

Introduction

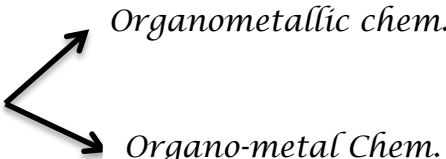
Inorganic chemistry is the study of the synthesis, reactions, structures and properties of compounds of the elements. Inorganic chemistry encompasses the compounds - both molecular and extended solids - of everything else in the periodic table, and overlaps with organic chemistry in the area of organometallic chemistry, in which metals are bonded to carbon-containing ligands and molecules. Inorganic chemistry is fundamental to many practical technologies including catalysis and materials (structural, electronic, magnetic etc.), energy conversion and storage, and electronics. Inorganic compounds are also found in biological systems where they are essential to life processes.

Due to the continuous increase in contributors to the science of chemistry, the chemical science has branched out into, among which we mention:

1. *Inorganic Chemistry.*
2. *Organic Chemistry.*
3. *Biological Chemistry.*
4. *Physical Chemistry.*
5. *Industrial Chemistry.*
6. *Analytical Chemistry.*
7. *Nuclear or Radioactive Chemistry.*
8. *Medical Chemistry.*
9. *Pharmaceutical Chemistry.*
10. *Environmental Chemistry.*
11. *Material Chemistry.*
12. *Theoretical Chemistry.*

First Stage

Due to the overlap and convergence between some of the above branches, other branches were formed, for example-:

1. Inorganic Chemistry + Organic Chemistry 
2. Inorganic Chemistry + Biochemistry \longrightarrow *Bio-Inorganic Chem.*
3. Inorganic Chemistry + Physical Chemistry \longrightarrow *Physical-Inorganic Chem.*
4. Inorganic Chemistry + Industrial Chemistry \longrightarrow *Industrial-inorganic Chem.*

Inorganic Chemistry

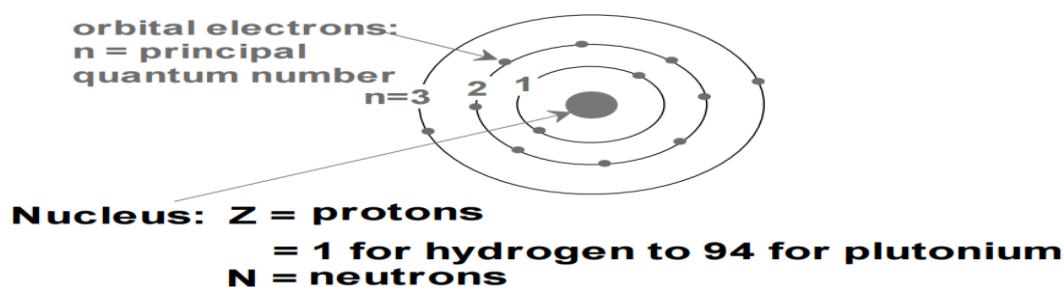
A generally-accepted definition of Inorganic Chemistry is the study of non-carbon molecules, or all the elements on the periodic table except carbon. But, this definition is not completely correct because the field of Inorganic Chemistry also includes organometallic compounds and the study of some carbon-based molecules that have properties that are familiar to metals (like conduction of electricity). This makes the field of inorganic chemistry very broad, and practically limitless.

Since the linguistic meaning of inorganic chemistry refers to what corresponds to (the opposite of) the linguistic meaning of organic chemistry, therefore we can know or find out the interests (interests) of this branch of chemistry by identifying the interests of the corresponding branch in meaning, i.e. the branch of chemistry. Membership. It can be said that organic chemistry is the chemistry (preparation, behavior, and reactions) of compounds of the positively charged four-carbon element (C^{+4}), which often contain a C-H bond, i.e., carbon-hydrogen. So, everything except the interests of organic chemistry falls under the interests of inorganic, and in another sense or expression, inorganic chemistry can be defined as the chemistry of all chemical elements and their compounds except the chemistry of the four-positively charged carbon element and its compounds.

Atomic Structure

The atom is composed of a central mass, which is the nucleus, which is positively charged, surrounded by electrons, and these electrons move around it, which constitutes the orbit. The shape of the orbit in which the electron rotates varies. The world Bohr and Rutherford thought that the orbit of the electron is circular, as shown in the figure below.

Bohr's Atom model



Atomic mass (A) = Z + N. Since nucleus are about 1840 times heavier than electrons.

But in general, the charge of the electron is negative, and the number of electrons is equal to the number of positively charged particles inside the nucleus (protons). In addition to the protons (P), there are neutrons (N), and their charge is neutral [(mass of the nucleus = number of P⁺ + number of N ((n±)]. The mass of the electron is not included in calculating the mass number or atomic weight of the atom because of the small weight or because the mass of the electron is too small to be calculated.

$$\text{(mass number)} = P + N$$

Mass of **P** = 1.673×10^{-27} Kg

Mass of **N** = 1.675×10^{-27} Kg

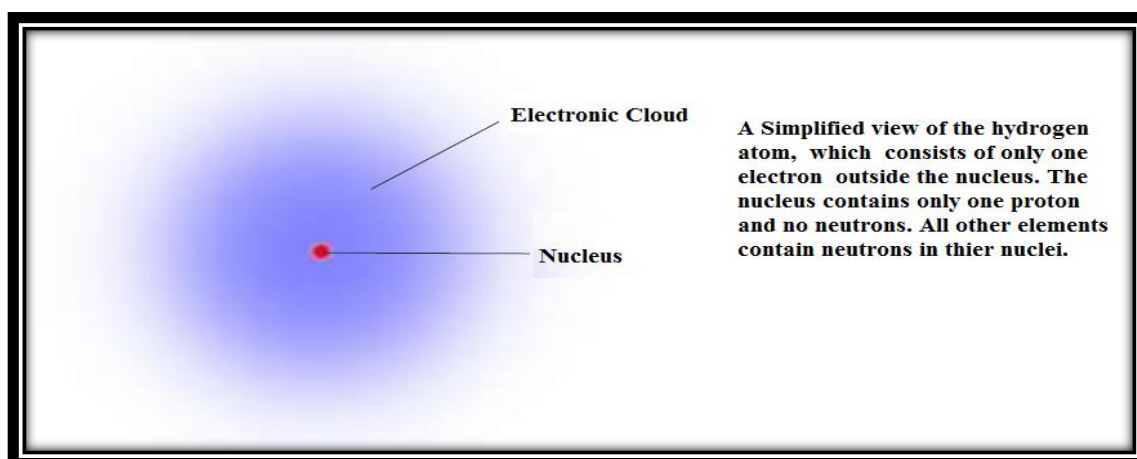
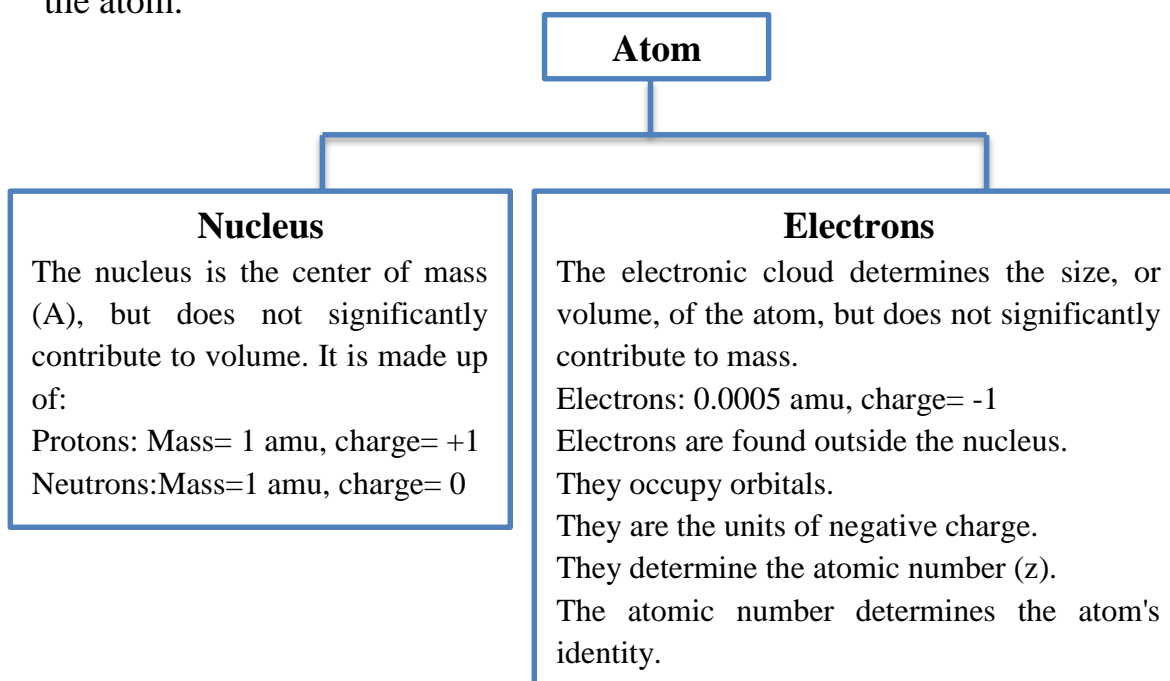
Mass number (A) = P + N

“Atomic weight = Sum of percentages of elements”

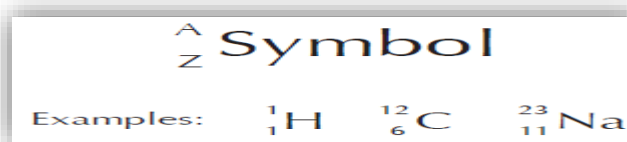
Each element has a fixed atomic number, but the mass number may vary as a result of the increase in the number of N. If the number of N increases over P, the presence of isotopes in one element increases.

First Stage

The following diagram summarizes the basic facts of the structure of the atom:



Elements in the periodic table are indicated by SYMBOLS. To the left of the symbol we find the **atomic mass (A)** at the upper corner, and the **atomic number (Z)** at the lower corner.



Electron trade constitutes the currency of chemical reactions. The number of electrons in a neutral atom (that is, the atomic number) gives the element its unique identity. **No two different elements can have the**

First Stage

same atomic number. The periodic table is arranged by order of increasing atomic number, which is always an integer. In contrast to the atomic number, **different forms of the same element can have different masses.** They are called **isotopes**. The following are representations for some of the isotopes of hydrogen and carbon.

| | | | |
|------------------|------------------|-------------------------|---------------------|
| ${}^1_1\text{H}$ | ${}^2_1\text{H}$ | ${}^{12}_6\text{C}$ | ${}^{13}_6\text{C}$ |
| regular hydrogen | deuterium | regular carbon, or C-12 | carbon-13, or C-13 |

Isotopic: They are isotopes in which the number of neutrons (N) exceeds the number of protons (P), which leads to instability of the element and becomes radioactive, subject to nuclear fission reactions or nuclear decay (half-life) such as radium, radon, and francium are very radioactive elements As well as heavy water D₂O (used in cleaning nuclear reactors).

The atomic mass reported in the periodic table for any given element is actually a **weighted average** of the masses of its isotopes as found in nature. Thus, the mass of carbon is reported as 12.01115 rather than 12.00000 because it contains the relative contributions of both isotopes. The natural abundance of carbon-12 is nearly 100%, whereas that of carbon-13 is only about 1%. The reported mass is slightly greater than 12.00000 because of the small contribution of carbon-13. Therefore, the mass number, as found in periodic tables, does not have to be an integer like the atomic number.

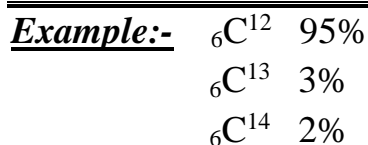
Example:- The % iron atom in isotopes Fe⁵⁴, Fe⁵⁶, Fe⁵⁷, Fe⁵⁸ are 5.8, 91.8, 2.1, 0.3 respectively, estimate the atomic weight of iron element?

Solution:-

$$\text{Average of Atomic Weight} = \frac{5.8 \times 54 + 91.8 \times 56 + 2.1 \times 57 + 0.3 \times 58}{100}$$

$$= 55.91$$

First Stage



$$\text{Atomic weight} = \frac{95 \times 12 + 3 \times 13 + 2 \times 14}{100}$$

***The numbers 14, 13, and 12 refer to the mass number.**

The average mass of atoms is called relative atomic weight or the atomic weight. The atomic weight is determined by the elemental analysis for example it has been found by mass spectrometric analysis.

Example:- The relative abundance of the various isotopic atomic of silicon (Si) element are 92.23% of ${}^{28}\text{Si}$, 4.67% of ${}^{29}\text{Si}$ and 3.10% of ${}^{30}\text{Si}$ calculate the atomic weight of silicon element?

Solution:-

$$\begin{aligned} \text{The atomic weight} &= \frac{92.23 \times 28 + 4.67 \times 29 + 3.1 \times 30}{100} \\ &= 28.085 \end{aligned}$$

No. of Avogadro

It is the number of atoms in one atomic number or the number of atoms in one molecular weight.

Number of Molecules = "Number of Avocadro N_A x Number of Moles"

Example:- How many atoms available in 18.998 (a.m.u), 4 (a.m.u) of F and H?

Solution:- no. of moles(F) = $\frac{W}{A.Wt} = \frac{18.9984}{18.9984} = 1 \text{ g/mole}$

$$\begin{aligned} \text{no. of Atoms} &= \text{no. of moles (F)} \times N_A \\ &= 1 \times 6.022 \times 10^{23} \text{ Atoms} \end{aligned}$$

$$\text{no. of moles (H)} = \frac{W}{A.Wt} = \frac{4.026}{1} = 4.026 \text{ g/mole}$$

First Stage

$$\begin{aligned}\text{no. of Atoms} &= \text{no. of moles}_{(H)} \times N_A \\ &= 4.026 \times 6.022 \times 10^{23} \\ &= 24.244572 \times 10^{23} \text{ Atoms}\end{aligned}$$

Q: *How many oxygen molecules (O₂) are there in 0.2 moles of O₂ gas?*

Q: *Find the no. of moles in 85g of carbon dioxide CO₂? and find the no. of molecules for this gas?*

Note:- *mass of one mole of atoms = atomic weight.*

mass of one mole of compound = molecules weight.

Atomic structure

The two scientists, Huygen and Maxwell, proved that light is generated as a result of the oscillatory movement of electrically charged bodies with the movement of the magnetic field, meaning that light waves are generated from two perpendicular electric and magnetic fields, and that visible light (Visible light) results from the oscillations of charged particles at a certain speed, and there are faster or slower oscillations to give unchanged light. Visible. Electromagnetic radiation includes:

Infrared rays (IR), visible rays (Vis), ultraviolet rays (UV), gamma rays (γ), x-rays (x-ray) and radio rays. Electromagnetic radiation waves travel in a vacuum at a speed of 3×10^{10} cm/s $\approx 2.998 \times 10^{10}$, 3×10^8 m/s. The speed of electromagnetic radiation changes depending on the type of medium.

Electromagnetic radiation has the following properties:

1. Wave length (λ) (Lambda).

It is the distance between two similar peaks of two successive waves, measured in units of distance.

$$\begin{aligned}1 \text{ cm} &= 10^{-2} \text{ m} = 10 \text{ mm} / 1 \text{ nm} = 10^{-7} \text{ cm} = 10^{-9} \text{ m} / 1 \text{ \AA} = 10^{-8} \text{ cm} = 10^{-10} \text{ m} / \\ 1 \mu\text{m} &= 10^{-6} \text{ m} = 10^{-4} \text{ cm}.\end{aligned}$$

2. Frequency (ν)

It is the number of oscillations per second or the number of vibrations per second. Its units are cycles/sec or Hz.

First Stage

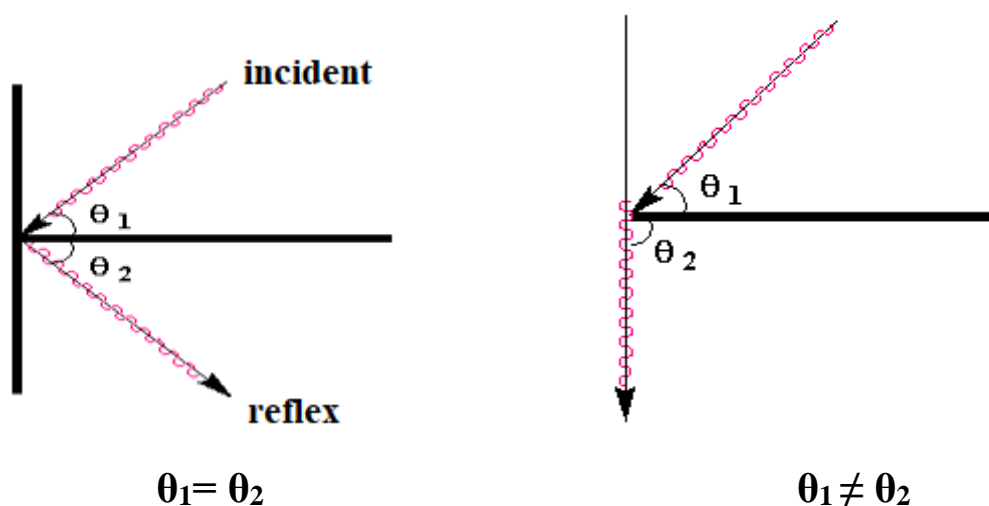
3. Velocity (C)

Frequency x Wavelength $C = \lambda \nu$

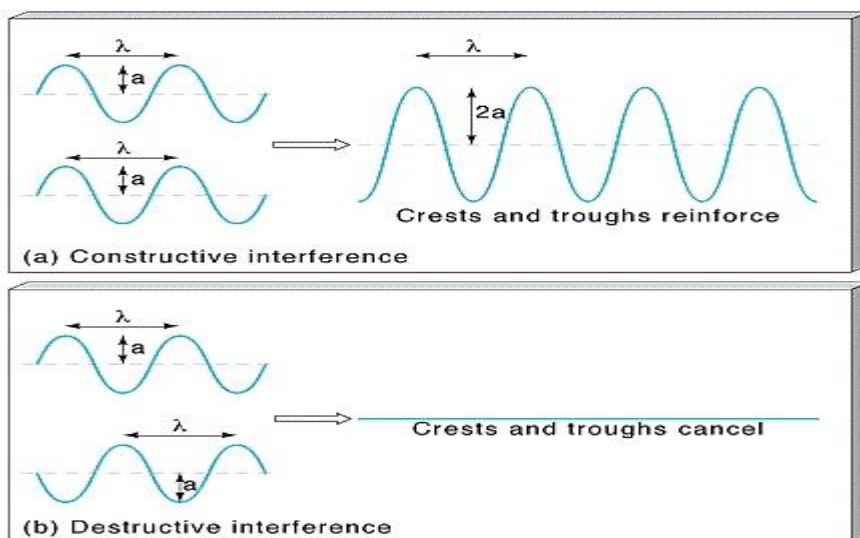
The wavenumber ν' is the inverse of the wavelength and its units are the inverse units of wavelength (cm^{-1}). $\nu' = 1/\lambda$.

Light has the properties of wave motion, which are:

- A:** 1- Reflection
 2- Refraction
 3- Diffraction



- B:** 1- Constructive interference.
 2- Destructive interference.



First Stage

As long as the atom exists, it is a particle with mass, and this particle is subject to Newton's laws of motion, which means that every particle has momentum, and this momentum is the product of mass multiplied by velocity.

(Momentum) $f = mv$ (Newton's law).

If these atoms suffer from reflection and diffraction, this means that they have wavelengths, so they have a wave characteristic, and since the electron is one of the components of this atom, therefore, it must be known whether this electron has mass or wave characteristics, or both.

The scientist Crook discharged a glass tube containing the gas of an element. When a high voltage is applied, the gas of this element will glow and move toward the anode electrode, and a dark space will appear near the cathode electrode, just as happens in neon tubes using a zinc sulfuric plate that glows in the same manner. This indicates that there are particles moving from the cathode electrode, called cathode rays, towards the anode electrode, and they collide with the screen, and when a barrier is placed between the screen and the cathode, they appear in the form of a black spot on the screen with the same size as the barrier. When you place a paper wheel in front of these rays, this paper wheel will rotate while it is exposed to the rays.

From this experience we conclude the following:

1. Cathodic rays are emitted when any type of gas is used for the elements.
2. Cathodic rays move in straight lines when they are emitted due to the barrier drawn on the screen.
3. These rays carry negative charges because they moved from the cathode to the anode.
4. These rays have a particle character, meaning they are negatively charged bodies because they were able to rotate the paper wheel as it passed towards these minutes that make up the cathode rays. These minutes were later called electrons by the scientist Thomson.

When high voltages are applied, the electrons accelerate, and as a result of the rise in temperature, these electrons emitted from the cathode will collide with the gas atoms of the element, leading to the ionization of these atoms and the emission of electrons, transforming into positive ions.

First Stage

When discharging under pressure, the electron beam moves in the direction from the negative electrode to the positive electrode. As for the spots, the strange blackness of the cathode is the result of non-ionization, while a glow occurs when the atoms of the element are ionized and electrons are emitted from its atoms. This experiment applies to all elements, so electrons are included in the composition of all elements.

The scientist Thomson measured the ratio $e / m = 1.76 \times 10^8 \text{ C/g}$. As for the charge of the "electron", it was measured by the scientist Millikan and was equal to $1.6 \times 10^{-19} \text{ C}$.

$$\therefore m = \frac{1.6 \times 10^{-19} \text{ C}}{1.76 \times 10^8 \text{ C/g}} = 9.1 \times 10^{-31} \text{ Kg}$$

Q: Estimate the number of coulombs carried by 20.1 g of chloride ion?

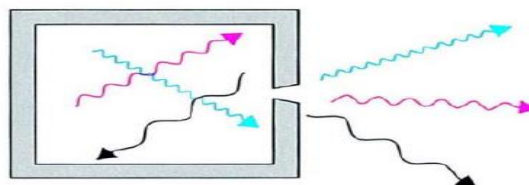
Solution:- $e/m = 1.76 \times 10^8$
 $e = m \times 1.76 \times 10^8$
 $e = 20.1 \times 1.76 \times 10^8$
 $= 21.29 \times 10^8 \text{ C}$

$$1 \text{ eV} = 1.662 \times 10^{-19} \text{ J}$$

Blackbody

Hot bodies emit radiation, which we experience as heat. As the temperature of an object is raised, it first glows a dull red, then changes to orange-yellow, and finally becomes **“white hot”**.

The radiation emitted by the opening is called blackbody or cavity radiation.



BlackBody Radiation and the Origin of Quantum Theory

Quantum theory came after primitive theories in explaining the nature of light and its physical behavior. One of these theories concerned itself with particles with a specific mass that move according to Newton's laws of motion, which is that light is a stream of small-sized particles called

First Stage

photons, which move in a vacuum with a speed equal to the speed of light. This theory, as we mentioned, was called the particle theory of the scientist Newton.

The other theory is the wave theory or Huygen's theory, which showed that light is waves that move in a continuous medium and are subject to the laws of wave motion, which result from the deflection of light. This phenomenon confirmed the deflection of light in a magnetic field. These theories, that is, the old theories, showed that the number of electrons and their energy are proportional to the intensity of the incident light. These theories failed to explain the phenomenon of radiation emitted by the black body. The ideal blackbody perfectly absorbs the rays and emits them equally, but the real blackbody is neither a complete absorber nor a complete emission, but in general, when heating any body, it will emit thermal radiation, as it is expected that the nature of this radiation depends on the temperature The body and the color gives an indication of the temperature of the radiating body. This thermal radiation is electromagnetic radiation with a specific wavelength longer than the wavelength of visible light. The scientist Vein has shown that the spectrum of a hot body is a continuous spectrum that has radiations of different wavelengths. The higher the temperature of the body, the higher the values of the frequencies of the emitted rays. This has been called Law by Wien's Law of Displacement.

An example of this is the change in the color of the piece of iron when its temperature is raised from red to orange, then to yellow, and in the end the piece of iron will become white. In 1879, Stevain calculated the rate of energy emission from the surface of the body according to the following relationship:

$$E = e \sigma T^4$$

E= energy of emitted

e= emitted

σ = stevain constant

T= Temp. in K

Gene and Rayleigh have combined the displacement law and Stephen's law with one law that states that the intensity of emitted

First Stage

radiation is directly proportional to the square of frequency and to the fourth power of absolute temperature.

$$I \propto \nu^2/T^4$$

Blackbody Radiation and Quantization of Energy

If a body is irradiated with radiation of a wavelength (λ), and a fraction $a(\lambda)$, of the radiation is absorbed the remainder being either reflected or transmitted. The absorbed fraction, $a(\lambda)$ is called the absorbance of a given body at wavelength (λ), clearly, the absorbance is the fraction of incident radiant energy absorbed per unit mass or thickness of an absorbance (or body). The fraction of the radiation reflected or transmitted respectively, the reflectance and the transmittance.

The sum of the absorbance, reflectance and transmittance is unity.

$$a(\lambda) + r(\lambda) + t(\lambda) = 1$$

$$\text{absorbance} + \text{reflectance} + \text{transmittance} = 1$$

However, a body for which the absorbance, $a(\lambda)=1$ for all wavelengths is a blackbody.

If a body is exposed to radiation with a wavelength λ and part of the radiation $a(\lambda)$ is absorbed by the body, then the rest of the radiation is either reflected or passes through the body and transmit. The absorbed part $a(\lambda)$ is called the absorbency of that body at a certain wavelength. It is clear that absorption is the absorbed portion of the energy of the components of the incident beam [or color] per unit mass or given thickness of the body capable of absorbing the beam. The part of the beam that is reflected or passes through the material or body is called the reflectance and the transmittance of a particular body, respectively.

The Definition and the Requirements of BlackBody

The idea or concept of the black body was brought by the Russian Gustav Khrechev in 1860 AD. A black body can be defined as a body or mass with a specific thickness that has the ability to absorb the entire beam [that is, all the wavelengths that make up the beam] falling on it. This means that the absorption capacity of the black body is equal to

First Stage

one. For this reason, a black body is an ideal source for studying the components of thermal radiation.

A BlackBody is an object or mass or device that completely absorbs all radiation that falls on it. Clearly, the Absorbance of the BlackBody is equal to one. This is why the blackbody is a good source for studying the components of Thermal Radiation.

German physicist Max Planck stipulated that three requirements or characteristics be present in a body in order for it to be called a black body or an ideal black body.

1. Allows all incident radiation to be absorbed. In other words, no radiation reflected or transmitted through the black body.

$$\begin{array}{ccccccc} \text{Transmittance} & + & \text{Reflectance} & + & \text{Absorbance} & = & 1 \\ 0 & + & 0 & + & \text{Absorbance} & = & 1 \end{array}$$

2. Possess a minimum thickness, which is adequate to absorb the incident radiation.
3. Satisfy server limitation upon scattering to prevent radiation from bouncing back a way.

BlackBody Radiation and Quantization of Energy

Any object or body at any temperature above absolute Zero will radiate to some extent, the intensity and frequency distribution of the emitted thermal radiation depending on the detailed structure and temperature of the used body or mass. For this reason, analyzing the intensity and frequency of the emitted thermal radiation requires detailed knowledge of the structure of the radiated body or object or mass to be specified or known. The simplest possible case is an idealized body which is a perfect absorber [its absorbance=1] and therefore, also a perfect emitter. The body meets these conditions are called a blackbody or blackbody.

A widely used model of a blockbody is a cavity (e.g. oven) with a very small controllable hole. The walls of the cavity are opaque to radiation. In addition, the cavity walls must absorb all entered radiation. This device (or cavity or blackbody) emits radiation having a wide range of wavelengths when it is heated. This thermal radiation is called a **blackbody** radiation, which are characteristic of the temperature and

First Stage

does not depend upon the properties of the cavity and the small hole. Clearly, the aim using a black body to produce a merely temperature dependent blackbody radiation and then Planck's spectrum.

After studying the blackbody radiation and its spectrum, Max Planck, in 1900, arrived to the following assumptions.

