time-independent and for one dimension.

$$\Psi = A \sin \frac{2\pi x}{\lambda}$$

► A: Amplitude

► λ : wavelength

► Ψ : wave amplitude for a given value of x

The first and the second derivatives:

- $\frac{d\Psi}{dt} = \frac{2\pi}{\lambda} A \cos\left(\frac{2\pi x}{\lambda}\right)$

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

$$\Rightarrow \frac{d^2\Psi}{dx^2} = -\frac{4\pi^2}{\lambda^2} \Psi \text{ (second order differential equation)}$$

To obtain the Schrodinger equation:

According to De Broglie: $\lambda = \frac{h}{mv}$ $d^2 = \frac{h^2}{m^2 v^2}$

$$\frac{d^2\psi}{dx^2} + \frac{4\pi^2 m^2 v^2}{h^2} \psi = 0$$

Schrodinger introduced the kinetic energy $E_k = \frac{1}{2}mv^2$

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2} E_k \psi = 0, \text{ where } E_k = E_T - E_P$$

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

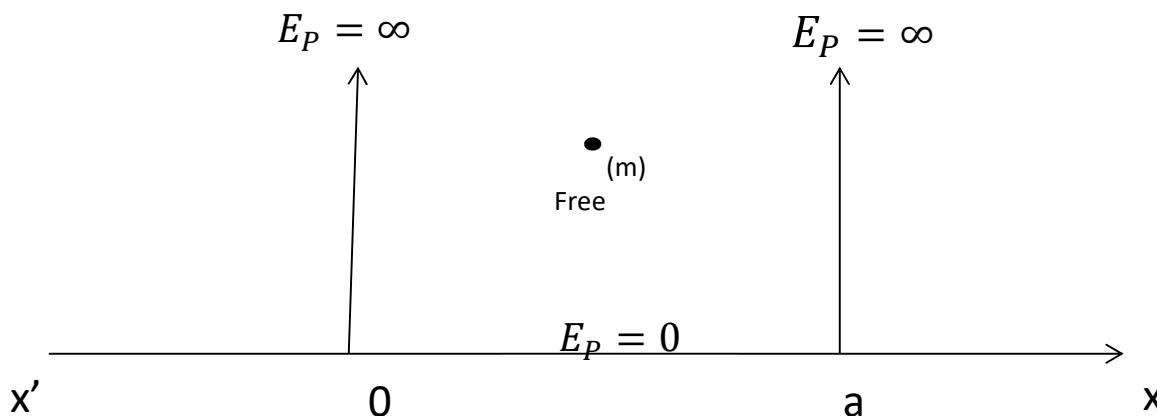
$$\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2} + \frac{8\pi^2 m}{h^2} (E - U) \psi = 0$$

If we multiply this equation by $-\frac{h^2}{8\pi^2 m}$ we obtain

$$-\frac{h^2}{8\pi^2 m} \Delta \psi + U \psi = E \psi$$

V-Applying $H(\psi) = E\psi$ to hypothetical situations

A) A free particle in a one dimension (1d) box



Conditions:

- ♥ Inside $E_P = 0$ (Free particle)
- ♥ Outside $E_P = \infty$
- ♥ For $x=0$ and $x=a$, $\Psi(0)=0$ and $\Psi(a)=0$, $\Psi^2(0)=0$ and $\Psi^2(a)=0$
- ♥ Electron is by itself (no attraction or repulsion) (No U).
- ♥ Electron moves between 0 and a.
- ♥ Electron doesn't touch 0 and a.

1) Quantization of energy of the electron

$\frac{d^2\Psi}{dx^2} + \frac{8\pi^2m}{h^2} E \Psi = 0$, outside the box the particle doesn't exist. Since $\Psi = \Psi(x)$

We set $\alpha^2 = \frac{8\pi^2m}{h^2} E$

The equation becomes: $\frac{d^2\Psi}{dx^2} + \alpha^2 \Psi = 0$ (second order differential equation).

It admits solutions: $\Psi = A \sin \alpha x + B \cos \alpha x$

▀ For $x=0 \Rightarrow \Psi^2(0) = 0$

$$\Rightarrow \psi(0) = 0 = A\sin 0 + B\cos 0 \Rightarrow B=0 \text{ and } A \neq 0$$

$$\Rightarrow \psi = A\sin \alpha x$$

$$\blacksquare \text{For } x=a \Rightarrow \psi^2(a) = 0$$

$$\Rightarrow \psi(a) = 0 = A\sin \alpha a, A \neq 0$$

$$\Rightarrow \sin \alpha a = 0 \Rightarrow \alpha a = n\pi, n=1,2,3\dots$$

$\triangleleft n \neq 0$, because if $n=0$, $a=0$.

$$\text{So } \alpha^2 a^2 = n^2 \pi^2 \Rightarrow \alpha^2 = \frac{n^2 \pi^2}{a^2}$$

$$\alpha^2 = \frac{8\pi^2 m}{h^2} E = \frac{n^2 \pi^2}{a^2}$$

$$\Rightarrow E_n = \frac{h^2}{8ma^2} n^2 = n^2 \cdot k \text{ (Energy is quantized by } n)$$

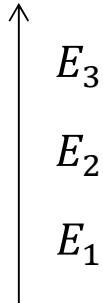
$$\blacksquare k = \frac{h^2}{8ma^2} \text{ (constant)}$$

uE diagram:

$$n=1 \Rightarrow E_1 = k$$

$$n=2 \Rightarrow E_2 = 4k$$

$$n=3 \Rightarrow E_3 = 9k\dots$$



$$\psi = A \sin \frac{n\pi}{a} x$$

To find $A \Rightarrow \psi$ satisfies a normalization conditions (for sure the particle inside the box)

$$\int_0^a \psi^2 dx = 1 \Rightarrow A^2 \int_0^a \sin^2 \alpha x dx = 1$$

$$\text{RECALL } \sin^2 \alpha x = \frac{1 - \cos 2\alpha x}{2}$$

$$\Rightarrow \frac{A^2}{2} \int_0^a (1 - \cos 2\alpha x) dx = \frac{A^2}{2} \left[x - \frac{\sin 2\alpha x}{2\alpha} \right]_0^a$$

$$\alpha = \frac{n\pi}{a}$$

$$\frac{A^2}{2} \left[x - \frac{\sin 2\frac{n\pi}{a}x}{2\frac{n\pi}{a}} \right]_0^a = 1$$

$$\frac{A^2}{2} [a - 0] = 1$$

$$A^2 = \frac{2}{a} \Rightarrow A = \sqrt{\frac{2}{a}}$$

$$\Rightarrow \psi = \sqrt{\frac{2}{a}} \sin \frac{n\pi}{a} x$$

$$\frac{d\psi}{dx} = 0 \Rightarrow \frac{n\pi}{a} \sqrt{\frac{2}{a}} \cos \left(\frac{n\pi}{a} x \right) = 0 \Rightarrow \frac{n\pi}{a} x = \frac{\pi}{2} + k\pi$$

$$\Rightarrow x = \frac{a}{2n} (1 + 2k) \text{ with } k = 0, 1, 2, 3, \dots \text{ and } 0 < x < a$$

$$\psi_{n_{\max \text{ or } \min}} = \sqrt{\frac{2}{a}} \sin \left(\frac{\pi}{2} + k\pi \right)$$

$$\text{If } k=0, 2, 4, \dots \Rightarrow \psi_n = \psi_{n_{\max}} = \sqrt{\frac{2}{a}}$$

$$\text{If } k = 1, 3, 5, 7, \dots \Rightarrow \psi_n = \psi_{n_{\min}} = -\sqrt{\frac{2}{a}}$$

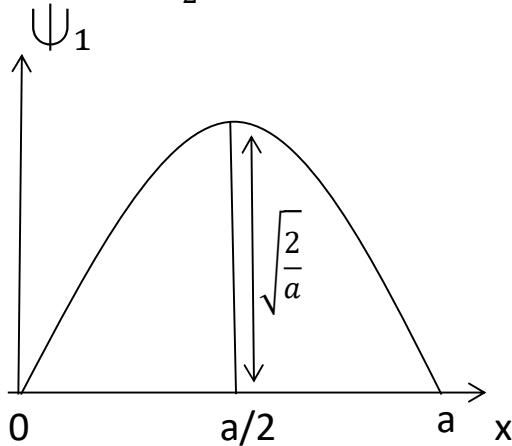
$$\Psi_{n_{max}}^2 = \frac{2}{a}$$

• n=1 : $\Psi_1 = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi}{a}x\right) \Rightarrow \Psi_1^2 = \frac{2}{a} \sin^2\left(\frac{\pi}{a}x\right)$

Extremum: $x = \frac{a}{2}(1 + 2k)$

$k=0 \Rightarrow x=\frac{a}{2}$ and $\Psi_{1_{max}} = \sqrt{\frac{2}{a}}$

$k=1 \Rightarrow x=3\frac{a}{2} > a$ (inacceptable)



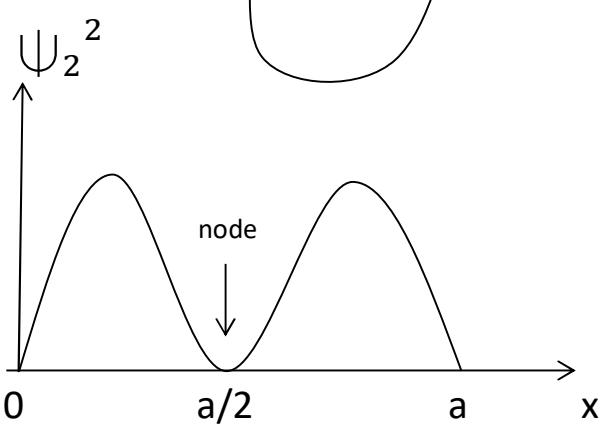
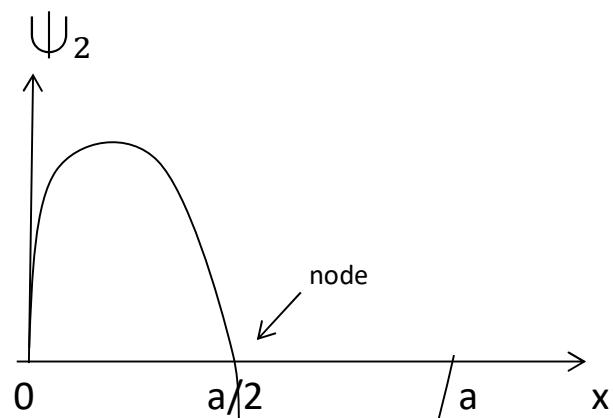
$n=2 : \Psi_2 = \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi}{a}x\right) \Rightarrow \Psi_2^2 = \frac{2}{a} \sin^2\left(\frac{2\pi}{a}x\right)$

Extremum: $x = \frac{a}{2} \cdot \frac{1}{4}(1 + 2k)$

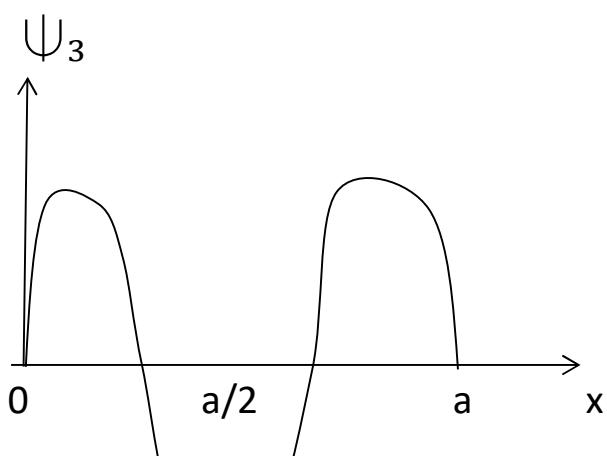
$k=0 \Rightarrow x=\frac{a}{4}$ and $\Psi_{2_{max}} = \sqrt{\frac{2}{a}}$

$$k=1 \Rightarrow x=3\frac{a}{4} \text{ and } \psi_{2min} = -\sqrt{\frac{2}{a}}$$

$$k=2 \Rightarrow x=5\frac{a}{4} > a \text{ (inacceptable)}$$

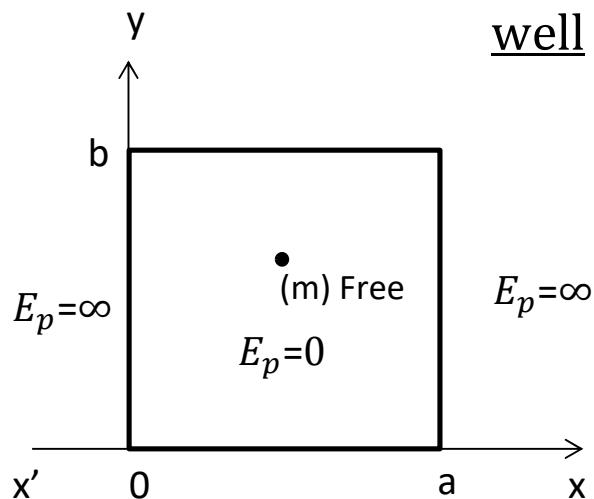


- $n=3 : \psi_3 = \sqrt{\frac{2}{a}} \sin\left(\frac{3\pi}{a}x\right) \Rightarrow \psi_3^2 = \frac{2}{a} \sin^2\left(\frac{3\pi}{a}x\right)$



$a/3$ $2a/3$

B) A free particle in a two-dimensional potential well



- ✓ Square: $a=b$
- ✓ Boundaries are forbidden

$$H(\Psi) = E \cdot \Psi$$

$$\Psi = \Psi(x, y)$$

separation of variables:

Two equations:

$$1) \% x: H(\Psi_x) = E_x \Psi_x$$

$$E_x = \frac{n_x^2 h^2}{8ma^2}$$

$$\Psi_x = \sqrt{\frac{2}{a}} \sin \frac{n\pi}{a} x$$

2) %y: $H(\Psi_y) = E_y \Psi_y$

$$E_y = \frac{n_y^2 h^2}{8ma^2}$$

$$\Psi_y = \sqrt{\frac{2}{b}} \sin \frac{n\pi}{b} y$$

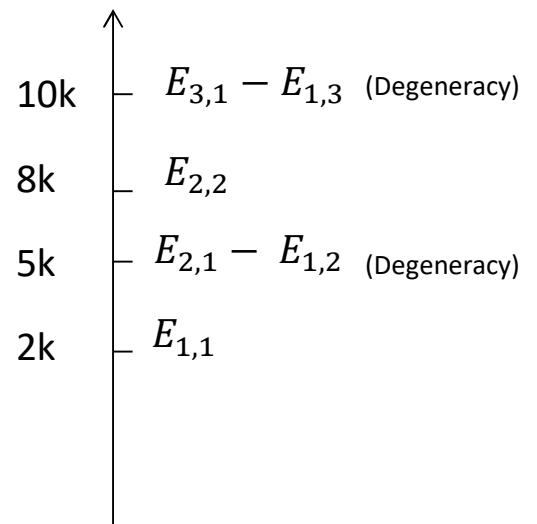
Final result: $E_{x,y} = E_x + E_y$

$$\Psi_{x,y} = \Psi_x \cdot \Psi_y$$

$$\text{Energy: } E_{x,y} = \frac{n_x^2 h^2}{8ma^2} + \frac{n_y^2 h^2}{8ma^2}$$

$$E_{x,y} = (n_x^2 + n_y^2) \frac{h^2}{8ma^2} = k(n_x^2 + n_y^2)$$

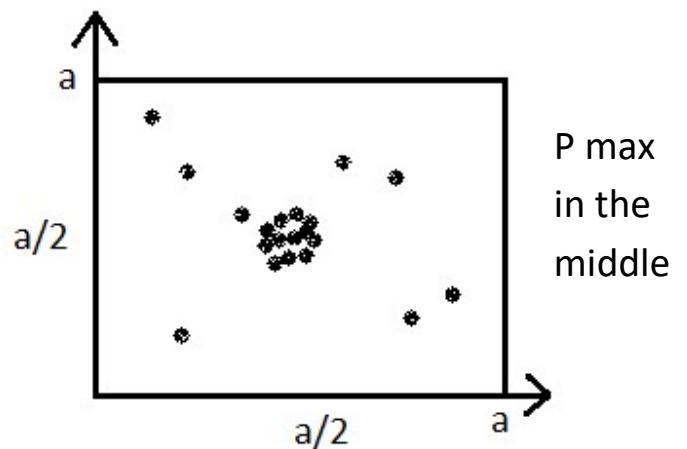
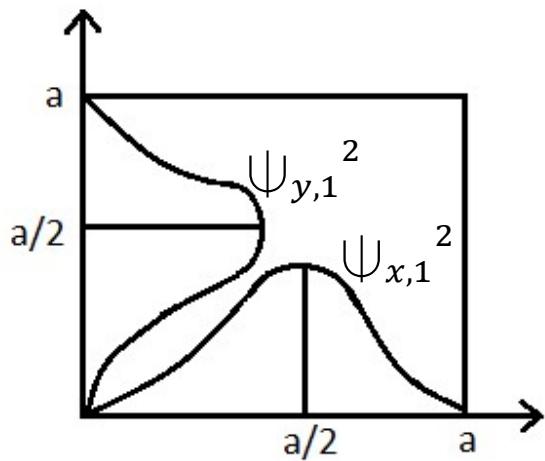
- $n_x = 1$ and $n_y = 1 \Rightarrow E_{1,1} = 2k$
- $n_x = 1$ and $n_y = 2 \Rightarrow E_{1,2} = 5k$
- $n_x = 2$ and $n_y = 1 \Rightarrow E_{2,1} = 5k$
- $n_x = 2$ and $n_y = 2 \Rightarrow E_{2,2} = 8k$
- $E_{1,3} = E_{3,1} = 10k$



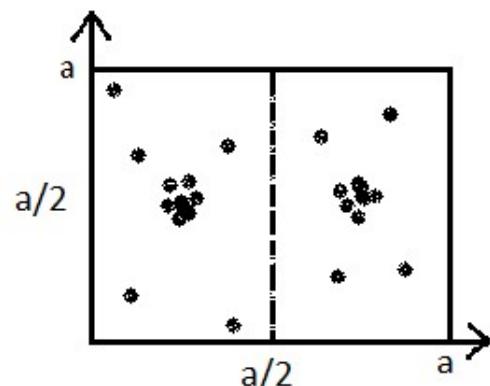
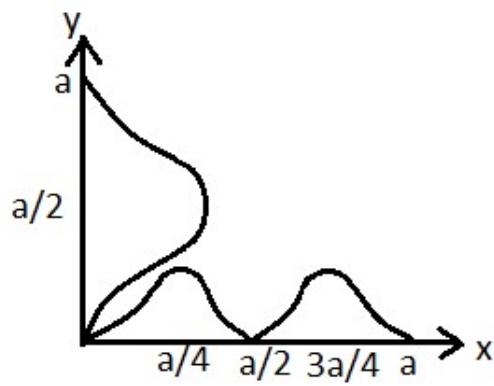
Probability: function $\Psi \Rightarrow \Psi^2$

- $n_x = 1 \Rightarrow \Psi_{x,1} = \sqrt{\frac{2}{a}} \sin \frac{\pi}{a} x \Rightarrow \Psi_{x,1}^2 = \frac{2}{a} \sin^2 \frac{\pi}{a} x$

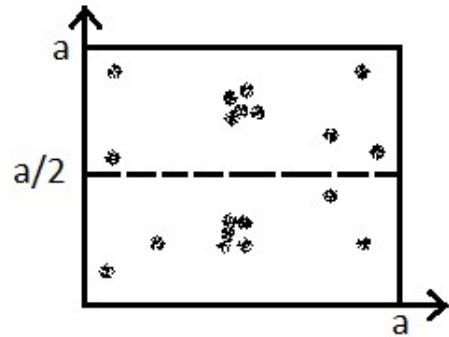
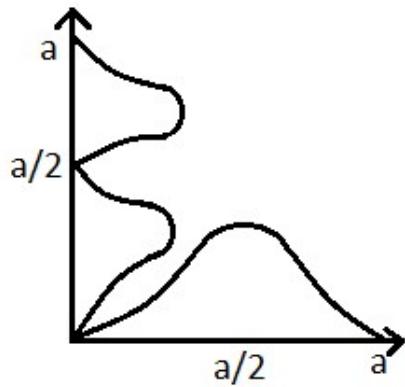
- $n_y = 1 \Rightarrow \Psi_{y,1} = \sqrt{\frac{2}{a}} \sin \frac{\pi}{a} y \Rightarrow \Psi_{y,1}^2 = \frac{2}{a} \sin^2 \frac{\pi}{a} y$



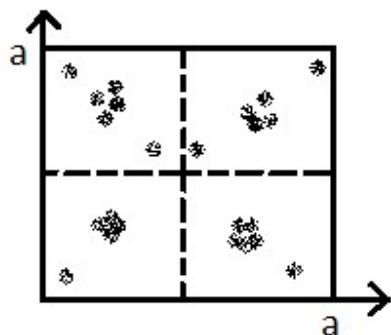
- $n_x = 2$ and $n_y = 1$



- $n_x = 1$ and $n_y = 2$



- $n_x = 2$ and $n_y = 2$



C) A free particle in a three-dimensional potential well

well

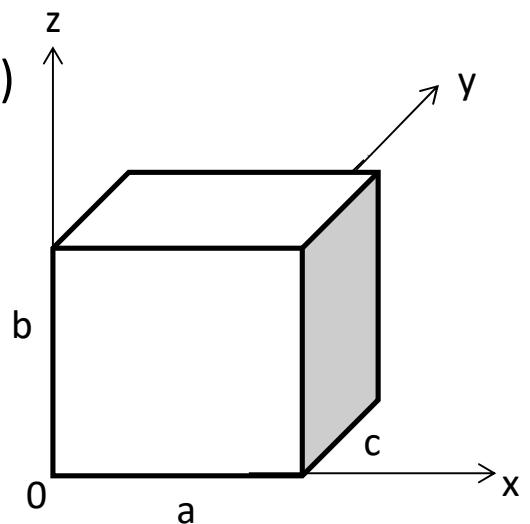
Cube $a=b=c$ (forbidden boundaries)

$$H(\Psi) = E \cdot \Psi$$

$$\Psi = \Psi(x, y, z)$$

separation of variables

Three equations %x %y %z

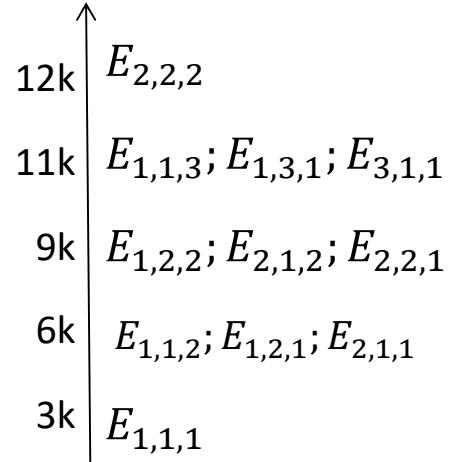


$$\begin{array}{ccc}
 n_x & & n_y \\
 \searrow & \downarrow & \swarrow \\
 \Psi_{x,y,z} = \Psi_x \cdot \Psi_y \cdot \Psi_z \\
 E_{x,y,z} = E_x + E_y + E_z
 \end{array}$$

- ✓ $H(\Psi_x) = E_x \cdot \Psi_x$
- ✓ $H(\Psi_y) = E_y \cdot \Psi_y$
- ✓ $H(\Psi_z) = E_z \cdot \Psi_z$
- ✓ $H = H_x + H_y + H_z$
- ✓ $E = E_x + E_y + E_z$

$$\begin{aligned}
 \Rightarrow E &= \frac{\hbar^2}{8ma^2} (n_x^2 + n_y^2 + n_z^2) \\
 \Rightarrow E &= k(n_x^2 + n_y^2 + n_z^2)
 \end{aligned}$$

- $n_x = n_y = n_z = 1 \Rightarrow E_{1,1,1} = 3k$
- $n_x = n_y = 1 \text{ and } n_z = 2 \Rightarrow E_{1,1,2} = 6k = E_{1,2,1} = E_{2,1,1}$
- $E_{1,2,2} = E_{2,1,2} = E_{2,2,1} = 9k$
- $E_{1,1,3} = E_{1,3,1} = E_{3,1,1} = 11k$
- $E_{2,2,2} = 12k$



Probability:

- ✓ **No node** $n_x = n_y = n_z = 1$
- ✓ $n_x = 2$ (one node); $n_y = n_z = 1$ (2 identical parts)

✓ Summary – Chapter III ✓

- ♥ $E = h \cdot \vartheta$ (théorie des quanta)
- ♥ $\Delta E = \Delta m \cdot c^2$ (nature corpusculaire)
- ♥ Formule de Broglie $\lambda = \frac{h}{mv}$ où $E = h \cdot \vartheta = mc^2$ c'est l'énergie d'un photon)
- ♥ Einstein → double nature aux photons
- ♥ Louis de Broglie → double nature à la matière

$$|\Delta v| \cdot |\Delta x| \cdot m \geq \frac{h}{4\pi}$$

♥ $m_{noyau} = \frac{1}{10000} m_{atome}$

- ♥ Schrodinger: $H(\Psi) = E \cdot \Psi$ (Il a lié les deux natures corpusculaire(m) et ondulatoire(Ψ))

Opérateur
Laplacien
 $\Delta(\Psi)$

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

Ψ : l'amplitude de l'onde associée à la particule.

