Electronic configuration of atoms

I.General

Classical (Newtonian) mechanics precisely studies the movements of macroscopic objects. The laws of this mechanics could not be extended to the microscopic scale.

Bohr's theory, which postulates that moving electrons describe orbits around the nucleus, failed due to the complexity of their movement.

Classical mechanics has not been able to provide explanations for certain phenomena that have been observed at this scale.

At this point new laws were needed that could govern the movement of such enormously small particles, which led to the laws of quantum mechanics.

II.Element of quantum mechanics

Classical mechanics describes moving objects as material points, whereas quantum mechanics describes moving objects as material waves.

1. Debroglie's postulate: 1924

Any moving particle of mass m moving at a speed v is associated with a wave of length λ such that: $\lambda = h/m.v$

λ represents the length of the wave.

h: Planck's constant ($h = 6.625.10^{-34}$ J.S)

m: the mass of the particle.

v: the speed of the particle.

Example:

Find the wave lengths of a tennis ball and an electron knowing that:

	Tennis ball	Electron
Mass(g):	200	2.10^{-31}
Speed (m/s) :	30	3.10^{8}

Answer: $\lambda Ball = 10^{-34} m$; $\lambda electron = 2.10^{-10} m$

We notice that the wave effect is negligible for the case of the ball but it is important with the example of the electron.

Conclusion: the wave effect only has meaning on the microscopic scale.

2. Heisenberg Uncertainty Principle: 1926

It is impossible to determine precisely the position and speed of a moving object at the same time on a microscopic scale.

If: Δx represents the uncertainty in the position and Δv the uncertainty in the speed, we have: $\Delta x . \Delta v \geq h/2\pi m$

The best we can do is to determine the probability of the presence of the electron at a point in space.

This is how the notion of orbit known in classical mechanics is replaced in quantum mechanics by the part of space where it is probable that the electron exists.

III. Concept of atomic orbital

The notion of orbit loses its meaning in quantum mechanics and will be replaced by the atomic orbital.

1. Schrödinger’s equation

The probability of the presence of the electron can be expressed using a function denoted ψ which represents the amplitude of the wave associated with the movement of the electron.

This function is the solution of a famous second order differential equation called the Schrödinger equation given by the expression:

$$\Delta\psi + (8\pi^2 m)/h^2 \cdot (E-V)\psi=0$$

$\Delta = \partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$: Mathematical operator called the Laplacian

E : Total energy of the system studied.

V : Potential energy.

Ψ :Wave function.

2. The atomic orbital

An atomic orbital is conventionally represented by a closed surface limiting the volume in which the probability of the presence of the electron is 95%.

Each atomic orbital is associated with three numbers n, l and m called quantum numbers:

The main quantum number: denoted n

It characterizes the energy level associated with the orbital.

$n \in \{1,2,3,4,5,6,7\}$

The secondary or azimuthal quantum number: denoted l

It characterizes the shape of the orbital ,$0 \leq l \leq n-1$.

l=0 Corresponds to the atomic orbital s.

l=1 Corresponds to the atomic orbital p.

l=2 Corresponds to the atomic orbital d.

$l=3$ Corresponds to the atomic orbital f.

The magnetic quantum number: denoted m.

It characterizes the orientation of the orbital in space, $-l \leq m \leq +l$.

Example :

$l=1$(p orbital)→ $m = -1,0,1$.

$m= -1$ Corresponds to the atomic orbital p oriented along the x axis, this is associated with the orbital p_x.

$m = 0 \rightarrow p_y$

$m = 0 \rightarrow p_z$

Generally speaking, the atomic orbital is always denoted nX_b

n: denotes the principal quantum number.

X: Symbol for the atomic orbital.

b: Coordinate axis symbol (x,y,z,xy,yz,xz,…)

Noticed :

An atomic orbital is always represented by a square which is called a quantum box.

3. The electron and the spin number

The rapid rotational movement of the electron around itself makes it possible to quantify its intrinsic angular momentum by associating it with a number called spin quantum number denoted S.

This number characterizes the orientation of the electron in a magnetic field.

$S = +1/2$ or $S = -1/2$ depending on the direction of rotation of the electron.

Noticed :

An electron is characterized by four quantum numbers n,l,m and s of which the first three characterize the orbital where probable its existence and the last quantifies its movement.

Example :

Atomic orbitals associated with energy levels characterized by:

n = 1, n = 2 and n = 3 and their quantum case representations.

n	layer	l	m	symbol	representation
1	K	0	0	1s (1A.0)	☐
2	L	0	0	2s (1A.0)	☐
		1	-1,0,1	2p:2px,2py,2pz (3A.O)	☐☐☐
3	M	0	0	3s (1A.0)	☐
		1	-1,0,1	3p: 3px,3py,3pz (3A.O)	☐☐☐
		2	-2,-1,0,1,2	3d:3dxy,3dyz,3dxz, $3dz^2$, $3d(x^2-y^2)$(5A.O)	

IV. The electronic structure of atoms

The arrangement of the Z electrons of an atom in its ground state around its charge nucleus +Ze obeys the following rules:

1. Rules for filling atomic orbitals

a. Klechkovsky rule (principle of stability)