- Assumptions reached by Max Planck:

1. Absorption and Emission of radiation arises from oscillators that change frequency. A change in an oscillator from a lower frequency to a higher frequency involves the absorption of energy. Whereas, energy is emitted as the frequency of an oscillator decreases (or changes from higher frequency to a lower frequency).
2. He assumed that the radiation could be subdivided into discrete bundles [or quanta] of Energy.
3. He proposed that the energy quanta is:

$$\mathbf{E \text{ quanta} = h\nu} \qquad \text{----- eqn. (1)}$$

This equation is latter known as plank's Equation. Where **h** is planck constant= 6.63×10^{-34} J. Sec. ν frequency and **E** quanta is the energy content of the quanta.

Propose the following: The quanta energy is expressed in equation (1) above. The above mathematical equation or relationship is known as Planck's equation, in which E quanta expresses the energy content of the quanta or particle from which the rays are formed, while ν and h are Planck's constant (the numerical value) and the frequency, respectively. It is worth noting that the physicist Planck was awarded the Nobel Prize for Physics in 1919 in appreciation of the important mathematical relationship he reached.

This mathematical relationship or Planck's equation reflects two important facts:-

- 1- The building unit of the beam, or quanta, has a specific energy content, or in other words, the quanta cannot have any energy content, and this is what is expressed by the energy quantity. This is the achievement for which Planck was awarded the Nobel Prize in Physics in 1999.
- 2- There is a direct relationship between energy and frequency.

First Stage

Because electromagnetic radiation is transverse wave [This means that moving wave consist of oscillations occurring perpendicular (right angle) to the directions occurring perpendicular (right angle) to the direction of energy transfer] is obey the relation:

$$\nu = \frac{c}{\lambda} \quad \text{----- eqn.(2)}$$

Where:

λ : is the wavelength.

C: is the speed of light and ν is the frequency.

Because electromagnetic rays represent a transverse wave [a transverse wave is defined as a moving wave or consisting of oscillations perpendicular to the direction of energy transfer or the direction of the axis of motion], it is represented or expressed by the following relationship:

Speed of light in empty space = frequency x wavelength

$$C = (\lambda) \times (\nu)$$

The above equation or relationship (Equation 2) can be rearranged as follows:

$$\nu = \frac{c}{\lambda} \quad \text{----- eqn.(3)}$$

By replacing ν in **Eqn.1** with $\frac{c}{\lambda}$. The following relationship is obtained:

$$E = \frac{hc}{\lambda} \quad \text{-----eqn.(4)}$$

Because $1/(\lambda) = \text{wavenumber } (\nu')$, the above equation can be rewritten as follows:

$$E = h'\nu c \quad \text{-----eqn.(5)}$$

From the above equations we can notice that the energy of a wave is related to a number of other wave properties such as frequency, wavelength, and wavenumber. What confirmed the validity of this relationship is the agreement of the theoretical calculations based on the above relationships with those relevant practical measurements.

Example: What is the molar energy associated with an atomic transition giving radiation at (Hz).

First Stage

Solution:-

$$E = h\nu NA$$

$$E = 6.626 \times 10^{-27} \text{ erg. } \cancel{\text{sec}} * 1 \frac{1}{\cancel{\text{sec}}} * 6.022 \times 10^{23} \text{ atom/mole}$$

$$E = 6.626 \times 10^{-27} \times 6.022 \times 10^{23}$$

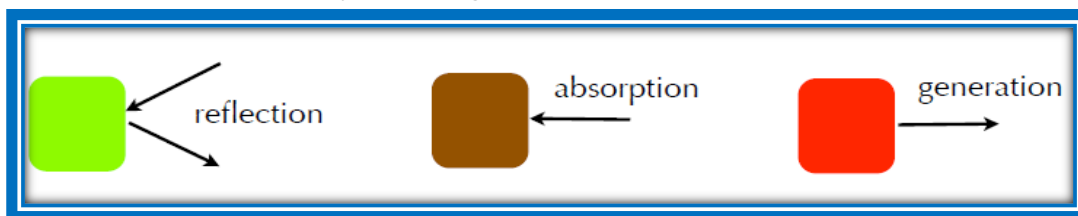
Example: What is the relationship between the electron volt (eV) and the wave length (λ) in nm of energy equivalent photon?

Solution:-

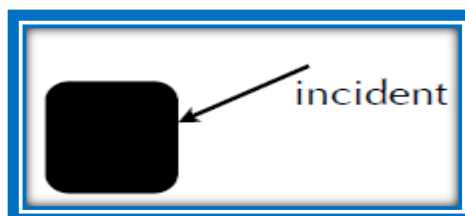
$$E = h c / \lambda.$$

Blackbody radiation

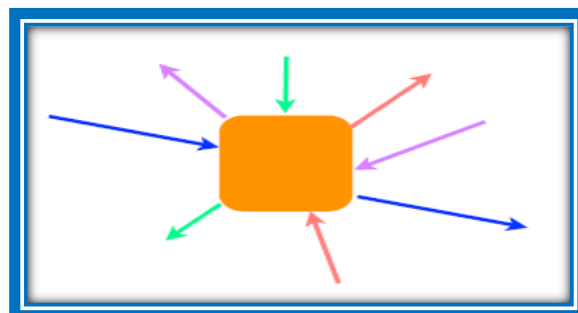
There are three ways that light interacts with matter:



In principle, all three things can be happening simultaneously. However, we see most things through reflection. If an object has no reflection, then, if there were no generation, it would appear to be absolutely black. We call it a blackbody. All incidents light are totally absorbed.



However, the blackbody can generate light. In fact, it must in order to maintain equilibrium.

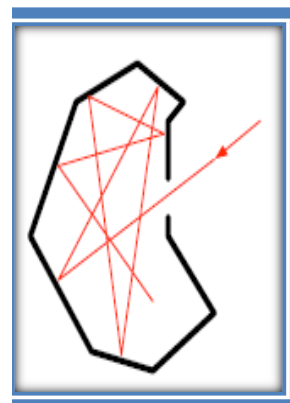


First Stage

According to Kirchhoff: The amount of radiation being absorbed at each and every frequency, will be exactly matched by outgoing radiation generated by the Blackbody.

Therefore, a perfect absorber of light must also be a perfect emitter of light. Because any blackbody is perfect emitter, every blackbody should have the same emission spectrum. When the Blackbody is heated to a given temperature, it will radiate EM energy, with an emission spectrum that is characteristic of the temperature. This makes it useful as laboratory standard in doing optics experiments. In the late 1800s, the study of black bodies was an important topic. Making a true blackbody is actually a bit tricky. Simply slapping some black paint over an object is not good enough, since that will not necessarily make the reflection go to zero.

The usual approach is to make a metallic cavity with a small hole. Any light from the outside hitting the hole will go inside and probably bounce around many times, eventually being absorbed by the walls of the cavity. The chances of the incident light being reflected directly back out the hole are very slim, assuming that some care was taken in the design of the cavity.

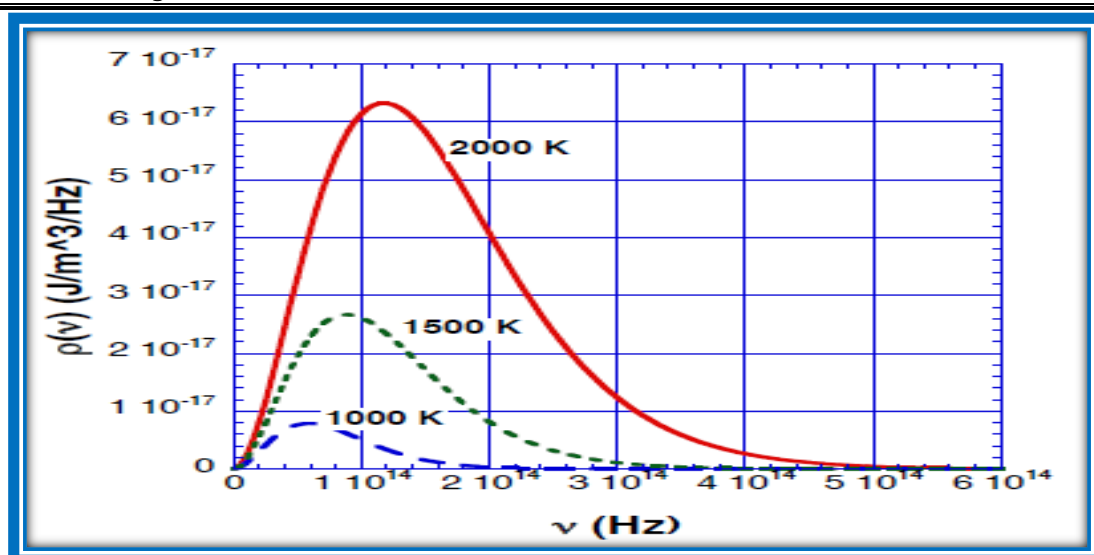


Any light being generated by the motion of the electrons in the walls of the cavity will bounce around many times before it may escape through the hole. (In fact, most of the internal light will simply be re-absorbed). In this way the hole acts like a blackbody, and the cavity is filled with Blackbody radiation. So, by heating the cavity structure up to a uniform temperature, you can observe blackbody radiation coming from the hole.

Blackbody Radiation Spectrum

As the Blackbody is heated, the total energy emitted increases (obviously) and the peak in the spectrum shifts to higher frequencies (shorter wavelengths).

First Stage



The properties of blackbody radiators had been determined experimentally by the end of the 1800s. The total EM power (integrated over all frequencies) radiated by a black body at a given temperature T is

$$P = \sigma AT^4$$

Where:

A: is the surface area of the Blackbody and σ is a constant equal to $5.67 \times 10^{-8} \text{ J/s/m}^2/\text{K}^4$. (**Stefan-Boltzmann law**)

However, since we usually work with a cavity, we can say the same thing by looking at the total EM energy density within the cavity.

$$\rho_T = \int_0^{\infty} \rho(\nu) d\nu$$

$$\rho_T = aT^4$$

Where: the constant a is equal to $7.56 \times 10^{-16} \text{ J/m}^3/\text{K}^4$.

Lastly, the peak frequency increases linearly with temperature, meaning that wavelength is inversely proportional to temperature.

$$\lambda_{\text{peak}} = w/T$$

Where: $w = 2.90 \times 10^{-3} \text{ m} \cdot \text{K}$ (This is Wien's Law.)

The experimental facts were not in dispute. These results had been measured in many laboratories by 1900. Trouble came though when theorists tried to explain the BB spectrum. This should have been a straightforward application of thermodynamics and EM theory.

- Use electromagnetics to determine the electromagnetic modes inside the cavity.

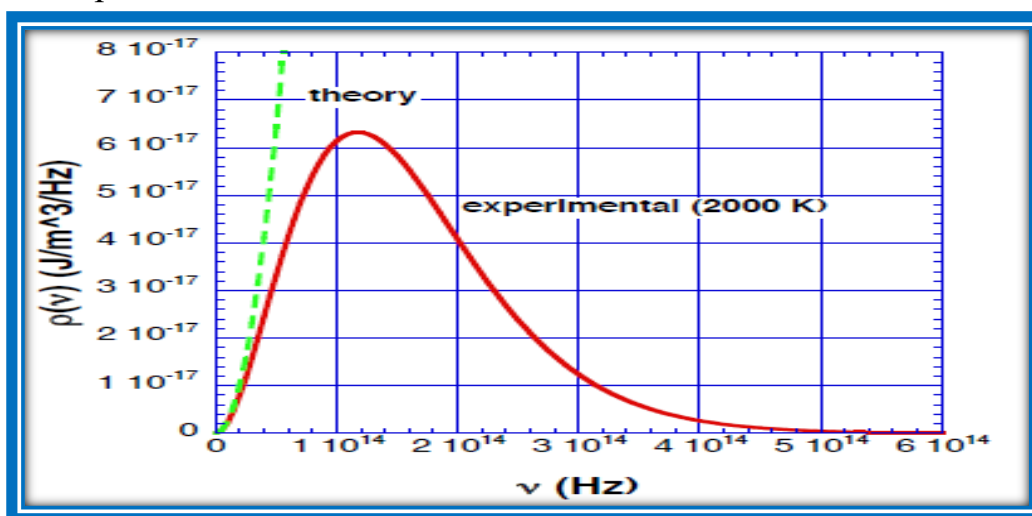
First Stage

- Use thermodynamics to determine the distribution of energy
- Underlying it all is the assumption that all energies are possible (a continuous distribution of energies).

The expression obtained using the classical theories were:

$$\rho(\nu) = \frac{8\pi kT}{c^3} \nu^2$$

Comparing the theoretical equation to the experimental results showed that the theory was a miserable failure. In fact, it predicted an infinite amount of energy being radiated (Referred to as the “ultraviolet catastrophe.”)



In 1900, Max Planck proposed a way to derive a suitable equation. To get there, he tossed aside the assumption that energies are continuously distributed. Instead assumed that the energy of EM modes in the cavity consisted of discrete packets. The energy of each packet was proportional to the frequency of the EM mode.

$$E = 0, h\nu, 2h\nu, 3h\nu, 4h\nu, 5h\nu, \dots \text{ etc.}$$

With this modification, the Planck's result was:

$$\rho(\nu) = \frac{8\pi h}{c^3} \frac{\nu^3}{\exp\left(\frac{h\nu}{kT}\right) - 1}$$

This matched the experimental results exactly, if h was chosen to have a value of 6.63×10^{-34} J.s. This was the first use of the notion of *quantization of energy*.

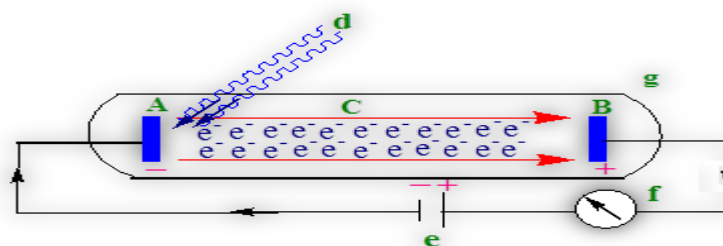
First Stage

Photoelectric effect (The Nature of Light)

In the 1800's, it was observed that when an electromagnetic radiation is shined on a substance [e.g. solid, gas or liquid] which is placed in an evacuated tube, an electric (electrons) current flows. This low-energy phenomenon of electromagnetic radiation -matter interaction and the subsequent emission of electrons is termed the photoelectric effect. So, **the photoelectric effect refers to the emission of electrons from a substance when it absorb an incident electromagnetic radiation. Electrons emitted in this manner may be called photoelectrons.**

An experimental set up for studying the photoelectric effect is shown below.

A diagram of the components used in the study of the phenomenon of electron emission by beam.

**Where:-**

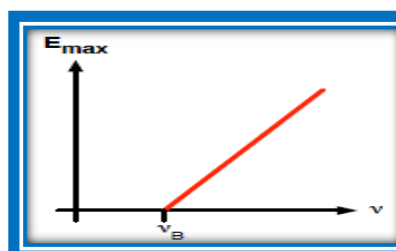
A, B: Metal Plates, **C:** Electron Current, **d:** Electromagnetic Rays.

f: Ammeter, **e:** electric cell and **g:** Evacuated tube.

There were two important observations:

1. The photocurrent is proportional to the intensity of the light.
2. The maximum energy of the emitted electrons is proportional to the frequency of the emitted light, and there is some minimum frequency below which no photocurrent is generated.

The second of these is puzzling, since according to classical EM theory, the frequency should play no role in the describing the energy transfer from light to electrons.

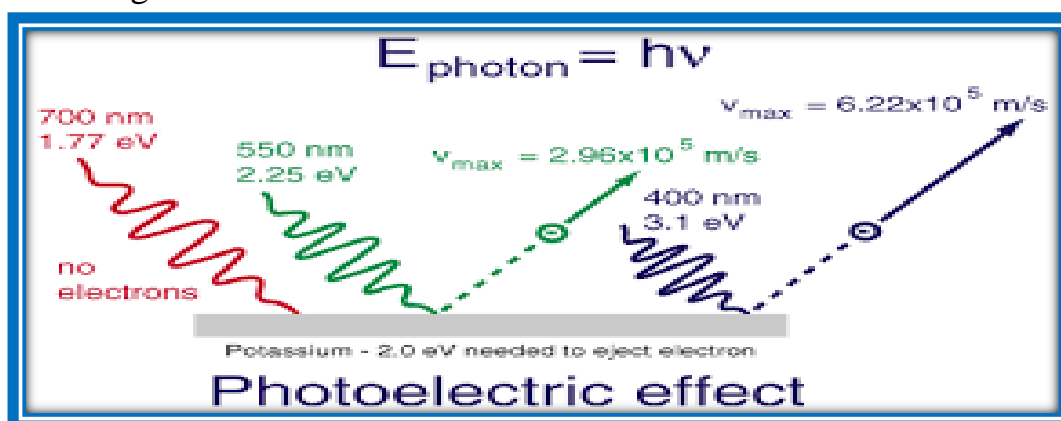


A plot of E_{\max} vs. frequency looked nearly the same for all metals used for the emitting electrode. Different metals would result in different minimum frequencies, but otherwise the curves were identical.

*First Stage***Below some of the results of photoelectric effect Experimental**

- The use of a bright light [higher intensity radiation] of a certain energy (or frequency) leads to an increase in the number of emitted electrons per time unit and the kinetic energy of the emitted electrons is not affected. This observation indicates that the number of emitted electrons [or electric current] is proportional to the intensity [or brightness] of the absorbed electromagnetic radiation [or light].
- the use of a dim light (or radiation) of a certain energy (or frequency) results in immediate emission of electrons but the number of emitted electrons is less than that observed when a brighter light was used. This observation indicates that the time is not an important factor for this phenomenon to occur.
- Increasing the frequency (or Energy) of the incident (or absorbed) light (or radiation) would lead to an increase in the kinetic energy of the emitted electrons. If, however, the frequency (ν) of the used radiation falls below a minimum value called the threshold frequency (ν_0), there would be no electrons emitted and no matter how intense the used radiation and how long the exposure are.

The diagram below shows in numerical values the relationship between the intensity and frequency of the incident beam and the kinetic energy of the emitted electron, as well as the effect of the threshold frequency (ν_0) on the possibility of electronic emission occurring.



We conclude from this that the energy of the incident photon must be sufficient to displace the electron from the influence of the nucleus, in addition to the electron gaining kinetic energy according to the following law:

First Stage

$$E = h\nu = h\nu_0 = W_0 + \frac{1}{2}mv^2$$

\swarrow \swarrow \searrow
 Critical frequency Work function Kinetic energy of the body

$$\frac{1}{2}mv^2 = h\nu - W_0$$

In other words, when a photon collides with the surface of a metal, the energy of the photon is transferred to one of the electrons in the metal. The electron gains this energy and is transformed from a low energy level to a high energy level. The electron is activated and gains kinetic energy. This kinetic energy is directly proportional to the frequency of the incident radiation, and the higher it is, the higher the photon energy.

$$h\nu = W_0 + \frac{1}{2}mv^2$$

The more active or ionizable the metal is, the lower the frequency required to displace electrons.

Example: Calculate the kinetic energy of the electron from potassium surface when $W_0 = 3.62 \times 10^{-12}$ erg by the incident light having the following wave lengths: 7×10^{-5} cm, 5.5×10^{-8} cm?

Solution:-

1- $C = \lambda\nu$

$$\nu = \frac{C}{\lambda} = \frac{3 \times 10^{10} \text{ cm/sec}}{7 \times 10^{-5} \text{ cm}}$$

$$\nu = 4 \times 10^{14} \text{ Hz}$$

$$\frac{1}{2}mv^2 = h\nu - W_0$$

$$= 6.62 \times 10^{-27} \times 4 \times 10^{14} - 3.62 \times 10^{-12}$$

2- $\nu = \frac{3 \times 10^{10}}{5.5 \times 10^{-8}} = 5 \times 10^{17} \text{ Hz}$

$$\frac{1}{2}mv^2 = 6.62 \times 10^{-27} \times 5 \times 10^{17} - 3.62 \times 10^{-12}$$

The ear of light is a stream of particle particles of photons that travel in a vacuum at the speed of light. Each photon has a specific energy, and radiation is a stream of particles that carry wave characteristics. This radiation can be deflected and can be divided into its components.

First Stage

In brief, the photoelectric effect experiment has three features which all explained easily by Einstein's assumption of the existence of quanta (or quantum).

- The photoelectric effect [or the kinetic energy of emitted electrons] depends on the energy or the frequency of the impinging or radiation. In addition, there exists some minimal frequency (or energy) below which the impinging radiation is unable to free electrons, whereas above that critical frequency, the photoelectric effect can be seen.

Question: - What happens if the energy of the beam or the frequency of the incident, impacted or absorbed by the material equals the minimum [or threshold frequency] of the material?

- The photoelectric current [the number of released electrons] is proportional to the intensity of the impinging radiation.
- There is basically no time delay between the liberation of electrons and the strike of the materials' surface by the radiation.

Einstein's Explanation for the Photoelectric effect

In the year 1905 AD, the German physicist Albert Einstein provided an explanation explaining the phenomenon of electronic emission from the surfaces of materials when an electromagnetic ray [or light] falls on them. It is worth noting that Einstein adopted in his interpretation some of the findings of his countryman, the physicist Max Planck, during his study of the phenomenon of black body thermal radiation.

Below are the most important aspects of Einstein's explanation of the photoelectric phenomenon:-

1. The electromagnetic radiation consists of a stream of fine particles or particles with a specific energy content [or as Planck said, the thermal radiation emanating from a black body consists of [quanta].
2. When these energy particles collide with atoms, molecules, or ions on the surfaces of objects, the energy content is transferred to the electrons of these materials, which may cause a noticeable increase in the energy of these electrons.
3. The electrons of materials are bound by a force of attraction to the rest of the components of matter. The least amount of energy that causes the forces of attraction to be broken and the electron to be released is

First Stage

called the work function. This term is widely used by physicists, while chemists use the term binding energy

Electron or W_0 to refer to the work function. Note that the work function or binding energy of an electron varies from one substance to another. This means that it is a physical property that distinguishes substances from one another.

In view of the foregoing, the effect or phenomenon of photoelectric emission can occur when the energy of the beam particles or quanta is greater than or equal to the electron binding energy W_0 of the surface of the material on which the beam falls, i.e.: $E_{\text{quanta}} \geq W_0$

However, the phenomenon or effect of photoelectric emission does not occur when: $E_{\text{quanta}} < W_0$. This explains why the phenomenon or effect of electronic emission does not occur in all cases.

4. Due to the diversity of electron binding energies for various materials, as well as the diversity of energies of beam particles [or quanta] with the diversity of electromagnetic rays, the kinetic energy E_{kin} of the electron or electrons liberated or emitted varies with the diversity of materials and rays falling on them.

The kinetic energy of the emitted electron is related to the electron binding energy and the energy of the beam particles by the following mathematical relationship:

$$E_{\text{quanta}} = E_{\text{kin}} + W_0$$

The above equation or relationship can be written in terms of the kinetic energy of the electron as follows:

$$E_{\text{kin}} = E_{\text{quanta}} - W_0$$

5. If the energy of the incident ray particles is greater or equal to the electron binding energy:

$$E_{\text{quanta}} \geq W_0$$

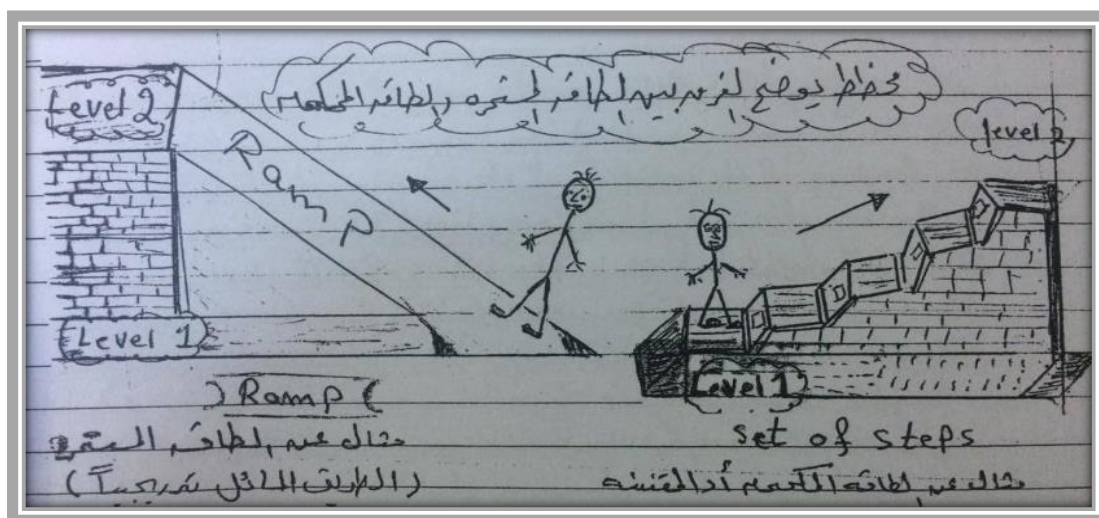
The phenomenon occurs when the ray touches the surface of the body or matter. Contrary to what was stated above, the phenomenon does not occur even if the surface of the body is exposed to radiation for a long period of time.

First Stage

6. Increasing the intensity or intensity of the appropriate electromagnetic beam [$E_{\text{quanta}} \geq W^{\circ}$ incident] leads to an increase in the number of emitted electrons. This direct relationship between the intensity or intensity of the beam of appropriate energy and the number of electrons emitted indicates that one electron absorbs one minute of beam [or quantum and its summation quanta].

It is clear from the above that the phenomenon or effect of photoelectric emission provides direct and convincing evidence of:

1. The particle or particle nature of electromagnetic radiation [or the formation of the radiation from objects or particles, which Max Planck called quanta, and its singular form is quantum].
2. The diversity of rays means the diversity of the energy content of their minute components, or in other words, the presence of more than one type of quantum.
3. Quantum energy and electron energy are specific quantities, and this is known as a quantum, or in other words, the quantum is a specific beam. It has a specific energy content and not any amount of energy or what is known as continuous energy.



In order to clarify or explain what is meant by the term quantized or regulated energy and what is meant by continuous energy, we try to understand what the following example or diagram above means and what is its relationship to the two terms mentioned previously.

First Stage

Quantized energy and continuous energy can be likened to the steps of a staircase and a gradually inclined road, respectively, and these two means connect two floors in two separate buildings. The inclined path corresponds to a continuous increase in energy, as a person can put his foot anywhere he wants and thus be at any height he wants and therefore can have any energy value he wants. As for the steps of the ladder, they correspond to quantized energy, as a person cannot place his foot in any place or point on the ladder, but there are specific areas or points with a specific energy height.

Although, Einstein made use of the assumption that electromagnetic radiation behaves as a particle, there is no denying of the validity of the experiment that show the electromagnetic radiation [e.g. light] behaves as a wave. Actually, light has characteristic of both waves and particles, the so called particle- wave duality. Experiment conditions will decide whether it behaves as a wave or as a particle.

For his explanation of photoelectric effect, Albert Einstein received the Noble Prize in physics in 1921. It is worth noting that in 1926, the American chemist G.N. Lewis, or simply Lewis, is a new name for quantum, which is the photon. Which is still used today.

Atomic Spectra

Electromagnetic Radiation Spectra and its Types

The radiation spectrum can be defined as an arrangement or display of lights, colors or other form of radiation separated according to their wavelengths, frequencies, or energies.

There are two types of spectra:

- 1- Emission spectrum.
- 2- Absorption spectrum.

Emission spectra can be obtained, i.e. this type of spectrum, by preparing the atoms of the element with sufficient energy, such as heating or exposing them to an electric arc or electrical discharge. This type is divided into:

- 1- Continuous spectrum
- 2- Band spectrum
- 3- Line spectrum

First Stage

1. **Continuous Spectrum**: is an emission spectrum that contains continuous unbroken distribution of all frequencies, wavelengths and color (or light). In other words, continuous visible spectrum has no dark (or black) or colored lines. Rainbow is an example of the continuous visible spectrum. In candescent blackbody (or blackbody radiation) gives a continuous visible spectrum (Planck's Spectrum).