Ψ^2 : indice de la probabilité de trouver la particule en une certaine position. D'où valeur exacte de la probabilité $P = \int \Psi^2 dv$

Où $dv = dx \cdot dy \cdot dz$

- ♥ Exemple d'opérateur: $\sqrt{-} ; \frac{d}{dx} ; \frac{d^2}{dx^2}$

- ♥ Démonstration de $H(\Psi) = E \cdot \Psi$ (opérateur Hamiltonien)

$$\left[\Delta(\Psi) + \frac{8\pi^2m}{h^2}(E - U)\Psi = 0 \right] \cdot \frac{-h^2}{8\pi^2m}$$

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

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

$$\Rightarrow H(\Psi) = E\Psi$$

♥ Uni-dimensionnel: $\frac{d^2\psi}{dx^2} + \frac{8\pi^2m}{h^2} E \cdot \psi = 0$

We set $\alpha^2 = \frac{8\pi^2m}{h^2} E$

$$\frac{d^2\psi}{dx^2} + \alpha^2 \psi = 0$$

$$\psi = A \sin \alpha x + B \cos \alpha x$$

$$\text{For } x=0 \Rightarrow \psi(0) = 0$$

$$\Rightarrow \psi(0) = 0 = A \sin 0 + B \cos 0 \Rightarrow B = 0 \text{ and } A \neq 0$$

$$\Rightarrow \psi = A \sin \alpha x$$

$$\text{For } x=a \Rightarrow \psi(a) = 0$$

$\Delta n \neq 0$, because if $n=0$, $a=0$.

$$\text{So } \alpha^2 a^2 = n^2 \pi^2 \Rightarrow \alpha^2 = \frac{n^2 \pi^2}{a^2}$$

$$\alpha^2 = \frac{8\pi^2m}{h^2} E = \frac{n^2 \pi^2}{a^2}$$

$$\Rightarrow E_n = \frac{h^2}{8ma^2} n^2 = n^2 \cdot k \text{ (Energy is quantized by } n)$$

Fonction d'onde $\psi: \psi = A \sin \alpha x = A \sin \frac{n\pi}{a} x$

$$\sum P = 1$$

$$\int_0^a \psi^2 dx = 1 \Rightarrow \int_0^a A^2 \sin^2 \frac{n\pi}{a} x dx = 1 = A^2 \int_0^a \frac{(1 - \cos 2\alpha x)}{2} dx$$

$$\Rightarrow \frac{A^2}{2} \left[x - \frac{1}{2\alpha} \sin 2\alpha x \right]_0^a = 1$$

$$\Rightarrow \frac{A^2}{2} \left[a - \frac{1}{2} \frac{n\pi}{a} \sin \left(\frac{2n\pi}{a} \cdot a \right) - (0 - \sin 0) \right] = 1$$

$$\Rightarrow A = \sqrt{\frac{2}{a}} \Rightarrow \psi = \sqrt{\frac{2}{a}} \sin \frac{n\pi}{a} x$$

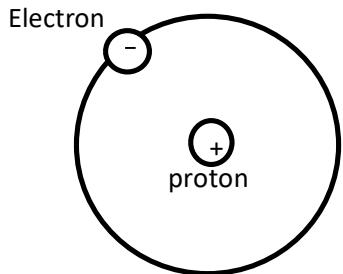
♥ Bi-dimensionnel:

$$E(x,y) = E = (x, y) = \frac{n_x^2 h^2}{8ma^2} + n_y^2 \frac{h^2}{8ma^2} = (n_x^2 + n_y^2)k$$

♥ Tri-dimensionnel:

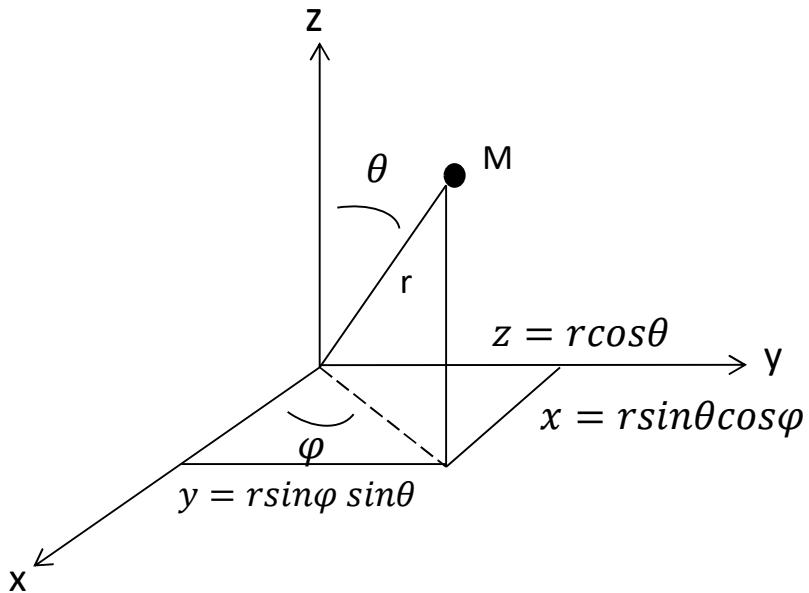
$$E(x, y, z) = (n_x^2 + n_y^2 + n_z^2)k$$

✓ Chapter IV- The H atom in Quantum Mechanics ✓



- Potential energy in the case of a hydrogen atom $U = -\frac{e^2}{4\pi\epsilon_0 r}$
- Potential energy in the case of a hydrogen like ion $U = -\frac{Ze^2}{4\pi\epsilon_0 r}$

I. Definition of the system:



- $\cos \theta = \frac{z}{r} \Rightarrow z = r \cos \theta$
- $\sin \theta = \frac{r'}{r} \Rightarrow r' = r \sin \theta$

- $\cos\varphi = \frac{x}{r'} \Rightarrow x = r'\cos\varphi = r\sin\theta\cos\varphi$
- $\sin\varphi = \frac{y}{r'} \Rightarrow y = r'\cos\theta = r\sin\theta\sin\varphi$

$$\Psi = \Psi(r, \theta, \varphi)$$

- ✓ $0 \leq r \leq \infty$
- ✓ $0 \leq \theta \leq \pi$
- ✓ $0 \leq \varphi \leq 2\pi$

II. Solving the Schrodinger equation

Separate $H(\Psi) = E \cdot \Psi$ to three different equations:

- $\%r: H(\Psi_r) = E \cdot \Psi_r$
 - $\%\theta: H(\Psi_\theta) = E \cdot \Psi_\theta$
 - $\%\varphi: H(\Psi_\varphi) = E \cdot \Psi_\varphi$
- $\Psi(r, \theta, \varphi) = \Psi_r \cdot \Psi_\theta \cdot \Psi_\varphi = R(r) \cdot \Theta(\theta) \cdot \Phi(\varphi)$
- $$= R(r) \cdot Y(\theta, \varphi)$$

R: radial wave function

θ: Site wave function

φ: Azimuthal wave function

$$P = \int_r \int_\theta \int_\varphi \Psi^2 \cdot dv, \text{ with } dv = dx \cdot dy \cdot dz \text{ and } dv \\ = r^2 \sin\theta \cdot dr \cdot d\theta \cdot d\varphi$$

$$P = \int_r \int_\theta \int_\varphi R^2(r) \cdot Y^2(\theta, \varphi) \cdot r^2 \sin\theta \cdot dr \cdot d\theta \cdot d\varphi$$

III. Results concerning the energy: The three quantum numbers n,l and m

$R(r)$ exists if and only if $n = 1, 2, 3 \dots n$

$\theta(\theta)$ exists if and only if $l = 0, 1, 2 \dots n - 1$

$\varphi(\varphi)$ exists if and only if $-l \leq m_l \leq +l$

$$E = \frac{-me^4}{8\varepsilon_0^2 h^2} \cdot \frac{1}{n^2}$$

each value of n corresponds to an energy level: volume
in space $n: 1, 2, 3, 4 \dots$ (layers)

1) The principle quantum number n

$n=1 \Rightarrow K$

$n=2 \Rightarrow L$

$n=3 \Rightarrow M$

$n=4 \Rightarrow N$

2) The angular momentum quantum number l

All the values of an integer between $0 \leq l \leq n - 1$

Each value of l corresponds to a sublevel within the level.

$n=1 \Rightarrow l=0$

$n=2 \Rightarrow l=0$ and $l=1$

$n=3 \Rightarrow l=0 ; l=1$ and $l=2$

$l=0$ s (sharp)

$l=1$ p (principal)

$l=2$ d (diffuse)

$l=3$ f (fundamental)

3) The magnetic quantum number m (m_l)

m: whole number +,-,0. All the values: $-l \leq m_l \leq +l$

Each value of m corresponds to a sub-sublevel (orbitals: volume in space)

$l=0 \Rightarrow m=0$

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

$l=2 \Rightarrow m=-2, m=-1, m=0, m=1, m=2$

n	level	l	sublevel	m	orbital	State n,l,m	symb ol	Energy
1	K	0	s	0	s	1,0,0	1s	-13.6/1
2	L	0	s	0	s	2,0,0	2s	-13.6/4
		1	p	-1	Py	2,1,-1	2Py	-13.6/4
				0	Pz	2,1,0	2Pz	-13.6/4
				1	Px	2,1,1	2Px	-13.6/4
3	M	0	s	0	s	3,0,0	3s	-13.6/9
		1	p	-1	Py	3,1,-1	3Py	-13.6/9
				0	Pz	3,1,0	3Pz	-13.6/9
				1	Px	3,1,1	3Px	-13.6/9
		2	d	-2	dxy	3,2,-2	3dxy	-13.6/9
				-1	dyz	3,2,-1	3dyz	-13.6/9
				0	dz ²	3,2,0	3dz ²	-13.6/9
				1	dxz	3,2,1	3dxz	-13.6/9
				2	dx ² -y ²	3,2,2	3dx ² -y ²	-13.6/9

Number of electrons

- Principal quantum number n

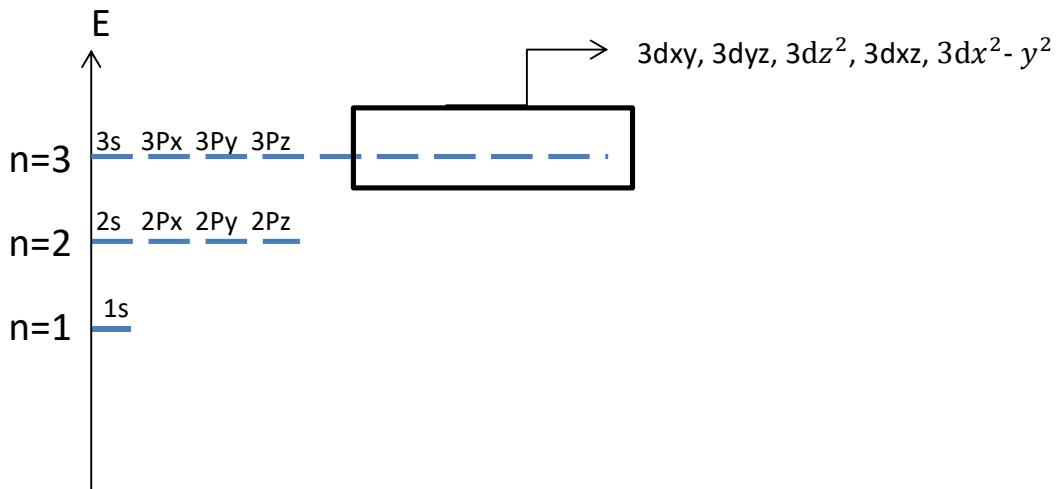
Letter	K	L	M	N	...
n	1	2	3	4	...
e^- capacity $2n^2$	$2e^-$	$8e^-$	$18e^-$	$32e^-$...

The energy is found equal to: $E_n = \frac{E_H Z^2}{n^2} eV$

Where $E_H = -13.54 eV$

- Angular momentum quantum number l

Letter	s	p	d	f	g	...
l	0	1	2	3	4	...
e^- capacity $2(2l+1)$	$2e^-$	$6e^-$	$10e^-$	$14e^-$	$18e^-$...



Degree of degeneracy n^2

Note: If you wanted to be absolutely 100% sure of where the electron is, you would have to draw an orbital the size of the Universe!

IV. Results concerning the wave function Ψ

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

Normalization condition: $\sum P = 1$

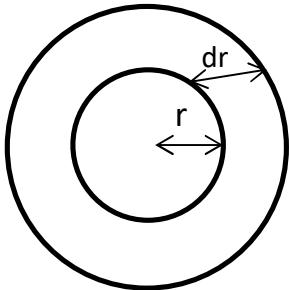
The total probability over all space is equal to 1

$$\int_{v_1}^{v_2} |\Psi|^2 d\nu = 1$$

In spherical coordinates:

$$P = \int_0^{\infty} r^2 \cdot R^2(r) \cdot dr \int_0^{\pi} \int_0^{2\pi} Y^2(\theta, \varphi) \cdot \sin\theta \cdot d\theta \cdot d\varphi = 1$$

The probability of finding the electron is: $4\pi r^2 R^2$



$$\begin{aligned} \text{Volume of spherical shell: } & \frac{4}{3}\pi(r + dr)^3 - \frac{4}{3}\pi r^3 \\ &= 4\pi r^2 dr \text{ (if } dr \text{ is small)} \end{aligned}$$

⇒ Radial probability distribution: $4\pi r^2 R^2 dr$

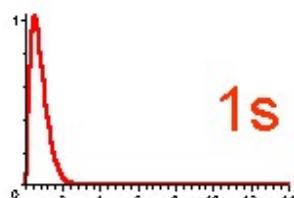
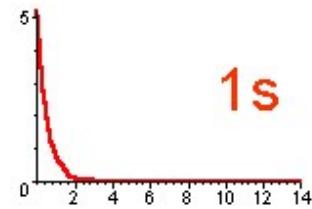
The probability of finding the electron between two spheres of radius r and $r+dr$.

V. Radial wave functions

1) Radial wave function of 1s

$$R_{1s} = \frac{2}{a^{3/2}} e^{-\frac{r}{a}} \text{ (radial wave)}$$

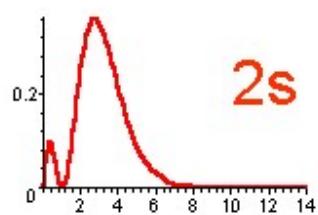
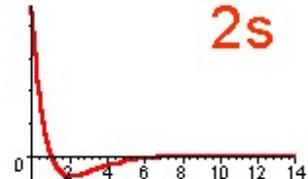
$$D = 4\pi r^2 R^2 \text{ (density)}$$



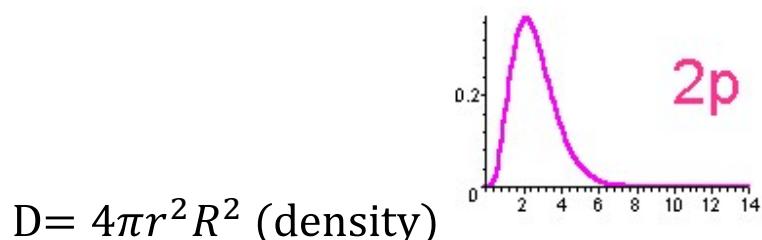
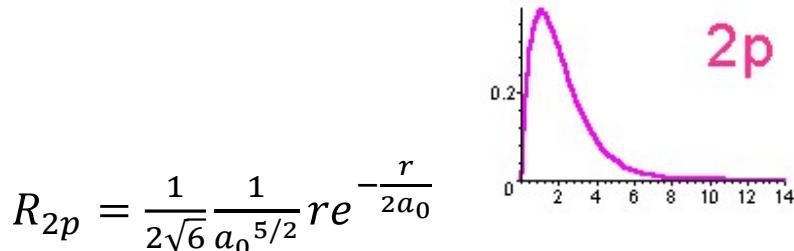
2) Radial wave function of 2s

$$R_{2s} = \frac{1}{\sqrt{2}} \frac{1}{a_0^{3/2}} \left(1 - \frac{r}{2a_0}\right) e^{-\frac{r}{2a_0}}$$

$$D = 4\pi r^2 R^2 \text{ (density)}$$

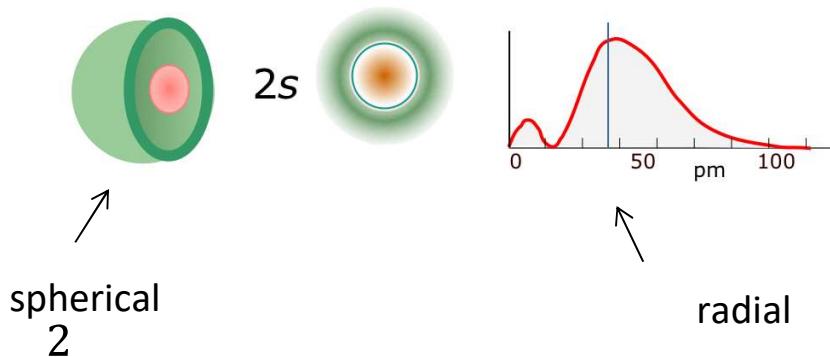
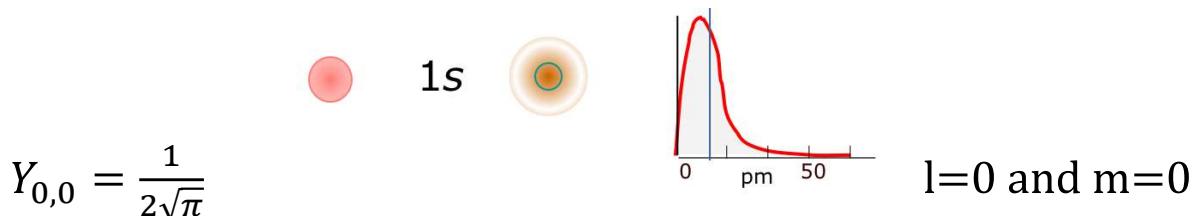