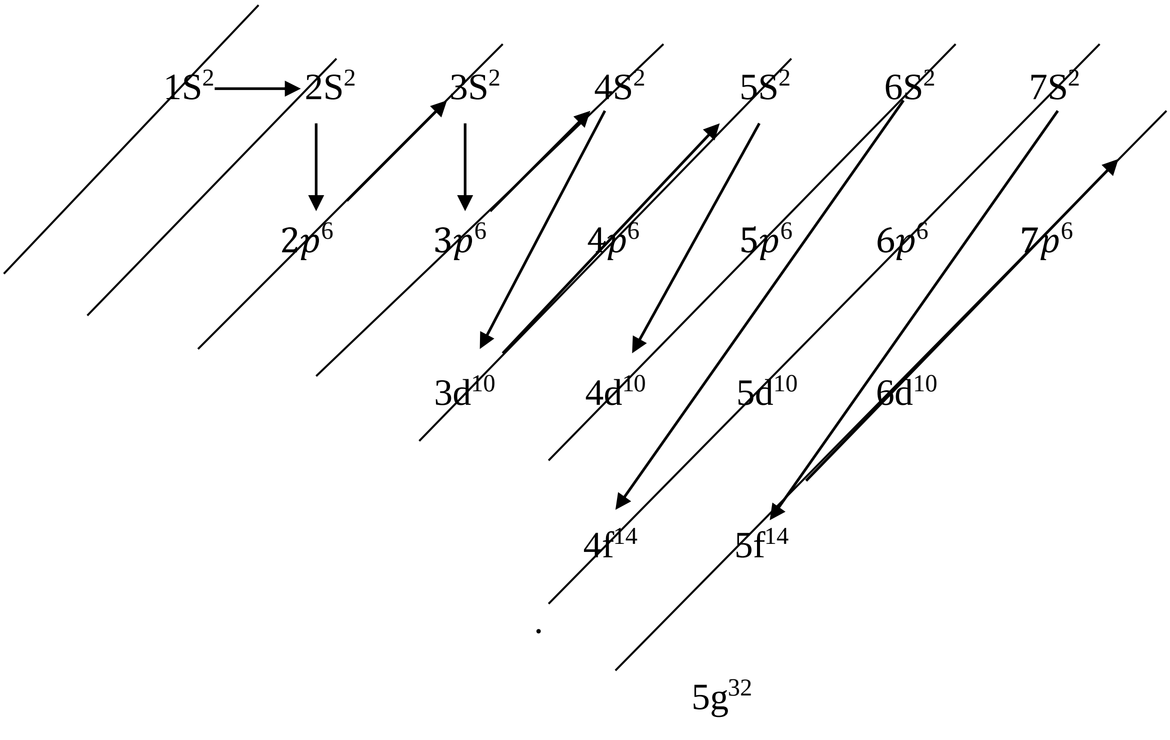
In the fundamental state, electrons occupy the lowest energy atomic orbitals, which gives the atom a minimum energy associated with maximum stability.

Noticed :

* The filling of the atomic orbitals is done in the increasing order of n+l.

* In the case where the sums n+l are equal, the filling is done in increasing order of n.

The order of filling of the atomic orbitals is done as shown in the following diagram, called **the Klechkovsky diagram.**



b. Pauli exclusion principle

Two electrons can never have their quantum numbers identical.

This leads, ultimately, to the fact that two probable electrons in the same atomic orbital must differ at least in their spin quantum number s.

Noticed :

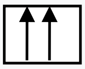
As a notation model, the electron moving in one direction in a positive direction is represented by an arrow pointing upwards (spin up) and downwards for a rotation of the electron in the opposite direction (spin down). .

Electron in spin up. ↑

Electron spin down. ↓

According to the Pauli exclusion principle:

Notation not allowed.



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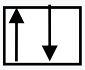

C. Hund's rule (high spin multiplicity rule)

The electrons are distributed in the atomic orbitals so as to occupy the maximum number of boxes in the level before completely saturating each orbital.

Let us distribute three electrons in quantum boxes.

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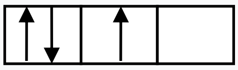

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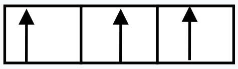


2.Representation of electronic structures

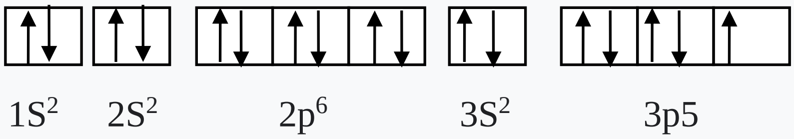
Example :

Let us take the case of the electronic representation of the atom of $_{17}$Cl.

$_{17}$ Cl : $1S^2$ $2S^2$ $2p^6$ $3S^2$ 3p5

We can also use the representation by quantum boxes

$_{17}$Cl:

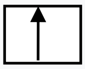


Noticed :

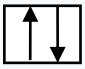
We often use the term “electronic configuration” or “electronic structure”

A quantum box can be noted, containing one electron or two electrons.

Vacant box



single electron



paired electrons

If in the electronic configuration of an atom all the electrons are paired the atom is said to be diamagnetic wheras if there is at least one single electron the atom is said to be paramagnetic.

The electrons in the internal layers are called internal or core electrons, whereas those in the external layers are called external or valence electrons, they determine the reactivity of the element (chemical properties).

Example :

Establish the electronic configuration of $_{29}$Cu.

Represent the external electrons by quantum boxes.

Is it a paramagnetic or diamagnetic atom ?