2. **Band spectrum**:

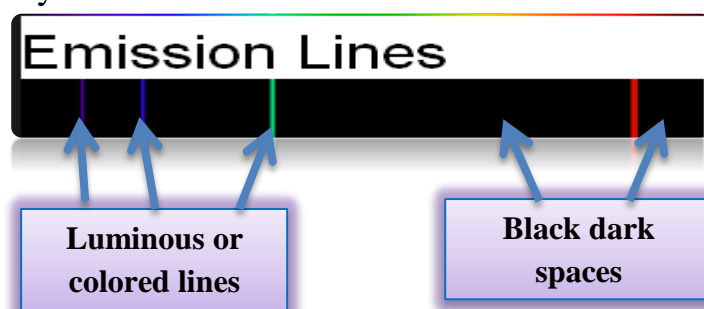
Band spectra contain a group of overlapping and entangled bands and are generated by radiation emitted by excited particles.

3. **Linear spectra**:

Linear Emission Spectrum The term linear emission spectrum is used to describe a spectrum that consists of a series of frequencies, wavelengths, or colored lines separated from each other. In the visible region of the electromagnetic spectrum the colored lines are separated from each other by dark, dark or black areas.

Emission Line Spectrum: This term used to describe the spectrum that is consisting of a series of separate frequencies, wavelengths or colored lines.

In the visible region of the electromagnetic spectrum, the colored lines are separated by dark or black areas.



Line spectra can be obtained when an electrical discharge occurs through the atoms of an element, provided that it is in the gaseous state and under low pressure. Light is emitted from the agitated metal atoms, and when the spectrum of this light is analyzed, it appears in the form of chains of spectral lines known as line spectra, and each line is

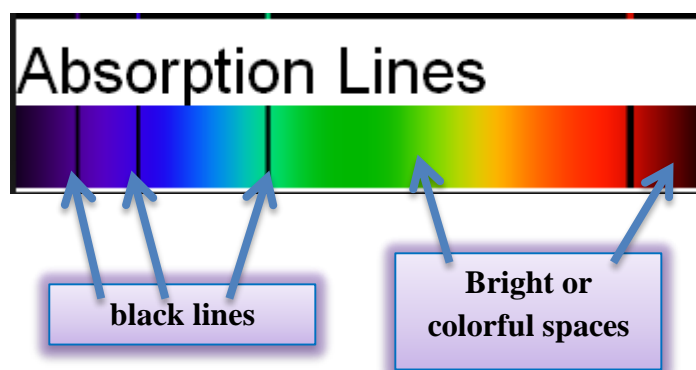
First Stage

characterized by a wavelength. Or a specific frequency, and each element has a specific linear spectrum. Some of these lines can be seen if they are located in the visible part of the spectrum when recorded on a photographic plate. This light comes from the transition of the energy level of electrons or electrons of atoms to a high energy level. When these electrons return to an energy level. The lower ones emit radiation at a different wavelength, and this method helps us to know the electronic arrangement in the atom. Just as every substance has an emission spectrum, every substance has its own absorption spectrum as well.

It should be noted that, in the emission line spectrum, the separate frequencies, wavelengths or colored lines are occurred at exactly the same wavelengths, frequencies, or dark or black lines in the absorption line spectrum. Thus, one thinks of the absorption spectrum as the continuous spectrum minus the emission spectrum. This can be expressed in an equation form.

Absorption spectrum= continuous spectrum- emission spectrum

Absorption line spectrum: is a spectrum that contains a block lines as a result of absorption of a certain wavelength by the media (eg. cool gas). As for the illuminated areas, they express radiation, frequencies, colors, or lights that are not absorbed by the medium through which the radiation passes.

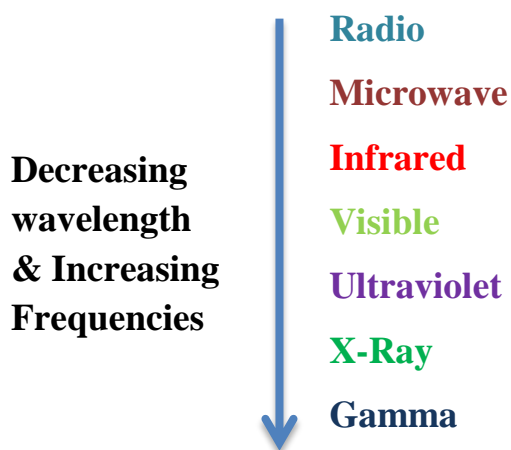


When light passes continuously through an atomic vapor of an element, the transmitted light has a decrease in wavelengths, and this results from the atoms of the element absorbing certain wavelengths of light to excite the electrons to high energy levels. Regions whose wavelengths have been absorbed by the model, and the absorption spectrum is used to characterize compounds.

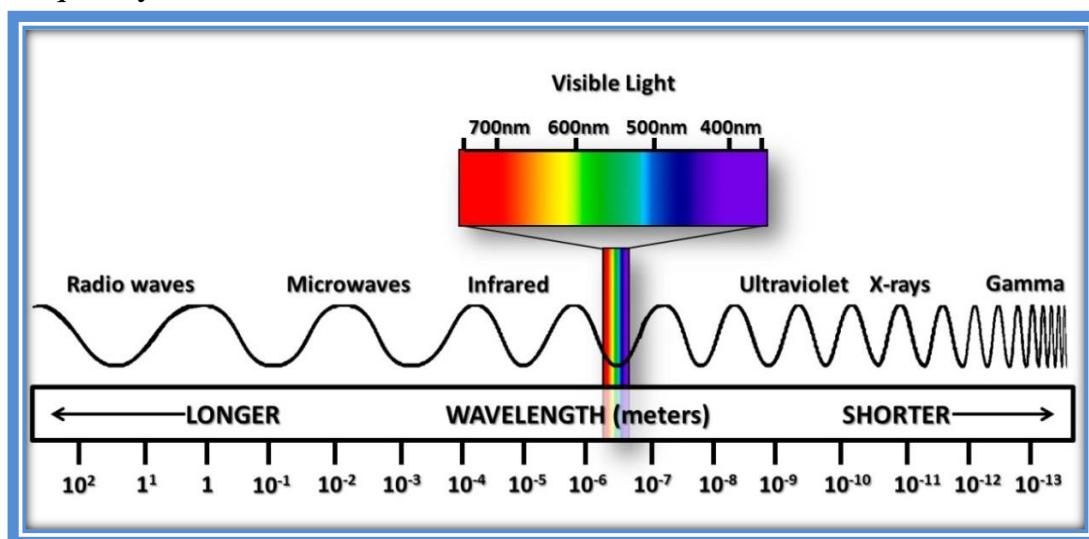
*First Stage**The Special Meaning of Electromagnetic Spectrum*

The electromagnetic spectrum may take a special meaning or definition as it expresses the spectrum that includes the entire range of frequencies or wavelengths known to man. It is clear that the continuous spectrum best represents this type or concept is the spectrum of sunlight. In scientific English, EM Spectrum is used to refer to the specific meaning of the electromagnetic spectrum.

The electromagnetic spectrum can be divided into parts where these parts are characterized by a certain range of frequencies or wavelengths.

The components or parts of the spectrum are:

The figure below shows the regions of the electromagnetic spectrum as well as the wavelengths λ (measured in angstroms or \AA) and the frequency measured in Hz.

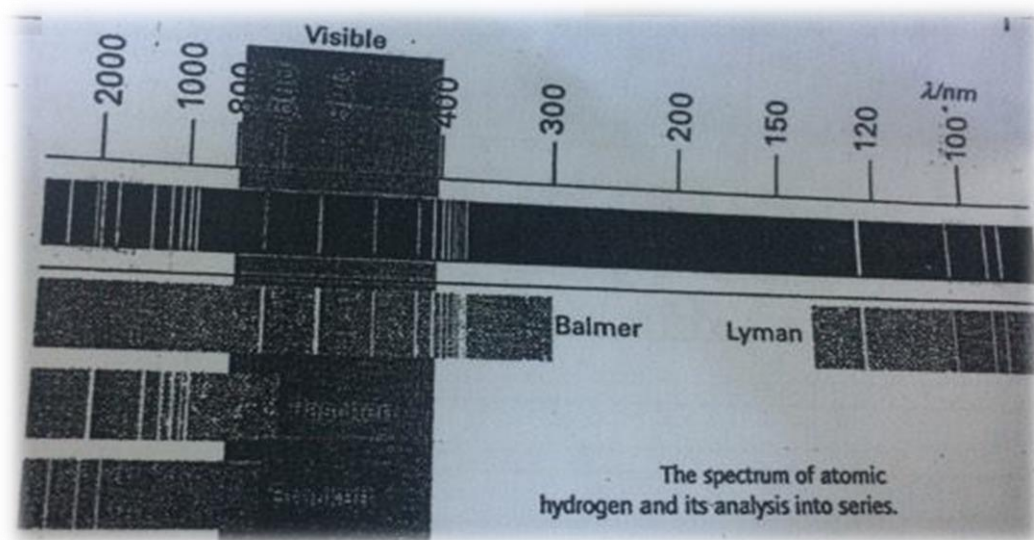


First Stage

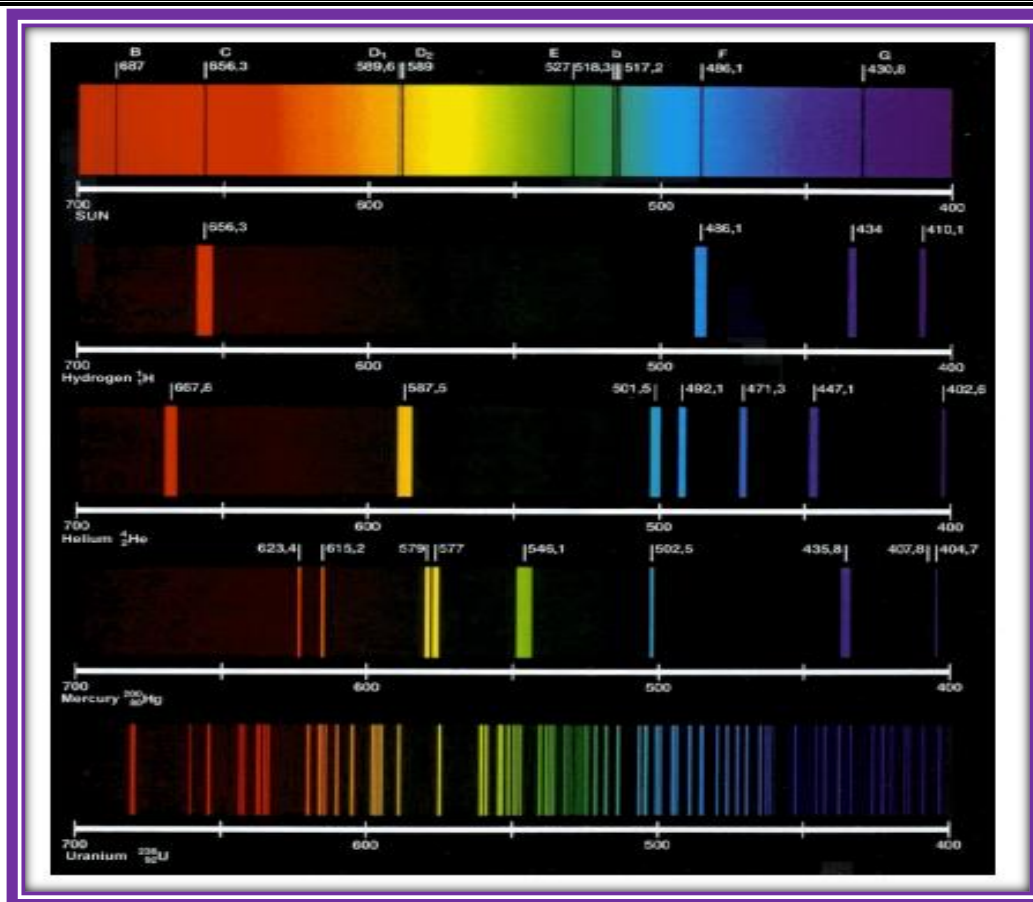
Clearly, EM spectrum extended from the frequencies (or wavelengths) used for modern radio communication ($\lambda=10^3$ m) to a gamma rays ($\lambda=0.1$ Å, or a fraction of the size of an atom). However, Radiations with a wavelengths between 380nm and 760 nm (nm=nanometer= 10^{-7} cm= 10^{-9} meter) are detected by human eye and perceived as visible light.

Atomic Emission Spectra of chemical Elements

Electromagnetic radiation is emitted when an electric charge passed through a gas sample of a chemical element. When the emitted radiation was allowed to pass through a prism or diffraction grating. A series of a single frequency radiation obtained. Some of these frequencies or are fallen in the visible, ultraviolet, and infrared regions of EM spectrum. The complete display of these frequencies is called atomic emission spectrum of an element. Each chemical element has an individual and characteristic emission line spectrum. For this reason, these spectra can be used to identifying various elements. Here is the complete atomic emission line spectrum of Hydrogen atom.



First Stage



Visible line emission spectra of a number of stoichiometric gases.

The above spectra are the atomic emission line visible spectra of some elements. Clearly, the simplest spectrum is that of hydrogen element. Hydrogen atom, however, is the simplest atom, because it has one electron. The hydrogen spectrum consists of a series of lines whose separation decreases in a perfect regular manner towards shorter wavelengths (higher energy). The spectra of all other chemical elements likewise consist of a series of lines. As the atomic number (or No. of electron) of an atom increases the number of the spectral lines and the overlapping between these lines are increased. For these reasons, they are not always so easily recognizable.

The apparent regularity of the line series of the hydrogen emission spectrum in the visible region was first mathematically formulated by the Swiss mathematician Johann Jakob Balmer or J.J. Balmer (1825-1898). He found the wavelengths of the visible lines, of the atomic emission spectrum of Hydrogen atom, can be described accurately by the following equation (Balmer Eqn.).

First Stage

$$\lambda = C \frac{n^2}{n^2 - 2^2}$$

Where:-

λ (or Lambda) = wavelength of the spectral line.

C= Balmer Constant= 3.645×10^{-7} m, and n= 3, 4, 5, ----- and so forth.

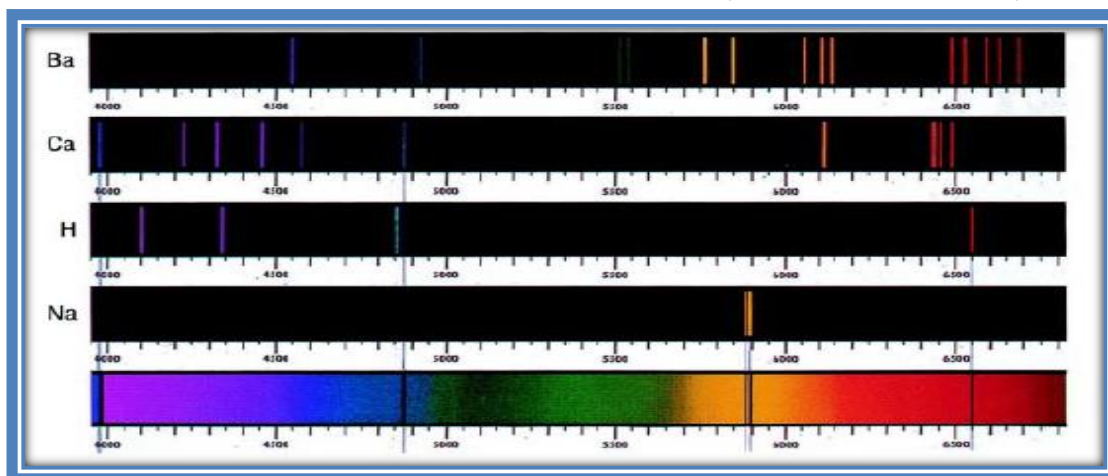
The first to express mathematically the state of regularity in the appearance of linear aggregates in the visible region of the emission spectrum of the hydrogen atom was the Swiss mathematician Jahan Jacob Palmer (born 1825 and died in 1898 AD), noting that he began his life as a teacher of mathematics in a Swiss school. Palmer found that the wavelengths of the visible atomic spectral lines of the hydrogen atom can be theoretically calculated or predicted using the following equation called the Palmer equation.

$$\text{Wavelength} = \text{Balmer's constant} \frac{(\text{Positive integer})^2}{(\text{Positive integer})^2 - 2^2}$$

Palmer's constant = 3.645×10^{-7} meters, λ = wave weight and the word (**lambda**), which is a Greek letter.

Line Spectra

The emission from a rarefied gas consists of sharp lines. Each elements has a characteristic set of lines that may be used to identify it.



Classical physics could neither explain these lines spectra nor fit them into any scheme.

Atomic Spectra of Hydrogen

The hydrogen atom was chosen to study the atomic structure because it is the simplest of the atoms and it has one electron. Thus, the levels between which this electron moves can be known, as well as knowing its distance from the nucleus, and this means that the linear spectrum can be studied for it.

By looking at the hydrogen atomic emission spectrum, someone can easily see that the hydrogen atomic emission spectrum contains other lines which are fallen outside the visible region of the EM spectrum. These lines of frequencies were not known to Balmer. These series of spectral lines are named of their discoverers.

When an electric discharge occurs in a tube containing hydrogen gas atoms, a glow will occur, and this light will be emitted through a prism in the spectroscopic device, so we will get a group of lines that appear in the form of groups of different wavelengths on a photographic plate.

These groups were later called sequences, and the first person to discover the emission lines of the hydrogen atom in the visible region was the world, Balmer. After that, the series were discovered by other scientists in other wavelengths, and these scientists were Brackett, Paschen, Pfund, and others.

Each group of emission lines represents electron transitions from a high energy level to a low energy level. The emitted energy has been calculated through an equation or a mathematical relationship, which is the Rydberg equation.

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

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

$R_H = 109678 \text{ cm}^{-1}$, $n =$ energy level or number.

The locations of the emission lines for the hydrogen atom can be determined from the series according to their locations, both according to their discoverers.

First Stage

Balmers Eqn. has a limited use, because it can be only used to calculate or predict the wavelengths of the lines of the visible spectrum of the hydrogen atom.

The nineteenth century Swedish spectroscopist **J. Rydberg Eqn.** is called **Rydberg's Eqn.** which can be used to calculate or predict all wavelengths that appear an atomic spectra [Emission or absorption] for hydrogen atom and hydrogen-like ions [Hydrogen-like ions are positive ions; cations, with only one electron, e.g. ${}_2\text{He}^+$, ${}_3\text{Li}^{2+}$.

$$1/\lambda = Z^2RH \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$$

Where: Z= atomic number.

RH=Rydberg Constant= $1.0973 \times 10^7 \text{ m}^{-1}$

$\lambda_{\text{vac.}}$ = The wavelengths of the light or radiation that is emitted in vacuum.

n_f and n_i are positive digits and $n_f > n_i$.

The Balmer equation is of limited use because it is only used to calculate or predict the frequencies of spectral lines appearing in the visible region of the hydrogen atom.

The Spectral Line Series are:**1- Lyman Spectral Series**

Its wavelengths lie in the UV region of EM spectrum (91.2 nm-122 nm). This spectral line series was named after its finder the American Physicist Theodor Lyman (1814-1954).

$n_1 = 1, \quad n_2 = 2, 3, 4 \text{ -----}$.

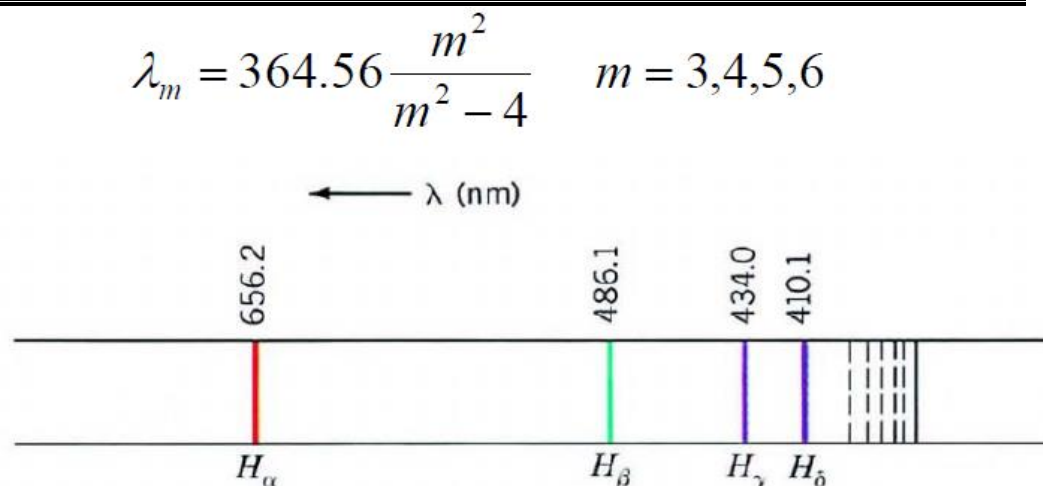
2- Balmer Spectral Series

The visible spectrum of hydrogen consists of four lines. In 1884, Balmer, a Swiss mathematics teacher, found that these wavelengths (in nm) could be represented by a single formula, called Balmer formula:

$n_1 = 2, \quad n_2 = 3, 4, 5 \text{ -----}$.

The wavelengths of the lines of this sequence lie in the visible region.

First Stage



3- Balmer series lines lie in the visible (Vis) region with a wavelength of 364-800 nm.

4- Paschen Spectral Series

Its wavelengths lie in the Infrared Region of the electromagnetic spectrum [820 nm → 1870]. This spectral series of lines named after its finder the German Physicist Louis Karl Paschen [1865-1947].

$$n_1 = 3, \quad n_2 = 4, 5, 6, \dots$$

5- Bracket Spectral Series

Its wavelengths lie in the IR region (or infrared region) of the EM spectrum [1460 nm → 4050 nm]. This spectral series was named after its discoverer the American Physicist Friedrich Brackett [1896-1988].

$$n_1 = 4, \quad n_2 = 5, 6, 7, \dots$$

6- Pfund Spectral Series

Its wavelengths lie in the IR region of the EM spectrum [2280 nm → 7460 nm]. This spectral series was named after the American Physicist August Herman Pfund [1879-1949].

$$n_1 = 5, \quad n_2 = 6, 7, 8, \dots$$

Example:- In the Lyman series, calculate the wave number $\bar{\nu}$, wave length λ and the frequency ν for the lines $n_2 = 4, 6, 8, \infty$?

Solution:-

$$\bar{\nu} = R_H \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) = \left(\frac{1}{1} - \frac{1}{16} \right) = 109677.9375$$

$$\bar{\nu} = \frac{1}{\lambda}, \quad \lambda = \frac{1}{\bar{\nu}} = \frac{1}{109677.9375}$$

$$= 9118 \times 10^{-9}$$

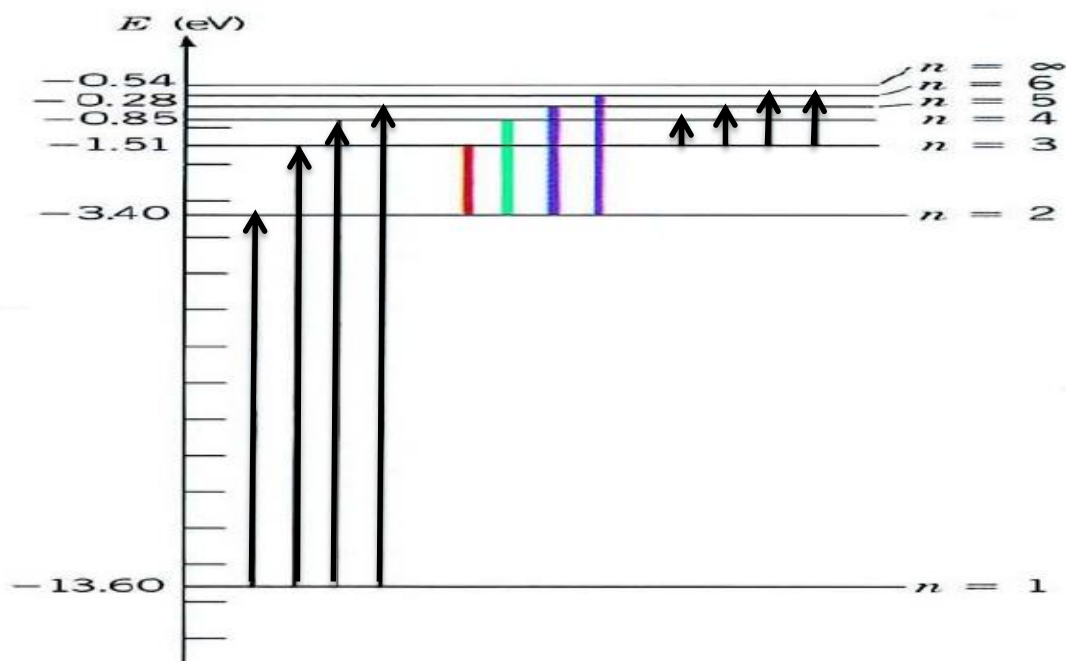
First Stage

$$c = \lambda \nu \rightarrow \nu = \frac{c}{\lambda} = \frac{3 \times 10^8}{9118 \times 10}$$

$$\nu = 3.29019$$

The Energy Level Diagram for Hydrogen (Z=1)

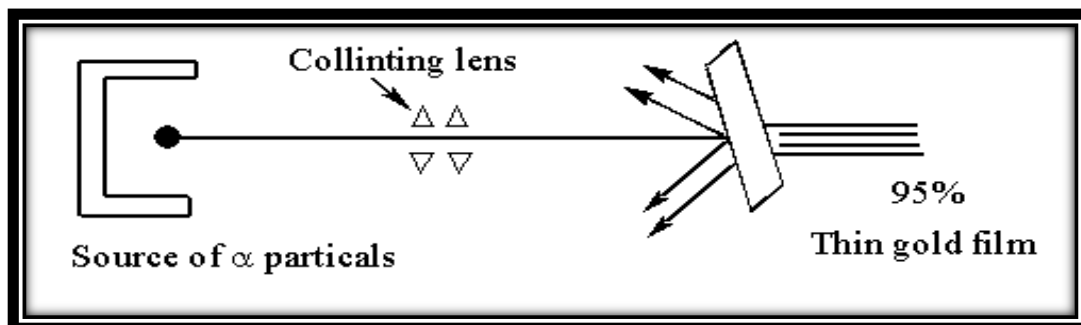
The photon energy must correspond exactly to the energy between two states involved in the transition.

*Interpreting the structure of the atom using linear spectra*

Among the questions raised by the linear emission spectrum and the Rydberg equation is why n is an integer? And what does $n=2$, $n=1$ ---- mean? Since the Rydberg equation includes all elements or applies to them, what is common between these elements to give such similarity, it becomes clear to us what is required to study the atomic structure on the basis of spectra. The scientist Thomson showed in 1898 that atoms consist of balls of positive charges to which electrons are attached in 1911. The scientist Rutherford noticed that when he conducted the experiment on alpha particles (the nucleus of the helium atom, He^{2+}), he did not know Rutherford said that the alpha particles are the nucleus of the helium atom, but he knew that it had a positive mass, so he applied a stream of alpha particles to a thin plate of gold placed in a direction perpendicular to the stream of alpha particles, since at that time

First Stage

Thomson's theory was accepted in the structure of the atom. Rutherford and the student who was conducting the experiment with him (Marsden) expected that all the alpha particles would pass through very quickly, penetrating the thin gold plate without any noticeable deviation, but what was observed was that 95% of the alpha particles were carried out.



Indeed, from the gold plate, but from time to time some of these minutes collide with the plate and return in the opposite direction. This means that if Thomson's assumption were correct, this number of minutes would not have bounced off. Rather, the thousand minutes pass from the plate without any obstruction, and for this reason Thomson's theory has become unacceptable.

Therefore, Rutherford assumed that the deviation that occurred shows that the atom has a dense positive charge, which is the nucleus, and is surrounded by a thin shell of electrons, and that the mass and charge of these electrons is concentrated in a very small space. Therefore, the scientist Rutherford demonstrated the ease with which most alpha minutes pass without obstruction because they pass through these spaces, but from time to time. Some positively charged alpha particles pass near the nucleus and a rapid and strong repulsion occurs. This explains that the electrons move around the nucleus in paths.