3) Radial wave function of 2p



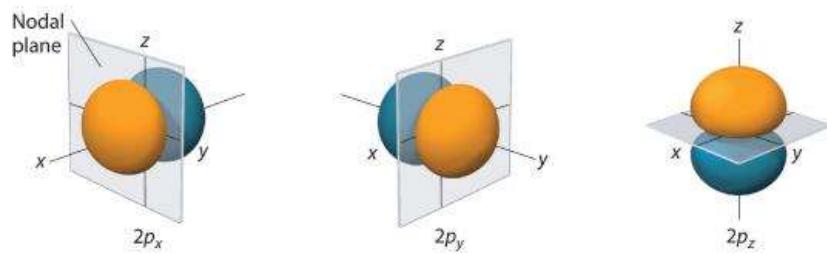
VI. Angular wave functions

1) Radial and spherical parts: Atomic orbital 1s and 2s

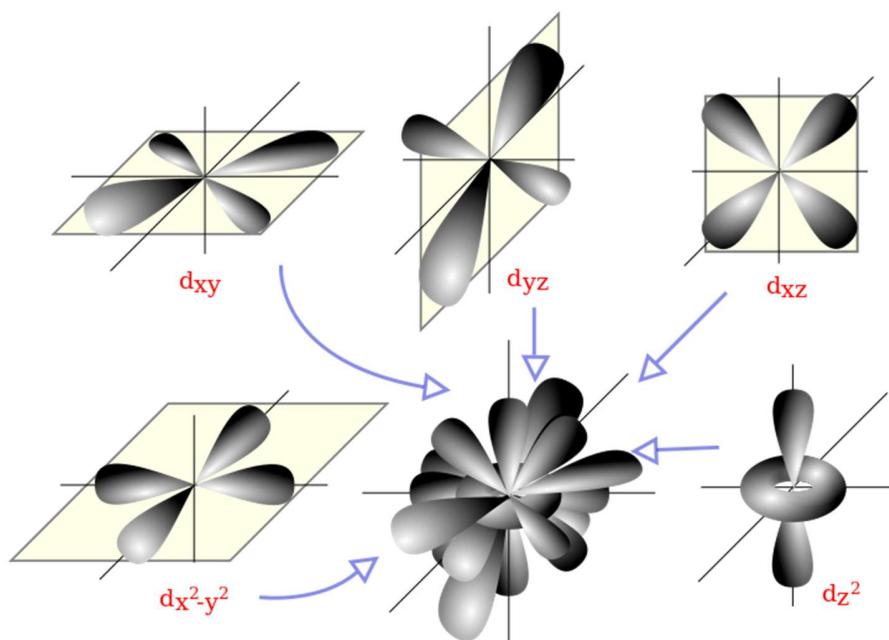
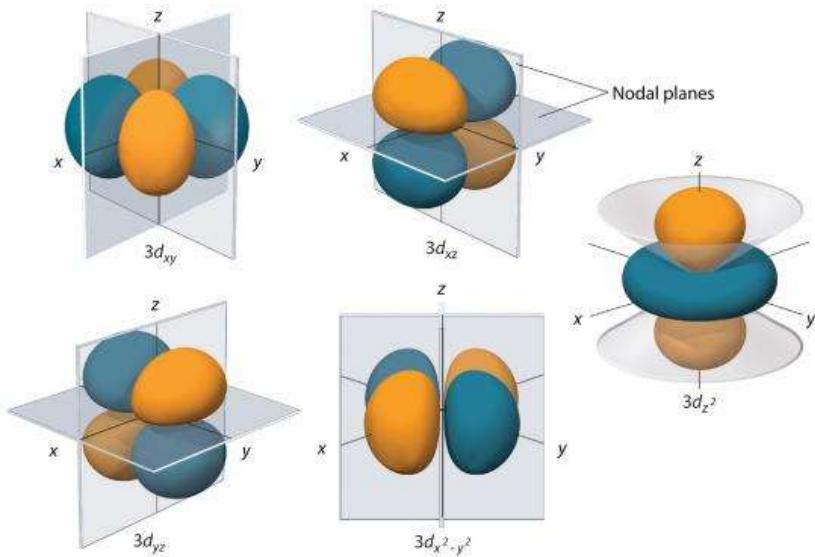


2) Spherical part: Atomic orbital 2p

$$2P_z: Y_{1,0} = \frac{\sqrt{3}}{2\sqrt{\pi}} \cos\theta \quad (\text{Rest of formulas in the summary})$$



3) Spherical part: Atomic orbital 3d



VII. The selection rule

Allowed transitions must satisfy:

$$\Delta l = \pm 1 \text{ and } \Delta m = \pm 1; 0$$

Transitions from $n = 1$ to $n = 2$

$$\begin{aligned} 1s(1,0,0) &\Rightarrow 2s(2,0,0) NO \\ 1s(1,0,0) &\Rightarrow 2Px(2,1,1) OK \\ 1s(1,0,0) &\Rightarrow 2Py(2,1,-1) OK \\ 1s(1,0,0) &\Rightarrow 2Pz(2,1,0) OK \end{aligned}$$

Transitions from $n = 2$ (take Px) to $n = 3$ (take 3d, $l=2$)

$$\begin{aligned} 2Px(2,1,1) &\Rightarrow 3dz^2(3,2,0) OK \\ 2Px(2,1,1) &\Rightarrow 3dxz(3,2,1) OK \\ 2Px(2,1,1) &\Rightarrow 3dyz(3,2,-1) NO \\ 2Px(2,1,1) &\Rightarrow 3d_{x^2-y^2}(3,2,2) OK \\ 2Px(2,1,1) &\Rightarrow 3dxy(3,2,-2) NO \end{aligned}$$

Transitions from $n = 2$ (take Py) to $n = 3$ (take 3d, $l=2$)

$$\begin{aligned} 2Py(2,1,-1) &\Rightarrow 3dz^2(3,2,0) OK \\ 2Py(2,1,-1) &\Rightarrow 3dxz(3,2,1) NO \\ 2Py(2,1,-1) &\Rightarrow 3dyz(3,2,-1) OK \\ 2Py(2,1,-1) &\Rightarrow 3d_{x^2-y^2}(3,2,2) NO \\ 2Py(2,1,-1) &\Rightarrow 3dxy(3,2,-2) OK \end{aligned}$$

Summary- Chapter IV

n	l	m_l	O.A.	Spherical part $Y(\theta, \varphi)$	Energy in eV
1	0	0	1s	$\frac{1}{2\sqrt{\pi}}$	$-13.6 Z^2$
2	0	0	2s	$\frac{1}{2\sqrt{\pi}}$	$-3.4 Z^2$
2	1	0	2Pz	$\frac{\sqrt{3}}{2\sqrt{\pi}} \cos\theta$	
2	1	1	2Px	$\frac{\sqrt{3}}{2\sqrt{\pi}} \sin\theta \cos\varphi$	
2	1	-1	2Py	$\frac{\sqrt{3}}{2\sqrt{\pi}} \sin\theta \sin\varphi$	
3	0	0	3s	$\frac{1}{2\sqrt{\pi}}$	
3	1	0	3Pz	$\frac{1}{2} \sqrt{\frac{3}{\pi}} \cos\theta$	$-1.51 Z^2$
3	1	1	3Px	$\frac{1}{2} \sqrt{\frac{3}{\pi}} \sin\theta \cos\varphi$	
3	1	-1	3Py	$\frac{1}{2} \sqrt{\frac{3}{\pi}} \sin\theta \sin\varphi$	
3	2	0	3dz ²	$\frac{1}{4} \sqrt{\frac{15}{\pi}} (3\cos^2\theta - 1)$	
3	2	1	3dxz	$\frac{1}{4} \sqrt{\frac{15}{\pi}} \sin 2\theta \cos\varphi$	
3	2	-1	3dyz	$\frac{1}{4} \sqrt{\frac{15}{\pi}} \sin 2\theta \sin\varphi$	
3	2	2	3d _{x²-y²}	$\frac{1}{4} \sqrt{\frac{15}{\pi}} \sin^2\theta \cos 2\varphi$	
3	2	-2	3dxy	$\frac{1}{4} \sqrt{\frac{15}{\pi}} \sin^2\theta \sin 2\varphi$	

Radial part: $R_{n,l}(r)$

$$\begin{aligned}
 R_{1,0} &= 2 \left(\frac{Z}{a_0} \right)^{\frac{3}{2}} e^{\frac{-Zr}{a_0}} \\
 R_{2,0} &= \frac{1}{\sqrt{2}} \left(\frac{Z}{a_0} \right)^{\frac{3}{2}} \left(1 - \frac{Zr}{2a_0} \right) e^{\frac{-Zr}{2a_0}} \\
 R_{2,1} &= \frac{1}{2\sqrt{6}} \left(\frac{Z}{a_0} \right)^{\frac{3}{2}} \frac{Zr}{a_0} e^{\frac{-Zr}{2a_0}} \\
 R_{3,0} &= \frac{2}{9\sqrt{3}} \left(\frac{Z}{a_0} \right)^{\frac{3}{2}} \left(3 - \frac{2Zr}{a_0} + \frac{2}{9} \left(\frac{Zr}{a_0} \right)^2 \right) e^{\frac{-Zr}{3a_0}} \\
 R_{3,1} &= \frac{4}{27\sqrt{6}} \left(\frac{Z}{a_0} \right)^{\frac{5}{2}} r \left(2 - \frac{Zr}{3a_0} \right) e^{\frac{-Zr}{3a_0}} \\
 R_{3,2} &= \frac{4}{81\sqrt{30}} \left(\frac{Z}{a_0} \right)^{3/2} \left(\frac{Zr}{a_0} \right)^2 e^{\frac{-Zr}{3a_0}}
 \end{aligned}$$

- Potential energy (atom): $U = -\frac{e^2}{4\pi\varepsilon_0 r}$ (ion): $U = -\frac{Ze^2}{4\pi\varepsilon_0 r}$

- 3 different forms of Schrodinger equations:

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

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

$$H(\Psi) = E\Psi \text{ (Hamiltonien operator)}$$

$$0 \leq r \leq \infty ; 0 \leq \theta \leq \pi ; 0 \leq \varphi \leq 2\pi$$

- $\Psi_{r,\theta,\varphi} = \Psi_r \Psi_\theta \Psi_\varphi = R(r).Y(\theta, \varphi)$

- $P = \int_r \int_\theta \int_\varphi \Psi^2 dv$

where $dv = dx dy dz$ and $dv = r^2 \sin\theta dr d\theta d\varphi$

$$P = \int_r \int_\theta \int_\varphi R^2(r). Y^2(\theta, \varphi) r^2 \sin\theta dr d\theta d\varphi$$

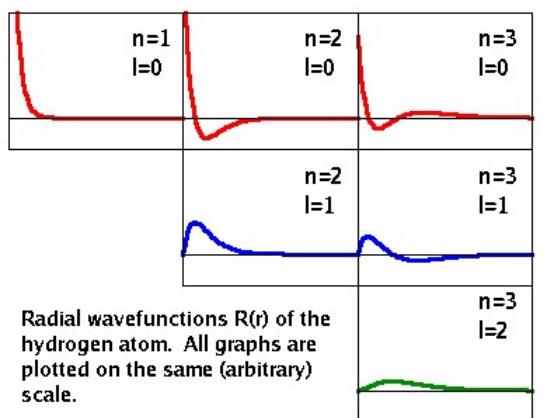
$$= 1, \text{ because } \sum P = 1$$

- Quantum numbers: $n=1,2,3\dots$; $0 \leq l \leq n-1$ ($l=0,1,2,3\dots$);
 $-l \leq m_l \leq l$ ($m_l = 0, \pm 1, \pm 2, \dots$)

✓Orbitals of the same quantum state belong to the same shell
(Shells are designated by letters K,L,M,N)

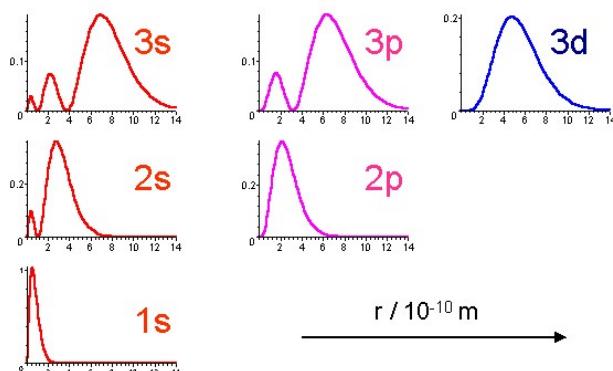
✓Orbitals of the same n and l , belong to the same subshell
($s, p, d, f, g \dots$)

- $E = \frac{-me^4}{8\varepsilon_0^2 h^2} \cdot \frac{1}{n}$
- s: shape; p: principal; d: diffuse; f: fundamental
- Degree of degeneracy = n^2
- Results concerning the radial factor $R(r)$:



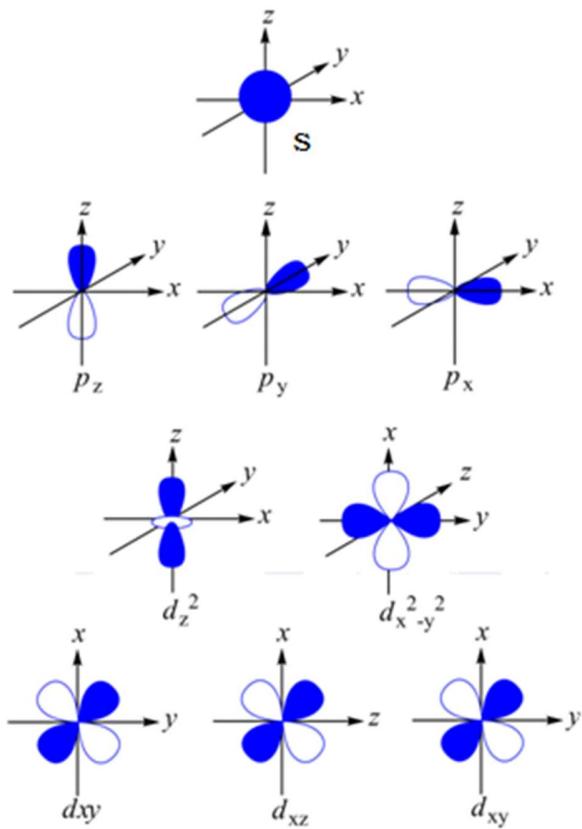
- The density:

$$\text{Electron density in atomic hydrogen } w(r) = r^2 [R_{nl}(r)]^2$$



2Px, 2Py, 2Pz each one of them is located on its axis.

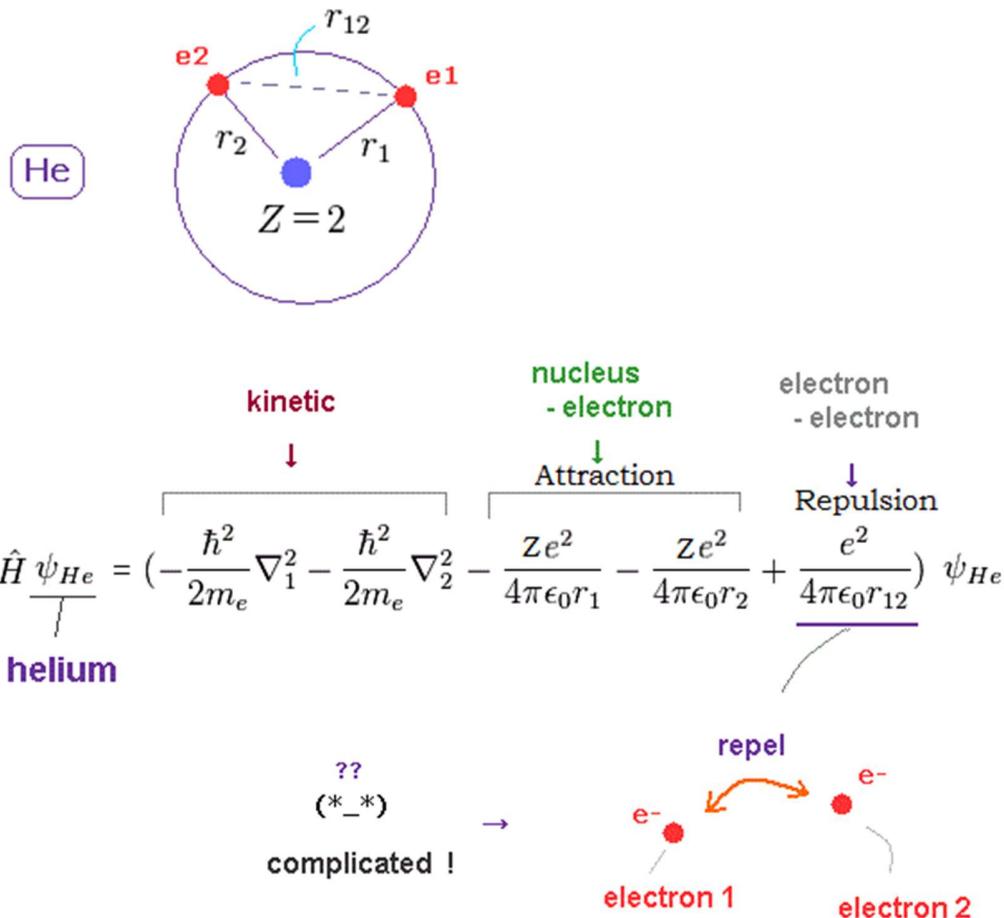
- Selection rule: $\Delta l = \pm 1$ and $\Delta m = \pm 1$ or 0
- $D(r) = 4\pi r^2 \psi^2$
- $\int_0^{+\infty} x^n e^{-x} dx = n! \Rightarrow r = 0$ (point node)
- $\int_a^b e^{-\lambda r} r^2 dr = \frac{-e^{-\lambda r}}{\lambda} (r^2 + \frac{2r}{\lambda} + \frac{2}{\lambda^2})_a^b$



✓ Chapter V- The Polyelectron atoms in quantum mechanics ✓

I. Quantum treatment

A) Helium Atom($Z=2$):



$$E_{He} = E_1 + E_2 = -108.8 \text{ eV} \text{ (calculation)}$$

$$\text{but } E_{He} = -79 \text{ eV} \text{ (exp.)}$$

$$\Rightarrow U = U_1 + U_2 + U_{12}$$

B) Approximation (screening or shielding effect)

SLATER RULES

$$U = U_1 + U_2 + U_{12}$$

$$U = \frac{-Ze^2}{4\pi\epsilon_0 r_1} + \frac{-Ze^2}{4\pi\epsilon_0 r_2} \Rightarrow \text{Introduce } \sigma \text{ where } Z^* = Z - \sigma$$

for He: $\sigma=0.30$

$$U = \frac{-(2-0.3)e^2}{4\pi\epsilon_0 r_1} + \frac{-(2-0.3)e^2}{4\pi\epsilon_0 r_2} = U_1' + U_2'$$

Two equations:

$$\begin{aligned} e_1^- : H(\psi_1) &= E_1 \psi_1 \text{ using } U_1' \\ &\Rightarrow U_1 \text{ and } E_1 \\ e_2^- : H(\psi_2) &= E_2 \psi_2 \text{ using } U_2' \\ &\Rightarrow U_2 \text{ and } E_2 \end{aligned}$$

$$E_1 = -13.6 (2-0.3)^2 = -39.3 \text{ eV}$$

$$E_2 = -13.6 (2-0.3)^2 = -39.3 \text{ eV}$$

$$E_{He} = E_1 + E_2 = -78.6 \text{ eV}$$

Z^* : Effective nucleus charge

$$E = -13.6 \frac{Z^{*2}}{n^2} \text{ eV}$$

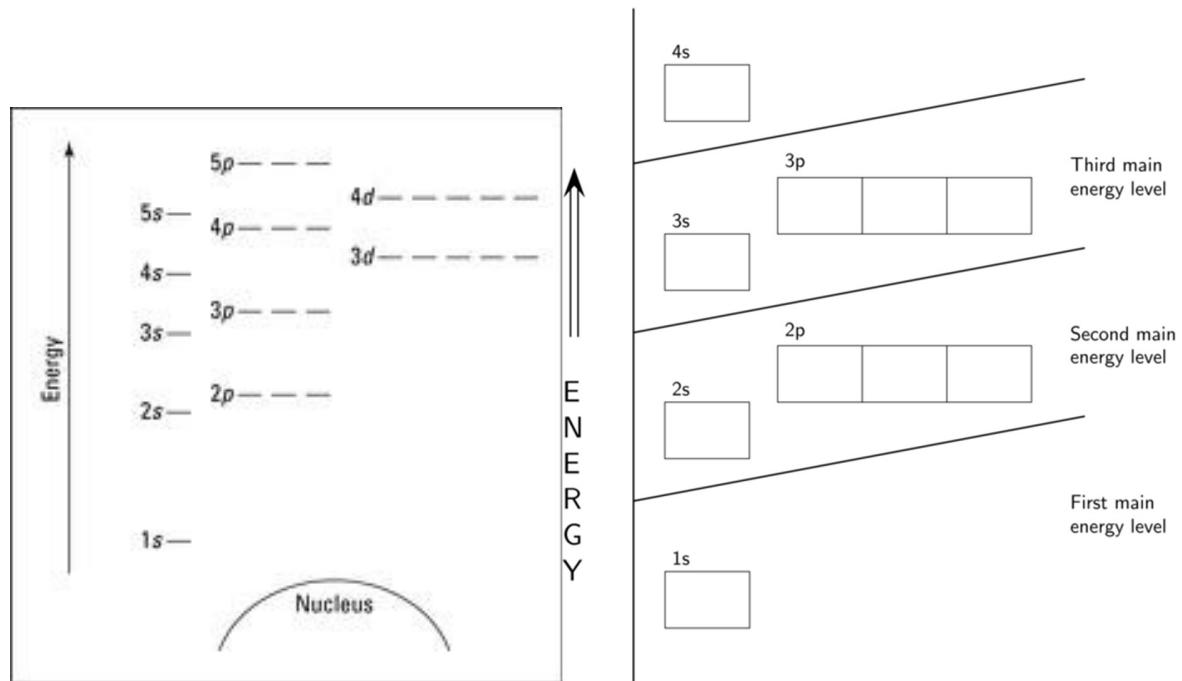
Generalization:

For an atom with N electrons: N equations.

$$\begin{aligned} e_1^- : H(\psi_1) &= E_1 \psi_1 \\ e_2^- : H(\psi_2) &= E_2 \psi_2 \\ &\dots \\ e_n^- : H(\psi_n) &= E_n \psi_n \end{aligned}$$

II. Energy diagram for multi-electron atoms(Kleschkowsky rule)

$1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 6s < 4f \dots$



III. Fourth quantum number: m_s

The electron has a permanent magnetic moment μ

- ☛ μ is quantized
- ☛ $\mu = -2 m_s \mu_B$ WITH $m_s = \pm \frac{1}{2}$ (m_s is the fourth quantum nb)
- ☛ μ_B is called the Bohr magneton
(represents a unit of magnetic moment)

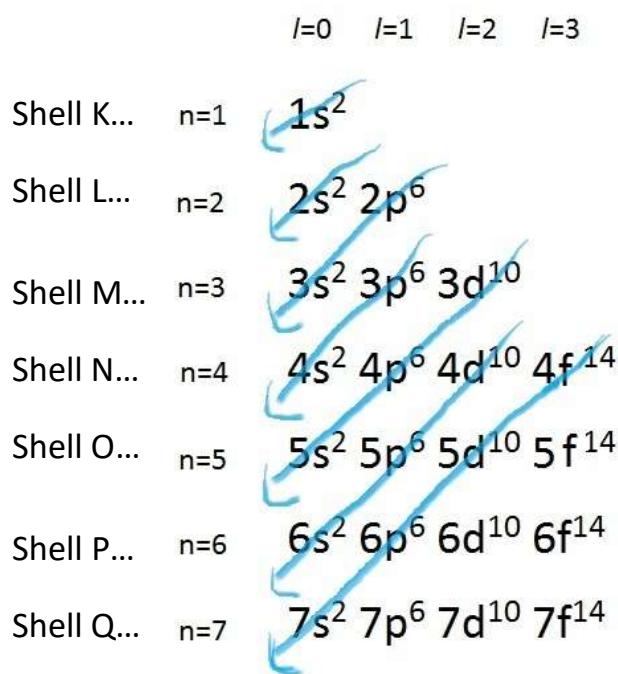
By convention:

- ☛ An electron with $m_s = +\frac{1}{2}$ is named α
- ☛ An electron with $m_s = -\frac{1}{2}$ is named β

⇒ Each electron in an atom is characterized by four quantum numbers. (n, l, m_l, m_s)

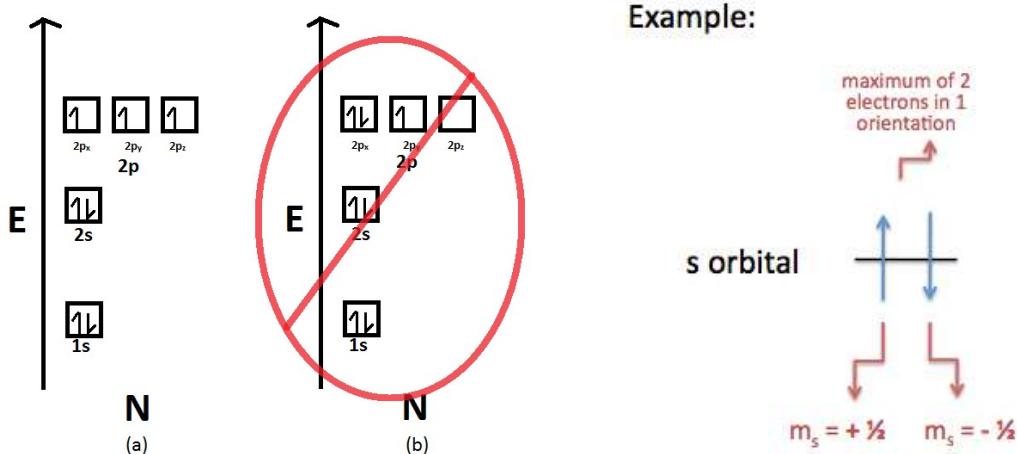
IV. Rules for writing the electron configuration for a polyelectron atom: Three rules

1) Aufbau principle



2) Pauli exclusion principle

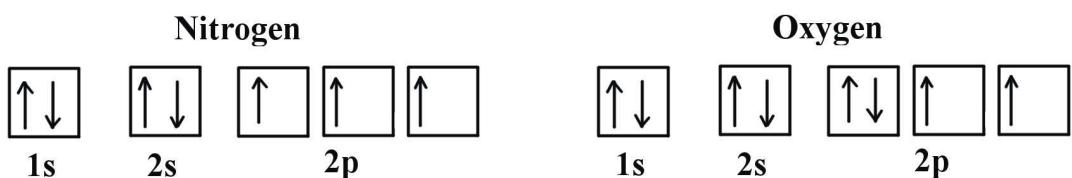
In the same atom, it is impossible to find two electrons having the same values of the 4 quantum numbers.