But the classical theory of electromagnetism shows that charged particles that pass around minutes opposite them in charge with a certain acceleration emit energy, and the rotation of electrons around the nucleus will lead to the emission of energy, and this will lead to lower levels of energy than the level in which it was. The nucleus and thus this movement becomes not abbreviated on a fixed orbit, but the orbit becomes helical and spinal until the electrons fall inside the nucleus, and for this reason Rutherford failed to explain the atomic structure or the structure of the atom.

First Stage

-Bohr interpreted Rutherford's experiment as he explained the emission spectral lines of the hydrogen atom only, and we will see later Bohr's failure to interpret the spectral lines of other elements.

Bohr's theory was mainly based on the theory of the scientist Max Planck and was based on two assumptions:

1. The electron of the hydrogen atom moves in a circular orbital path around the positively charged nucleus without radiating energy, and the classical theory of electromagnetism does not apply to atomic particles.
2. As long as the electron is moving in a circular path, this means that it has angular momentum equal to multiples of Planck's constant and divided by twice the constant ratio.

$$\begin{aligned} \text{Angular momentum} &= mvr, & mvr &= \frac{nh}{2\pi} \\ & & &= \frac{nh}{2\pi} \end{aligned}$$

Where:-

r = radius of the orbit

v = the speed of the electron

h = Planck's constant

n = positive integer

If there is no external force, the angular momentum remains constant, and there are an infinite number of possible circular paths for the presence of the electron in the hydrogen atom, and the radius of the path (**n**) or the radius of each of these paths are according to the value of (n), or in other words, the lower the value (**n**) The radius of the orbit decreases.

However, despite the multiple circular paths, there are no values for the angular momentum between the successive values of integers, meaning that the angular momentum of the electron depends entirely on the values of **n**, which are specific quantized values and nothing else, and therefore (**n**) is considered quantum no. Any quantum number, which is an integer and does not allow passage between these values. This shows that when an electron absorbs energy and is present at **n=1** or **n1**, this electron can move to another circular path with higher energy, or vice versa, and the difference between the two paths is whether it is absorption energy or emission energy. In the sense of this:

$$\Delta E = hv$$

First Stage

The scientist Bohr calculated the π (path radius) and the energy of the electron within the electron path of the hydrogen atom and similar atoms, as well as calculating the Rydberg constant.

If you want to calculate q, it can be known from the following law:

$$r = \frac{n^2 h^2}{4\pi^2 m z e^2} \Rightarrow r = \frac{n^2 h^2}{4\pi^2 m e^2} \quad \text{for H atom } Z=1$$

$$r = \frac{h^2}{4m\pi^2 e^2} \approx a^\circ \approx 0.529 \times 10^{-8} \text{ cm} = 0.529 \text{ \AA}$$

When $n=1$ for H_2

$$(H_2) \quad r = n^2 a^\circ$$

$$r = n^2 a^\circ / Z$$

(For similar atoms)

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

$$E_k = \frac{1}{2} mv^2 \quad E_p = \frac{-Ze^2}{r}$$

$$E_T = \frac{-Ze^2}{r} + \frac{1}{2} mv^2$$

$$E_n = \frac{-2 \pi^2 m e^4 z^2}{n^2 h^2} \quad (\text{for Hydrogen atom and similar atom})$$

For Hydrogen atom \Rightarrow

$$E_n = \frac{-2 \pi^2 m e^4}{n^2 h^2}$$

$$J = \frac{2 \pi^2 m e^4}{h^2}$$

$$E_n = \frac{-J}{n^2}$$

$$E_n = \frac{-2 \pi^2 m e^4 Z^2}{n_1^2 h^2}$$

$$E_n = \frac{-2 \pi^2 m e^4 Z^2}{n_2^2 h^2}$$

$$\Delta E = \frac{2 \pi^2 m e^4 Z^2}{n_1^2 h^2} - \frac{2 \pi^2 m e^4 Z^2}{n_2^2 h^2}$$

$$\Delta E = \frac{2 \pi^2 m e^4 Z^2}{h^2} (1/n_1^2 - 1/n_2^2)$$

First Stage

$$E = h\nu = hc\nu'$$

$$hc\nu' = \frac{2\pi^2 me^4 Z^2}{h^2} (1/n_1^2 - 1/n_2^2)$$

$$\nu' = \frac{2\pi^2 me^4 Z^2}{h^3 c} (1/n_1^2 - 1/n_2^2)$$

$$\nu' = R_H (1/n_1^2 - 1/n_2^2)$$

which $R = \frac{2\pi^2 me^2}{h^3 c} (Z^2=1)$

$$\nu' = R_H(Z)^2 (1/n_1^2 - 1/n_2^2)$$

(For similar atoms)

So, the processes of emission of spectral lines in the hydrogen atom in series are energy differences in the ground state of the hydrogen atom. The location of the electron is at $n=1$, and if a white light is shone on it, for example, this electron will move to a higher energy level as a result of the absorption of energy.

Example: Calculate the first five Bohr radii for hydrogen atom?

Solution:-

- 1- $r = 0.529 \text{ \AA}$ $n=2,3,4,5$.
- 2- $r = n^2 a_0 = 4 \times 0.529 = 2.116 \text{ \AA}$
- 3- $r = n^2 a_0 = 9 \times 0.529 = 4.761 \text{ \AA}$
- 4- $r = n^2 a_0 = 16 \times 0.529 = 8.464 \text{ \AA}$
- 5- $r = n^2 a_0 = 25 \times 0.529 = 13.225 \text{ \AA}$

Example:- Calculate the five lowest energy levels of the hydrogen atom (in ergs units)?

Solution:

$$1- E_n = \frac{-2\pi^2 me^4}{n^2 h^2} = \frac{-2(3.14)^2 \times 9.1 \times 10^{-31} \times (1.6 \times 10^{-19})^4}{1 \times (6.626 \times 10^{-27})^2}$$

$$2- E_2 = \frac{-2\pi^2 me^4}{(2^2)h^2} =$$

$$3- E_3 = \frac{-2\pi^2 me^4}{(3^2)h^2} =$$

First Stage

$$1- E_4 = \frac{-2 \pi^2 m e^4}{(4^2) h^2} =$$

$$2- E_5 = \frac{-2 \pi^2 m e^4}{(5^2) h^2} =$$

Example: Calculate the wave no. (ν) of photon of light will excited an electron from $n=1$ to $n=4$ energy level of H. atom?

Solution:

$$\begin{aligned} \nu &= R_H \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \\ &= 109678 \text{ cm}^{-1} \left(\frac{1}{1} - \frac{1}{16} \right) \\ &= 109678 \text{ cm}^{-1} (0.9375) \\ &= 102823.725 \text{ cm}^{-1} \end{aligned}$$

Example: Calculate the wave no. and the frequency of the first Lyman transition?

Solution:

$$\begin{aligned} \nu &= R_H \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \\ &= 109678 \text{ cm}^{-1} \left(\frac{1}{1} - \frac{1}{4} \right) \\ &= 109678 \times 0.75 = 822585 \text{ cm}^{-1} \\ \lambda &= \frac{1}{\nu} = \frac{1}{822585} = 1 \times 10^{-6} \text{ cm} \\ \nu &= \frac{c}{\lambda} = \frac{3 \times 10^{10}}{1 \times 10^{-6}} = 3 \times 10^4 \text{ (Hz)} \end{aligned}$$

Example: Calculate the ionization energy of the He^+ when $n_1=1$, $n_2=\infty$?

Solution:

$$\begin{aligned} \nu &= R_H(Z)^2 \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \\ &= 109678 \times 4 \left(\frac{1}{1} - \frac{1}{\infty^2} \right) \\ &= 4067053 \times (1-0) \\ &= 4067053 \text{ cm}^{-1} \\ \lambda &= \frac{1}{4067053} \text{ cm} \end{aligned}$$

First Stage

$$\nu = \frac{c}{\lambda} = \frac{3 \times 10^{10}}{4067053} = 3 \times 4067053 \times 10^{10} \text{ (Hz)}$$

$$= 21432510 \times 10^{10} \text{ (Hz)}$$

$$E = h\nu = 6.626 \times 10^{-27} \times 2143251 \times 10^{11}$$

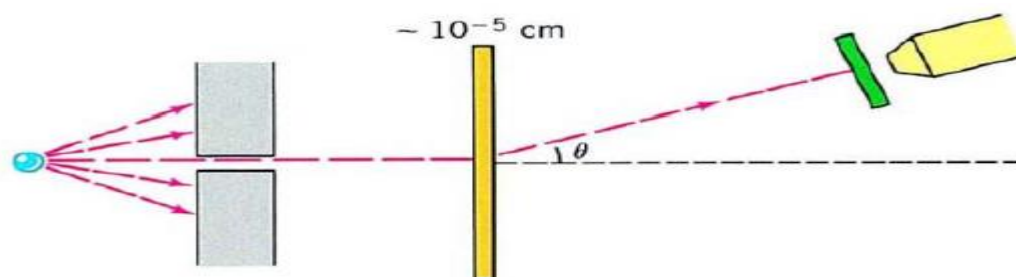
$$= 14201181.1 \times 10^{-16} \text{ erg.}$$

Example:- What is the radius of the first Bohr orbit for He⁺? (Z=2)

Solution: $n^2 a_0 / Z = \frac{1 \times 0.529}{2}$
 $= 0.2645 \text{ cm.}$

Atomic Models

In the 19th century, there was considerable chemical and physical evidence for the existence of atoms, but nothing was known about their structure. Thomson suggested that an atom consists of a positively charged sphere in which electrons were embedded. (The model was not satisfactory). In 1909, Rutherford studied the scattering of alpha particles by a very thin gold foil as shown below.



The Bohr Model

What is the stationary state? We need a quantum condition that restricts the allowed values of the orbital radius. It was realized only later that this is a fundamental aspect of quantum theory, and so it serves as our “third” postulate: *The angular momentum of the electron is restricted to integer multiples of $h/2\pi$.*

First Stage

$$\text{Angular momentum } mvr = n\hbar \Rightarrow v = \frac{n\hbar}{mr}$$

$$\text{Energy } \frac{1}{2}mv^2 = \frac{ke^2}{2r} \Rightarrow r_n = \frac{n^2\hbar^2}{mke}$$

The total energy of the n th orbit is

$$E_n = -\frac{mk^2e^4}{2\hbar^2} \left(\frac{1}{n^2}\right) = -\frac{13.6}{n^2} \text{ eV}$$

Bohr's Atomic Model

Following Rutherford's experiment in 1911, Niels Bohr studied the emitted light of the hot hydrogen gas (or hydrogen excited atom) using spectrograph, which separates different wavelengths of light (just like a simple prism). After a series of experiments, Bohr made the following assumptions, which led to the convincing explanation of atomic emission spectrum of hydrogen atom and to new atomic model, which is called Bohr's atomic model or shells model.

The assumptions are:

1. In an atom, electrons move around the nucleus in circular energy defined discrete orbits (or shell) under the influence of the electrostatic columbic attraction of the nucleus. In other words, electron could any present in certain allowed, energy defined, circular, and discrete orbit (or shells). These orbits (or shell) are found at various distances from the nucleus. They are called energy sheels or energy level s and are labelled with positive integer number $n=1,2,3,4,---$ and so forth. The orbit with the lowest integer number is the nearest to the nucleus and given the number 1 (or $n=1$). The 2nd lowest shell is given the number 2 ($n=2$) and so on .the highest orbit or shell (the farthest the nucleus) is given the value of ∞ or infinity ($n=\infty$).
2. In the absence of an electromagnetic radiation with the correct amount of energy, the energy state of an atom or electrons are describe as Ground State, which can be defined as the lowest energy state of the atom and its electron (or electrons) occupied the lowest possible energy shells or orbits. If an atom absorbs electromagnetic radiation (or energy) , the energy states of the atom and its electron (s) as excited states, which can be defined as the energy states, which can be defined as the energy states of atom and electrons when their energy content are higher than the energy content of the ground state.

First Stage

3. Like the Einstein's theory and the photoelectric effect, the electron's jump between various orbits or shells requires a discrete and appropriate amount of energy (specific photon) to be lost or absorbed. This is due to the fact that the electron can only exist in quantized energy state or shell or orbit.
4. The electrons can only orbit stably, without radiating. This type of movement represents a special state of circular motion (orbiting) and is called stationary state; consequently, the orbit is called stationary orbit. In these stationary states, the electron's acceleration does not result in radiation or energy loss as required by classical electromagnetic theory. So no change in the energy of the orbiting electron.
5. Electron can only gain or lose energy by jumping from one allowed stationary orbit (or state or shell) to another allowed stationary orbit. This movement (or jumping) between two allowed stationary orbits requires absorbing or emitting electromagnetic radiation with a frequency, ν (or energy E) determined by the energy differences between stationary orbits.

$$E = h\nu \quad \text{Planck's Eqn.}$$

$$\Delta E = E_f - E_i$$

$$\Delta E = h\nu_f - h\nu_i = h(\nu_f - \nu_i).$$

Where:

E_f and ν_f are the energy and the frequency of the final orbit (the orbit where the electron moves to) while E_i and ν_i are the energy and the frequency of the initial orbit (the orbit occupied by the electron before the electron moves to a different orbit).

Electrons can only gain or lose (lose) energy by jumping or moving from one allowed static orbit to another allowed static orbit. These transitions or movement between two permitted orbits or shells require the absorption or loss of an electromagnetic beam (or energy) with a wavelength determined by the amount of difference in energy of the two static orbits or shells.

This is what Planck's equation shows:

$$E = h\nu$$

$$\Delta E = E_f - E_i = h\nu_f - h\nu_i = h(\nu_f - \nu_i).$$

First Stage

ν_f, E_f indicate the energy and frequency of the shell or orbital to which the electron has moved. ν_i, E_i represent the energy and frequency of the orbital or shell from which the electron moved.

In addition, Emission of electromagnetic radiation can only occur when an electron moves from a higher energy stationary orbit to a lower energy stationary orbit. In reverse process, absorption of electromagnetic radiation by the moving electron is required. As a result, the numerical value of ΔE is positive for energy absorbing process [$\Delta E = E_f - E_i = +\text{Value}$].

In view of the above mentioned Bohr's Assumptions, the linear spectrum can be interpreted as follows:

- Spectral lines are the result of the emission (loss) or absorption (gain) of an electromagnetic beam (or energy) accompanied by electronic transfer between shells or orbits of varying energy separated from each other. Electrons cannot exist, move, or move outside these shells or orbits of specific energy. Therefore, these shells or orbits can be described as energy levels.

The location of the different spectral lines expresses the energy difference or frequency between the energy levels to which the electron is transferred. The separation or divergence of these spectral lines from each other supports the above conclusion regarding the separation or divergence of the energy levels from each other.

In the case of the atomic emission spectrum of the excited hydrogen atom, the following linear spectral groups were identified:

a- Lyman Spectral Lines Series

This group of spectral lines results from electronic transitions from different energy levels exclusively to the first energy level. Therefore, $n_i = 1$ always, while $n_f = 2, 3, 4, 5, \dots, \infty$, where n_f represents the level the final energy level or the electron is transferred to, while n_i represents the initial energy level or the electron is transferred from. The lines of this group lie in the ultraviolet region of the electromagnetic spectrum (EM spectrum).

First Stage**b- Balmer Spectral Lines Series**

This group of spectral lines is caused by the fall of electrons of various energies to the second energy level exclusively. That is, $n_i = 2$ always while $n_f = 3, 4, 5, 6, \dots, \dots, \infty$.

The Balmer spectral group consists of six lines. The four lines whose wavelengths range between 400 → 700 (nm) are located in the visible region of the electromagnetic spectrum, while the other two lines, whose wavelengths are 397 and 365 nanometers, are located in the ultraviolet region of the electromagnetic spectrum.

The transitions produced for the four colored lines from the Balmer spectral group are as follows:

| n_f | n_i | color | Wavelength (nm) |
|-------|-------|--------|-----------------|
| 3 | 2 | Red | 656 |
| 4 | 2 | Cyan | 486 |
| 5 | 2 | Blue | 434 |
| 6 | 2 | Violet | 410 |

c- Paschen Spectral lines Series

The Paschen spectral group results from electronic transitions from the energy levels $n_f = 4, 5, 6, \dots, \dots, \infty$ to the energy level $n_i = 3$ exclusively. All wavelengths of the lines of this group fall in the infrared region of the electromagnetic spectrum (EM Spectrum).

d- Brakett Spectral lines Series

This group of spectral lines results from electronic transitions from the energy levels $n_f = 5, 6, 7, \dots, \dots, \infty$ exclusively to the fourth energy level $n_i = 4$. The wavelengths of the lines of this group fall in the infrared region of the electromagnetic spectrum.

e- Pfund Spectral lines Series

The Pfund group lines result from electronic transitions from $n_f = 6, 7, \dots, \dots, \infty$ exclusively to the $n_i = 5$ energy level. Its wavelengths fall within the infrared region of the electromagnetic spectrum.

Due to the diversity of n_f values with the diversity of the above-mentioned spectral line groups, Rydberg's Equation can be written or rewritten to calculate the wavelength of each line of one spectral group.

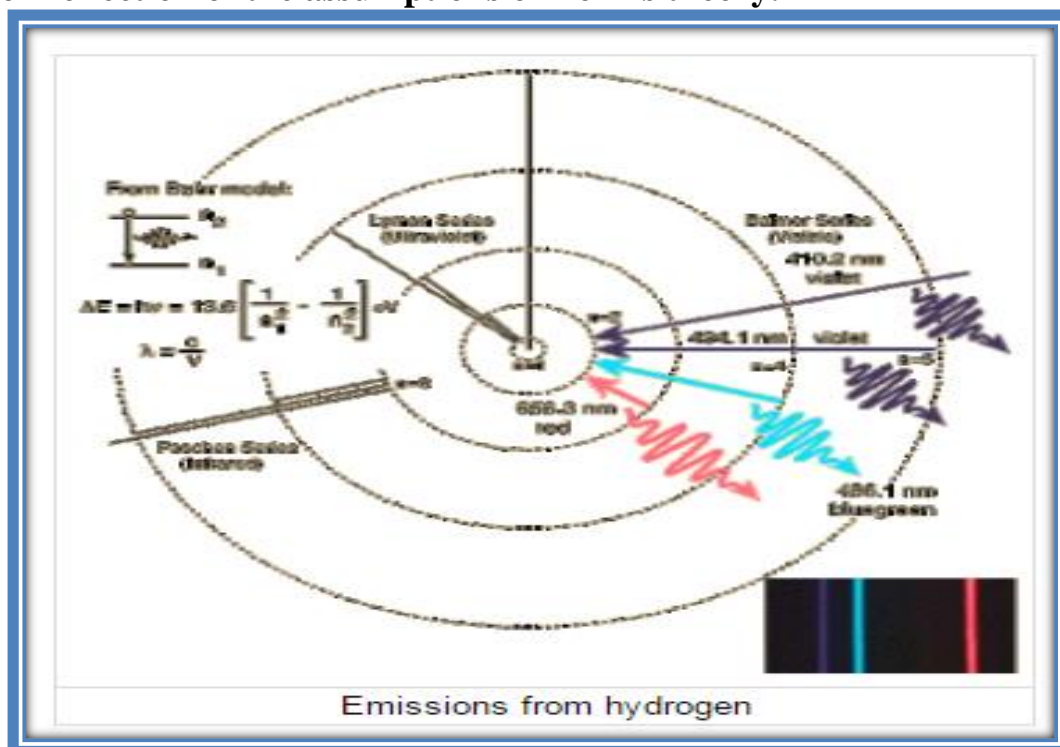
First Stage

- a- Lyman Series : $\frac{1}{\lambda} = R_H Z^2 \left(\frac{1}{1^2} - \frac{1}{n_i^2} \right)$
- b- Balmer Series : $\frac{1}{\lambda} = R_H Z^2 \left[\frac{1}{2^2} - \frac{1}{n_i^2} \right]$
- c- Paschen Series : $\frac{1}{\lambda} = R_H Z^2 \left[\frac{1}{3^2} - \frac{1}{n_i^2} \right]$
- d- Brackett Series : $\frac{1}{\lambda} = R_H Z^2 \left(\frac{1}{4^2} - \frac{1}{n_i^2} \right)$
- e- Pfund Series : $\frac{1}{\lambda} = R_H Z^2 \left(\frac{1}{5^2} - \frac{1}{n_i^2} \right)$

- One of the features of the emission spectrum of a hydrogen atom is the presence of black or dark areas separating the colored lines. In addition, these dark areas gradually diminish with the increase in line frequencies or the discrepancy in the wavelengths of the colored line.

According to Bohr's hypotheses, the dark spaces are due to the existing spaces that show the various energy levels that are not occupied by electrons. The diminishing of these dark spaces is attributed or refers to the diminishing of the areas of these spaces in the direction of colored lines with short wavelengths [or in other words, in the direction of the violet color].

The atom diagram or atom structure shown below is Translation or reflection of the assumptions of Bohr's theory.



First Stage**Bohr's Corresponding Principle**

Classical physics is very successful in dealing with a large number of phenomena. Bohr felt that when a newer, more general, theory is proposed, its predictions should **reduce** to the classical result when the appropriate limit is taken. This requirement that the results of a new theory correspond, in the limit, to classical physics is called the **correspondence principle**. For example, at large quantum number the physics becomes to classical.

Example: Calculate the wavelength of the radiation associated with electron's jump from n=4 to n=2 in an excited hydrogen atom. Is the radiation emitted by the atom? Explain your answer.

Answer:

$$\Delta E = E_2 - E_1$$

$$E_2 = -2.18 \times 10^{-18} \text{ J } \left(\frac{1}{2^2} \right)$$

$$E_4 = -2.18 \times 10^{-18} \text{ J } \left(\frac{1}{4^2} \right)$$

$$\Delta E = -2.18 \times 10^{-18} \text{ J } \left(\frac{1}{2^2} - \frac{1}{4^2} \right)$$

$$\Delta E = 4.09 \times 10^{-19} \text{ J}$$

Since the change in energy is (- = ΔE) or a negative quantity, the transition from $n_4 \leftarrow n_2$ is accompanied by the emission of a beam or the release of energy.

Question: Can the beam emitted above be seen or not? Give a reason for your answer.

$$E = \Delta E = h\nu$$

$$\nu = \frac{E}{h} = \frac{4.09 \times 10^{-19} \text{ J}}{6.63 \times 10^{-34} \text{ J}\cdot\text{s}} = 6.17 \times 10^{14} \text{ S}^{-1}$$

Look at the numerical value of frequency, as it does not contain a negative sign, while the value of E does.

$$c = \lambda\nu$$

$$\lambda = \frac{c}{\nu} = \frac{3.00 \times 10^8 \text{ ms}^{-1}}{6.17 \times 10^{14} \text{ s}^{-1}} = 4.87 \times 10^{-7} \text{ m}$$

Because 1m = 10 nm.

$$\lambda = 487 \text{ nm (or } 4.87 \times 10^2 \text{ nm)}$$

First Stage

Some aspects of Bohr's Model Failure (or Limitation)

Although Bohr's Model successfully accounted for the atomic emission line spectrum of Hydrogen atom, the model or the theory failed to:

- 1- Explain the line spectra of atoms containing more than one electron.
- 2- Explain the splitting of spectral lines in a magnetic field [Zeeman effect] and electric field [Stark effect].
- 3- The dual character of electron as explained on the basis of DeBroglie concept, which indicates that the electron has particle and wave characteristics, Bohr treated the electron only as a particles.
- 4- Bohr's theory violates the Heisenberg uncertainty principle.

Quantum Theory

Energy is not constantly emitted, radiated, or absorbed, but objects radiate or absorb energy in specific quantities that depend on the wavelength absorbed or emitted. If the assumption of scientists Jane and Reilly is correct, this means that space will be full of ultraviolet rays, X-rays, and other radiation. However, upon practical application, it was found that the long, low-frequency wavelengths emitted follow these laws, but after that we reach a certain peak, and upon reaching higher frequencies (shorter wavelengths), the intensity of the incident radiation will decrease. This contradicts the law, which does not expect a peak, but rather a continuous increasing relationship. The scientist Max Planck solved this contradiction and assumed that energy is not continuous energy, or in other words, that energy does not radiate or be absorbed continuously, but rather objects absorb energy and emit it in the form of units called quanta or photons, and that the energy of each photon is directly proportional to the frequency of the photon.

$$E \propto \nu$$

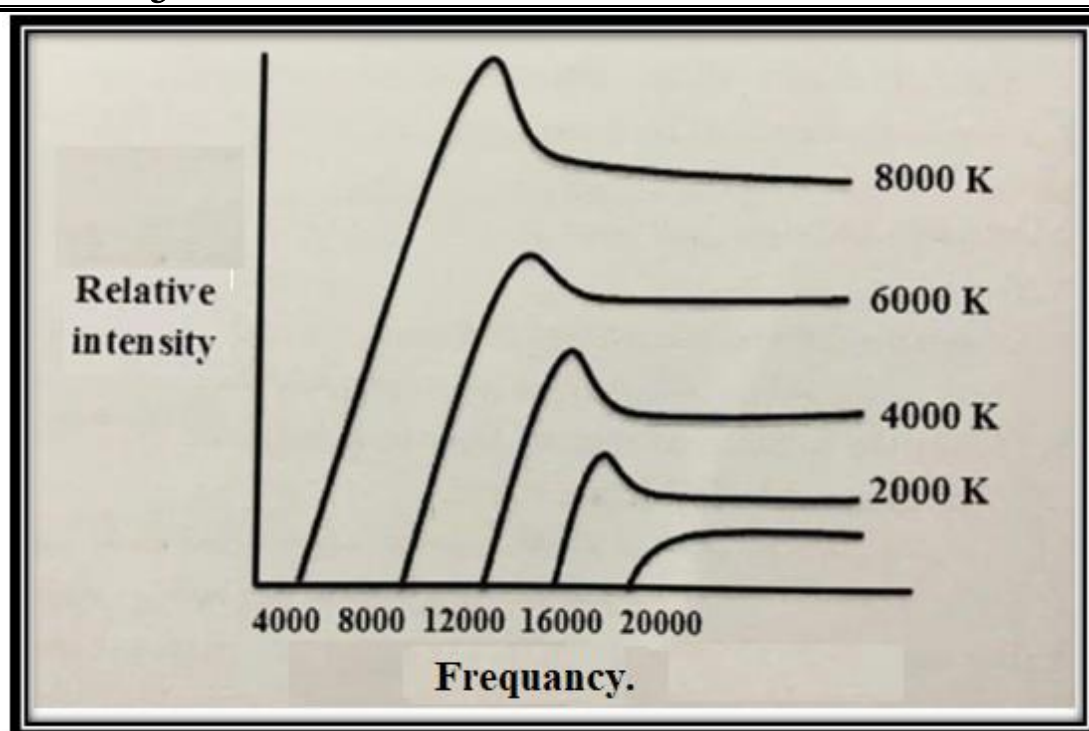
$$E = h \nu \text{ ---- (1)}$$

E= energy J.erg.er.

ν = frequency

h= plank's constant = 6.626×10^{-27} erg.sec or 6.626×10^{-34} J.sec.

First Stage



This phenomenon is explained based on the quantum theory of the scientist Max Planck, where the atoms of the body are at a certain temperature at different levels of energy, and these atoms are distributed over the levels so that most of the atoms occupy energy levels, which are medium-peak, but when moving to high frequencies the number of these atoms diminishes, so the The increase in radiation results from an increase in the number of excited atoms, meaning that the reason for the slope of the curve from the top is the decrease in the number of atoms that have high energy that can lead to the emission of high-energy or high-frequency radiation. When temperatures increase, the high-energy atoms increase, so the radiation intensity shifts to higher frequency.

This shows that:-

As the energy of the radiation increases, as explained by quantum theory, the frequency increases. In other words, we conclude from this theory: Energy increases with frequency, not with intensity of incident radiation.

$$C = \lambda \nu \quad \text{-----(2)}$$

$$\nu = C/\lambda \quad \text{-----(3)}$$

$$E = h C/\lambda \quad \text{-----(4)}$$

$$E = hc'\nu, \quad \nu = 1/\lambda$$

First Stage

Example: Determine the frequencies in Hz and wave number of electromagnetic radiation of the following wave length:

- 1- 1.0 Å.
- 2- 500 μm.
- 3- 4.4 nm.
- 4- 4.89 m.

Solution:

- | | |
|---|--|
| 1- $\nu = 1/\lambda = 1/1 \times 10^{-10}$ | $\nu = c/\lambda = 3 \times 10^8 / 1 \times 10^{-10} = 3 \times 10^{18}$. |
| 2- $\nu = 1/\lambda = 1/5 \times 10^{-4}$ | $\nu = c/\lambda = 3 \times 10^8 / 1 \times 10^{-6}$. |
| 3- $\nu = 1/\lambda = 1/4.4 \times 10^{-9}$ | $\nu = c/\lambda = 3 \times 10^8 / 1 \times 10^{-9}$ |
| 4- $\nu = 1/\lambda = 1/4.89$ | $\nu = c/\lambda = 3 \times 10^8 / 4.89$. |

Some Principle of Quantum Mechanics Theory

By the mid-1920s, it had become apparent that by Bohr model could not be made to work. The model is, however, important because it showed that the observed quantization of energy in atoms could be explained by making rather simple assumptions. Bohr's model paved the way to the current theory of atomic. However, a totally new approach was needed. Three physicist were at the forefront of this effort: the German physicist and Nobel Prize laureate in physics Werner Heisenberg(1901-1976), Louis Vector de Broglie (1892-1987), French physicist and Noble Prize Louis laureate in physics in 1929, and the Austrian physicist and Nobel Prize in Physics in 1933 Erwin Schrodinger (1887-1961). The approach they developed became known as wave mechanics, or more commonly, Quantum Mechanics.

Matter and Waves

De Broglie showed that every particle's movement is linked to wave motion, or in other words, that there are waves accompanying the movement of particles or objects. These waves are not electromagnetic waves, so they are called minute waves or physical waves, and it shows that the wavelength of moving particles is inversely proportional to momentum.

$$\lambda \propto \frac{1}{\rho} \propto \frac{1}{mv} \quad \rho = \text{momentum} \quad \rho = mc$$

$$\lambda = \frac{h}{mv} \Rightarrow \lambda = \frac{h}{\rho} \quad \rho = mv$$

First StageThe Proof:

$$E=h\nu\text{-----}(1), E=mc^2\text{-----}(2)$$

$$h\nu = mc^2 \Rightarrow h \frac{c}{\lambda} = mc^2$$

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

$$\frac{h}{\lambda} = mc, \quad \rho = \frac{h}{\lambda}$$

Because $\rho = mc$

$$\lambda = \frac{h}{\rho}$$

So, every body with a mass m and a speed C has accompanying waves and a connection to it that can be measured from momentum. The less the mass of the body, the longer the accompanying waves increase.

Example: Calculate the wavelengths associated with an electron travelling at one tenth the speed of light?

$$\lambda = \frac{h}{mc}$$

$$\begin{aligned} &= \frac{6.626 \times 10^{-27}}{9.1 \times 10^{-31} \times 0.3 \times 10^{10}} \\ &= \frac{6.626 \times 10^{-5}}{2.73} = 2.42 \times 10^{-5} \text{ cm} \end{aligned}$$

David Sind noticed that a beam of electrons falling on a nickel plate is reflected and deflected, and this is a wave characteristic, and this indicates that particles have wave characteristics.

Q: Calculate the energy in erg, frequency, momentum, wavelength of an electron that has been accelerator to yield energy of 50000 eV.?

Q: Calculate the momentum of photon whose frequency is $6 \times 10^{14} \text{ sec}^{-1}$?

It is clear from the de Broglie equation that as the mass of a body increases, the wavelength accompanying its movement decreases, so that we reach a wave that is difficult to measure, but because the electron has a very small mass, the wave accompanying its movement can be measured, meaning: instead of the electron's path being circular, it rotates in the form A series of waves moving within a path or that: A circular path is a group of waves. In order for the circular path to be stable, the

First Stage

waves must reinforce each other so that they form standing waves within a circle with a radius, and the circumference of the circle for the path that Bohr assumed is the number of its constituent waves. If n is the location of the electron or the path, then the number of wave's represents the circumference of the circle, and Bohr's theory can be modified according to de Broglie:

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

$$n\lambda = 2\pi r$$

$$n\lambda = \frac{n h}{p} = \frac{n h}{mv} = 2\pi r$$

$$\frac{n h}{2\pi} = mvr$$

$$V = \frac{n h}{2\pi m r} \quad \text{Electron velocity within a de Broglie orbital.}$$

In this case, the de Broglie equation determined the electron's speed, angular momentum, and position in the Bohr orbit at the same time. The DeBroglie Equation can be explained as follows:

It was put forward by a young French doctoral student Louis DeBroglie in 1924, that any particle travelling with a linear momentum (mv) should have a wavelength λ given by the relation (or Equation):

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

Whereas:-

λ = wavelength of particle

“Note that wavelength is a characteristic of waves”.

h = plank constant.

v = velocity of practical.

m = mass of particle.

“Note that mass is a characteristic of particulate matter”.

Since the mass of the practical is inversely related to the wavelengths, then it is expected that for a given value of the velocity (v), smaller particles will have a large wavelengths. The display of wave property by a practical occurs when the practical is bounded in a region, which has dimensions that are comparable to the natural wavelength of the practical.

First Stage

The diameter of a ground state Hydrogen atom is about 1 \AA ($=10^{-10} \text{ m} = 100 \text{ pm}$). An electron travelling with a speed of one – third the speed of light has a natural wavelength of about 7 pm . This, therefore, suggests that an electron bounded within the hydrogen atom (or other atoms) will display wavelike properties. In the light of the above discussion, it becomes very clear that an electron could exhibit properties of both particle and wave. This phenomenon is referred to as wave-particle Duality.

Wave-Particle Duality of Light

Wave nature: Young's double-slit interference and single slit diffraction.

Particle nature: Photoelectric effect and Compton scattering.

What is the true nature of light?

Light exhibits a **wave-particle** duality. Depending on the experiment performed, it will behave either as a particle, or as a wave. Generally speaking, at lower frequency it behaves like a wave, while at higher frequency it acts like a particles. This observation is crucial in that it suggests that wave properties should become very important for smaller particles. This therefore means that classical mechanics is not able to explain the motion of very small particles. To account for the wave-like nature exhibited by these small particles a new theory is required, wave mechanics is the tool of choice.

This observation is very important because it indicates that wave characteristics become very important for very small and moving particles. This means that the laws and theories of traditional mechanics are unable to explain the movement of a very small particle body. To explain the wave nature exhibited by very small particles, wave mechanics is the tool of choice to explain the wave characteristics of very small bodies.

The Heisenberg Uncertainty Principle (HUP)

Heisenberg's inaccuracy principle: (It is not possible to determine the location and momentum of a body at the same time) the path of the electron (e) cannot be determined because the path of (e) depends on the energy levels that have major and secondary levels. To know the path of the electron in the atom, we must focus on two concepts.

First Stage

1. The electron is a particle that has mass despite its small weight.
2. The movement of the electron is a wave movement in its paths, and when a beam of electrons is projected and passes through a prismatic grating or a crystal (a crystal of nickel or gold), diffraction occurs from the path of this beam, and in this case it resembles light in its wave nature, as light is waves, as The speed of light $C = 3 \times 10^{10}$ cm/sec.

Photon energy = frequency x Planck's constant

$$E = h\nu \quad \leftarrow \quad E \propto \nu$$

Whereas:

h = (Planck's constant).

E = (Photon energy).

ν = (frequency).

The wave motion of light depends on:

1-Frequency ν : It is the number of oscillations per second and depends on the wavelength λ wavelength unit's cm, Å or nm.

$$\nu = c/\lambda \quad \text{the speed of wave propagation.}$$

2- Wavelength: It is the distance between two identical ends of two successive waves. The energy of a photon is directly proportional to the frequency.

$$E \propto \nu$$

$$E = h \nu$$

Whereas :

$$h = 6.6 \times 10^{-34} \text{ J. Sec.}$$

This rule appeared, which states the following:

The position and momentum of any particle cannot be determined exactly at the same time.

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

Δx = uncertainty in position

Δp = uncertainty in momentum

First Stage

If we could measure the position accurately, then accurate information about momentum would not be available, and vice versa.

Because an electron has wave-like properties, it becomes impossible to know exactly, at the same time, either the momentum (or energy) and the position of an electron in an atom. This statement is called the Heisenberg Uncertainty Principle (or HUP).

If \mathbf{x} and (\mathbf{mv}) are the position and momentum of an electron respectively and $\Delta\mathbf{x}$ and $\Delta(\mathbf{mv})$ are their respective uncertainties then, by the **HUP**, we get the above inequality relationship. Where \mathbf{h} is Planck's constant (as shown above for the numerical value and its units), \mathbf{m} and \mathbf{v} are the mass and displacement of the electron, respectively.

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

Where:-

\mathbf{h} , Planck's constant = 6.626×10^{-34} JS (or $\text{Kg m}^2 \text{S}^{-1}$) and,

\mathbf{m} , mass of the electron = 9.11×10^{-31} Kg.

\mathbf{v} , velocity of the electron.

If you look closely at the above inequality, it can be seen that the right side is a constant, which is to say that, the product of the uncertainties cannot be less than the value of $\mathbf{h}/4\pi$.

In addition, the more accurately we know an electron's energy or momentum [$\Delta(\mathbf{mv})$ is very small], the less accurately we know its position ($\Delta\mathbf{x}$ is very large) and vice versa.

This uncertainty exists for all systems. For the earth-moon system where the mass of the moon is 7.4×10^{22} kg, the uncertainty is so small, but is significant in the case of microscope particle such as proton-electron system where the mass of the electron 9.11×10^{-31} Kg. This implies that the path of the electron cannot be calculated with a reasonable degree of accuracy.

This includes the following:- The location, path, or orbit of the electron cannot be determined with a reasonable degree of accuracy.

The energy of spectral lines can be measured with great precision, in turn allowing precise determination of the energy of electrons in atoms. This precision in energy also implies precision in momentum [$\Delta(\mathbf{mv})$ is small], therefore according to Heisenberg uncertainty principle or HUP,

First Stage

there is a large uncertainty in the location (or position) of the electron in atom (Δx is large). These concepts mean that it is not appropriate to treat electron (or a moving microscopic particles) as simple particle with their motion describe precisely, but we must instead consider the wave properties of electron, characterized by a degree of uncertainty in their positions. In other word, instead of being able to describe precise orbit or shall of electron, as in Bohr Model, we can only describe orbital, an actual region that describe the probable location of electron. The probability of finding the electron at a particular point in space of the atom is called the electron density.

Example: An electron is travelling at a speed of 10^8 cm/sec if the Bohr radius is equal to 0.529×10^{-8} cm and if the error in this measurement is 0.001×10^{-8} cm. calculate the uncertainty (error) in the momentum of the electron?

Solution:-

$$\begin{aligned} p &= mv = 9.1 \times 10^{-28} \text{ g} \times 10^8 \text{ cm/sec.} \\ &= 9.1 \times 10^{-20} \text{ g cm sec}^{-1}. \end{aligned}$$

$$\Delta x. \Delta p \geq \frac{h}{4\pi}$$

$$\Delta x. \Delta p \geq \frac{h}{4\pi} = \Delta p \geq \frac{6.626 \times 10^{-27} \text{ erg}}{4\pi \times 10^{-11}}$$

$$\Delta p = 6.7 \times 10^{-16} \text{ g. cm. sec}^{-1}.$$

So the amount of error in momentum is approximately a thousand times as large as the momentum itself, which means that it is not possible to measure momentum or speed. That is, the speed values are default values.

An Introduction to the Schrodinger Wave Equation

We have seen from the above that the Frenchman de Broglie established the idea that the electron has wave properties after the electron was described as being a body or a minute. Following the same way of thinking as de Broglie, in 1926 and 1927, both Schrodenger and Heisenberg separately issued or announced the results of their studies, which took into account the wave properties of the electron. Despite the apparent difference between the mathematical techniques and methods used by Schrodenger and Heisenberg, it soon became clear that their treatment or mathematical equations were equivalent in any case. We will

First Stage

touch upon some concepts of the Schrodinger differential wave equation, which is widely used in presenting and explaining the modern theory of atomic structure. Note that it may be called wave mechanics, quantum mechanics theory, quantum equation, or wave equation.

Schrodinger Equation

Schrödinger relied on the world's de Broglie equation, which describes the movement of electrons in the form of waves to form the circular path. And for the scientist Bohr as well, at the same time, he relied on the principle of inaccuracy of the scientist Heisenberg, which cannot determine both the position of the electron and its momentum at the same time. To solve this problem, and in order to know the position of the electron and its momentum at the same time, which in turn is related to knowing the energy of the electron, the scientist Schrodinger used the wave function ψ to determine The energy of the electron in the atom and the different energy levels in one atom, and this means that there are different values of the wave function, and according to the endurance of the lowest energy, it represents the energy of stability, the Ground state, and the electron can be excited to rise to a higher energy excited state. The wave function does not exist in nature and its practical measurement is based on measuring ψ^2 , which gives an absolute value that can be used practically and is referred to as the potential relative density or probability distribution, which is the probability that the electron will be located in relation to the nucleus according to its distance from the nucleus relative to the three axes **x, y, z**.

So, for the hydrogen atom, a choice was made within the axes of the poles inside a sphere or inside a circle, and this location can also be determined by the angles at which the location is and the distance of the electron from the nucleus according to the angle function and the diagonal function, so we obtain a three-dimensional image, which in this case appears in the form of a cloud because it represents a possibility. The spread of the presence of the electron in space, and this is completely different from finding the location of the electron in sharp lines, such as the Bohr orbit, for example, because the electron has become more likely to be found anywhere from ϕ , Θ , R . Therefore, in this case, the name of the circular path, “orbit,” is replaced with the word “non-circular path” or

First Stage

“orbital,” which is also the case. It means an electron cloud, and it also represents the energy state, and it also represents the energy level. So the concept became clear between Schrodenger and Bohr’s idea of the location of the electron.

The scientist Bohr determined the location of the electron in the circular path, which has a radius. For example, the radius of the circular path of the electron of the hydrogen atom in the state of stability is **0.529 x 10⁸**, while Schrödinger, who relies on the principle of inaccuracy, imagined that there is no sharp circular path, but rather that the electron of the hydrogen atom is in the state of stability It is a spherical cloud, the center of this cloud is **0.529 x 10⁸** away from the nucleus, but the presence of electron density and its extension beyond this point is called electron density, so if this probability of presence is high, then the electron density is high and vice versa. Although the lowest energy level in the hydrogen atom is the spherical electron density, this does not mean that all spherical electron clouds may take different forms according to ϕ , Θ , r .

Quantum mechanics delivers better model

- Schrödinger equation time dependent:

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right) + U\Psi = i\hbar \frac{\partial \Psi}{\partial t}$$

- In atom stationary states, time independent Schrödinger equation:

$$\Psi(x, y, z, t)^2 \quad \text{Probability density}$$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{2m}{\hbar^2} (E - U)\psi = 0$$

- Solving this equation for Coulomb potential:

$$\psi(x, y, z)^2 \quad \text{Probability density}$$

$$U = -\frac{e^2}{4\pi\epsilon_0 r}$$

First Stage

The most important features of the Schrödinger equation are:

- 1- Use the mathematical expression known as the wave function, symbolized by ψ [a Greek letter pronounced psi and written in English as psi]. This mathematical function is used to determine the three-dimensional location and movement of the electron in the atom. Therefore, when using x-ray or Cartesian coordinates to describe the location and movement of the electron, the wave function is written as ψ_{xyz} . However, when using polar or spherical coordinates, the wave function is written as $\psi_{r\theta\phi}$.
- 2- It takes or treats the properties or binary nature of the electron or the wave properties known as microwave-wave. This described the electron or the wave properties of the electron as a standing wave.
- 3- Ombining the energy E and the position and movement of the electron ψ , this is considered a response to Heisenberg's imprecision principle.
- 4- Below are some expressions or forms of the Schrodenger equation.

The Schrodinger equation, of which the wave function is a solution, is:

a) using the Cartesian coordinates

$$E\psi_{xyz} = \frac{-h^2}{8\pi^2 me} \left(\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2} \right) \psi + V\psi$$

The above equation can be written as follows:

$$E\psi_{xyz} = \frac{-h^2}{8\pi^2 me} \nabla^2\psi + V\psi \quad \text{-----Eqn.1}$$

∇^2 Is called Laplacian operator of ψ .

$$\nabla^2 = \left(\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2} \right).$$

b) Schordinger Equation, applies to on electron moving in one direction, can be written shown below.

$$E_{(x)}\psi_{(x)} = \frac{-h^2}{8\pi^2 me} \frac{d^2\psi_{(x)}}{dx^2} + V_{(x)}\psi_{(x)} \quad \text{-----Eqn.2}$$

In light of what was written above, the electron or the equation that describes the electron or the equation that classifies the electron describes an electron moving along the **x** axis.

First Stage

The previous equation corresponds to the equation given in classical physics, which is:

Potential energy + kinetic energy = total energy

Or:

$$E = K + V$$

So $E_{\psi(x)}$ represents the total energy, $V_{(x)} \psi(x)$ the potential energy and the rest of equation 2 represents the kinetic energy.

c) Schrodinger Equation for free electron.

Schrodinger equation for a free electron [i.e., an electron that is not part of the atom].

$$E_{(x)}\psi(x) = \frac{-h^2 d^2 \psi(x)}{8 \pi^2 m e dx^2}$$

This means that the total energy of the free electron is equal to the kinetic energy, knowing that the potential energy of the free electron, which is not part of the atom, is zero.

d) Because the potential energy, v, of the electron in the field of nucleus is equal to $-ze^2/r$.

$$E\psi = \frac{-h^2}{8 \pi^2 m e} \nabla^2 \psi + \left(\frac{-ze^2}{r} \right) \psi$$

Where:

m= electron mass.

E= total electrical energy.

z= atomic number [for Hydrogen atom, Z=1]

e= electronic charge.

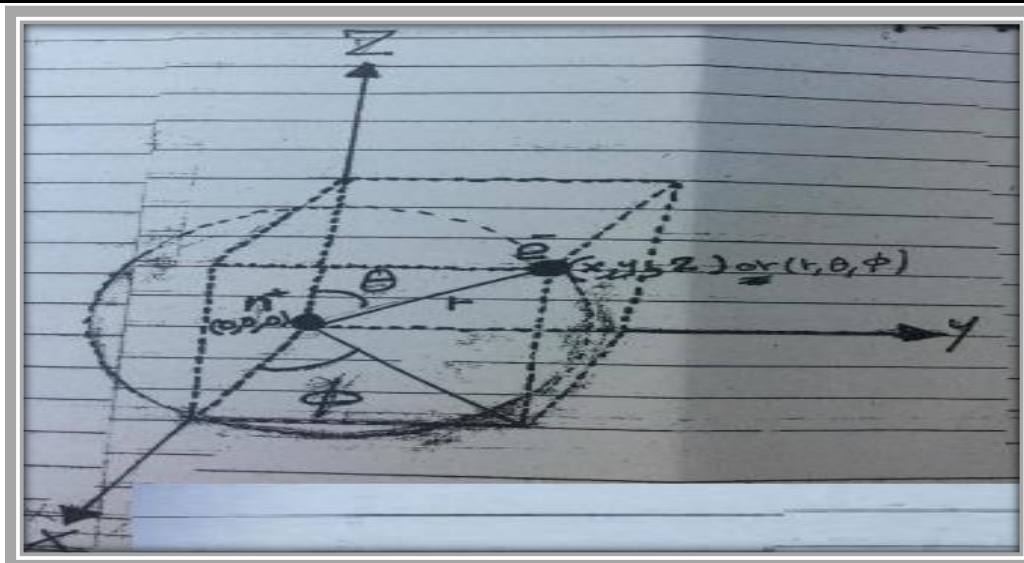
r= distance between the electron and the nucleus.

h= plank constant.

and using polar coordinates,

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d\psi}{dr} \right) + \frac{1}{r^2 \sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\psi}{d\theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{d^2 \psi}{d\phi^2} + \frac{8 \pi^2 m e}{h^2} \left(E + \frac{ze^2}{r} \right) \psi = 0$$

First Stage



A diagram showing the location of the electron relative to the location of the nucleus.

(0, 0, 0) Where the location can be determined using the Cartesian coordinates z , y , x or the polar or spherical coordinates ϕ , θ , r .

Note: Schrodinger used the above formula to find ψ for the electron of the hydrogen atom.

Solution of Schrodinger wave equation for hydrogen atom gives the allowed energy level and the corresponding wave function.

Wave function, ψ , and the probability density ψ^2

The wave function is defined as a mathematical expression that includes all information related to the movement of the electron as well as the location of the electron in the atom or space. Since the space occupied by the electron is called the orbital [or atomic orbital in the case of atoms]. It can be said that the wave function, or sometimes called the state function, gives a complete description of the atomic orbital. Note that the atomic orbital does not mean the Bohr orbit or the concept of the orbit, shell, or energy level that came in the Bohr Theory of atomic structure.

According to Heisenberg uncertainty principle, which involves using it to determine the location of the electron and its energy at the same time, the atomic orbital is redefined as the three-dimensional space or place in which the electron is possible.

First Stage

Schrodener and Max Born [a German-British physicist who won the Nobel Prize in Physics] proposed the following:

The probability of finding an electron at a particular location in space is proportional to the square of the wave function ψ^2 at that location in space. The numerical quantity of ψ^2 is called the electron potential density or electron probability density. To calculate the probability density throughout space, the following integral expression or equation is used, which indicates that the probability density of an electron or the spread of an electron in space cannot be more than one.

$$\int_{\text{All the space}} \psi^2 d\tau = 1 \quad \text{OR} \quad \int_{-\infty}^{\infty} \psi^2 d\tau = 1$$

τ is pronounced tau and $d\tau$ means very small.

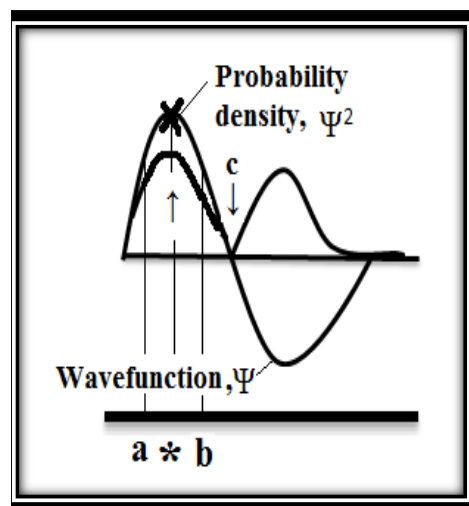
The following diagram shows the relationship between ψ and ψ^2 , as well as the field that represents the highest probability density and the point at which the probability of the existence of an electron is **zero**, or in other words the point at which the numerical quantity of the probability density, or ψ^2 , equals **zero**.

The b-a space represents the highest probability.

*The point that represents the highest intensity

Possibility = the probability point of finding an electron.

c: represents zero probability density and thus represents the point at which there is no possibility of an electron.



The Results of Solving Schrodinger Wave Equation

Fortunately, chemists do not need to understand how to solve the Schrodener wave equation in order to use its results for energy [the energy of the electron, the energy of the energy level or the energy of the orbital] and the wave function [the position and nature of the electron's

First Stage

motion]. This means that the chemist is interested in understanding the results of solving the equation, not the way in which the equation is solved.

For the hydrogen atom **H**. And ions similar to the hydrogen atom [such as the lithium ion ${}^3\text{Li}^{+2}$], which is characterized by the presence of only one electron, the solution of the Schrödinger equation in an accurate and precise manner is considered possible. The hydrogen atom and atoms similar to it may be described as simple atoms and ions. When solving the Schrodener equation, it was found that obtaining an acceptable solution for the wave function requires defining the energy in one of the quantities expressed by the following equation:

$$E_n = -2.178 \times 10^{-18} \text{ J } (Z^2/n^2).$$

Where **J** stands for joule (unit of measurement of energy), **Z** is the atomic number of an atom or simple ion [hydrogen atom or hydrogen-like ion], **n** takes positive integer values such as 1,2,3,4,5,-----, -----, ∞ . Since **z=1** for the hydrogen atom, the above mathematical relationship can be rewritten as shown below, which expresses the energy levels of the hydrogen atom exclusively. This equation is exactly the Bohr equation. So it remains called Bohr's equation:

$$E_n = -2.178 \times 10^{-18} \text{ J } (1^2/n^2).$$

What was mentioned above indicates and confirms:

- 1- What Einstein reached [the phenomenon of photoelectric emission] and Bohr's theory of atomic structure regarding the quantization of energy.
- 2- Like the quantization of wave functions, meaning that the electrons or atomic orbitals are located at certain specific dimensions or spaces that have a specific energy content. In other words, wave functions cannot exist anywhere in space or the atomic structure, but rather they exist in space that has an amount of energy that is consistent with the matmetical equation above

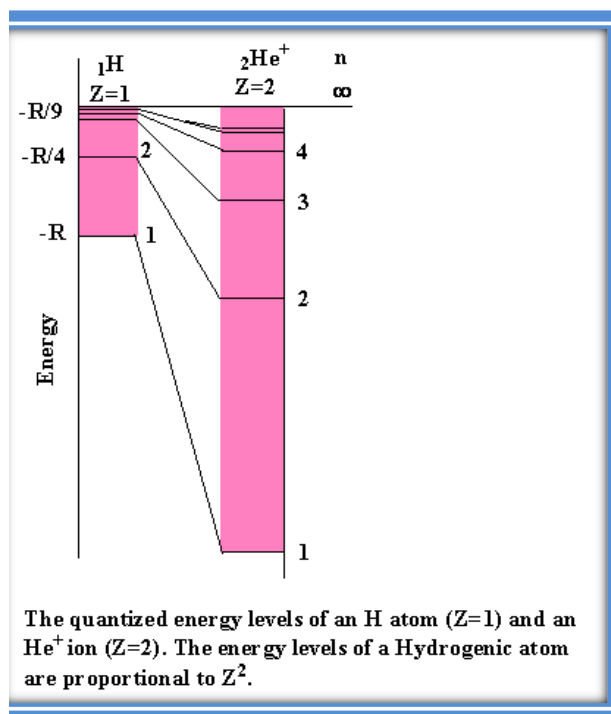
Looking at the above equation, it can be said that energy and the wave function depend on the numerical value of the positive integer **n**, which, according to what was stated in the texts of the Schrodener equation, is called the principal quantum number.

It expresses the lowest energy state [that is, the energy state in which the lone electron of the hydrogen atom or hydrogen-like ions occupies the

First Stage

first energy level [$n=1$] in the ground state. Based on the Bohr equation, the numerical value of the ground state energy of the hydrogen atom is equal to -2.178×10^{-18} Joules, while the numerical value of the ground state energy of the ions similar to the hydrogen atom varies with the atomic number of the ions similar to the hydrogen atom, but it can be said that the energy of the ground states of the ions similar to the hydrogen atom is lower or more negative than -2.178×10^{-18} joules.

For example, the ground state energy of the helium ion ${}^2\text{He}^+$, which is similar to the hydrogen atom, but with the atomic number of helium $Z = 2$, is equal to $-4(-2.178 \times 10^{-18})$ J, that is, four times lower than the energy of the ground state of the hydrogen atom. This explains to us the difference in levels Energy in each of ${}^2\text{He}^+$, ${}^1\text{H}$ shown in the following figure :



It is clear from the above and from the figure that the energy levels in the hydrogen atom and in hydrogen-like ions do not lie at the same distance from the center of the atom or ion. However, if the energy of the hydrogen atom and ions similar to it is less negative [i.e. less than -2.178×10^{-18} J for the hydrogen atom... [The atom or ion is described as being in the excited or excited state. In any case, there is one numerical value that expresses the ground state of the hydrogen atom and one numerical value that expresses the ground state. Conversely, there is more than one numerical value that expresses the excited state of an atom. Hydrogen (less negative than -2.178×10^{-18} joules) and more than one numerical value expressing the excited state of a given ion.