State	Principal quantum number <i>n</i>	Orbital quantum number <i>ℓ</i>	Magnetic quantum number <i>m_ℓ</i>	Spin quantum number <i>m_s</i>	Maximum number of electrons
1s	1	0	0	$+\frac{1}{2}, -\frac{1}{2}$	2
2s	2	0	0	$+\frac{1}{2}, -\frac{1}{2}$	2
2p	2	1	-1,0,+1	$+\frac{1}{2}, -\frac{1}{2}$	6
3s	3	0	0	$+\frac{1}{2}, -\frac{1}{2}$	2
3p	3	1	-1,0,+1	$+\frac{1}{2}, -\frac{1}{2}$	6
3d	3	2	-2,-1,0,+1,+2	$+\frac{1}{2}, -\frac{1}{2}$	10

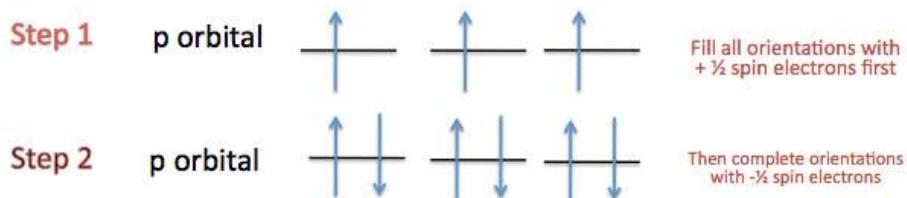
- PS:**
- ✓ Orbital is represented by \square
 - ✓ Electron is represented by \uparrow or \downarrow
 - ✓ \square Vacant
 - ✓ $\frac{1}{2}$ filled $\boxed{\uparrow}$
 - ✓ Saturated $\boxed{\uparrow\downarrow}$

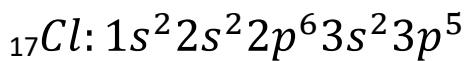
3) Hund's rule



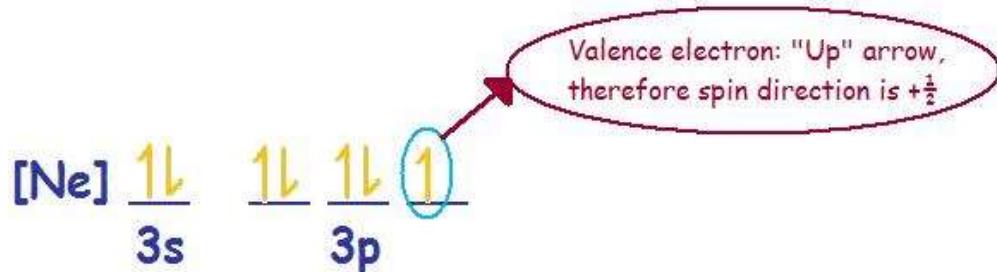
Example of Hund's Rule:

p orbital with 6 electrons

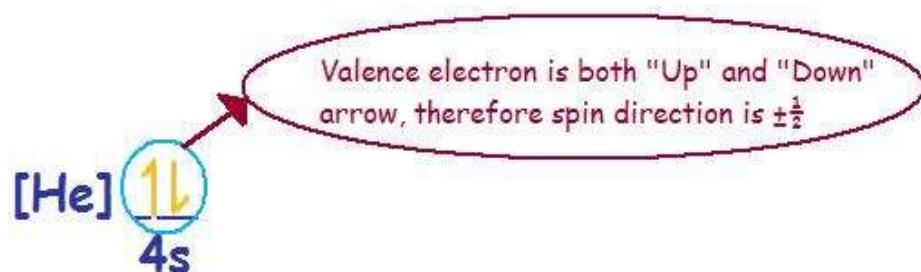




Electronic Configuration [Ne] 3s² 3p⁵



Ca: Electronic Configuration [He] 4s²



Anomalous configurations are in the summary

V. Periodic table

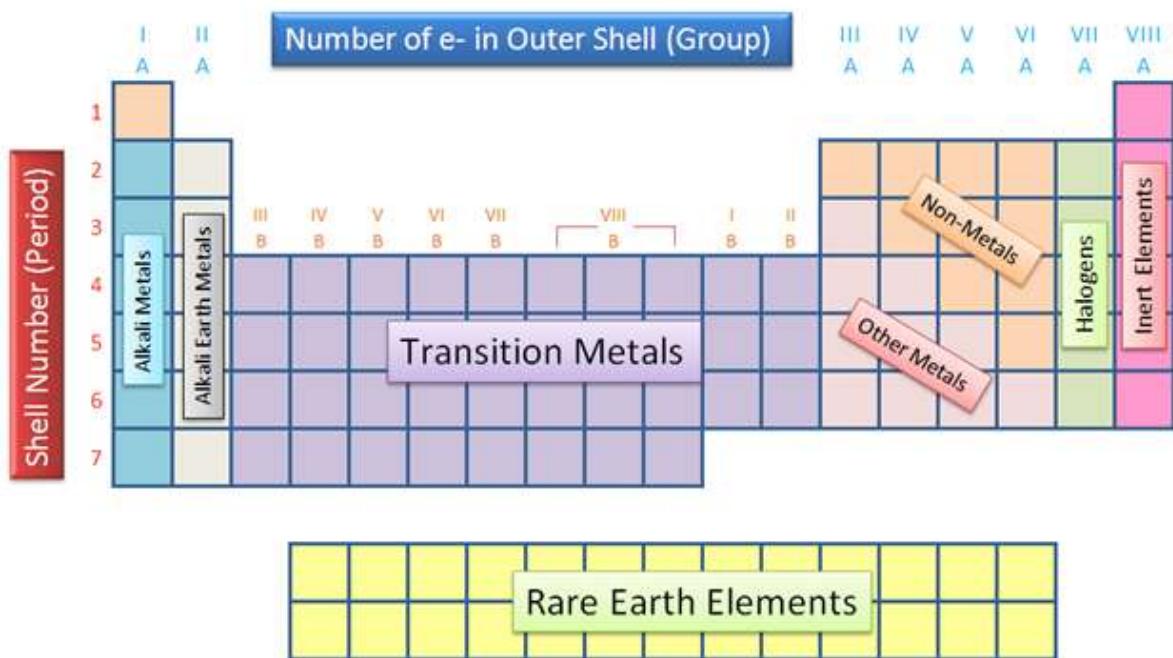
History:

- English chemist John Newland saw that elements should be arranged in *octaves*.
- Mendeleev, in 1869, arranged 63 elements in a table of 8 columns according to increasing order of their atomic masses, in a way that elements of same column have *similar properties*.
- In 1872, Mendeleev first published his table.
- The only fundamental difference between the current version of the periodic table and that of Mendeleev is that it lists the elements in order by atomic number rather than by atomic mass.

- In 1887, Mendeleev made an ascent in a balloon to study a total eclipse of the sun.
- Structure of the Periodic table 7 rows(7 periods), 18 columns(18 groups).
- After $_{92}\text{U}$: transuranium elements (artificial)

The diagram illustrates the structure of the periodic table and atomic orbitals. The main table is organized into groups: IA, IIA, IIIA, IVA, VA, VIA, VIIA, VIIIA, IIIA, IVA, VA, VIA, VIIA, VIIIA, IIIA, IVA, VA, VIA, VIIA, VIIIA. The Lanthanide and Actinide series are shown as rows below the main table. The atomic orbitals diagram above the table shows the filling of orbitals across seven periods (rows 1-7). The nonmetals are indicated by a vertical line pointing from the top of group VIA down to the bottom of the Lanthanide series.

IA																VIIIA		
1 H 1.01	II A															2 He 4.00		
3 Li 6.94	4 Be 9.01															10 Ne 20.18		
11 Na 22.99	12 Mg 24.30	III B	IV B	V B	VI B	VII B	VIII B	VIII B	I B	II B	III A	IV A	V A	VIA	VII A	VIIIA		
19 K 39.1	20 Ca 40.08	21 Sc 44.96	22 Ti 47.88	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.89	29 Cu 63.55	30 Zn 65.38	31 Ga 69.72	32 Ge 72.59	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80	
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (98)	44 Ru 101.1	45 Rh 102.9	46 Pd 106.4	47 Ag 107.9	48 Cd 112.4	49 In 114.8	50 Sn 118.7	51 Sb 121.8	52 Te 127.6	53 I 126.9	54 Xe 131.3	
55 Cs 132.9	56 Ba 137.3	57 La 138.9	58 Hf 178.5	59 Ta 181.0	60 W 183.8	61 Re 186.2	62 Os 190.2	63 Ir 192.2	64 Pt 195.1	65 Au 197.0	66 Hg 200.6	67 Tl 204.4	68 Pb 207.2	69 Bi 209.0	70 Po (209)	71 At (210)	72 Rn (222)	
87 Fr (223)	88 Ra 226.0	89 Ac (261)	104 Rf (262)	105 Db (263)	106 Sg (262)	107 Bh (265)	108 Hs (266)	109 Mt (266)										
* Lanthanide Series				58 Ce 140.1	59 Pr 140.9	60 Nd 144.2	61 Pm (145)	62 Sm 150.4	63 Eu 152.0	64 Gd 157.2	65 Tb 158.9	66 Dy 162.5	67 Ho 164.9	68 Er 167.3	69 Tm 168.9	70 Yb 173.0	71 Lu 175.0	
** Actinide Series				90 Th 232.0	91 Pa 231.0	92 U 238.0	93 Np 237.0	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (260)	



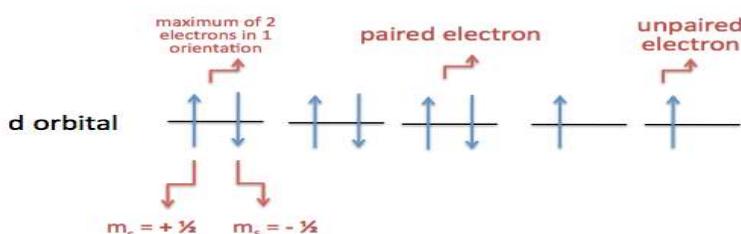
S.No	Group	Name
1	I A	Alkali metals ont tendance à donner leur électron périphérique (s^1)
2	II A	Alkaline earth metals ont tendance à donner leurs 2 électrons périphériques sauf Be
3	III A	Boron family
4	IV A	Carbon family, Presque tous les éléments ont tendance à partager leurs électrons
5	V A	Nitrogen family ont tendance à capter des électrons
6	VI A	Oxygen family ont tendance à capter des électrons
7	VII A	Halogens ont tendance à capter des électrons
8	Zero	Noble gases sont très inertes, très stables, leur couche périphérique est saturée

MAGNETIC PROPERTIES

Paired electrons \Rightarrow No magnetic properties \Rightarrow Diamagnetic

Unpaired electrons \Rightarrow Magnetic properties \Rightarrow Paramagnetic

Example :



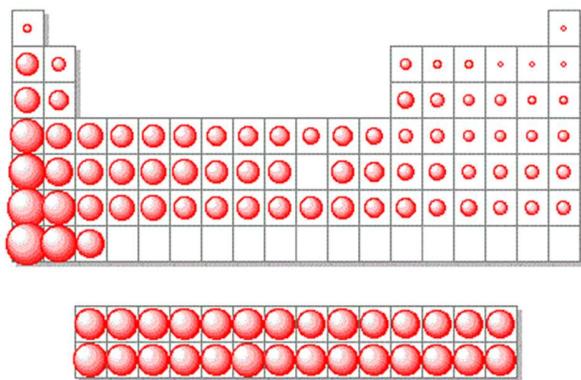
This is **paramagnetic** because there exists one or more unpaired electrons.

VI. Periodic trends of properties in the periodic table

1. Atomic radius

Period: decreases from left to right

Group: decreases from bottom to top



2. Ionic radius

Just like the atomic radius.

There are two cases:

• An atom loses an electron N_{protons} becomes $> N_{\text{electrons}}$

⇒ Attraction between the nucleus and the electrons increases

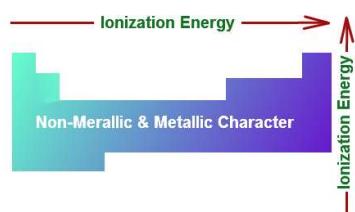
⇒ Ionic radius decreases

• An atom gains an electron N_{protons} becomes $< N_{\text{electrons}}$

⇒ Attraction between the nucleus and the electrons decreases

⇒ Ionic radius increases

3. Ionization energy

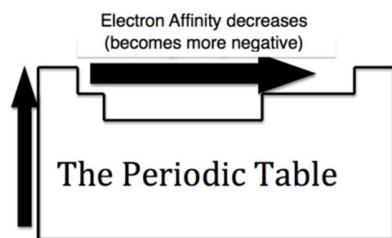


Energy required to remove an electron from a gaseous atom; the atom is assumed to be in its ground state.



Series of ionization energies ($\text{IE}_1, \text{IE}_2, \dots$)

4. Electron affinity



Release of energy when accepting e^-

5. Electronegativity

Electro negativity has the same variation as electro affinity.

VII. Effective nuclear charge and Slater's rule

	$n' < n-1$	$n' = n-1$	$n' = n$	$n' > n$
$1s$	-	-	0.3	0
n_s, n_p	1	0.85	0.35	0
n_d, n_f	1	1	0.35	0

Ruthenium atom: Ru: Z = 44

$(1s^2) (2s^2 2p^6) (3s^2 3p^6) (3d^{10}) (4s^2 4p^6) (4d^7) (5s^1)$

$$S(1s^2) = 1 * 0.35 = 0.35$$

$$S(2s^2 2p^6) = 7 * 0.35 + 2 * 0.85 = 4.15$$

$$S(3s^2 3p^6) = 7 * 0.35 + 8 * 0.85 + 2 * 1.00 = 11.25$$

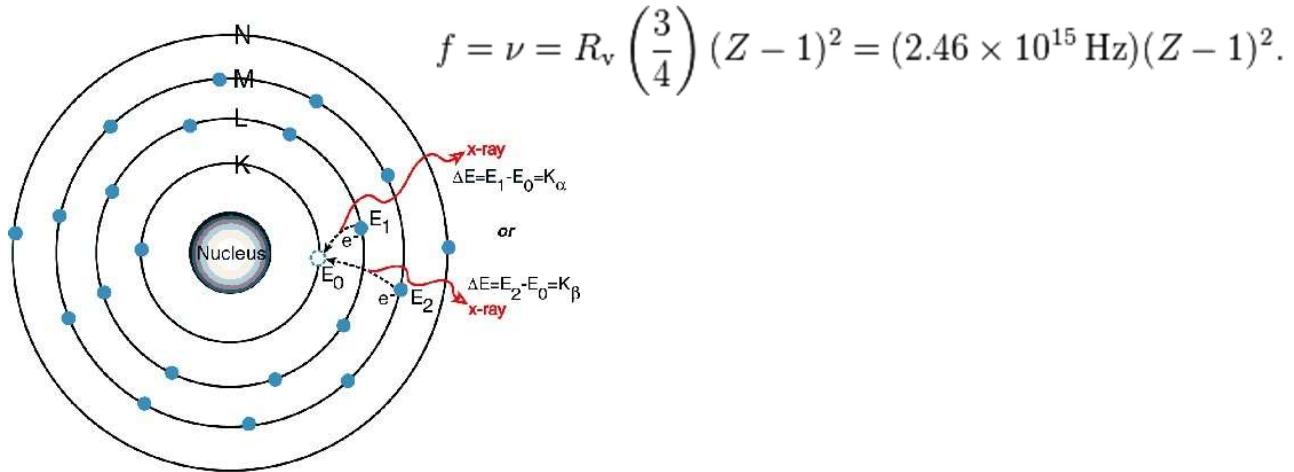
$$S(3d^{10}) = 9 * 0.35 + 8 * 1.00 + 8 * 1.00 + 2 * 1.00 = 21.15$$

$$S(4s^2 4p^6) = 7 * 0.35 + 18 * 0.85 + 8 * 1.00 + 2 * 1.00 = 27.75$$

$$S(4d^7) = 6 * 0.35 + 8 * 1.00 + 18 * 1.00 + 8 * 1.0 + 2 * 1.00 = 38.1$$

$$S(5s^1) = 15 * 0.85 + 18 * 1.00 + 8 * 1.00 + 2 * 1.00 = 40.75$$

VIII. X-RAYS-Moseley's law



NOMENCLATURE OF ELEMENTS WITH Z>110

- 0: nil
- 1: un
- 2: bi
- 3: tri
- 4: quad
- 5: pent
- 6: hex
- 7: hept
- 8: oct
- 9: enu
- 10: enn

Summary- Chapter V

- $U = U_1 + U_2 + U_{12}$

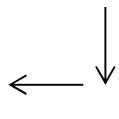
- Effective $Z^* = Z - \sum \sigma$

- $E = -13.6 \frac{Z^{*2}}{n^2} \text{ eV}$

- $m_s = \pm \frac{1}{2}$

- ✓ Vacant 
- ✓ $\frac{1}{2}$ filled 
- ✓ Saturated 

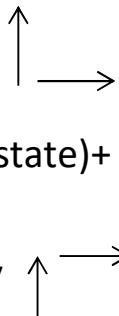
- Atomic radius



- Ionization energy ↑ →



- Electron affinity



- Electronegativity ↑ →

- Paired electrons Diamagnetic

- Unpaired electrons Paramagnetic

- s(1 square), p(3), d(5), f(7)

- Moseley's law $\sqrt{\vartheta} = \sqrt{\frac{3}{4} R_H C (Z - 1)}$

- Groupes I et II ont tendance à donner des électrons périphériques sauf Be
Groupes V, VI et VII captent des électrons
Groupe IV partage ses électrons
(L'hydrogène est une exception dans le groupe IA)
- 0: nil; 1: un; 2: bi; 3: tri; 4: quad; 5: pent; 6: hex; 7: hept; 8: oct; 9: enu; 10: enn
- Anomalous electron configurations(Z=24, 29, 41, 42, 44, 45, 46, 47, 57, 78, 79, 89,)
 - 1) $_{24}\text{Cr}$: $4s^13d^5$ (chrome)
 - 2) $_{29}\text{Cu}$: $4s^13d^{10}$ (cuivre)
 - 3) $_{41}\text{Nb}$: $5s^14d^4$ (niobium)
 - 4) $_{42}\text{Mo}$: $5s^14d^5$ (molybdene)
 - 5) $_{44}\text{Ru}$: $5s^14d^7$ (ruthenium)
 - 6) $_{45}\text{Rh}$: $5s^14d^8$ (rhodium)
 - 7) $_{46}\text{Pd}$: $5s^04d^{10}$ (palladium)
 - 8) $_{47}\text{Ag}$: $5s^14d^{10}$ (argent)
 - 9) $_{57}\text{La}$: $6s^24f^05d^1$ (lanthane)
 - 10) $_{78}\text{Pt}$: $6s^14f^{14}5d^9$ (platine)
 - 11) $_{79}\text{Au}$: $6s^14f^{14}5d^{10}$ (or)
 - 12) $_{89}\text{Ac}$: $7s^26d^1$ (actinium)

✓ Chapter VI- Chemical bonds ✓

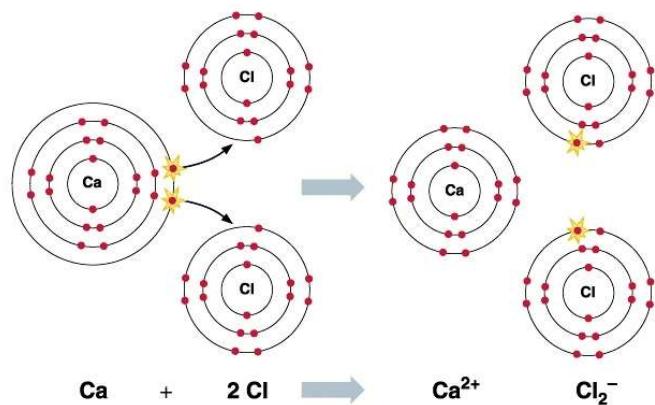
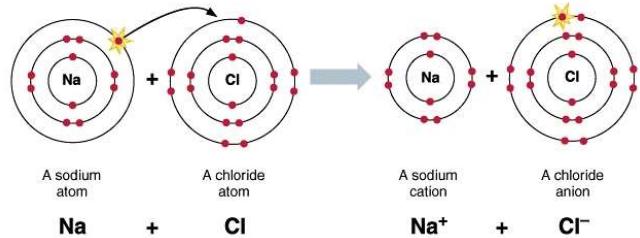
❖ Introduction

In general, the formation of a chemical bond lower the energy of a system. Experience has shown us that we can classify the bonds into 7 different types, the 3 are of major importance.