The reason for the multiple values of excited states for a hydrogen atom and for a specific ion similar to a hydrogen atom is due to the

First Stage

multiple energy levels [$n=2,3,4, \dots, \infty$] in which an excited or excited electron can exist. Note that the energy level occupied by the electron depends on the energy of the electron. Therefore, it can be said that each atom of a chemical element in the ground state or excited state has its own energy diagram that shows the arrangement of the various energy levels and their distance from each other, as well as their distance from the center of the atom or ion. The reason for this is due to the diversity of atomic numbers of various atoms and ions, knowing that there are no two atoms of two different chemical elements that have the same atomic number.

Modifying Bohr world theory and quantum numbers

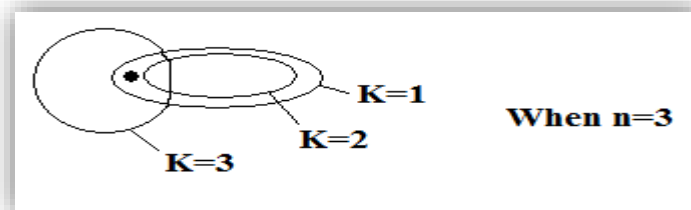
When the spectrometers advanced and became more accurate, the linear emission spectrum of the hydrogen atom was examined again, and it was found that the shape of the single line of the spectrum was found, which is a group of accurate and close lines, and this means that the main line is principle quantum no. (**n**) Or the main quantum number is a set of secondary lines, meaning that the main energy level n is secondary levels of energy, and this indicates that the electron moves between these lines that are close in energy, and if the resulting linear emission spectrum is placed under the influence of a magnetic field as The scientist Zeeman did, these lines separate from each other and form other groups, and this is called the Zeeman effect. These results contradict the theory of the world Bohr, which identified electronic transitions and made them permissible between $n_3, n_2, n_1 \dots$ or between the main shells or the main energy levels, and thus determined the momentum of the electron.

Sommer Field modification of Bohr's theory of the hydrogen atom

Sommer Field showed, based on quantum theory, the possibility of dividing the n principal energy levels into elliptical orbits in addition to the circular path. The scientist Field also explained the Zeeman effect by saying that the difference between the elliptical and circular paths is that in a circle the angle of rotation Θ changes and the radius remains constant while the elliptical path changes. It contains both the angle of rotation and the radius, which necessitated the introduction of a secondary quantum

First Stage

number in addition to the primary quantum number. This number is called **K** and is called the azimuthal quantum number no. The shape of this path, which is in the form of an elliptical orbit, and the scientist Sommer explained that each value of n has an equal number of integer values for the values of k . This means that if the value of $n = 3$, then **K** has three values, which are 1, 2, and 3. Therefore, the circular path has the form It is when $K=n$



This means that energy levels that differ in quantum number K and are similar in quantum number n have small differences in energy, so the transfer of an electron between these orbitals causes the appearance of additional spectral lines. This theory only succeeded in interpreting the spectral lines of the hydrogen atom and similar atoms, but it failed in analyzing the emission lines of atoms containing a large number of electrons, and it failed in studying their circular properties, so the secondary quantum number (K) was replaced by a secondary quantum number called (ℓ) ℓ =Secondary quantum no. So the value of $\ell=K-1$.

Zeeman Effect

When a magnetic field is applied in the spectrometer to the lines of the spectrum, the secondary levels separate into other, more precise lines, so this world introduced a third quantum number, which is the magnetic quantum number (m_ℓ) magnetic quantum no. It describes the direction of the secondary levels relative to the applied magnetic field, and its value depends on the value of the secondary quantum number ℓ .

$$m_\ell = +\ell \text{ --- } 0 \text{ --- } -\ell.$$

When: $n=1 \rightarrow \ell = n-1 = 1-1=0.$

$$m_\ell = +\ell \text{ --- } 0 \text{ --- } -\ell=0$$

When: $n=2 \rightarrow \ell = 0,1$

When $\ell=0 \rightarrow m_\ell = 0.$

$$\ell=1 \rightarrow +1, 0, -1.$$

First Stage

When: $n=3 \rightarrow \ell=0,1,2$

When $\ell=0 \rightarrow m_\ell = 0$.

$\ell=1 \rightarrow +1, 0, -1$.

$\ell=2 \rightarrow +2, +1, 0, -1, -2$.

The values of ℓ has identified with certain labels denoted by letters called spectral letters because they relate to the linear emission spectrum, and they represent energy levels:

| | | | |
|--------------|----------|---|-------------|
| When: | $\ell=0$ | S | Sharp |
| | $\ell=1$ | P | primary |
| | $\ell=2$ | d | diffuse |
| | $\ell=3$ | f | fundamental |

And since n is a number of ℓ values, then the angular momentum values that Bohr defined as $\frac{nh}{2\pi}$ became angular momentum determined by ℓ values as well, and the angular momentum became equal to $nh/2\pi$. The magnetic field and these values become $+\ell \frac{nh}{2\pi} \dots -0 \frac{nh}{2\pi} \dots +\ell \frac{nh}{2\pi}$. As for the number of m_ℓ values, they are equal to $2\ell + 1$ ear when $\ell=0$.

When: $\ell=0 \rightarrow m_\ell = 1 \text{ S}(0)$.
 $\ell=1 \rightarrow m_\ell = 3 \text{ P}(+1, 0, -1)$.
 $\ell=2 \rightarrow m_\ell = 5 \text{ d}(+2, +1, 0, -1, -2)$.
 $\ell=3 \rightarrow m_\ell = 7 \text{ f}(+3, +2, +1, 0, -1, -2, -3)$.

This means, for example, that the secondary level of type **d**, for example, is under the influence of the magnetic field. It separates into five orbitals, giving five vectors according to the direction of the magnetic field applied to these five orbitals, because these orbitals were equal in energy before the magnetic field was applied, but they differ in energy after the field was applied magnetic on it. These values and levels that have been reached show and support the scientist Heisenberg's interpretation of the principle of inaccuracy, as well as support the scientist Schrodenger.

So, in the hydrogen atom or multi-electron atoms, the electron movement is determined in terms of m , ℓ , n , and these three values include the diagonal and angular wave functions together. With the advancement of spectrometer devices, in addition to the (m_ℓ) lines that appear when a magnetic field is applied, these lines were separated into doubles, in which each pair has two different energies, one in the direction

First Stage

of the magnetic field and the other opposite the direction of the magnetic field. These very fine lines represent the movement of the electron around its axis under the influence of the magnetic field, and this movement has another quantum number. The fourth quantum number is called the Permin quantum number, spin quantum no. (m_s) and takes the values $m_s = -1/2, +1/2$. Since this movement also has momentum, the values of angular momentum are according to the number of twist quantum in terms of $\frac{h}{2\pi}$, so momentum is $\pm \frac{1}{2} \frac{h}{2\pi}$.

Electron Energy Levels by Four Quantum Numbers

1- Principle Quantum no. (n)

It is the orbit that determines the total energy of the main shell and also determines the distance of the electron from the nucleus. It takes the following integers:

$$n=1,2,3,4,-----, \infty.$$

These shells are called according to the following names:

When: $n= 1$, 2 , 3 , 4 , 5 , 6
 K_2 L_8 M_{18} N_{32} O P

Every prime quantum number contains a number of orbitals, which can be known from the following law:

no. of orbitals= n^2

That all the values of the minor quantum number ℓ for any principal quantum number n are equal in energy before the magnetic field is applied or when it is empty, but it differs in energy when the magnetic field is applied, and as the values of ℓ increase, its energy increases according to $\ell = 0, 1, 2, 3$:

S < P < d < F

Each principal quantum number carries a maximum number of electrons, which can be known from the following equation:

no. of electrons = $2n^2$.

2- Secondary Quantum no. (ℓ)

It is the number that determines the secondary energy level and also determines each path, and its value begins according to the following law: $\ell=0 ---, n-1$.

When: $n=1 \rightarrow \ell=0$
 $n=2 \rightarrow \ell=0,1$

First Stage**The values of ℓ are used to obtain the following:**

- 1- Calculating the orbital angular momentum, which is a vector and constant value within one secondary plane.

$$n\ell = \sqrt{\ell(\ell + 1)} \frac{h}{2\pi}$$

This does not mean that the electron is at rest when the momentum = 0, but the resultant angular momentum = 0 because the momentum is the value of its vector and represents the angular momentum $\mu\ell$ resulting from the movement of the electron around the nucleus in the secondary level ℓ .

$$\text{When: } \ell=1 \rightarrow \mu_\ell = \sqrt{\ell(\ell + 1)} \frac{h}{2\pi} = \sqrt{\frac{2h}{2\pi}}$$

$$\text{When: } \ell=2 \rightarrow \mu_\ell = \sqrt{2(2 + 1)} \frac{h}{2\pi} = \sqrt{\frac{6h}{2\pi}}$$

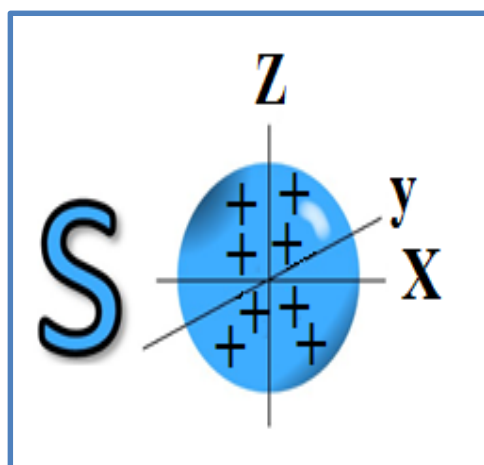
2- Determine the shape of the secondary orbitals.

The shape of the secondary orbital is determined by knowing the probability of the electron being present through the wave function determined by the angular function and the diagonal function, that is, depending on r , Θ , ϕ with x , y , z , which is represented by the number of electrons from the center of the atom and the angles it forms with the axes. This is done by determining for the knots formed by the electron movement and extracted from the following equation:

$$\text{no. of lobes} = \ell$$

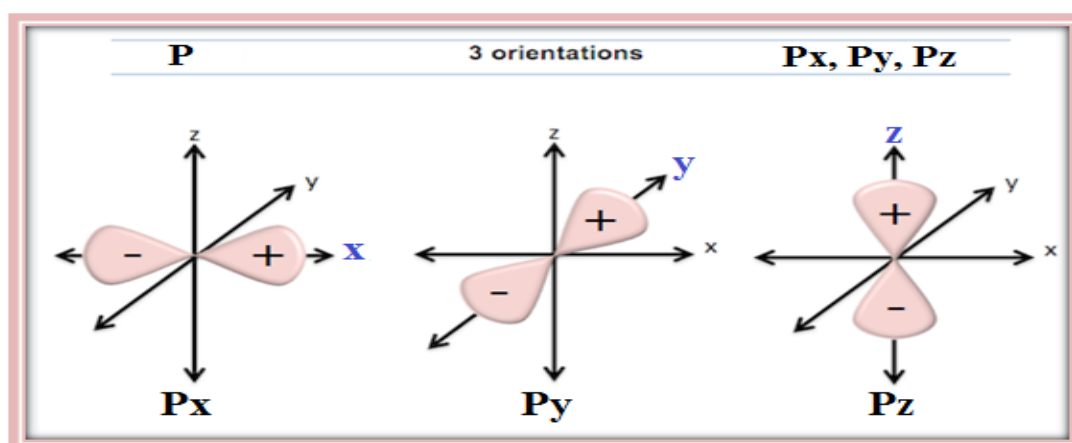
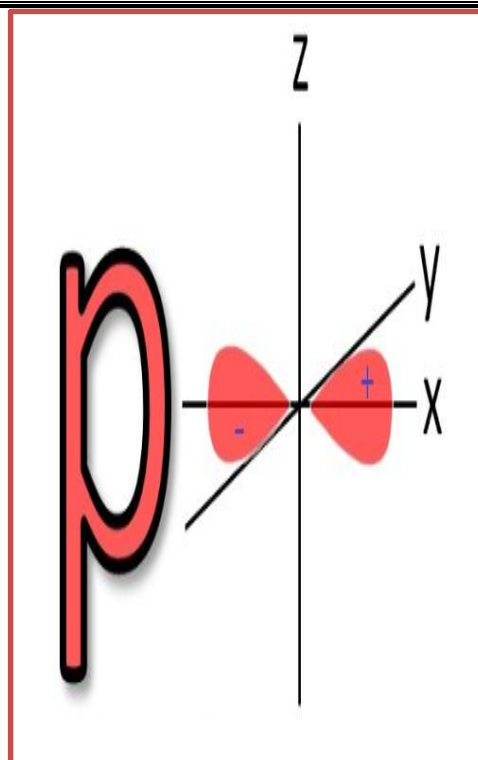
It exists within the three axes: x , y , z .

If $\ell = 0$, then the number of nodes = 0 and the orbital is of the S type and its shape is spherical or circular, meaning that it has a diagonal function only, and since the resultant of its angular momentum = zero, it is regular symmetric within the three dimensions or axes, and regular symmetry is given the symbol (g) (gerada) and when $\ell = 1$, then the number of nodes = 1.



First Stage

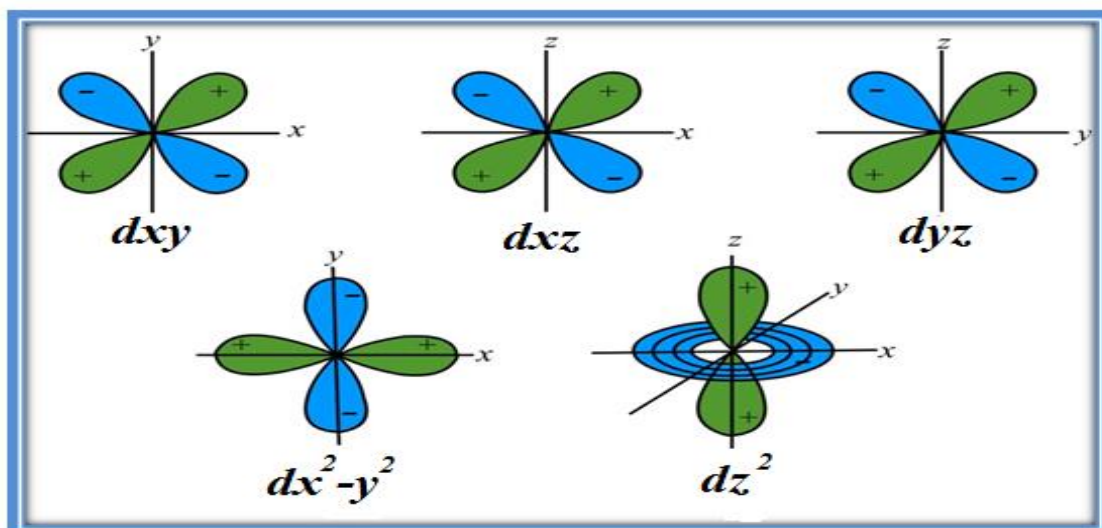
The orbitals of the secondary level are of the p type, and their number is three orbitals called Pz, Py, Px, each of which has a node, meaning that the probability of the presence of the electronic density is in the following form, that is, the sign of the wave function changes, and the symmetry is non-spherical, and the probability of the presence of the electronic density and its distribution changes with the change of the angular function and the function. The diagonal is within the Cartesian axes x, y, z for each orbit, and the three (p) orbitals are distributed perpendicular to the three axes:



Orbitals (p) do not have spherical symmetry, but consist of orthogonal lobes of asymmetric sign in the wave function and are symbolized by (u) (ungerada), i.e. the wave function sign changes for each orbital of the p orbitals.

When $\ell = 2$, then the number of orbitals of the secondary level (d), and it has five orbitals, each containing two nodes, that is, for each orbital of the d orbitals, it contains two orthogonal nodes. Opposite to each other, they are symmetrical, that is, the symmetry becomes of the type g, and it is as in the p orbitals, the wave function changes with $m\ell$, ℓ , r, and the shape of the four d orbitals is identical or similar.

First Stage



As for the fifth orbital, dz^2 , it is located on the z axis. The electronic density, or the presence of the wave function, is as large as possible on the z axis above and below the axis, and the electronic density is less on the $Wave dz^2-x^2, dz^2-y^2$. When $\ell = 3$, the number of nodes = 3, meaning that the wave function is unified by the values of ϕ , Θ , r , and the wave function has irregular symmetry (ungerada). Every principal quantum number (n) contains a number of orbitals, which can be known from the following equation:

$$\text{no. of orbital} = n^2, \text{ When } n=1$$

All values of the secondary quantum number ℓ for any primary quantum number n are equal in energy before the magnetic field is applied or if they are empty.

- 3- The secondary quantum number ℓ determines the energy of the electron in the secondary energy level.

$$\text{When } \ell = 0, 1, 2, 3, 4 \\ s < p < d < f$$

- 4- Each secondary energy level contains a maximum number of electrons depending on the principal quantum number. no. of electron = $2n^2$.

Since each secondary level contains a number of orbitals, which = $2L + 1$, these electrons for each secondary level are distributed among the orbitals so that each orbital does not take more than two electrons.

- 5- Since each principal quantum number n contains a number of secondary levels, the determination of the energy of any electron is based on the principal quantum number n formed by the secondary

First Stage

levels. In other words, the identity of the secondary energy level is defined by the principal quantum number.

- 6- The probability of the presence of an electron relative to the radius r or the presence of the electronic density follows the rule $n-l$.

Know the following rules:

- 1- Pauli's rule 2- Hund's rule

Pauli's Rule: It is not possible for two electrons in one atom to have the same four quantum numbers. Therefore, one orbital cannot occupy more than (2), where the spin quantum number is (-1/2, +1/2) i.e. it has one spindle motion.

Pauli's exclusion principle

If in the same system, no two electron can have the same set of quantum numbers; consequence in each of Schrödinger's orbitals, we have a maximum of two electrons, one "spin up" the other "spin down" in each orbital.

The Pattern used to assign electrons to energy levels

| | $l=0$ | $l=1$ | $l=2$ | $l=3$ | $l=4$ | $l=5$ |
|----------------|-------|-------|-------|-------|-------|-------|
| | (s) | (p) | (d) | (f) | (g) | (h) |
| n= 1(K) | 2 | | | | | |
| n= 2(L) | 2 | 6 | | | | |
| n= 1(M) | 2 | 6 | 10 | | | |
| n= 1(N) | 2 | 6 | 10 | 14 | | |
| n= 1(O) | 2 | 6 | 10 | 14 | 18 | |
| n= 1(P) | 2 | 6 | 10 | 14 | 18 | 22 |

Note: 2, 6, 10, 14---refer to the number of electron in the energy level.

First Stage

| | | |
|-----------------|-------------|---|
| 3s ¹ | electron 11 | $n = 3, l = 0, m_l = 0, m_s = +\frac{1}{2}$ or $-\frac{1}{2}$ |
| 2p ⁶ | electron 10 | $n = 2, l = 1, m_l = +1, m_s = -\frac{1}{2}$ |
| | electron 9 | $n = 2, l = 1, m_l = +1, m_s = +\frac{1}{2}$ |
| | electron 8 | $n = 2, l = 1, m_l = 0, m_s = -\frac{1}{2}$ |
| | electron 7 | $n = 2, l = 1, m_l = 0, m_s = +\frac{1}{2}$ |
| | electron 6 | $n = 2, l = 1, m_l = -1, m_s = -\frac{1}{2}$ |
| | electron 5 | $n = 2, l = 1, m_l = -1, m_s = +\frac{1}{2}$ |
| 2s ² | electron 4 | $n = 2, l = 0, m_l = 0, m_s = -\frac{1}{2}$ |
| | electron 3 | $n = 2, l = 0, m_l = 0, m_s = +\frac{1}{2}$ |
| 1s ² | electron 2 | $n = 1, l = 0, m_l = 0, m_s = -\frac{1}{2}$ |
| | electron 1 | $n = 1, l = 0, m_l = 0, m_s = +\frac{1}{2}$ |

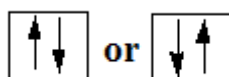
The complete set of quantum numbers for each of the 11 electrons in sodium.

The exclusion rule can be expressed as:

No more than two electrons may occupy a single orbital and if two electrons do occupy a single orbital, then their spins must be paired. By "Paired", we mean that one electron spin must be spin up (\uparrow) and the other spin down (\downarrow); the pair is denoted $\uparrow\downarrow$ or $\downarrow\uparrow$.

Another way of expressing the Pauli Exclusion Principle is to note that, because an electron in an atom is describe by four variable quantum number; $n, \ell, m\ell, m_s$, No two electrons can have the same four quantum numbers.

There is only one orbital in the $n=1$ quantum shell, from Pauli exclusion principle, a maximum of two electrons can be accommodated in it. Using the symbol of **S** orbital with maximum number of electron can be written as **1S²** or **1S^{↑↓}** represented box (or square) and arrow as:

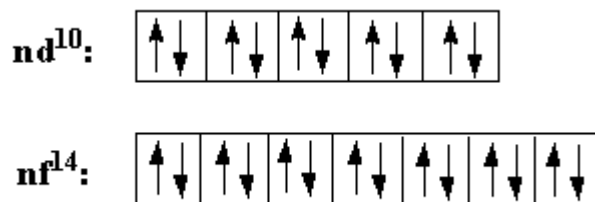


Thus, the three orbitals in a **P** subshell can accommodate six electron, **nP⁶** (**nP_x², nP_y², nP_z²**) or (**nP_x^{↑↓}, nP_y^{↑↓}, nP_z^{↑↓}**) or using the Box and arrow as:



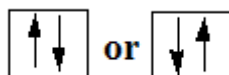
First Stage

The five and seven orbitals in **d** and **f** subshells can accommodate a total of ten and fourteen electrons respectively:



There is one orbital in the quantum shell n=1, according to the Pauli Exclusion Principle, the maximum number of electrons that can occupy or inhabit that single orbital is two electrons.

Using the orbital symbol S, the orbital containing the highest number can be expressed as 1S² or 1S^{↑↓}, or we can represent it using a square or box shape with an arrow as follows:



So: The three orbitals of the P-type secondary shell accommodate a total of six electrons, as in the above methods in which the shell is written with the electrons. The five and seven orbitals of each of the secondary shells, **nf** and **nd**, accommodate the maximum number of ten and fourteen electrons, respectively, because they are opposites, and we express them in writing or schematically using the square or arrow shape.

(Hund's Rule of Maximum Multiplicity)

When more than orbital with the same energy are available, electrons would occupy separated orbitals and do so with parallel spins. By convention, the unpaired electrons are represented as having spin up.

- **P-type subshell with two electrons.**

Two electrons in secondary shell as p-type (or np²)



- **d-type subshell with five electrons.**

Five electrons in secondary shell as p-type (or np²)



- **P-type subshell with four electrons.**

Four electrons in secondary shell as p-type (or np²)



*First Stage***The rule states:**

When there is more than one orbital with the same energy (the same numerical value of the two quantum numbers n , ℓ) available, the electrons are distributed individually and in parallel over these orbitals. It is agreed that the parallel spin of individual electrons is represented by the symbol for a spin opposite to the direction of rotation of the clock hand, or \uparrow , or according to the English term, spin up.

Examples and orbital and electron diagrams (box and arrow) illustrate some aspects of the rule. This rule bears the name of the German physicist F.H. HUND.

The rule requires that electrons be placed in separate degenerate orbitals so as to give the maximum total spin (S) possible (or the maximum number of parallel spins).

This rule can be understood in term of weaker repulsive forces that exit between electron occupying different regions of space (electrons in different orbital) than between those occupying the same region of space (electrons in the same orbital). The requirement of parallel spins of electron that do occupy different orbitals is a consequence of a quantum mechanical effect called **Spin Correlation**. Spin correlation is the tendency for two electrons with parallel spins to stay a part from one another and hence to repel each other less. Lowering of electrostatic repulsion between electrons results in a low energy-content of an atom. Therefore, this rule is a consequence of the lowest energy rule.

Hund's rule requires that electrons be placed or distributed in an unpaired manner in independent orbitals of equal energy as much as possible in order to give so as to give the highest possible numerical value for the total spin, which is denoted by S [where $S_x = ms_1 + ms_2 + ms_3 + \dots + ms_x$, where x refers to the number of single (unpaired) electrons in the atom] or the largest number of unpaired electrons with parallel spins.

The reasons that led to the formulation of this rule can be understood by understanding the force of electrostatic repulsion that exists between negatively charged electrons. The repulsion between electrons that occupy different regions of space (or orbitals separated from each other)

First Stage

weakens or decreases, while the electrostatic repulsion between paired electrons that occupy the same space or region of space (i.e., they occupy the same orbital) strengthens or increases. In addition, Hund's rule requires that unpaired electrons occupying separate orbitals have a parallel spin, as this is a requirement of the so-called spin correlation effect, which is a specialty of the theory of quantum mechanics.

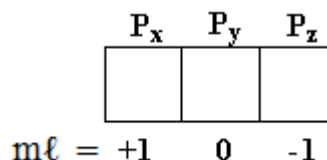
The Permian bonding effect is known as the tendency of two electrons with parallel spins to stay away from each other and thus have less repulsion. The decrease in electrostatic repulsion between electrons results in a reduction in the energy content of the atom. Based on the above, this rule is one of the results of the low energy rule. It is obituary which of degenerate orbitals of the P, d, and f is occupied first, but it is common to adopt either:

a) The alphabetical order, for:

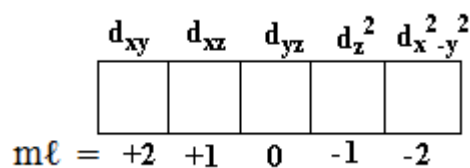
- P-type subshell, the order of filling is: P_x , P_y , and P_z .
- d-type subshell, the order of filling is: d_{xy} , d_{xz} , d_{yz} , d_x^2 , $d_x^2-y^2$.

b) The orbital filled first is the one with the highest positive value of the magnetic quantum number, $m\ell$ and the going to successive lower values, **a** and **b** methods are identical as shown below.

- **P-type subshell.**



- **d-type subshell.**



The order of filling

The system of distributing electrons to equal-energy orbitals (or which of these equal-energy orbitals is filled or occupied by electrons first) is described. Arbitrarily or randomly, in other words, it does not matter who fills it first because they are equal in energy, but it is common to adopt one of the two methods:

First Stage

- a) According to the sequence of letters of the alphabet $z \rightarrow y \rightarrow x$.
- b) The orbital that is filled first with electrons and separately as much as possible is the one that has the highest positive value of the magnetic quantum number m_l , followed by the lowest and lowest. Note that the two methods **a** and **b** are identical.

The multiplicity is either:

- a) The number of unpaired electron (**u**) plus one, **or**
 b) $2S+1$, where **S** is the total spin.

What is meant by multiplicity is:

- a) The number of unpaired electrons (**u**) plus one.

Multiplicity = u+1

Where u= unpaired of electron.

Or b) **Multiplicity = 2S+1**

When: $S = \text{Total spin}$.

When there are one to six electrons in **P** orbitals (or subshell). The best arrangements and the highest multiplicity are those given in the following tabulated form.

| No. of the best electron arrangement | No. of unpaired electrons | Multiplicity | | |
|--|---------------------------|--------------------|------------|--------------|
| | | $2S+1$ | u+1 | Total |
| 1 \uparrow $\underline{\quad}$ $\underline{\quad}$ | 1 | $2(1/2) + 1$ | $1+1$ | 2 |
| 2 \uparrow \uparrow $\underline{\quad}$ | 2 | $2(1/2+1/2) + 1$ | $2+1$ | 3 |
| 3 \uparrow \uparrow \uparrow | 3 | $2(1/2+1/2+1/2)+1$ | $3+1$ | 4 |
| 4 $\uparrow\downarrow$ \uparrow \uparrow | 2 | $2(1/2 + 1/2) + 1$ | $2+1$ | 3 |
| 5 $\uparrow\downarrow$ $\uparrow\downarrow$ \uparrow | 1 | $2(1/2)+ 1$ | $1+1$ | 2 |
| 6 $\uparrow\downarrow$ $\uparrow\downarrow$ $\uparrow\downarrow$ | 0 | $2(0)+ 1$ | $0+1$ | 1 |

Any other arrangement of electrons results in fewer unpaired electrons and lower of multiplicity.

First Stage**2- Magnetic quantum number ($m\ell$)**

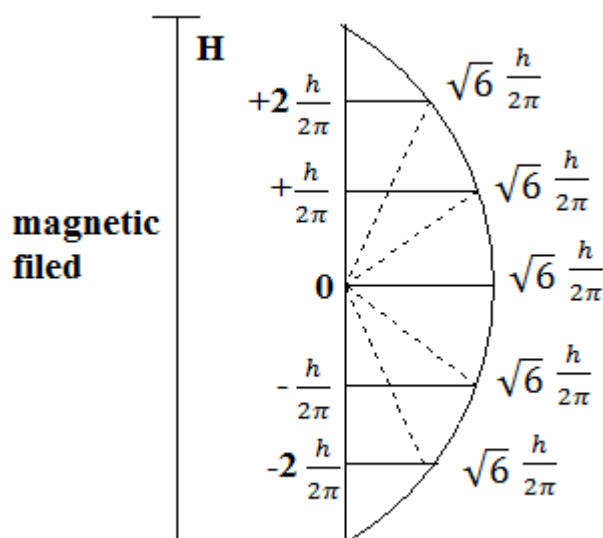
The magnetic quantum number $m\ell$ determines the direction of the orbitals in the secondary levels ℓ . When the external magnetic field is applied, as we showed previously, the value of the orbital angular momentum is constant within the designated secondary level ℓ . This means that all three **p** orbitals each carry an orbital angular momentum whose value is equal to:

$\mu_{\ell} = \sqrt{\ell(\ell + 1)} \frac{h}{2\pi}$ (momentum), whether it is of the type **p_x**, **p_y**, **p_z**, and each of the five **d** orbitals carries an orbital angular momentum of value $\mu_{\ell} = \sqrt{\ell(\ell + 1)} \frac{h}{2\pi}$ whether d_{z^2} , $d_{x^2-y^2}$, d_{yz} , d_{xz} , d_{xy} .

All of these orbitals are equal in energy before the magnetic field is applied, but if the magnetic field is applied, the energy of these orbitals will change and differ among themselves according to their response in the direction of the applied magnetic field or opposite to the direction of the magnetic field, so the values of the orbital angular momentum become in terms of $m\ell$, or in other words in terms of the effect of the magnetic field, they become: The following figure:

When $\ell=0$ s $m\ell=0$ $\mu_{m\ell}=0$
 When $\ell=1$ p $m\ell=+1, 0, -1$ $\mu_{m\ell} = \frac{h}{2\pi}, 0, -\frac{h}{2\pi}$

As shown in the following figure:

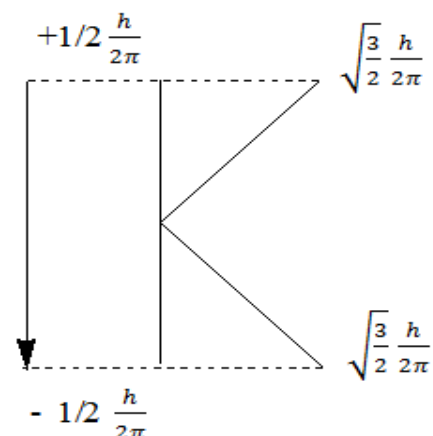


*First Stage***3- Spin quantum number (m_s)**

The number of quantum spins (m_s) is determined by the change in the direction of the angular momentum of the electron's movement around its axis when the magnetic field is applied. This momentum is calculated from the following law:

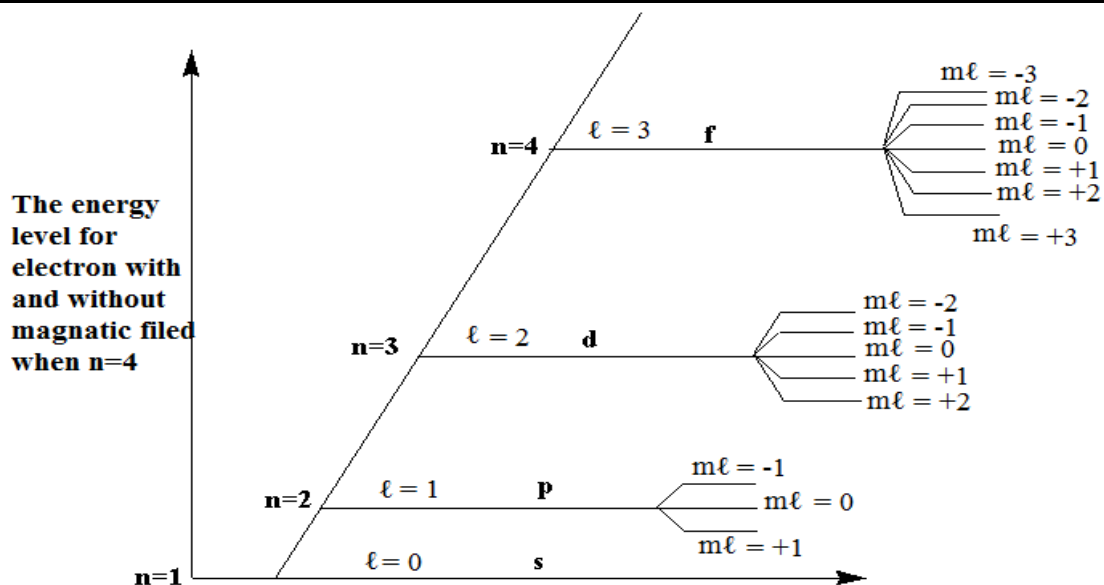
$$\begin{aligned}\mu_s &= \sqrt{s(s+1)} \frac{h}{2\pi} \\ &= \sqrt{\frac{1}{2} \left(\frac{1}{2} + 1\right)} \frac{h}{2\pi} \\ &= \sqrt{\frac{3}{2}} \frac{h}{2\pi}\end{aligned}$$

It is a constant value before the magnetic field is applied, but when the magnetic field is applied, it affects the spin of the electron, so the value of the angular momentum becomes, in general, $-1/2 \frac{h}{2\pi}$, $+1/2 \frac{h}{2\pi}$.



The positive value is the lowest energy, and the negative value is the highest energy. The four quantum numbers are what determine the energy of the electron in atoms, whether it is an **H** atom or other multi-electron atoms, because they represent the distribution of electrons on the atom from the lowest energy to the highest energy in the orbitals belonging to the secondary levels that are composed. For major envelopes or major energy levels.

First Stage



So, an orbital can be defined physically as: a vacuum space with a shape in which the probability of spreading the electronic density is high, and it is determined by the value of the square of the wave function Ψ^2 relative to the radius, which determines the location of the electron or the square of the wave function Ψ^2 , and it depends on the values of m_l , l , r .

1eV = 1 volt.

1eV = 1.602×10^{-19} J = 1.602×10^{-12} erg

J = Kg m² Sec⁻²

erg = g cm² Sec⁻²

$$\left. \begin{array}{l} \text{J} = \text{Kg m}^2 \text{Sec}^{-2} \\ \text{erg} = \text{g cm}^2 \text{Sec}^{-2} \end{array} \right\} \begin{array}{l} h = 6.62 \times 10^{-34} \text{ Kg. m}^2. \text{sec}^{-1} \\ = 6.62 \times 10^{-27} \text{ g.cm}^2.\text{sec}^{-1} \end{array}$$

erg = 6.2416×10^{-11} eV

e = 1.602×10^{-19} Colom

e = 4.8×10^{-10} e.s.u (electron static unit).

Quantum Numbers

Once again, information about the wave functions (or orbitals) is obtained from Schrodinger wave Equation, which can be set up and solved exactly or approximately. The equation can be solved exactly for an one-electron system (e.g ${}_1\text{H}$, ${}_2\text{He}^+$, ${}_3\text{Li}^{++}$).

Solving the equation is required the imposition of a set of certain conditions, thus only acceptable solutions can be obtained. These conditions, thus only acceptable solutions can be obtained. These conditions or requirements are known as quantum numbers (or Boundary Condonations).

First Stage

As a result, each of the wave function obtained by solving the Schrodinger wave equation for a hydrogenic atom or ions is uniquely labelled (or governed) by a set of three quantum numbers. These numbers are designated n , ℓ , and $m\ell$.

- $\color{red}{+}$ $\color{blue}{-}$ **n** : is called the Principle Quantum Number .
- $\color{red}{+}$ $\color{blue}{-}$ **ℓ** : is called the Secondary Quantum Number.
- $\color{red}{+}$ $\color{blue}{-}$ **$m\ell$** : is called the magnetic Quantum Number.

The Four Quantum Numbers

The quantum numbers are parameters that describe the distribution of electrons in the atom, and therefore its fundamental nature. They are:

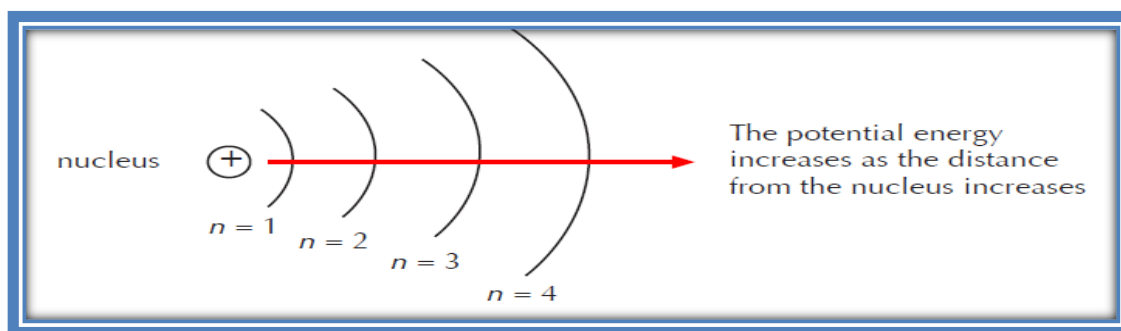
1. **Principle Quantum Number (n)**: Represents the main energy level, or shell, occupied by an electron. It is always a positive integer, that is $n = 1, 2, 3 \dots$
2. **Secondary Quantum Number (ℓ)** : Represents the energy sublevel, or type of orbital, occupied by the electron. The value of ℓ depends on the value of n such that $\ell = 0, 1, \dots n-1$. This number is sometimes also called azimuthal, or subsidiary.
3. **Magnetic Quantum Number ($m\ell$)**: Represents the number of possible orientations in 3-D space for each type of orbital. Since the type of orbital is determined by ℓ , the value of $m\ell$ ranges between $-\ell$ and $+\ell$ such that $m\ell = -\ell, \dots, 0, \dots, +\ell$.
4. **Spin Quantum Number (m_s)**: Represents the two possible orientations that an electron can have in the presence of a magnetic field, or in relation to another electron occupying the same orbital. Only two electrons can occupy the same orbital, and they must have opposite spins. When this happens, the electrons are said to be paired. The allowed values for the spin quantum number m_s are $+1/2$ and $-1/2$.

According to Heisenberg's **uncertainty principle**, it is impossible to know the electron's velocity and its position simultaneously. The exact position of the electron at any given time cannot be known. Therefore, It is impossible to obtain a photographic picture of the atom like we could of a busy street. Electrons are more like fast-moving mosquitoes in a swarm that cannot be photographed without appearing blurred.

First Stage

The uncertainty about their position persists even in the photograph. An alternative picture of the swarm can be obtained by describing the area where the mosquitoes tend to be concentrated and the factors that determine their preference for certain locations, and that's the best we can do. The quantum numbers provide us with a picture of the electronic arrangement in the atom relative to the nucleus. This arrangement is not given in terms of exact positions, like the photograph of a street, but rather in terms of probability distributions and potential energy levels, much like the mosquito swarm.

The potential energy levels are described by the main quantum number n and by the secondary quantum number ℓ . The probability distributions are given by the secondary quantum number ℓ and by the magnetic quantum number $m\ell$. The now outdated solar system model of the atom allows us to visualize the meaning of the potential energy levels. The main energy levels, also called shells, are given by the main quantum number n .



The Relationship between Potential Energy and Stability is Inverse

As the potential energy of a system increases, the system's stability is more easily disrupted. As an example, consider the objects on the earth. Objects that are positioned at ground level have lower potential energy than objects placed at high altitudes.

The object that is placed at high altitude, be it a plane or a rock at the top of a mountain, has a higher "potential" to fall (lower stability) than the object that is placed at ground level. Systems tend towards lower levels of potential energy, thus the tendency of the plane or the rock to fall. Conversely, an object placed in a hole on the ground does not have a tendency to "climb out" because its potential energy is even lower than the object placed at ground level. Systems do not naturally tend towards states of higher potential energy. Another way of saying the same thing is to say that systems tend towards states of higher stability. In the case of

First Stage

the electrons in the atom, those at lower levels of potential energy (lower shells, or lower n) are more stable and less easily disrupted than those at higher levels of potential energy.

Chemical reactions are fundamentally electron transfers between atoms. In a chemical reaction, it is the electrons in the **outermost shell** that react, that is to say, get transferred from one atom to another. That is because they are the most easily disrupted, or the most available for reactions. The outermost shell is the marketplace where all electron trade takes place. Accordingly, it has a special name. It is called the **valence shell**. Now, the solar system model of the atom is outmoded because it does not accurately depict the electronic distribution in the atom. Electrons do not revolve around the nucleus following elliptical, planar paths. They reside in 3-D regions of space of various shapes called orbitals.

An orbital is a region in 3-D space where there is a high probability of finding the electron

An orbital is, so to speak, a house where the electron resides. Only two electrons can occupy an orbital, and they must do so with opposite spin quantum numbers m_s . In other words, they must be paired.

The type and shape of orbital is given by the secondary quantum number ℓ . As we know, this number has values that depend on n such that $\ell = 0, 1, \dots, n-1$. Furthermore, orbitals are not referred to by their numerical l values, but rather by small case letters associated with those values. Thus, when $\ell = 0$ we talk about *s* orbitals. When $\ell = 1$ we talk about *p* orbitals. When $\ell = 2$ we talk about *d* orbitals, and so on. In organic chemistry, we are mostly concerned with the elements of the second row and therefore will seldom refer to ℓ values greater than ℓ . We will be talking mostly about *s* and *p* orbitals, and occasionally about *d* orbitals in reference to third row elements.

Since the value of ℓ depends on the value of n , only certain types of orbitals are possible for each n , as follows (only the highest energy level is shown for each row of elements):

First Row Elements: $n = 1$, $\ell = 0$ only *s* orbitals are possible, denoted as **1s orbitals**.

Second Row Elements: $n = 2$, $\ell = 0$ *s* orbitals are possible, denoted as **2s orbitals**, $\ell = 1$ and *p* orbitals are possible, denoted as **2p orbitals**.

First Stage

Third Row Elements: $n = 3$, $\ell = 0$ s orbitals are possible, denoted as **3s orbitals**,

$\ell = 1$ **p** orbitals are possible, denoted as **3p orbitals**,

$\ell = 2$ and **d** orbitals are possible, denoted as **3d orbitals**.

Finally, the orientations of each orbital in 3-D space are given by the magnetic quantum number $m\ell$. This number depends on the value of ℓ such that $m\ell = -\ell, \dots, 0, \dots, +\ell$. Thus, when $\ell = 0$, $m\ell = 0$. There is only one value, or only one possible orientation in 3-D space for s-orbitals. That stands to reason, since they are spherical. In the case of p-orbitals $\ell = 1$, so $m\ell = -1, 0$, and $+1$. Therefore, there are three possible orientations in 3-D space for p-orbitals, namely along the x , y , and z axes of the Cartesian coordinate system. More specifically, those orbitals are designated as px , py , and pz respectively. The principle quantum number, **n** is related to the size and energy of the orbital. The size and energy of a given type increases. The principle quantum number, **n** is essentially assumed in the Bohr's Model of Hydrogen.

The Secondary quantum number, ℓ , is related to the shape of wave function (or atomic orbital).

The magnetic quantum number, $m\ell$, is related to the orientation of a given orbital in space.

The above mentioned set of three quantum numbers are used to specify a given atomic wave function (or orbital).

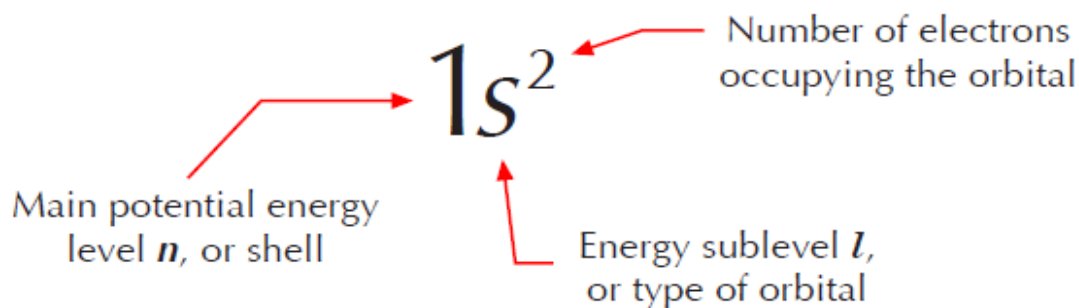
In addition, there is no two orbitals, in a given atom or ion, can have exactly the same set of three quantum numbers. For this reason, the three quantum numbers can be used to differentiate between various orbitals in an atom or ion.

The group referred to above, consisting of three quantum numbers, is used to determine or determine the atomic wave function (or orbital). In addition, there are no two orbitals or wave functions in a given atom or ion that have exactly the same set of three quantum numbers. For this reason, the three quantum numbers can be used to distinguish between atomic wave functions or atomic orbitals in a particular atom or ion.

First Stage

Electronic Configuration

To indicate the electronic configuration of the atom, that is to say, where the electrons reside, we use the following notation.

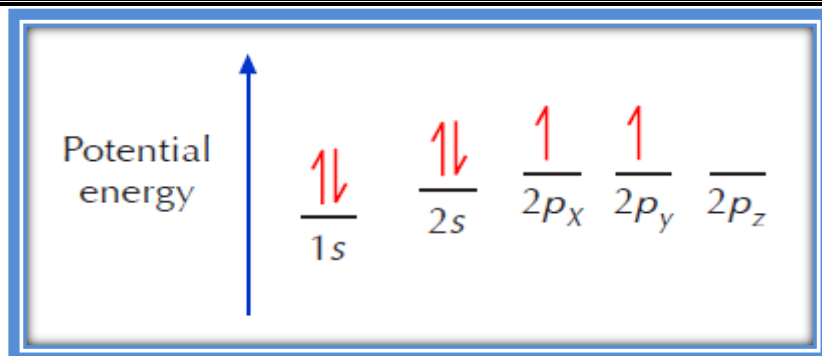


Given a periodic table, all we need to know to write the electronic configuration for a given atom is the atomic number Z , which tells us the number of electrons in the neutral atom. We start by writing the first potential energy level ($n=1$), then the possible types of orbitals in this level (s , p , etc.), and then the number of electrons occupying that orbital, which is always either 1 or 2. It will always be 2 unless Z is an odd number and we're down to the last electron in the valence shell. The electronic configurations for the nonmetals of the second row are shown below.

| | | | | |
|----------|----|--------|--------------------------------------|---|
| BORON | B | $Z=5$ | $1s^2, 2s^2, 2p_x^1$ | Total of 5 electrons, 3 in the valence shell |
| CARBON | C | $Z=6$ | $1s^2, 2s^2, 2p_x^1, 2p_y^1$ | Total of 6 electrons, 4 in the valence shell |
| NITROGEN | N | $Z=7$ | $1s^2, 2s^2, 2p_x^1, 2p_y^1, 2p_z^1$ | Total of 7 electrons, 5 in the valence shell |
| OXYGEN | O | $Z=8$ | $1s^2, 2s^2, 2p_x^2, 2p_y^1, 2p_z^1$ | Total of 8 electrons, 6 in the valence shell |
| FLUORINE | F | $Z=9$ | $1s^2, 2s^2, 2p_x^2, 2p_y^2, 2p_z^1$ | Total of 9 electrons, 7 in the valence shell |
| NEON | Ne | $Z=10$ | $1s^2, 2s^2, 2p_x^2, 2p_y^2, 2p_z^2$ | Total of 10 electrons, 8 in the valence shell |

We can also write electronic configurations where electrons are shown as half-arrows and potential energy levels are shown as horizontal dashes positioned at different heights to indicate those levels. The following diagram shows the electronic configuration for carbon.

First Stage

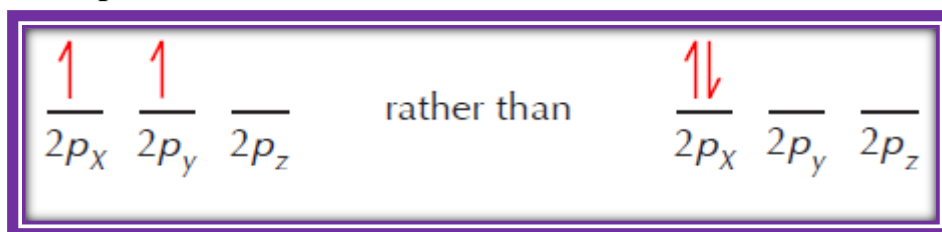


The half-arrows shown together in opposite directions indicate that the electrons are paired. Single arrows indicate unpaired electrons. Notice that an empty orbital does not mean that such orbital does not exist. It only means there are no electrons in it. Given the right circumstances, it could hold electrons. This is in opposition to an orbital whose existence is not possible. For example, *d* orbitals are not possible for second row elements and therefore are nonexistent in those elements. Orbitals which are of exactly the same energy, such as the $2p_x$, $2p_y$, and $2p_z$ orbitals, are said to be degenerate.

In writing electronic configurations, we follow the **Aufbau principle**, **Hund's rule**, and the **Pauli exclusion principle**.

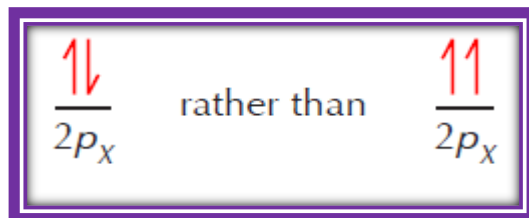
The **Aufbau principle** (German for *building up*) makes reference to the process of building an atom from the ground up. That is to say, the manner in which electrons are placed in the atom one by one. We start by placing the first electron at the lowest potential energy level, which is the $1s$ orbital, and then following with the rest of the electrons always placing them at the lowest available level of potential energy. In other words, electrons always go into orbitals with the lowest possible energy.

Hund's rule says that when electrons go into degenerate orbitals, they occupy them singly before pairing begins. That's the reason why in the carbon atom shown in the previous page, the electrons in the $2p_x$ and $2p_y$ orbitals are placed one in each orbital, unpaired, rather than two in one orbital and paired.



First Stage

Finally, the Pauli exclusion principle states that only electrons with opposite spins can occupy the same orbital. In other words, if two electrons must go into the same orbital, they must be paired. In the example shown above we have:



Acceptable Solutions of wave function and Their Meaning in Relation to Atomic Structure

A- A hydrogen atom or ion in the ground state

Solutions to the Schrodinger equation for a hydrogen atom or ion in the ground energy state show that there is only one acceptable solution. The wave function for this plausible solution is described or expressed as Ψ_{100} . The numbers **0, 0, 1** symbolize the three quantum numbers **m ℓ , L, n** that restrict the acceptable solution to a wave function or a hydrogen atom ion in the lowest energy states.

Semantics or what does the above solution mean?

1. The existence of one energy level corresponding to one orbital.

Due to the presence of the atom or hydrogen ion in the ground energy state, this energy level represents the lowest energy level and the closest to the nucleus, and is symbolized by the principal quantum number $n=1$.

2. Since the function does not depend on the secondary quantum number ($L=0$) and the magnetic quantum number ($m\ell=0$), the mathematical expression for this function is devoid of the angular function. Therefore, the space, space, or orbital occupied by the electron can be described as spherical and is symbolized by the symbol **s** (small letter).

3. This orbital (i.e., **s**) forms the only subshell, which in turn forms the first main energy shell ($n=1$). It has been agreed that the symbol for the secondary shell should be written in a way that shows the numerical value of the primary shell (the value of n) followed by the symbol for the secondary shell. Therefore, the expression or symbol

First Stage

that indicates the only secondary shell in the hydrogen atom in the ground state is **1s** [note that **s** is a lowercase letter].

The quantum numbers $m_l=0$, $L=0$, $n=1$ are used to describe **1s** orbitals. If we want to describe the electron that occupies the **1s** orbital, we must use a fourth quantum number, which is the Permin magnetic quantum number m_s . It was agreed that the only electron occupying the **1s** orbital would be given the value $m_s=+1/2$, or that it would be symbolized by α or the upward arrow \uparrow . Accordingly, the complete description [or metaphor of the title] for the residence of an electron in an atom or hydrogen ion in the lowest energy state is as follows:

$$m_s=+1/2, \quad m_l=0, \quad L=0, \quad n=1$$

B: There is also a hydrogen atom or ion in the excited state.

Some general notes:

- 1- No. of orbital in a specification; $n=n^2$.
- 2- Orbitals with the same values of **n** and **l** form subshell. It is common practice to refer to each subshell by a letter s, p, d, f, g, h, ----. For most purpose, we need consider only s, p, d, f subshell. Number of subshells is equal to the numerical value of the related principle quantum number.

Example: If $n = 2$, then the number of secondary shells = 2, and so on.

- 3- Number of orbitals in each type of subshell is equal to $2L+1$.

For example:

- **s- type subshell :**
 $2L+1 = 2 \times 0 + 1 = 1$, one orbital.
 Because, $L=0$ for s-type subshell.
- **p- type subshell :**
 $2L+1 = 2 \times 1 + 1 = 3$ orbitals.
 Because, $L=1$ for p-type subshell.
- **d- type subshell :**
 $2L+1 = 2 \times 2 + 1 = 5$ orbitals.
 Because, $L=2$ for d-type subshell.
- **f- type subshell :**
 $2L+1 = 2 \times 3 + 1 = 7$ orbitals.
 Because, $L=3$ for f-type subshell.

First Stage

4- The orbitals of p, d, and f subshell can be distinguished by the magnetic quantum number; m_L , which can have the $2L+1$ integer values. These Values are ranging from $+L$ down to $-L$ including zero.

To explain how the numerical values of m_l used to label the orbital by the square shape.

- **P-type subshell**

$$l=1$$

$$m_l = +1, 0, -1$$

$$\text{No. of orbitals} = 3$$

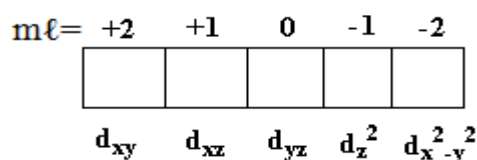


- **d-type subshell**

$$\text{No. of orbitals} = 5$$

$$m_l = +2, +1, 0, -1, -2$$

$$l=2$$



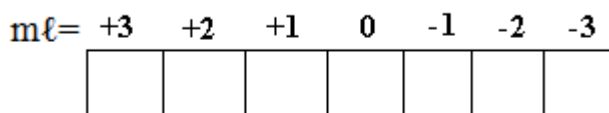
The numerical values of m_l mean that each orbital of d-subshell has different orientation in space.

- **f-type subshell**

$$\text{No. of orbitals} = 7$$

$$l=3$$

$$m_l = +3, +2, +1, 0, -1, -2, -3$$

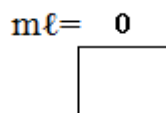


- **s-type subshell**

$$\text{No. of orbitals} = 1$$

$$l=0$$

Value of $m_l = 0$, this means one symmetrical orientation in space.



Note: The S-type orbital is spherically symmetric and does not have diverse space extensions. Rather, it has a homogeneous or spherical symmetric space extension.

First Stage

The sequence of orbital energies for the hydrogen atom is shown in the figure below. It will be noticed that the energies of orbitals are negative. This implies that energy of the hydrogen atom, whether the atom in the ground state ($n=1$) or an excited state ($n \geq 2$), is lower than the energy of the isolated electron or electron that is widely separated from the nucleus ($n = \infty$). The figure indicates that, for the hydrogen atom, the s, p, d, and f orbitals of a particular quantum shell are of equal energy. In other words, the energy of the orbitals is defined completely by the principle quantum number n .