1. Ionic
2. Covalent
3. Metallic

I. Ionic bonding

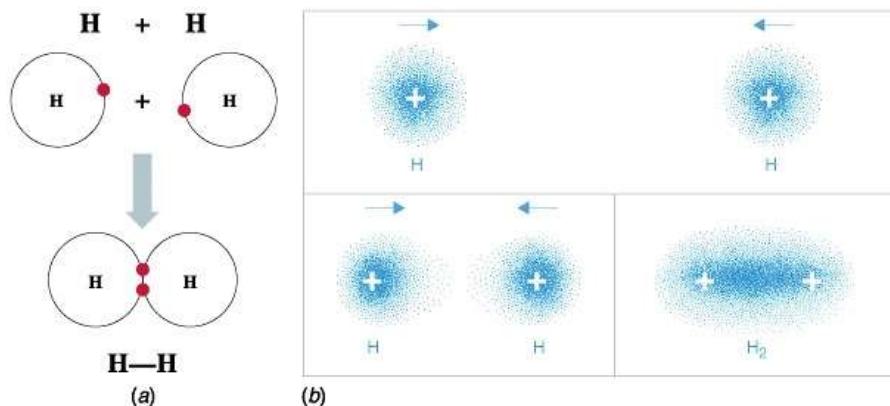
Both atoms also end up with a charge, one negative, and the other positive. We call the positive charged atom a **cation(groups IA, IIA, IIIA)**, and the negatively charged one, an **anion(groups VA, VIA, VIIA)**.



II. Covalent bonding

Theory proposed by G.N. Lewis and I. Langmuir. A type of bond that is intermediate between ionic and metallic is the covalent bond where atoms in groups (or molecules) of 2 or more share electrons.

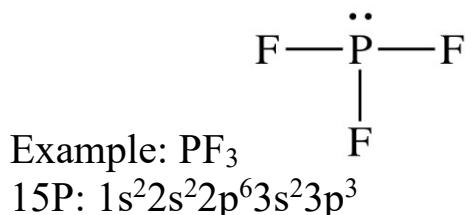
- These groups of atoms are quite stable and do not react easily.
- The most important covalent bond is formed with carbon. We could think of some C giving up 4 e⁻ and others accepting 4 e⁻, or all the carbons give up 4 e⁻ into a sea to form a metal, but this just does not happen. Instead, the electrons are shared along individual bonds.
- Organic chemistry is the study of the carbon bond.



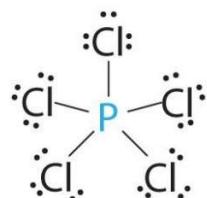
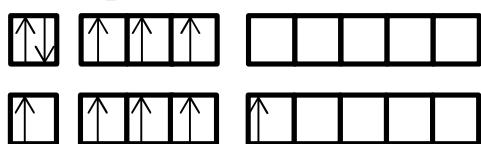
A. Simple rules for covalent bond formation

1. The energy of the electron in A is close to the energy of the electron in B. (A and B are two atoms) (If it's not close \Rightarrow Ionic)
2. Atomic orbitals must have the same sign to form a bond. (ψ function in phase)
3. As a consequence of the Pauli Exclusion Principle, the two electrons occupying the same region of space, have opposite spins.
4. Each atom will have to apply octet rule(8 electrons on outermost shell) (A groups of the P.T., except H) (exceptions B and Be). Sum of A.O.=sum of (bond pairs+lone pairs)





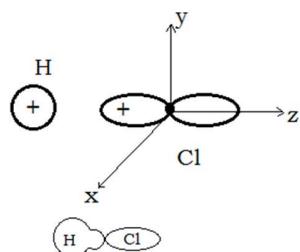
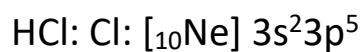
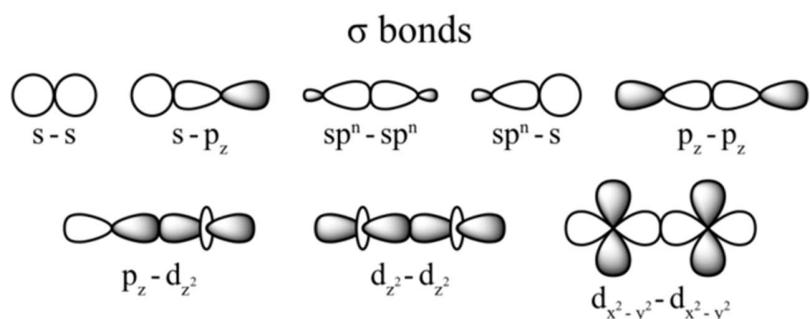
5. In d orbitals we have more than 8 electrons.



6. The new shape of the bonds will allow the reduction of repulsion.
 7. The energy of the obtained system is lower than that of the separated atoms

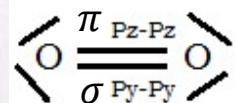
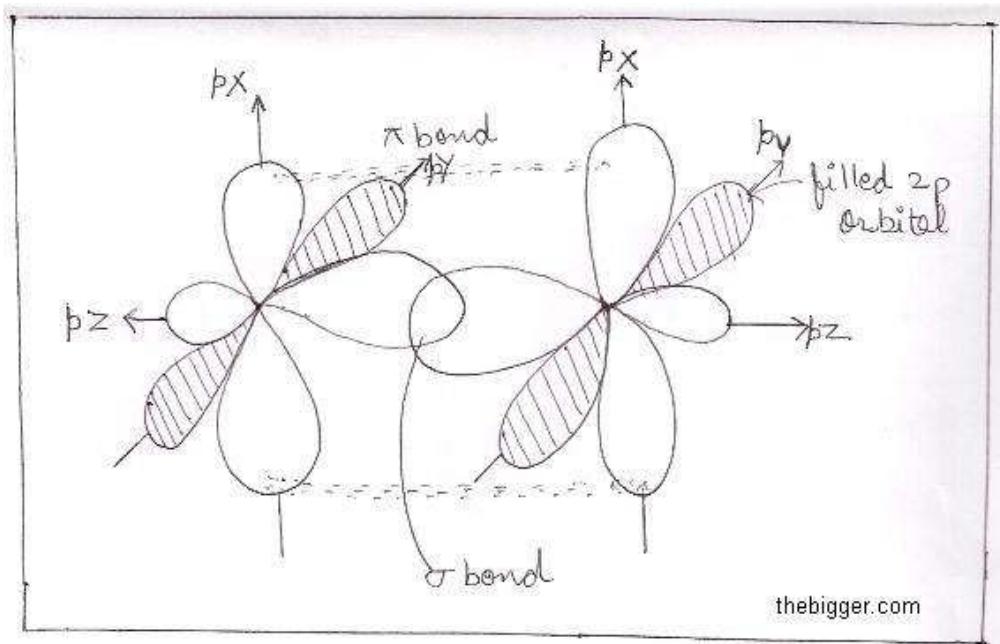
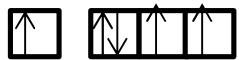
B. σ and π bonds

Examples of molecules: H_2 . σ bond happens between one end of an atom and an end of another atom.



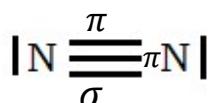
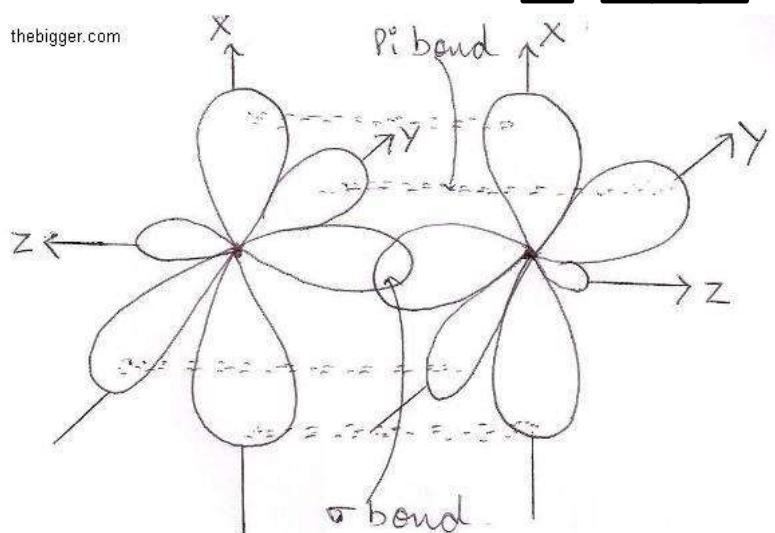
π bonding: side by side (lateral)

ex: O₂ with ₈O: [He] 2s²2p⁴

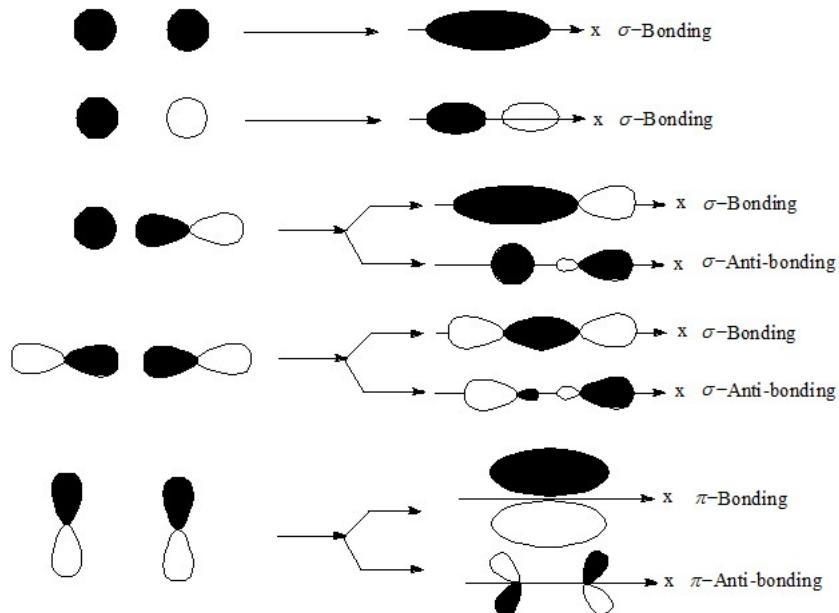


Formation of oxygen molecule by overlapping of the two half-filled p-orbitals of each oxygen atom

Ex: N₂ with ₇N: [He] 2s²2p³



Formation of nitrogen molecule



C. Molecular orbital theory

Two waves in the same space may be constructive(++,--) or destructive(-+,+-).

Constructive \Rightarrow In phase \Rightarrow A.O. same-sign \Rightarrow Positive overlap
 Destructive \Rightarrow Out of phase \Rightarrow A.O. opposite-signs \Rightarrow Negative overlap

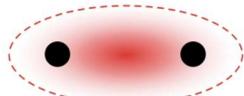
Atomic orbitals that overlap \rightarrow s and p (will be studied)

Two types of Molecular orbitals may be produced (σ and π)

σ bond

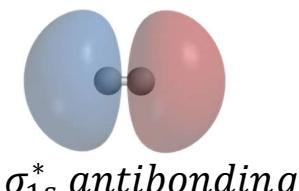
σ bonds are obtained when: 2s orbitals overlap

$\sigma - \text{bonding}$



σ_{1s} bonding

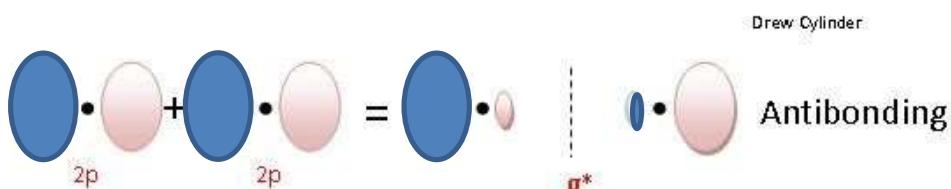
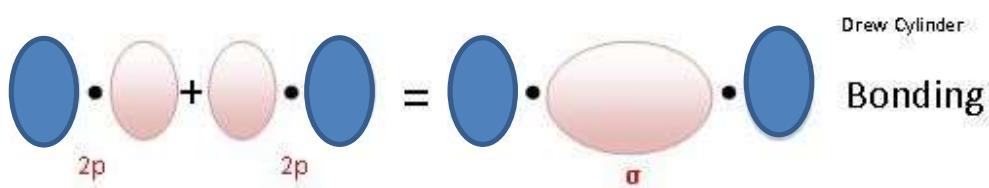
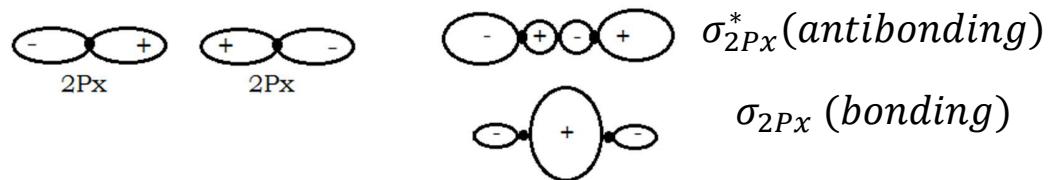
$\sigma - \text{antibonding}$



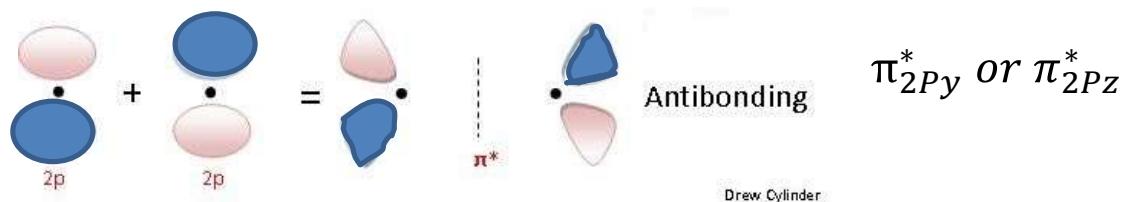
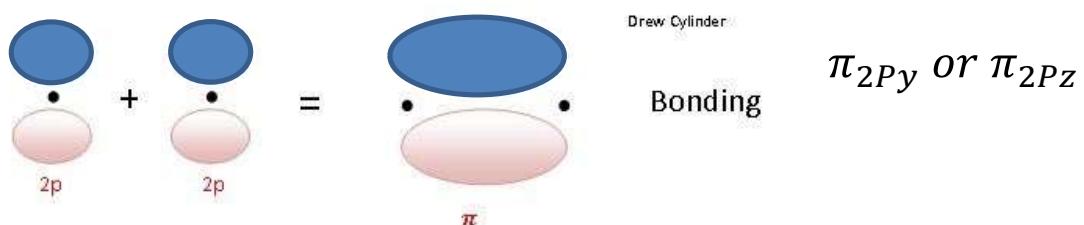
σ_{1s}^* antibonding

The star * denotes an antibonding orbital.

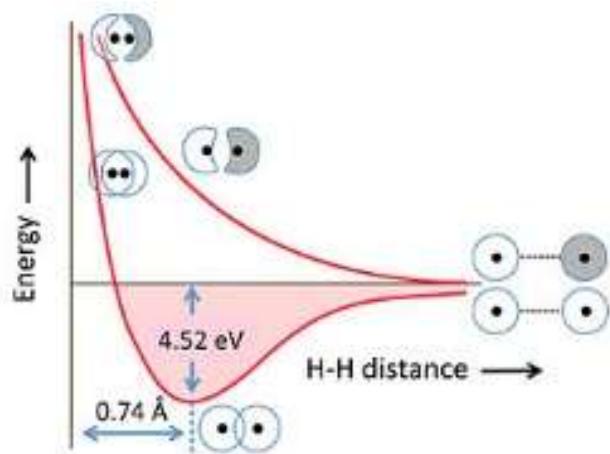
σ bonds are obtained when: 2p orbitals overlap



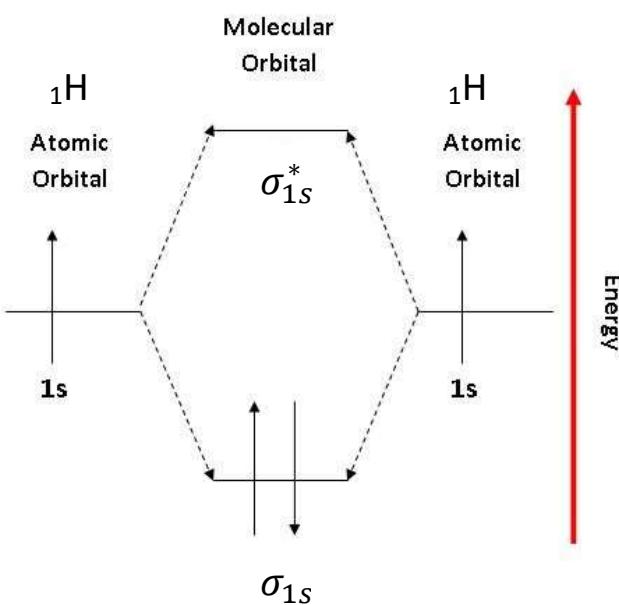
π bond



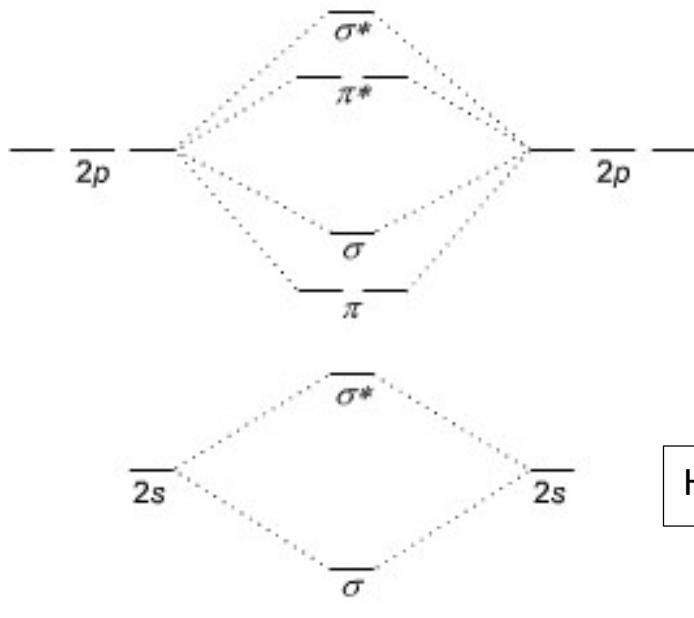
H₂



Energy diagram



- σ bonds are more stable than π bonds.
- *Bonding orbitals have lower energy than antibonding orbitals.*
- *There are two degenerate bonding π orbitals and two degenerate antibonding π orbitals.*



Homonuclear diatomic molecules

$$E_{\sigma_{2P}} < E_{\pi_{2Py}} = E_{\pi_{2Pz}}$$

Bond order and Bond stability

The Bond order is the difference between the number of bonding electrons and the number of antibonding electrons divided by 2.

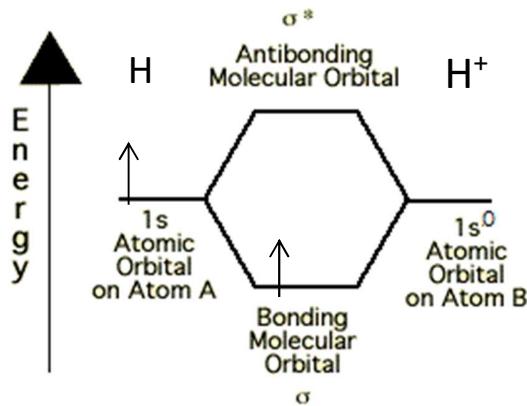
It may be equal to zero which means the molecule does not exist.

It may be a fractional number which means the molecule presents an odd number of valence electrons or has resonance.

Examples: H₂

Electron configuration: σ_{1s}^2

$$\text{B.O.} = (\text{nb of bonding e}^- - \text{nb of antibonding e}^-)/2 = \frac{2-0}{2} = 1$$

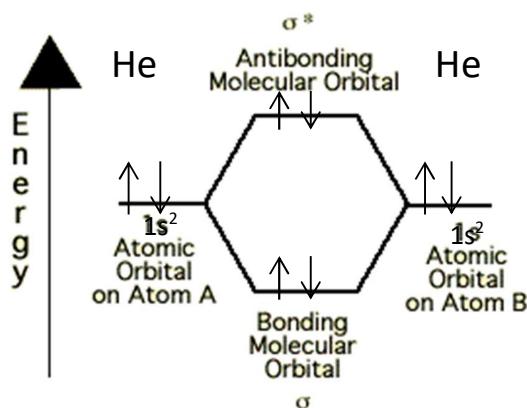


Electron configuration: σ_{1s}^1

$$B.O. = \frac{1}{2}$$

$\Rightarrow B.O.(H_2) > B.O.(H_2^+)$ so H_2 is more stable & Length.B.(H_2) < L.B.(H_2^+)

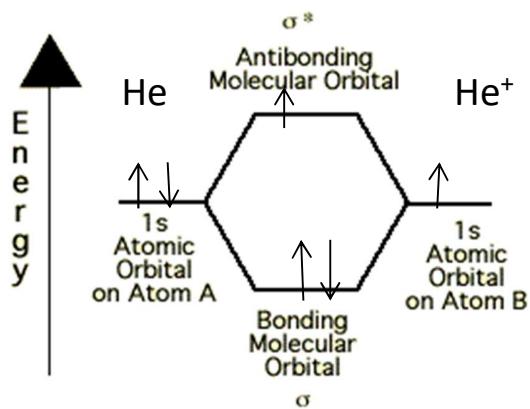
Examples of molecular orbital energy level diagram, bond order and magnetic properties



Electron configuration: $\sigma_{1s}^2, \sigma_{1s}^{*2}$

B.O. = 0, molecule does not exist.

He_2^+ :

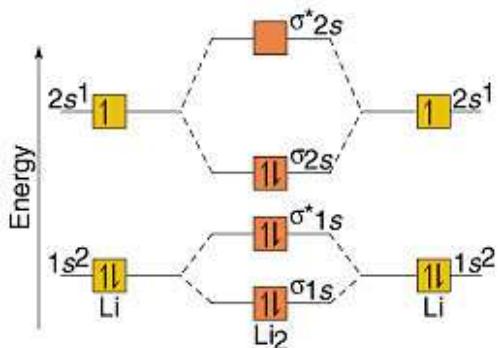


Electron configuration: $\sigma_{1s}^2, \sigma_{1s}^{*1}$

Paramagnetic

$$\text{B.O.} = \frac{1}{2}(2 - 1)$$

Li_2 :



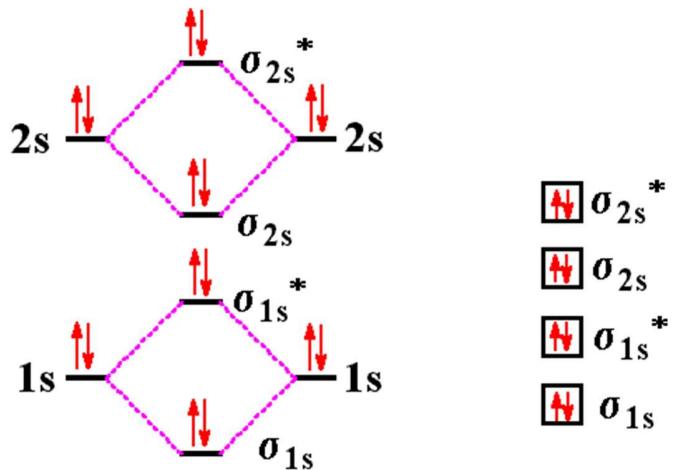
Electron configuration: $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2$

Diamagnetic

$$\text{B.O.} = \frac{1}{2}(2 + 2 - 2) = 2$$

Be₂:

A Shorthand

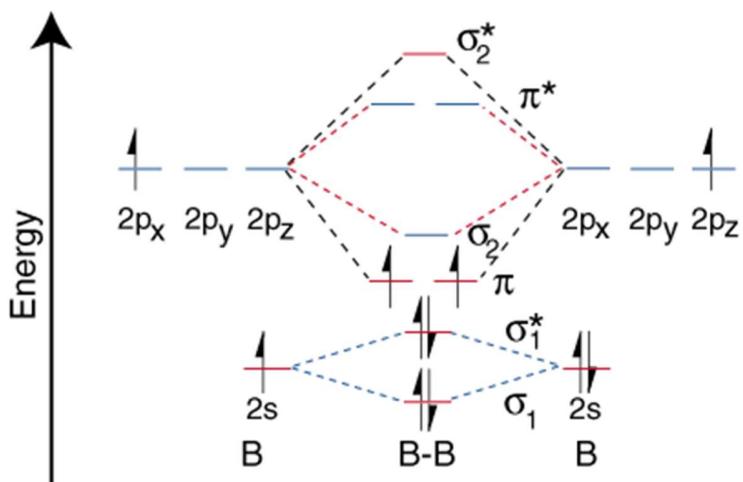


Electron configuration: $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}$

B.O.=0

EXCEPTIONS: B₂, C₂, N₂

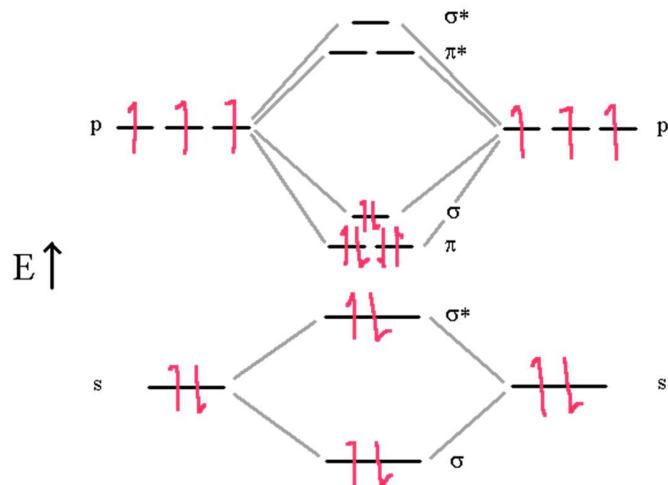
B₂:



Electron configuration: $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \pi_{2p}^2$

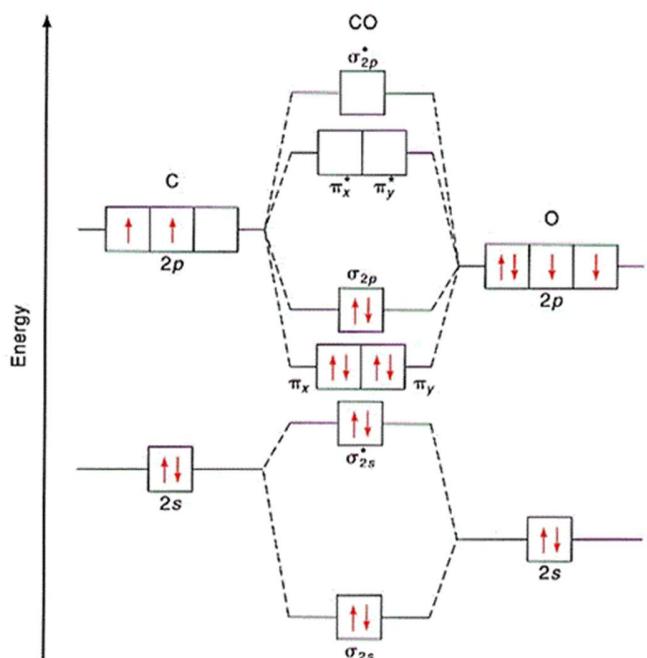
B.O.=1

N₂:



Diatomeric heteronuclear molecules: type AB

Anomalous configurations: CO, CN⁻, BO⁺

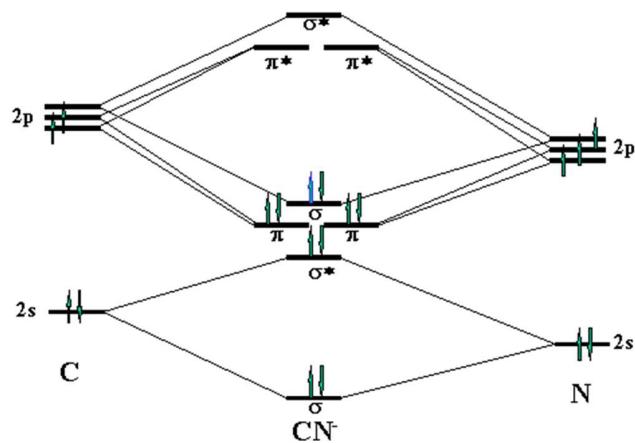


Electron configuration: $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \sigma_{2p}^2, \pi_{2p}^4$

Diamagnetic

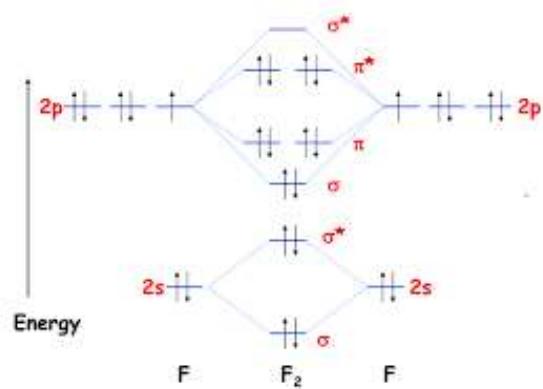
$$\text{B.O.} = \frac{10 - 4}{2} = 3 \text{ very stable}$$

CN⁻:

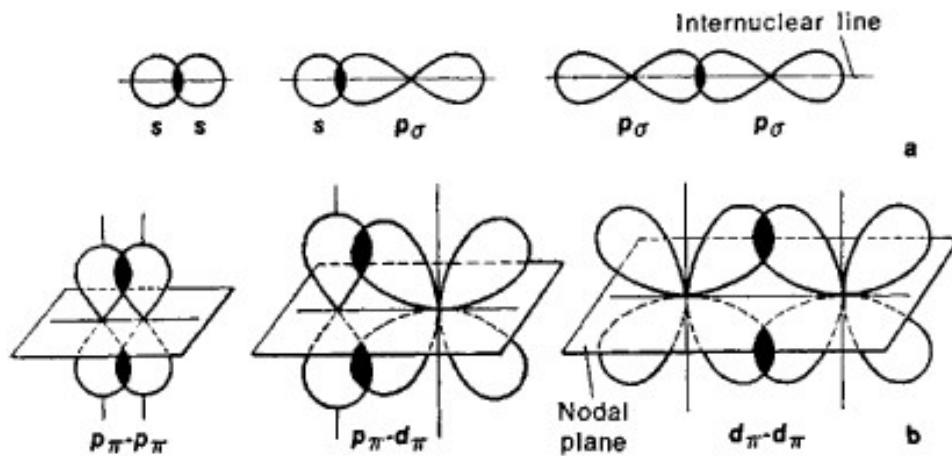


B.O.: 3 very stable

F₂:



Summary-Chapter V



- In general, a formation of a chemical bond lowers the energy of a system.
- Theory of covalent bonds proposed by Lewis and Langmuir.
Rules are:
 1. Between two atoms A and B, E_A is close to E_B
 2. The considered atomic orbitals may have the same sign to form a bond
 3. The two electrons occupying the same region of space, have opposite spins(Pauli)
 4. Sum of the A.O. = Sum(bond pairs+lone pairs)
 5. In the case of atoms with a d A.O., central atom more than 8 electrons in its valence shell.
 6. Lone pairs and bond pairs will be adjusted in a way to minimize the repulsion.
 7. Molecules have lowest energy (maximum number of bonds) (And because the energy of the obtained system is lower than that of the separated atoms)

- The combination of atomic orbitals form “Molecular orbitals”
- Two waves may be constructive(in phase, positive overlap) and destructive(out of phase, negative overlap)
- Positive overlap is the formation of a bonding molecular orbital
- Negative overlap is the formation of an antibonding molecular orbital
- Two types of molecular orbitals will be studied
 σ bonds and π bonds.
- You have to know:

σ bonds are more stable than π bonds

Bonding orbitals have lower energy than antibonding orbitals

There are two degenerate bonding π orbitals and two degenerate antibonding π orbitals.

$$\text{Bond Order} = \frac{\sum \text{bonding } e^- - \sum \text{antibonding } e^-}{2}$$

- B.O.(H₂) > B.O.(H₂⁺) so H₂ is more stable & Length.B.(H₂) < L.B.(H₂⁺)
- If B.O. is zero, the molecule does not exist.
B.O.= $\frac{n}{q}$, the molecule exists but not stable (Paramagnetic or has resonance)
- B.O.=number (like 1) Diamagnetic
- Exceptions B², C², N², CN⁻, CO, BO⁺

✓ Chapter VII- Polyatomic molecules ✓

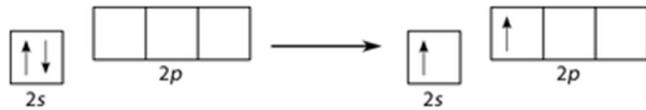
I. Hybridization theory

It's a combination between atomic orbitals (s and p) to form hybrid orbitals to form bonds.

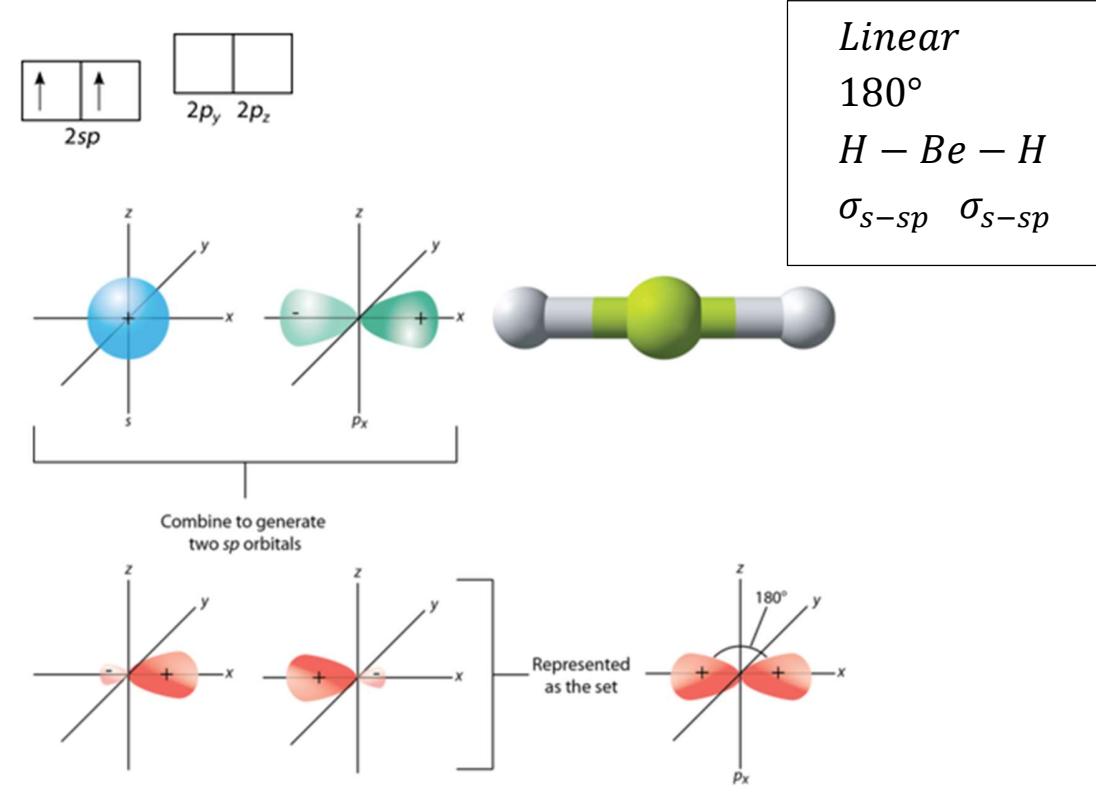
1. Hybridization of type sp: molecule BeH₂



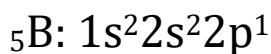
A beryllium hydride (BeH₂) molecule is predicted to be linear by VSEPR.



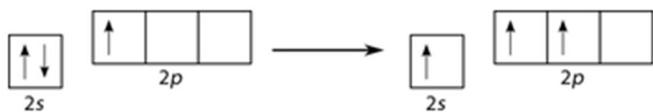
The occupied orbitals are then hybridized, and the result is a pair of *sp* hybrid orbitals.



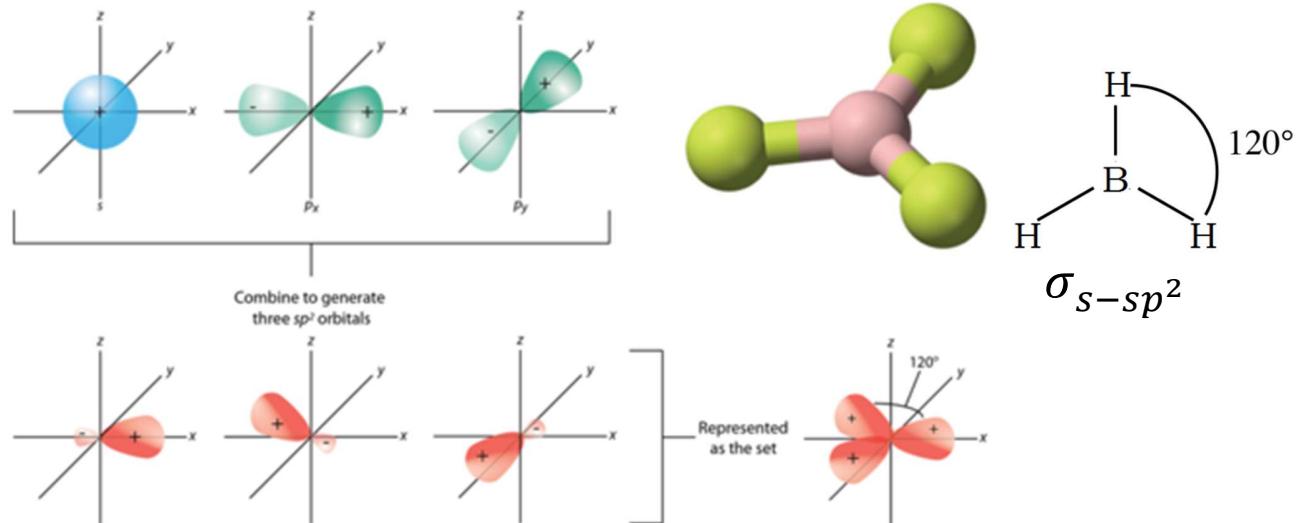
2. Hybridization of type sp^2 : molecule BH_3



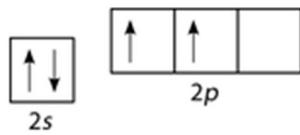
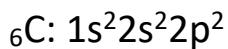
Boron trifluoride (BH_3) is predicted to have a trigonal planar geometry by VSEPR.

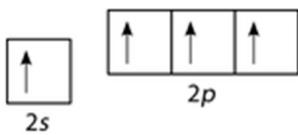


This is followed by hybridization of the three occupied orbitals to form a set of three sp^2 hybrids, leaving the $2p_z$ orbital unhybridized.

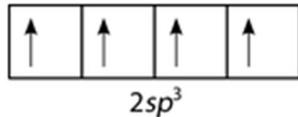


3. Hybridization of type sp^3 : CH_4

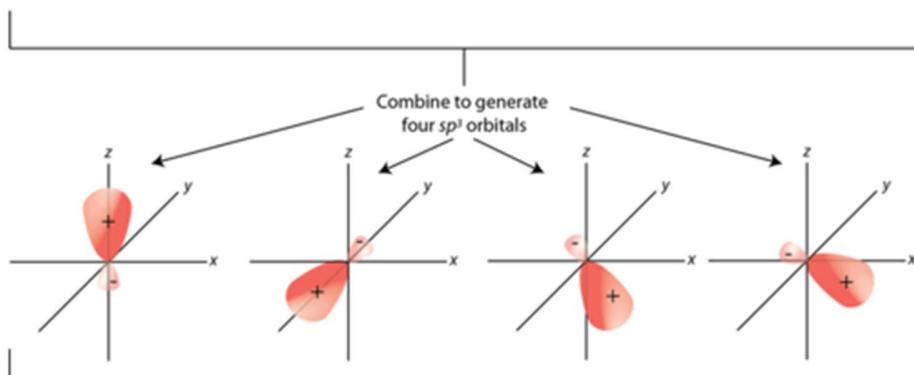
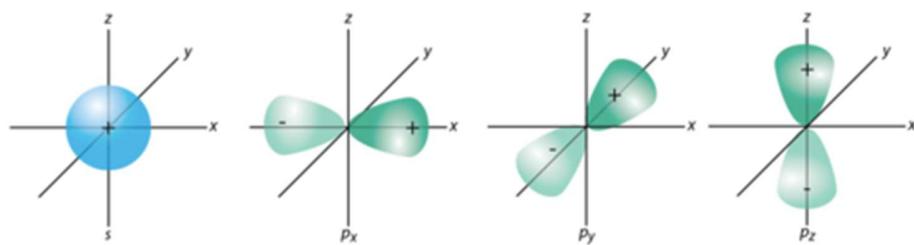




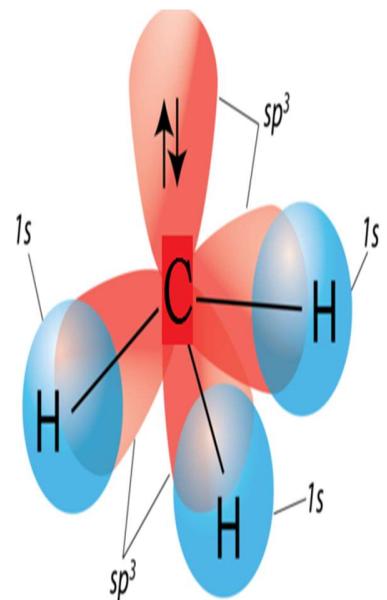
In the current case of carbon, the single $2s$ orbital hybridizes with the three $2p$ orbitals to form a set of four hybrid orbitals, called sp^3 hybrids.



sp^3
Tetrahedron
 $109^\circ.28'$

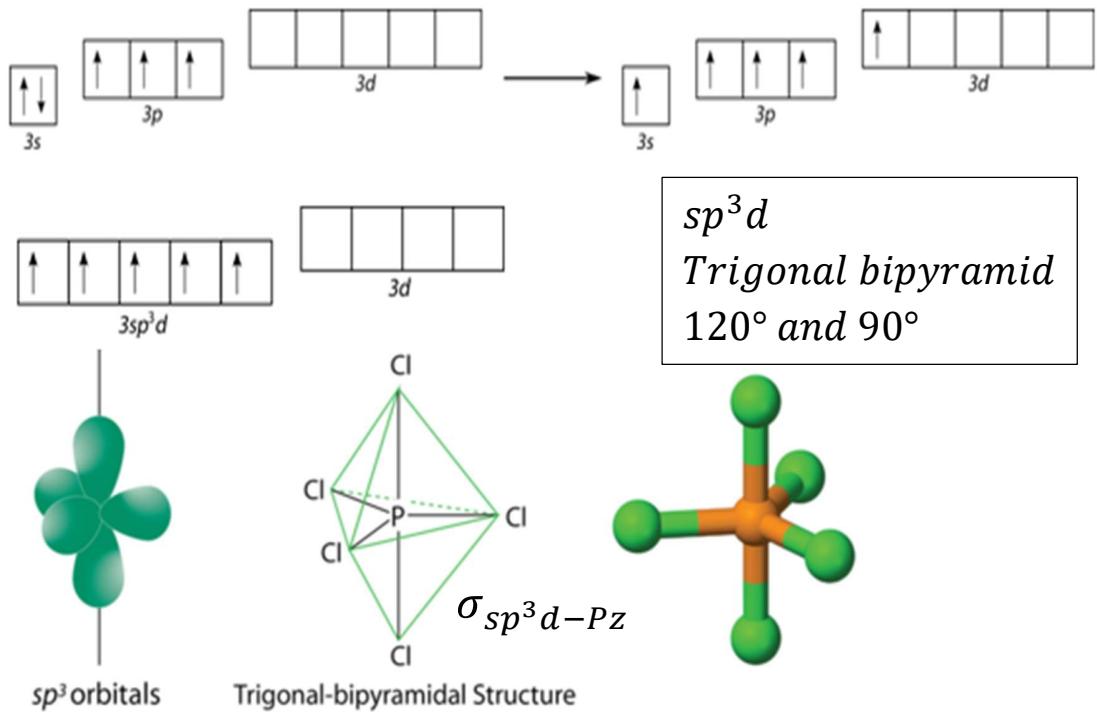


Represented as the set

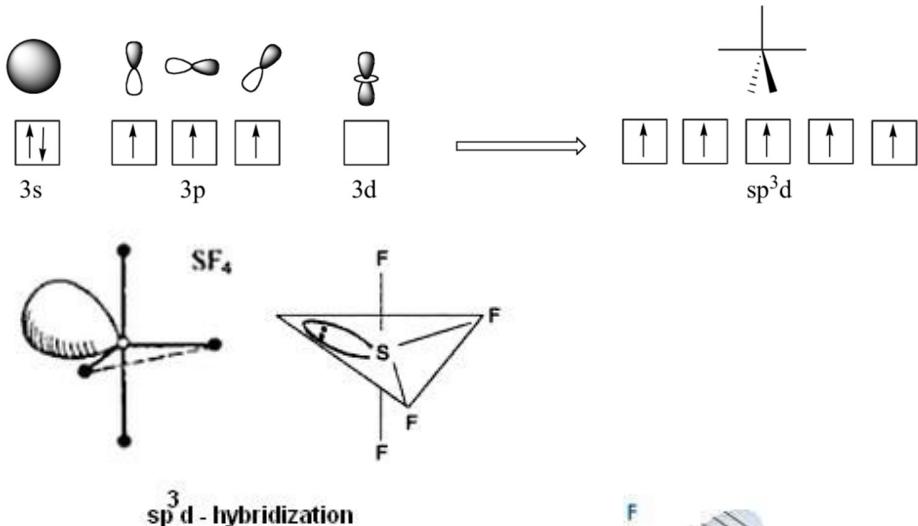


4. Hybridization of type sp^3d : PCl_5 , SF_4 , ClF_3 , XeF_2

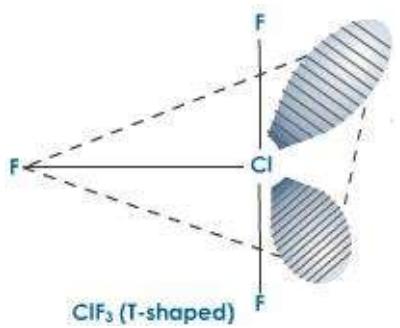
$_{15}P$: $[_{10}Ne] 3s^2 3p^3 3d^0$

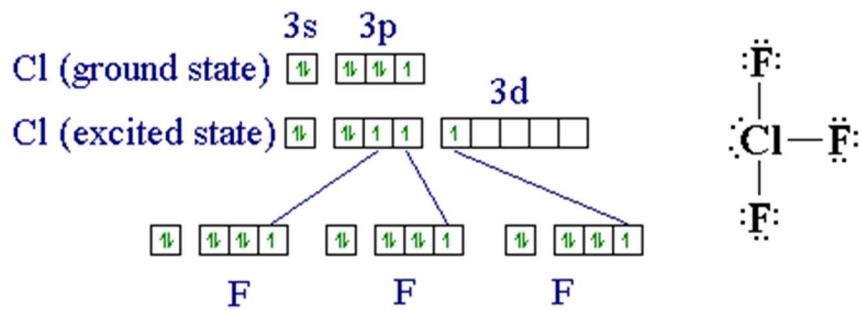


$_{16}S$: $[_{10}Ne] 3s^2 3p^4 3d^0$

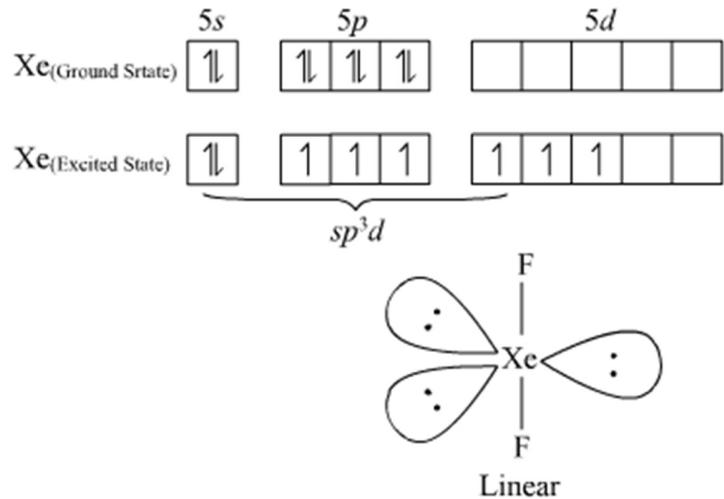
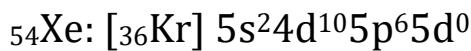


$_{17}Cl$: $[_{10}Ne] 3s^2 3p^5 3d^0$





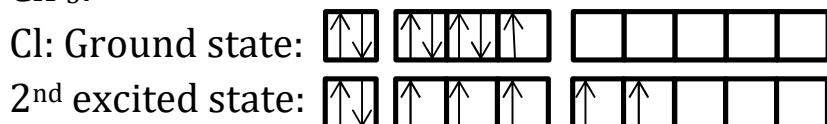
Trigonal bipyramidal in shape of T



Linear shape

5. Hybridization of type sp^3d^2 : ClF_5 , SF_6 , XeF_4

ClF_5 :

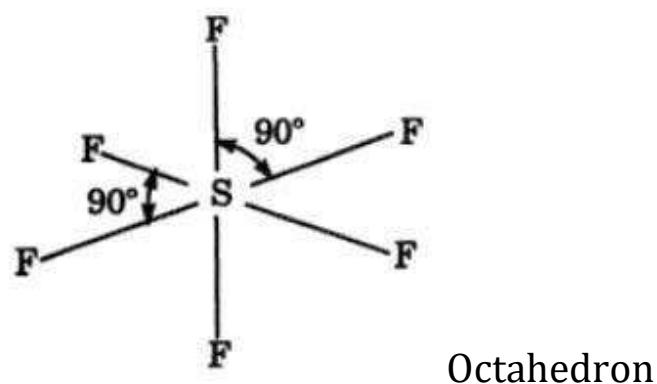


S: $[_{10}\text{Ne}] 3s^2 3p^4 3d^0$

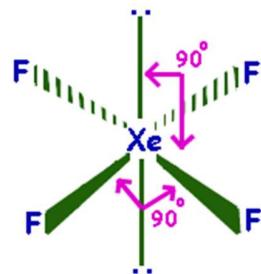
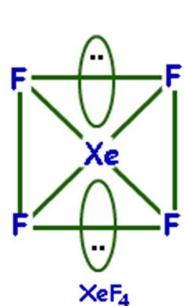
Cl: Ground state



2nd excited state



Xe:



Square shape

6. Hybridization of type sp^3d^3 : ClF_7 , XeF_6

Cl: Ground state:



3rd excited state:



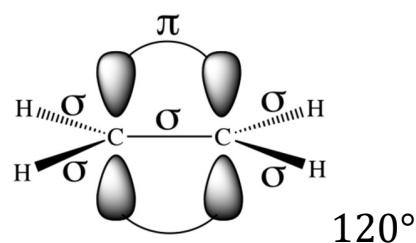
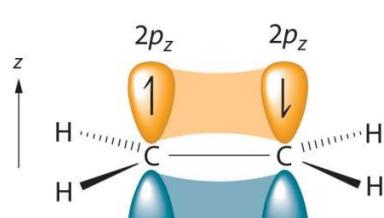
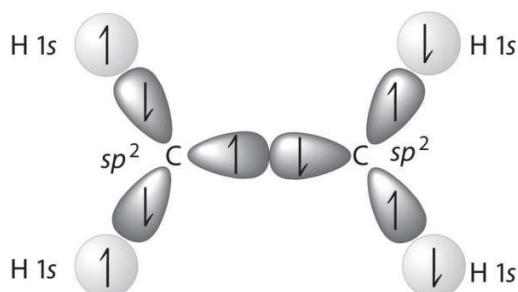
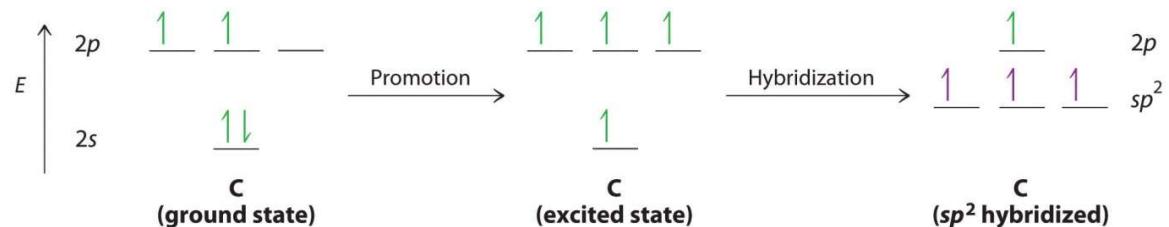
sp^3d^3

Bipyramid pentagonal

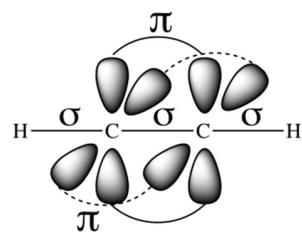
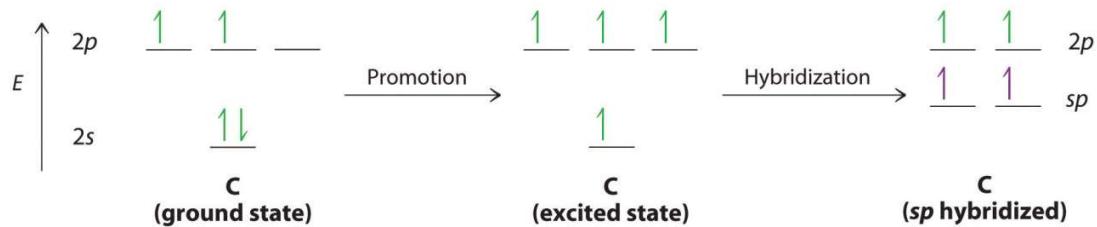
$72^\circ + 90^\circ$

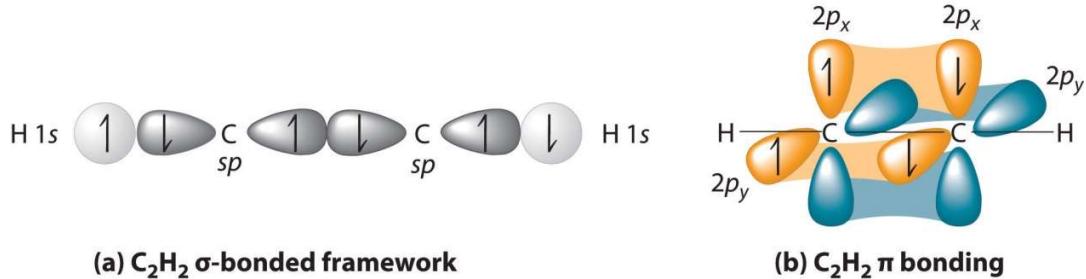
Other examples: C₂H₄, C₂H₂

C₂H₄:



C₂H₂:



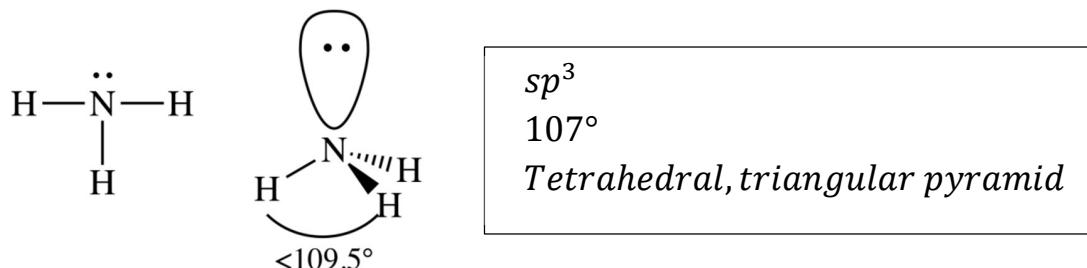


Particular cases: NH_3 and H_2O

NH_3 :

${}^7\text{N}$: $[\text{He}]2\text{s}^22\text{p}^3$

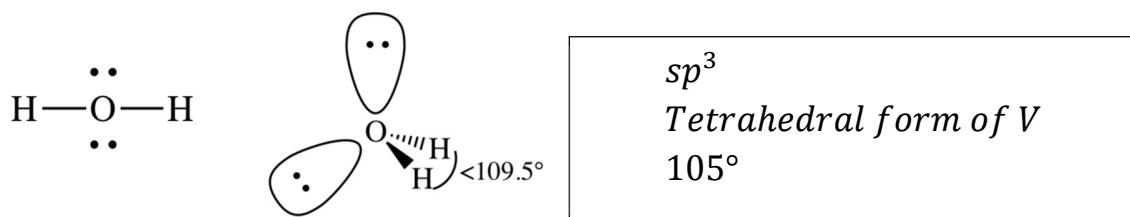
Ground state:



H_2O :

${}^8\text{O}$: $[\text{He}]2\text{s}^22\text{p}^4$

Ground state:



II. Theory of the valence shell electron pair repulsion VSEPR

Repulsion:

- Bond angle
- Nature/ type of electron pair surrounding the central atom
(Non bonding pairs “N” and Bonding pair “B”)

Max repulsion: between 2 N

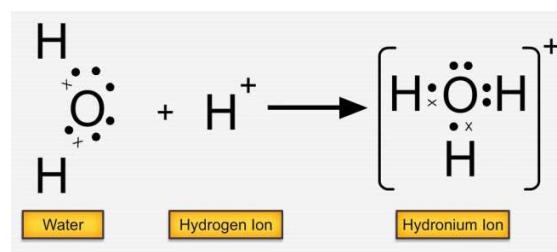
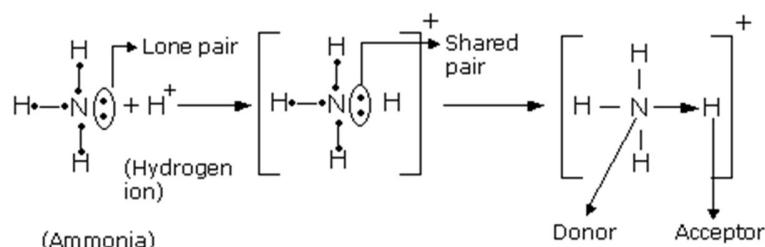
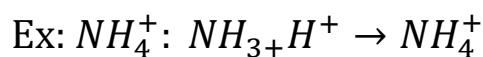
Ave repulsion: between 1 N and 1 B

Min repulsion: between 2 B

III. Coordinate covalent bond

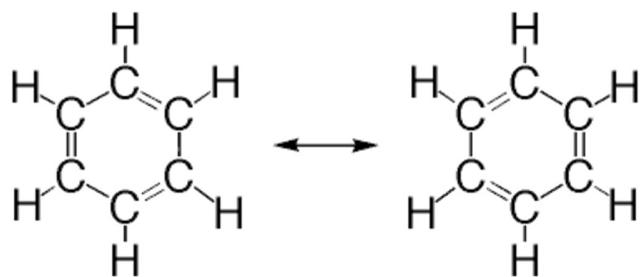
Two conditions:

- An atom having a lone pair
- Another atom with a vacant orbital



IV. Resonance (delocalized π electrons)

Benzene C₆H₆:

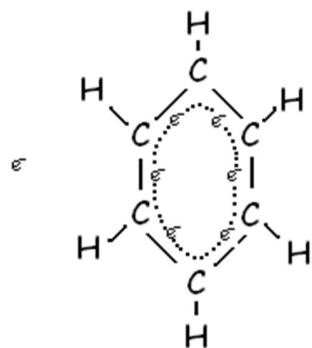


$$C - C \ 1.46 \text{ \AA}^\circ$$

$$C = C \ 1.33 \text{ \AA}^\circ$$

Scientists found that it is a regular hexagon.

6e⁻ of the 3 π bonds that are moving.

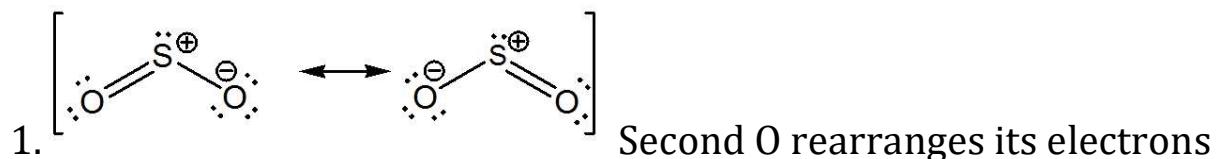


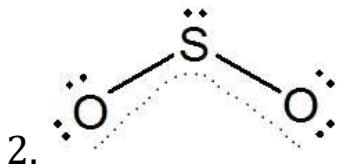
$$-C \ \frac{\pi}{\sigma} \ C - C \ \frac{\pi}{\sigma} \ C -$$

SO₂:

₈O: [He] 2s²2p⁴

₁₆S: [Ne] 3s²3p⁴





Scientists found that both bonds are equal.

V. Polarity of bonds- Polarity of molecules

Polarity of bonds

Ex: H•—•H: pure covalent bond: non polar. Electron shared equally.

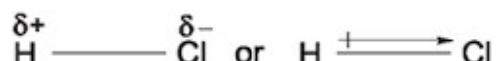
Ex: Na^+ ; Cl^- : *ionic bond*



The bonded electron pair is

Ex: attracted towards the Cl atom.

Polar covalent bond with a certain % of ionic character



Creation of a dipole

Vector goes from $\delta+$ to $\delta-$ (dipole moment

vector) $\vec{\mu}$: *dipole moment*

Partial charge: $|\delta| < |e|$

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

μ in C.m

$q \approx 10^{-19}$ in C

$\Phi \approx 10^{-1}$ in m

$$1D = \frac{1}{3} \cdot 10^{-2} \text{ C.m} = 3.3 \cdot 10^{-30} \text{ C.m}$$

$$|\vec{\mu}| = 4.8 \cdot \delta \cdot l$$

μ in D

δ in e

l in A°

$$q = \delta \cdot e$$

Exercise: distance $l = 1.28 \text{ A}^\circ$

$$|\vec{\mu}| = 1.03 \text{ D}$$

% of ionic character in HCl?

$$\mu = 4.8 \cdot \delta \cdot l$$

$$\Rightarrow \delta = \frac{1.03}{4.8 \cdot 1.28} = 0.17 \text{ e}$$

$$\% \text{ of ionic character} = \left| \frac{\delta}{e} \right| \cdot 100 = \left| \frac{0.17 \text{ e}}{e} \right| \cdot 100 = 17\%$$

If the difference of electromagnetivity increase, the % of ionic character increase

Non-polar bond: $\delta = 0$

Ionic bond $\delta = 1$

Covalent bond: $0 < \delta < 1$

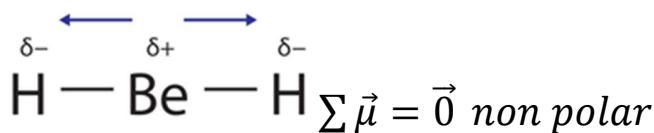
1 kJ/mol = 4.18 kcal

F > O > Cl > N > Br > I > S > C > H

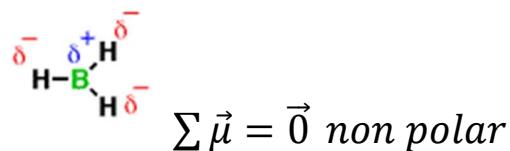
Polarity of molecules

- A molecule is polar if: $\sum \vec{\mu} \neq \vec{0}$
- A molecule is non polar if: $\sum \vec{\mu} = \vec{0}$

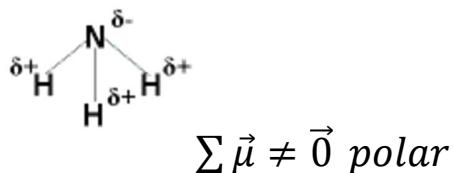
BeH₂:



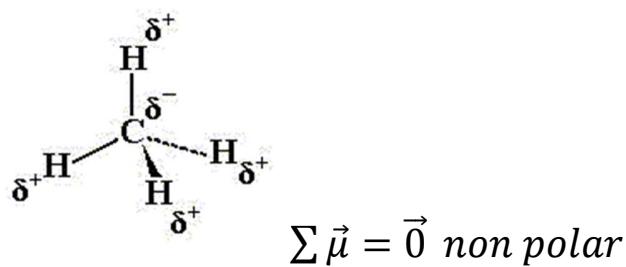
BH₃:



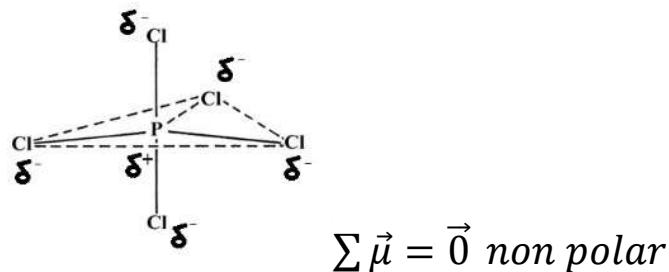
NH₃:



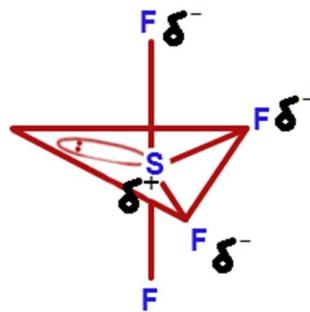
CH₄:



PCl₅:



SF₄:



VI. PAULING electronegativity scale

Fluorine F: $X_F = 3.98$

- A is more electronegative than B
- $X_A - X_B = 0.102\sqrt{\Delta_{AB}}$
- $\Delta_{AB} = E_{A-B} - \sqrt{E_{A-A} - E_{B-B}}$

Ex: HF → X_H

$$X_F - X_H = 0.102\sqrt{\Delta_{HF}}$$

$$\Delta_{HF} = E_{H-F} - \sqrt{E_{F-F} \cdot E_{H-H}}$$

$$X_F = 3.98$$

$$E_{H-F} = 566 \frac{KJ}{mol}$$

$$E_{F-F} = 158 \frac{KJ}{mol}$$

$$E_{H-H} = 436 \frac{KJ}{mol}$$

$$X_F - X_H = 0.102\sqrt{566 - 244} = 1.83$$

$$X_H = 2.15$$

VII. Formal charge of an atom in a molecule

It is equal to the number of outermost electrons (at ground state)

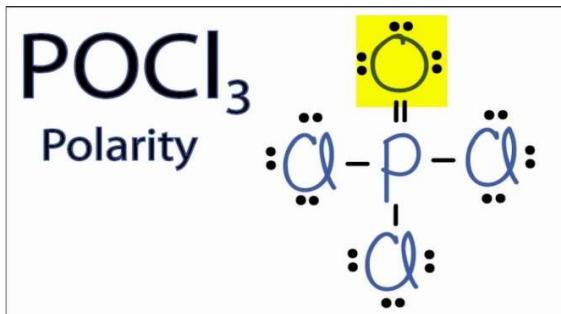
- Number of electrons of lone pairs
- Number of bonds

Ex: POCl_3

^{15}P : $[\text{Ne}] 3s^2 3p^3$

^8O : $[\text{He}] 2s^2 2p^4$

^{17}Cl : $[\text{Ne}] 2s^2 2p^5$



P: $5-0-4=1$

Cl: $7-3(2)-1=0$

O: $6-3(2)-1=-1$

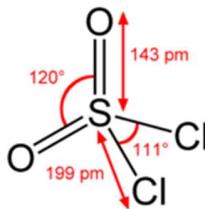
Sum=0 \Rightarrow Charge of molecule

Ex: SO_2Cl_2

${}_{16}\text{S}$: $[{}_{10}\text{Ne}]3s^23p^4$

${}_{17}\text{Cl}$: $[{}_{10}\text{Ne}]3s^23p^5$

${}_8\text{O}$: $[{}_{2}\text{He}]2s^22p^4$



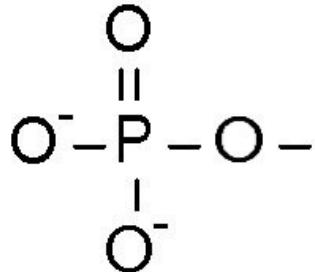
S: $6 - 0 - 4 = 2$

Cl: $7 - 3(2) - 1 = 0$

O: $6 - 3(2) - 1 = -1$

$\Rightarrow \text{Sum} = 2 + 0 - 1(2) = 0$

Ex: PO_4^{3-}

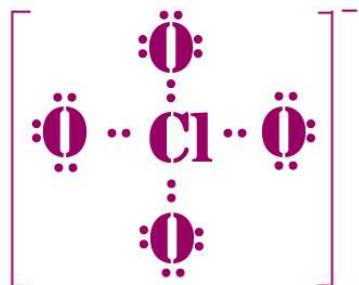


P: $5 - 0 - 4 = 1$

O: $6 - 3(2) - 1 = -1$

Sum: $1 - 1(4) = -3$

Ex: ClO_4^-

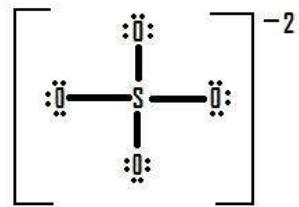


$$Cl: 7 - 0 - 4 = 3$$

$$O: 6 - 3(2) - 1 = -1$$

$$Sum: 3 - 1(4) = -1$$

Ex: SO_4^{2-}



$$S: 6 - 0 - 4 = 2$$

$$O: 6 - 3(2) - 1 = -1$$

$$Sum = 2 - 1(4) = -2$$

Ex: CO_3^{2-}

✓ Summary-Chapter VII ✓

- $1D = \frac{1}{3} \cdot 10^{-2} \text{ C.m} = 3.3 \cdot 10^{-30} \text{ C.m}$
- $1 \text{ kJ/mol} = 4.18 \text{ kcal}$
- $q = \delta \cdot e$
- $|\vec{\mu}| = 4.8 \cdot \delta \cdot l$
- $|\vec{\mu}| = q \cdot l$
- $\% \text{ of ionic character} = \left| \frac{\delta}{e} \right| \cdot 100 = \left| \frac{0.17e}{e} \right| \cdot 100 = 17\%$

If the difference of electromagnetivity increase, the % of ionic character increase

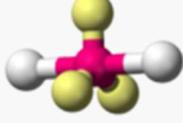
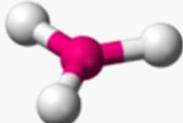
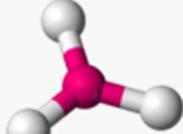
- Non-polar bond: $\delta = 0$
Ionic bond $\delta = 1$
Covalent bond: $0 < \delta < 1$
- A molecule is polar if: $\sum \vec{\mu} \neq \vec{0}$
- A molecule is non polar if: $\sum \vec{\mu} = \vec{0}$
- A is more electronegative than B
- $X_A - X_B = 0.102 \sqrt{\Delta_{AB}}$
- $\Delta_{AB} = E_{A-B} - \sqrt{E_{A-A} - E_{B-B}}$
- $\mu_{H_2O} = 2\mu_{OH} \cos\left(\frac{\alpha}{2}\right)$
- Formal charge = number of outermost e^- – number of e^- of lone pairs – number of bonds
- $\lambda = \frac{h}{mv} \text{ Broglie}$
- $|\Delta x| |\Delta v| m \leq \frac{h}{4\pi} \text{ Heisenberg}$
- $mvr = \frac{nh}{2\pi}$
- $M = \frac{m+m_e^-}{1+\frac{m}{M_{noyau}}}$

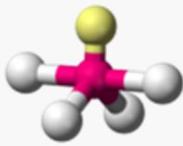
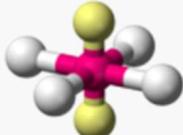
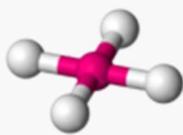
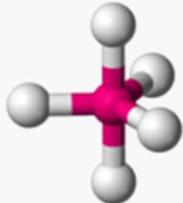
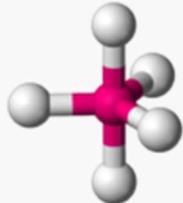
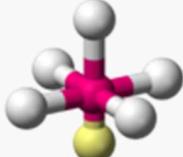
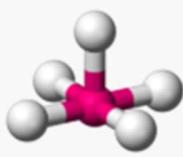
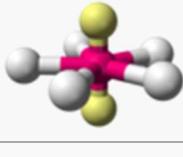
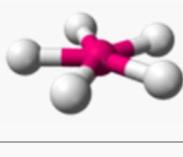
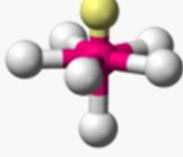
- $v = \frac{z}{n} \cdot \frac{e^2}{2\epsilon_0 h}$
- $\frac{1}{2}mv^2 = v \cdot e$

VSEPR Notation	Name of Molecular Geometry (Shape)	Bond Angle	Polar or Nonpolar Molecule?
AB₂	linear	180°	nonpolar*
AB₃	trigonal planar	120°	nonpolar*
AB₂E₁	bent	<120°	polar
AB₄	tetrahedral	109.5°	nonpolar*
AB₃E₁	trigonal pyramidal	<109.5°	polar
AB₂E₂	bent	<109.5°	polar

VSEPR Notation	Name of Molecular Geometry (Shape)	Ideal Bond Angle(s)	Polar or Nonpolar Molecule?
AB₅	trigonal bipyramidal	90°, 120°	nonpolar
AB₄E₁	seesaw	90°, 120°	polar
AB₃E₂	T-shaped	90°	polar
AB₂E₃	linear	180°	nonpolar
AB₆	octahedral	90°	nonpolar
AB₅E₁	square pyramidal	90°	polar
AB₄E₂	square planar	90°	nonpolar

Molecule Type	Shape ^[12]	Electron arrangement ^[12]	Geometry ^{#[12]}	Examples

AX₂E₀	Linear			BeCl ₂ , HgCl ₂ , CO ₂
AX₂E₁	Bent			NO ₂ ⁻ , SO ₂ , O ₃ , CCl ₂
AX₂E₂	Bent			H ₂ O, OF ₂
AX₂E₃	Linear			XeF ₂ , I ₃ ⁻ , XeCl ₂
AX₃E₀	Trigonal planar			BF ₃ , CO ₃ ²⁻ , NO ₃ ⁻ , SO ₃
AX₃E₁	Trigonal pyramidal			NH ₃ , PCl ₃
AX₃E₂	T-shaped			ClF ₃ , BrF ₃
AX₄E₀	Tetrahedral			CH ₄ , PO ₄ ³⁻ , SO ₄ ²⁻ , ClO ₄ ⁻ , XeO ₄

AX₄E₁	Seesaw (also called disphenoidal)			SF ₄
AX₄E₂	Square planar			XeF ₄
AX₅E₀	Trigonal bipyramidal			PCl ₅
AX₅E₁	Square pyramidal			ClF ₅ , BrF ₅ , XeOF ₄
AX₅E₂	Pentagonal planar			XeF ₅ ⁻
AX₆E₀	Octahedral			SF ₆ , WCl ₆
AX₆E₁	Pentagonal pyramidal			XeOF ₅ ⁻ , IOF ₅ ²⁻

AX₇E₀	Pentagonal bipyramidal			IF ₇
AX₈E₀	Square antiprismatic			IF ₈ ⁻ , ZrF ₈ ⁴⁻ , ReF ₈
AX₉E₀	Tricapped trigonal prismatic (as drawn) OR capped square antiprismatic			ReH ₉ ²⁻

✓ Chapter VIII-Intermolecular forces (bonds of weak energy) ✓

There are two kinds of intermolecular interactions:

- Van der Waals forces can be of three types:
 - Keesom interactions
 - Debye interactions
 - London Dispersion Forces

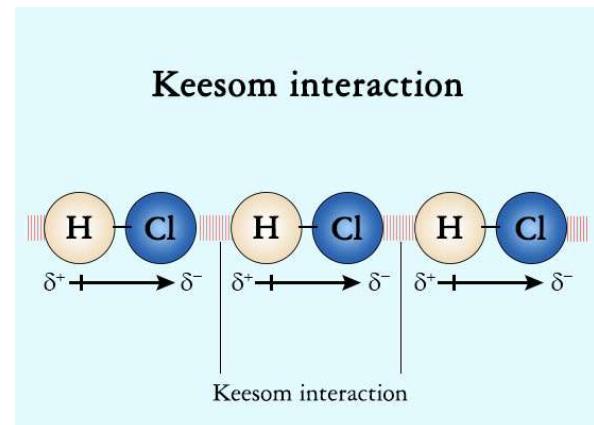
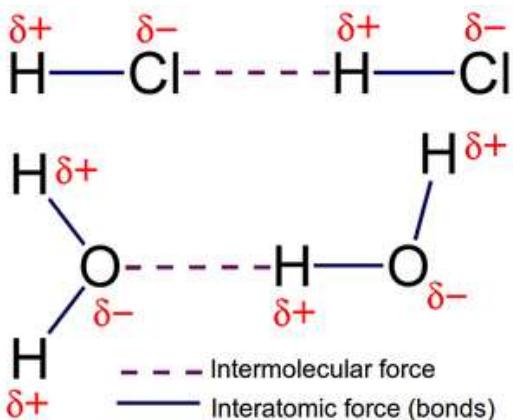
- Hydrogen Bonding

I. Van der Waals forces(or interactions):

1. Permanent dipole moment interactions(Keesom):

When two polar molecules (permanent dipoles) are near each other, a dipole-dipole interaction is developed between them

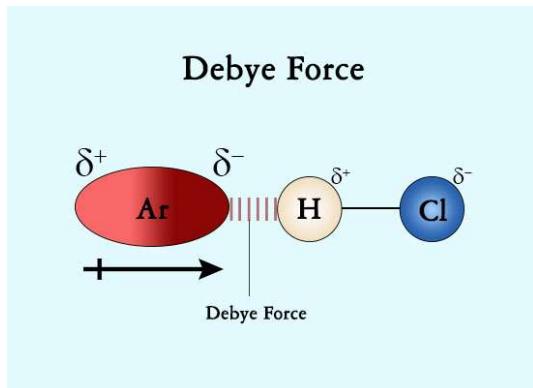
Example: HCl



2. Interactions between permanent dipoles and induced dipoles(Debye):

Put a non-polar molecule in an electric field.

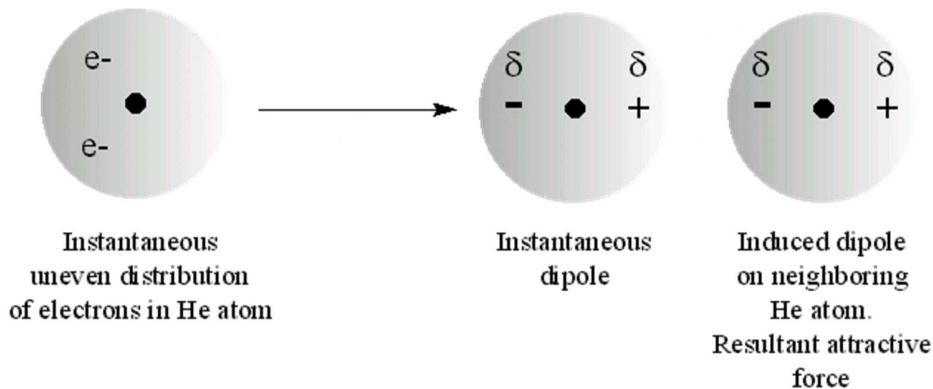
Put a non-polar molecule with a permanent dipole.



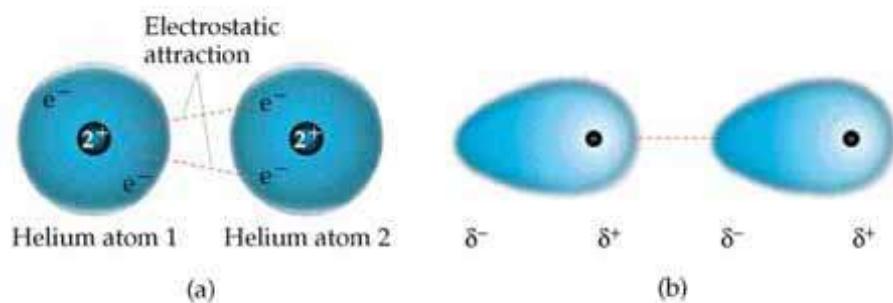
(If I want to make them closer, I have to increase the pressure and decrease the temperature)

3. Interactions between instantaneous dipoles and induced dipoles (London Dispersion forces)

Everytime, even it's non-polar with non-polar



At any instant t , we have instantaneous dipole



Polarizability: The tendency to create the separation of atoms.

Polarizability is easier with larger atoms or molecules.

Van der Waals intermolecular forces are weak. Factors affecting on forces are size and molecular mass.

These atoms are non-polar.

Halogen	Molecular Weight (amu)	Boiling Point (K)	Noble Gas	Molecular Weight (amu)	Boiling Point (K)
F ₂	38.0	85.1	He	4.0	4.6
Cl ₂	71.0	238.6	Ne	20.2	27.3
Br ₂	159.8	332.0	Ar	39.9	87.5
I ₂	253.8	457.6	Kr	83.8	120.9
			Xe	131.3	166.1

These atoms are non-polar.

*Van der Waals bonds increase with Boiling point and Melting point
As molecule increase (Molecular mass) Boiling Point and Melting Point*

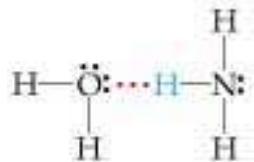
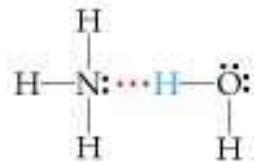
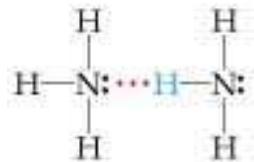
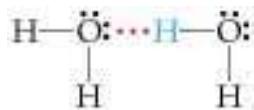
Substance	Molecular Weight (amu)	Dipole Moment, μ (D)	Boiling Point (K)
Propane, CH ₃ CH ₂ CH ₃	44	0.1	231
Dimethyl ether, CH ₃ OCH ₃	46	1.3	248
Methyl chloride, CH ₃ Cl	50	1.9	249
Acetaldehyde, CH ₃ CHO	44	2.7	294
Acetonitrile, CH ₃ CN	41	3.9	355

	Dipole moment (D)	Energies (kJ/mol)			
		Keesom	Debye	London	Total
Ar	0	0.000	0.000	8.5	8.5
CO	0.12	0.0004	0.008	8.7	8.7
HI	0.38	0.025	0.112	25.83	25.96
HBr	0.78	0.685	0.50	21.90	23.08
HCl	1.03	3.30	1.00	16.80	21.10

London is proportional to the size of a molecule.

Difference of Electronegativity is proportional to the dipole moment.

II. Intermolecular Hydrogen bonding



$$E_{H-bonding} > E_{VOW\ bonding}$$

Two conditions:

- One of the three atoms: N,O,F
- One H atom bonded to N,O or F

Ex: $\text{H}_2\text{O}, \text{HF}, \text{NH}_3 \dots$

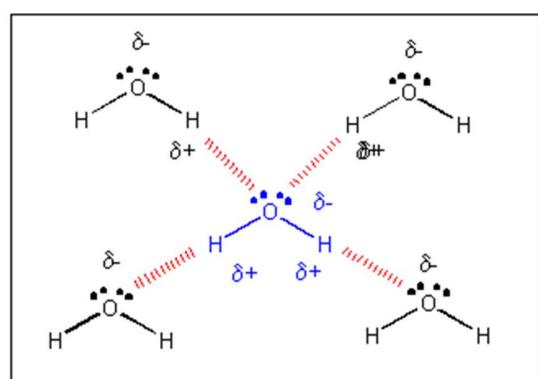
Alcohols $\text{CH}_3 - \text{OH}$

$$\text{H}_2\text{Te} > \text{H}_2\text{Se} > \text{H}_2\text{S} \text{ (Boiling Point)}$$

Ex:

As we heat ice, H bonds will be destroyed.

At 100°C all H bonds are destroyed.



Comparison Boiling points

CH_4 and CH_3OH

CH_4 non polar (London)

CH_3OH (Hydrogen bonding)

$$\text{B.P.}(\text{CH}_3\text{OH}) > \text{B.P.}(\text{CH}_4)$$

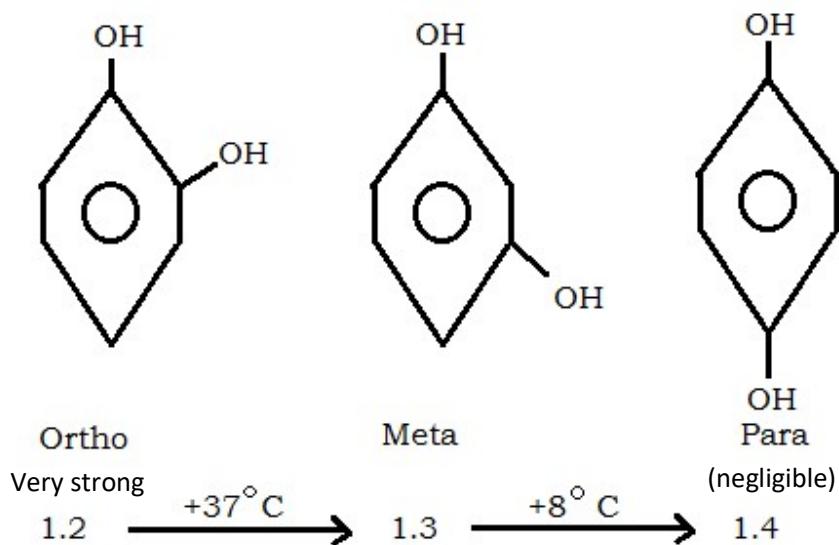
CH_3OH and CH_3CH_2OH

Hydrogen bonding, but the size of CH_3CH_2OH bigger than the size of CH_3OH

$$B.P.(CH_3OH) < B.P.(CH_3CH_2OH)$$

III. Intra molecular H bonding

Ex: $C_6H_4(OH)_2$ dihydroxybenzene: 3 isomers



⇒ Intermolecular Hydrogen bonding increases the boiling point.

⇒ Intramolecular Hydrogen bonding decreases the boiling point.

IV. Viscosity and surface tension

Intermolecular forces affect many physical properties:

- Viscosity
- Surface tension

Viscosity

Liquids	Viscosity (Poise)	Type of IM attraction
Water	1.002	H-bonding & London
Tetrachloromethane	0.969	London
Olive oil	84	London
Oleic acid	25	London
Glycerine	1490	H-bonding & London

Surface tension

Describes the resistance, that a liquid has, to an increase in its own surface area.

If the intermolecular forces between liquid molecules are strong:

- The molecules will be more attracted to each other
- The forces at the surface pull inward leading to a reduction in the liquids surface area
 - thus: a more spherical shape
 - Liquid with a high surface tension

Example: $\text{Hg} > \text{H}_2\text{O}$

⇒The stronger the intermolecular forces are, the stronger the surface tension is!

✓ Chapter VIII-Summary ✓

- Van der Waals forces can be of three types:
 - Keesom interactions(permanent dipoles)
 - Debye interactions (Interactions between permanent dipoles and induced dipoles)
 - London Dispersion Forces (Interactions between instantaneous dipoles and induced dipoles)
- Hydrogen Bonding (One of the three atoms: N,O,F ; One H atom bonded to N,O or F)
- Polarizability: The tendency to create the separation of atoms. Polarizability is easier with larger atoms or molecules.
- Van der Waals intermolecular forces are weak. Factors affecting on forces are size and molecular mass.
- *Van der Waals bonds increase with Boiling point and Melting point As molecule increase (Molecular mass) Boiling Point and Melting Point*
- London is proportional to the size of a molecule. Difference of Electronegativity is proportional to the dipole moment.
- Intermolecular Hydrogen bonding increases the boiling point. Intramolecular Hydrogen bonding decreases the boiling point.

Final exam bonus

Subject: The experiment that contradicts Einstein

Location: Metropolis Switzerland

- 1) The Swiss researchers have made an achievement by an experiment that could verify that two distant photons over 10 km maintain contact. Two photons emitted by this source excited by a laser behave like a “couple” despite the distance that separates them, demonstrating the principle of the quantum coherence.

- 2) This experience contradicts:
 - The Heisenberg uncertainty principle, since we know the speed and position of each of the electrons.
 - Einstein’s special relativity that no information can travel faster than the speed of light.

- 3) The outcome of this experiment is useful in quantum cryptography (transfer of information using a long distance photon) which would ensure military confident near-perfect crypts messages).