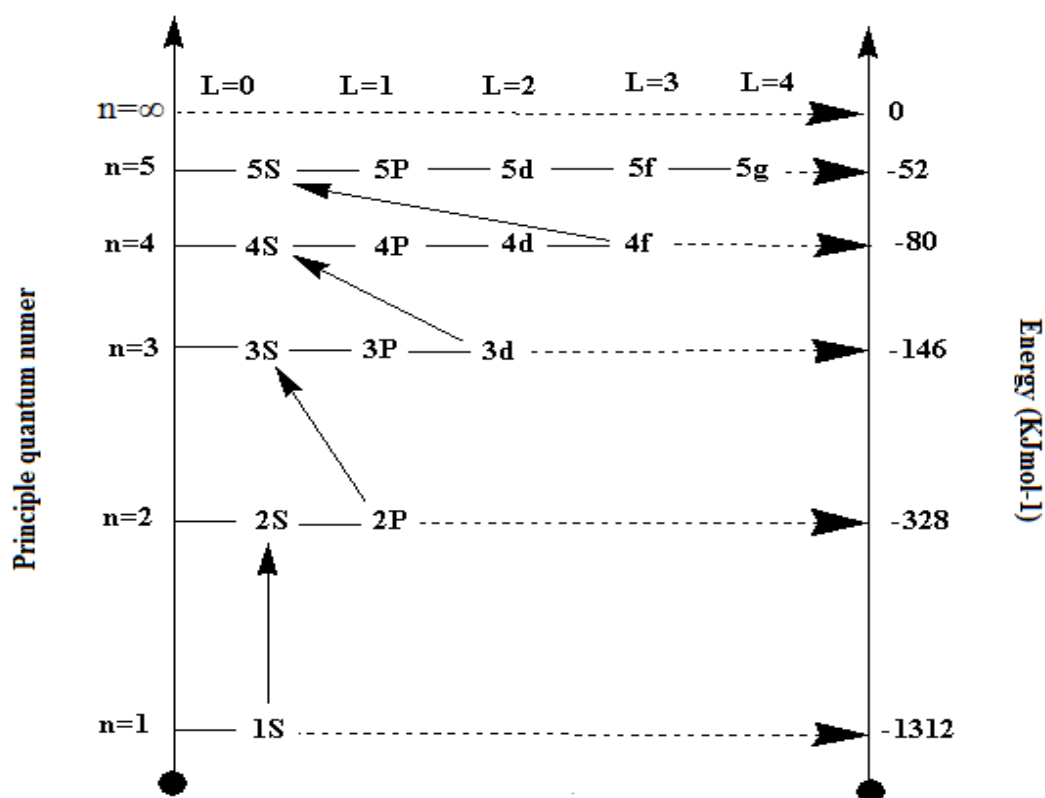
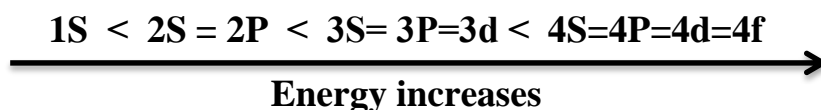


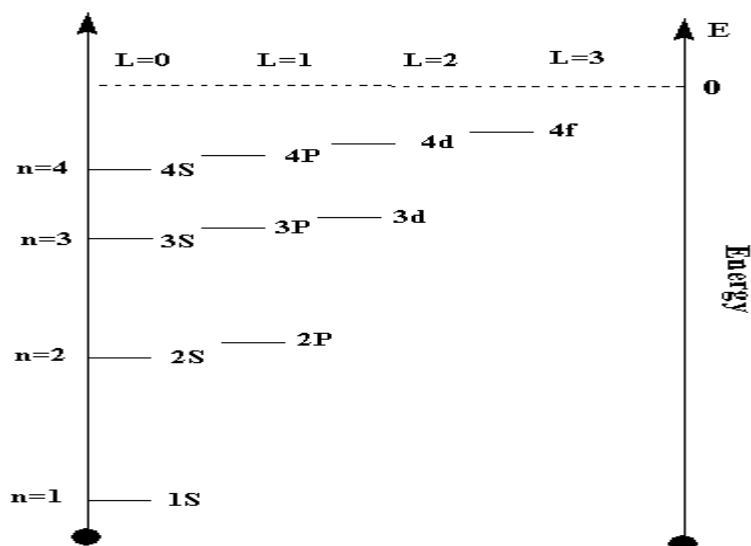
Figure: some electronic energy level in the hydrogen atom. Note that the energy of the n^{th} level is equal to $-1312/n^2 \text{ KJmol}^{-1}$. As n increases, the orbitals become larger and the electrons are further from the nucleus. By Coulomb's law, this results in a lowering of electron binding energy.



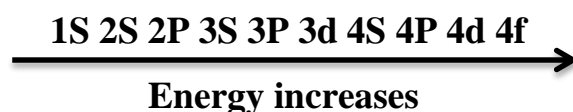
The above sequence of several different energy states (or orbitals or subshells) can be written as shown below.

First Stage

In all other atoms [multi-electron atoms or ions]. The energy of each orbital or subshell depends on both n and L ; the effect of this on the sequence of orbital energies for the light elements is shown in the Figure. This partial dependence of the energy on the secondary quantum number (ℓ) will be discussed later on.



The above sequence of orbital energy levels can be written as shown below.



Determination of Secondary Energy Levels and the Rules for Determination Ground State Electronics Structure

Sequence of energy levels and rules for determining the electronic structure of an atom in a stable state based on the four quantum numbers.

It depends on the following factors -:

1. In stable atoms, the distribution of electrons begins from low energy levels until we reach high energy levels. For example, in the H atom, in the ground state, the electron is located in the principal quantum number level when $n = 1$ within the secondary level $\ell = 0$, that is, located in the **1S** orbital and in every There is a large group of orbitals available in an atom, similar to what happens in an **H** atom. All atoms have one **1S**, one **2S**, three **2P**, five **3d**, and seven **4f**. It has the same shapes as we mentioned in the hydrogen atom, and it is spherical, S and P, consisting of two lobes, and d, consisting of four lobes, no

First Stage

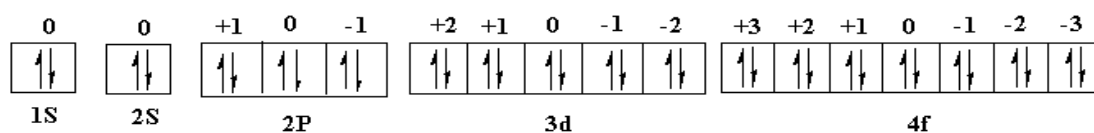
matter how different the atoms are, but their sizes and energy differ with the values of the principal quantum number n .

$$1n < 2n < 3n < 4n < 5n \rightarrow \text{increase of energy}$$

$$1S < 2S \ 2P < 3S \ 3P \ 3d < 4S \ 4P \ 4d \ 4f \rightarrow \text{increase of size}$$

But when we start filling with electrons, we must identify the low-energy secondary levels first. We inevitably reach the higher-energy levels, and this is done by relying on the values of m_s , m_l , and ℓ .

- Electronic distribution at the beginning by giving the electron to the atom containing the nucleus of the element gradually one after the other from the lowest energy secondary orbitals in one shell, the lowest energy level, until we reach the high-energy orbitals. One orbital can bear no more than two electrons.



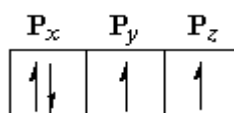
- The filling or distribution of electrons in the secondary levels belonging to the main shells is according to the equation $(n+\ell)$. As this value increases, the energy level of the electron increases and it becomes farther from the nucleus. As this value decreases, the energy level of the electron increases and it becomes farther from the nucleus. As this value decreases, it becomes Closest to the nucleus and lowest energy level, filling is from the lowest value of $n+\ell$ to the highest value. If two electrons are present, the values of $n+\ell$ are different, starting with the lower value and then moving up. For example, if one electron has a value of $n+\ell=1$ and another has a value of $n+\ell=2$, this means that the first must enter the 1S orbital and the other must enter the 2S orbital.
- After we have determined the secondary energy level, we must know that the orbitals of a single secondary level are equal in energy, but according to the values of m_l , they will be different in the directions due to the shedding of the magnetic field. Also, two important rules must be followed, which are based on the values of m_l , n , ℓ that are determined for the electron's energy mentioned previously. They are:

First Stage

Pauli Exclusion Rule: This rule states that each secondary orbital holds or occupies only two electrons at a maximum, such that their spiral motions are opposite, or in other words, no two electrons in one secondary orbital can have the same four quantum numbers.

Hund's rule: It states that electrons are distributed individually among secondary orbitals of equal energy as much as possible and do not pair unless forced to do so. After that, electrons are added to reach the required limit. This results from the repulsion that occurs between the electrons, so they must be far apart from each other.

For example, if we have the secondary level 2P containing three or four electrons, then the electrons are initially distributed as follows:



Each of them has an electron, then the fourth electron comes and enters P_x and pairs with the electron previously present in P_x . This is done because the pairing at the beginning leads to an increase in the energy of the atom as a result of the repulsion that occurs between the paired electrons, while the single distribution from the beginning leads to a decrease in the energy of the atom.

Examples:

1- When $n=2$ energy levels, which ℓ values fill first?

$$\ell = n-1 \text{ ----- } 0 \rightarrow \ell = 0, 1.$$

$$n + \ell = 2 \qquad n + \ell = 3$$

∗ $\ell = 0$ fill first.

2- Which orbital will first when $n=3, \ell=2$ or $n=4, \ell=0$?

If the values of $n+\ell$ for different orbitals are equal, the orbital with the lowest energy is the one with the lowest value for n .

Example: When $n=4, \ell=1, n=4, \ell=0$ which will fill first?

For first orbital $\rightarrow n+\ell = 4+1=5$

Second orbital $\rightarrow n+\ell = 4+0=4$ the second orbital will fill first.

First Stage**Magnetic Property**

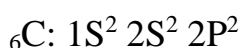
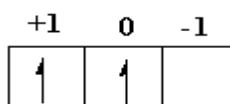
In each orbital there are one or two electrons. If the electron is alone, its rotation around its axis generates a magnetic field. However, if there is another electron with it, the field of each one of them cancels the magnetic field generated by the other electron. In other words, the orbital generates a magnetic field if it contains an electron. One, while an orbital does not generate a magnetic field if it contains two electrons. Any atom or molecule that contains one or more single electrons in an orbital or orbitals has a characteristic called paramagnetic. However, if the atom or molecule does not contain a single electron, then it possesses a characteristic (diamagnetic).

Examples & Questions:

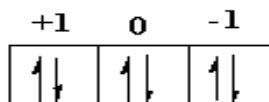
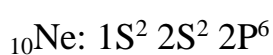
- Find the four quantum no.s of the last electron of the following atoms in ground states? H, He, Li, N, C, O, F and Ne.

Solution:

$$n=1 \quad \ell=0 \quad m\ell=0 \quad m_s = +\frac{1}{2}$$



$$n=2 \quad \ell=1 \quad m\ell=0 \quad m_s = +\frac{1}{2}$$



$$n=2 \quad \ell=1 \quad m\ell = -1 \quad m_s = -\frac{1}{2}$$

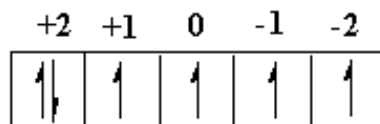
First Stage

- Find the four quantum No.s of the last electron in each of the following element or ions in their ground states? Co, Co⁺³, S, Sc, Mn⁺², Fe⁺², Rb, In, Br⁻¹ and Cr.

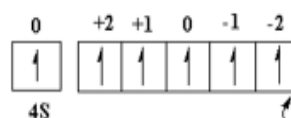
Solution:



n=3 ℓ=2 mℓ=+2 m_s= - $\frac{1}{2}$



n=4 ℓ=2 mℓ= -2 m_s= + $\frac{1}{2}$

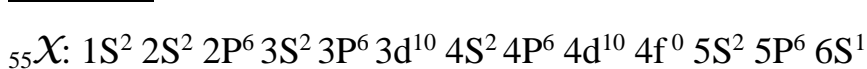


the last electron

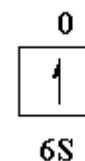
This is half saturated.

Q: Determine the four-quantum no.s of the valance electron of the following atomic no.s of atoms? 55, 19, 82, 49 and 86.

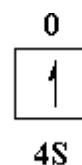
Solution:



n=6 ℓ=0 mℓ=0 m_s= + $\frac{1}{2}$



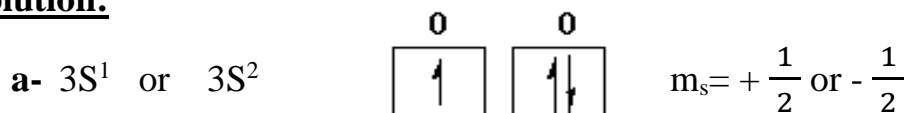
n=4 ℓ=0 mℓ=0 m_s= + $\frac{1}{2}$



Q: Classify the electron that has following Q.no.s and find the probable missing qu. no. s?

- a/ n=3 ℓ= 0 mℓ= 0
 b/ n=4 ℓ= 2
 c/ n=4 ℓ= 2 mℓ= +1

Solution:



b- 4d¹, or 4d² or 4d³ or---- 4d¹⁰ There are several possibilities.

First Stage

$$c- 4d^2 \text{ or } 4d^7 \quad m_s = +\frac{1}{2} \text{ or } -\frac{1}{2}$$

| | | | | | | | | | | |
|----|----|---|----|----|--|----|----|---|----|----|
| +2 | +1 | 0 | -1 | -2 | | +2 | +1 | 0 | -1 | -2 |
| ↑ | ↑ | | | | | ↑↓ | ↑↓ | ↑ | ↑ | ↑ |

Q: Find the atomic no. of the element who's the last electron have the following Quantum no.s?

- 1- $n=4 \quad \ell=0 \quad m\ell=0 \quad m_s = +1/2.$
- 2- $n=3 \quad \ell=1 \quad m\ell=+1 \quad m_s = +1/2.$
- 3- $n=4 \quad \ell=1 \quad m\ell=0 \quad m_s = -1/2.$
- 4- $n=5 \quad \ell=1 \quad m\ell=+1 \quad m_s = -1/2.$
- 5- $n=3 \quad \ell=2 \quad m\ell=+1 \quad m_s = -1/2.$
- 6- $n=4 \quad \ell=3 \quad m\ell=+1 \quad m_s = -1/2.$

Solution:

1- $X = 1S^2 2S^2 2P^6 3S^2 3P^6 4S^1 3d^0.$ Atomic no. = **19** $X = K.$

2- $X = 1S^2 2S^2 2P^6 3S^2 3P^1.$ Atomic no. = **13** $X = Al.$

3- $X = 1S^2 2S^2 2P^6 3S^2 3P^6 4S^2 3d^0 4P^5.$ Atomic no. = **35** $X = Br.$

4- $X = 1S^2 2S^2 2P^6 3S^2 3P^6 4S^2 3d^{10} 4P^6 4d^{10} 4f^0 5S^2 5P^4.$

Atomic no. = **52** $X = Te.$

5- $X = 1S^2 2S^2 2P^6 3S^2 3P^6 4S^0 3d^7.$ Atomic no. = **27** $X = Co^{+2}.$

6- $X = 1S^2 2S^2 2P^6 3S^2 3P^6 3d^{10} 4S^2 4P^6 4d^{10} 4f^7 5S^2 5P^6 6S^2 5d^1.$

Atomic no. = **64** $X = Gd.$

Electronic Configuration of many Electron Atoms

The purpose of this topic is to explain how electrons are arranged around the nucleus. As a result, you will learn how to write a correct electron configuration for a given many-electron atom in its ground state.

The importance of electron configuration is due to the fact that electrons are so important in chemistry. The way in which electrons are arranged around the nucleus plays a crucial role in determining the chemical reactivity of all atoms.

In addition, Knowledge of the electron configuration of different atoms is useful understanding the structure of the periodic table of elements.

First Stage

electron configuration is also useful for describing the chemical bond that hold atoms together.

In quantum chemistry, the arrangement of electrons of an atom or molecules in atomic or molecular orbital is known as the electron configuration. For example, the electron configuration of hydrogen atom $1S^1$ or $1S^\uparrow$ or $\boxed{\uparrow}$

The most stable arrangement of electrons is called the ground state electron configuration, in which all of the electrons in an atom are occupied the lowest energy orbitals possible.

Electron configuration was first conceived of under Bohr model of the atom, and it is still common to speak of shells and subshells despite the advances in understanding of the quantum mechanical nature of electrons. The "Aufbau" principle [Aufbau is a German word, which means building up or construction] was an important part of **Bohr's original concept of electron configuration it may be stated as:** a maximum of two electrons are put into orbitals in the order of increasing orbital energy: the lowest energy orbitals are filled before electrons are placed in higher energy orbitals.

The modern form of the "Aufbau" or building up principles are:

1- Orbitals are filled in the order of increasing $n+l$. To explain this point, let us consider the order of filling of various subshells in shell 3 (or $n=3$). For $n=3$, there are three different subshell, namely 3S, 3P, and 3d. According to the above Aufbaue rule, 3s must be filled first, followed by the filling of 3P, and then 3d. This order is in line with $n+l$ rule.

| Shell (n) | Subshell | $n+l$ | |
|--------------|----------|---------|---|
| 3 | S | $3+0=3$ | ↓ The order of filling = the order of energy increases. |
| 3 | P | $3+1=4$ | |
| 3 | d | $3+2=5$ | |

2- Where two orbitals have the same value of $n+l$, they are filled in order of increasing **n**.

For example, 2P must be filled before 3S, although both have the same $n+l$, which is equal to 3, because 2P has the smaller **n** than the 3S.

*First Stage***The modern formulation of the Aufbau principle or atomic structure is:**

1. Orbitals are filled with electrons in increasing order by the sum of $n + \ell$ [where n is the principal quantum number and ℓ is the secondary quantum number]. To explain or clarify this rule, we will study the system of filling the secondary shells of the third major shell ($n = 3$).

According to principle (1) above of Aufbau's rule, the orbital or secondary shell 3s is filled first, then followed by 3P and finally 3d. This is consistent with principle (1) above, "look at the $n+\ell$ values that correspond to the 3S, 3P, and 3d secondary shells."

2. When two orbitals share the same numerical value of $n+\ell$, these orbitals are filled according to the increase in the value of n , i.e. whoever has lower n (lowest energy) fills first.

Example: 2P fills in before 3S even though they both have the same value of $n+\ell$, so why 2P has a smaller value of n than 3S.

This gives the following order for filling the orbitals:

1S 2S 2P 3S 3P 4S 3d 4P 5S 4d 5P 6S 4f 5d 6P 7S 5f 6d 7P



Filling is done according to the direction shown.

Graphically, the orbital diagram for electron filling, showing increasing energy from 1S orbital down to 7P orbital.

The rule is to start at the beginning of each arrow, and then follow it all of the way to the end, filling in subshells that it passes through.

How to write an Electronic Configuration

Basically, three rules are required to write a correct electron configuration.

- 1- The Aufbau Principle
- 2- HUND'S RULE
- 3- Pauli Exclusion Principle

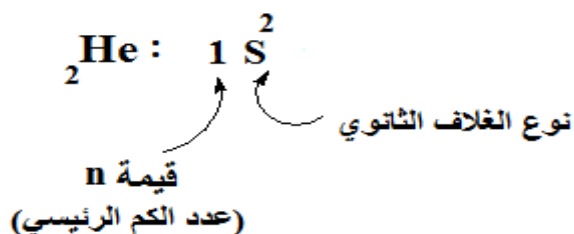
Now we try to write the electronic arrangement of multiple atoms according to the rules mentioned above.

mass No. → 4
Atomic No. → 2 **He**

- Helium atom (the helium atom contains two electrons).

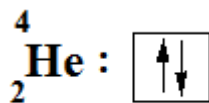
First Stage

Since the carrying capacity of one orbital is two electrons, both electrons occupy one atomic orbital at the lowest energy levels. Returning to the orbital filling diagram, it can be said that the two electrons occupy the **1S** secondary shell (or orbital). Accordingly, the electronic arrangement of the helium atom is as shown below:



The formula for writing the electron configuration above is called the Standard Electron Configuration. The electronic arrangement can be expressed in what is called an orbital diagram, which consists of a square shape to indicate the orbital and an arrow to indicate the electron.

Therefore, the electronic arrangement of the helium atom, according to the orbital diagram, is:



Based on the idea of electronic arrangement, it can be said that the S-type orbital of the helium atom is similar in shape only to the orbital of the hydrogen atom in the ground state. It is worth noting that the size of the **1S** orbital of the helium atom is smaller than the size of the 1S orbital of the hydrogen atom. This is due to the larger charge of the nucleus of the helium atom compared to the nucleus of the hydrogen atom. The increase in the positive charge of the nucleus leads to an increase in the force of electrostatic attraction between the nucleus and the **1S²** electrons, which leads to the shrinkage of the orbital.

Question: Is the **1S** energy of a hydrogen atom equal to the **1S** energy of a helium atom? And why?

Question: Is the radius of a hydrogen atom equal to the radius of a helium atom? And why?

First Stage

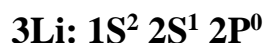
• **Lithium metal atom ${}_3\text{Li}$**

Because of the conflict with Pauli's rule, we cannot imagine that the electronic arrangement of the lithium atom in the ground state is 1S^3 .

So how are the electrons distributed in the lithium atom?

1. Only two electrons occupy the 1S orbital or secondary shell, the only component of the first main shell, $n=1$.
2. The third electron occupies one of the secondary shells (2S) or (2P) that make up the second main shell, $n=2$.

Since the energy of 2S is less than the energy of 2P , the third electron occupies 2S . The above is the standard electronic arrangement for the lithium metal atom.

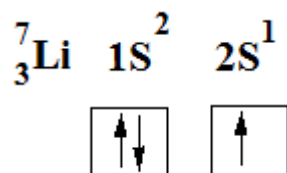


Or we just write:



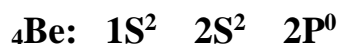
This is because 2P has no electrons.

By combining the standard electronic arrangement with the electronic arrangement using the orbital diagram, the following can be written:



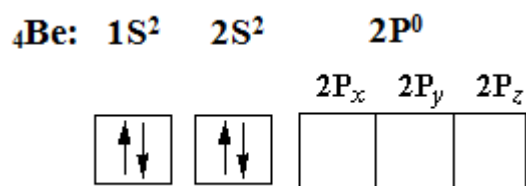
• **Beryllium atom ${}_4^9\text{Be}$**

Returning to the orbital filling diagram and the previously mentioned rules, the standard electronic arrangement of the beryllium atom is.



By combining the above method, which is the most widely used method, with the orbital chart, we get:

First Stage



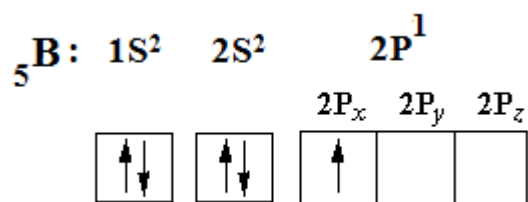
Note: We can dispense with writing **2P** because it is devoid of electrons.

- **Boron atom** ${}_{5}^{11}\text{B}$

Boron has a standard electron configuration of :



Combining the above with the orbital diagram:



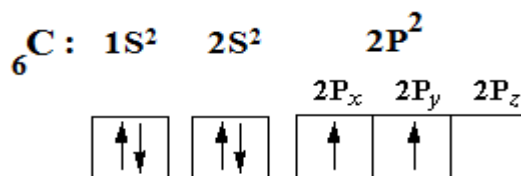
Note: The three orbitals of the secondary shell **2P** are described as being of equal energy, “Degeneration Orbitals”. Therefore, the fifth electron of the boron atom can be placed in any one of them. However, it was agreed that the distribution of electrons among the orbitals of the multi-orbital secondary shells **f**, **d**, **p** should be according to the alphabetical sequence. This is why we put the fifth orbital of boron **2P_x**.

- **Carbon atom** ${}_{6}^{12}\text{C}$

The distribution of electrons in the carbon atom is as follows:

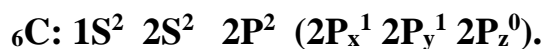


Combining the above with the arrangement called the orbital diagram gives:

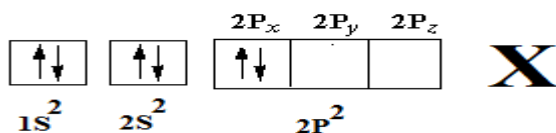


First Stage

To explain the distribution of electrons over the three orbitals of the secondary shell, the standard electronic arrangement can be written as follows:



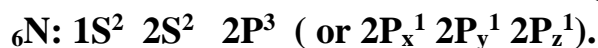
Question: Why can't the orbital diagram for carbon be written as follows?



- Nitrogen atom ${}^7_4\text{N}$

It can be noted that the nitrogen atom has only one electron more than the carbon atom. Therefore, the first six electrons in the nitrogen atom are distributed in the same correct way used to distribute the electrons in the carbon atom. As for the seventh electron, it will occupy the orbital 2P_z , which is one of the components of the secondary shell 2P , which in turn is one of the components of the second main shell $n=2$.

Therefore, the standard electronic arrangement of the nitrogen atom is:



This can be illustrated pictorially using an orbital diagram.



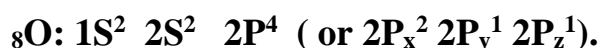
The numbering 1→7 above shows the way the electrons are distributed to the secondary shells and orbitals.

Question: State and give the name of the rule that states that electrons are distributed as individually as possible among orbitals of equal energy that form a given secondary shell or an orbital with a diverse space direction?

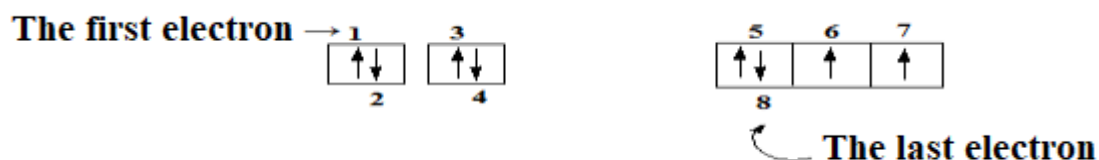
First Stage

- Oxygen atom ${}^{16}_8\text{O}$

The oxygen atom has eight electrons, and the first seven electrons are distributed in the same way as the seven electrons of the nitrogen atom. This is entirely consistent with Hund's rule of maximum versatility. As for the eighth electron, electron number **5** will participate in the work of the $2P_x$ orbital, but the direction of its movement or spin will be opposite to the fifth electron, and this is what is required by Pauli's exclusion rule.



According to the orbital chart.



Question: (a) Calculate the total atom spin of atoms ${}_6\text{C}$, ${}_7\text{N}$, ${}_8\text{O}$?

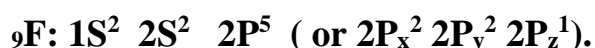
(b) Use the above results and calculate the multiplicity of the atoms above.

(c) Use the four quantum numbers m_s , m_l , l , n to describe the last electron in atoms ${}_6\text{C}$, ${}_7\text{N}$, ${}_8\text{O}$.

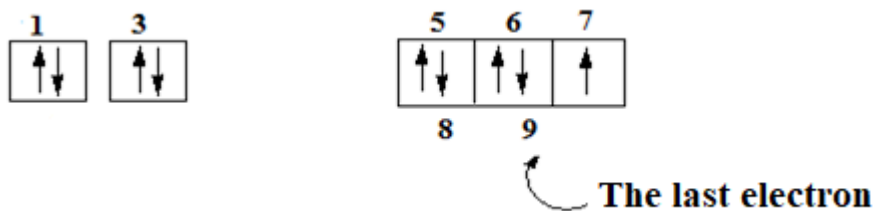
- Fluorine atom ${}^{19}_9\text{F}$

Fluorine has nine electrons. The first eight electrons are distributed or arranged around the nucleus as shown above in the oxygen atom. As for the ninth electron, it will be occupied with the sixth electron, the orbital $2P_y$, which is one of the orbitals of the secondary shell $2P$ which in turn forms with $2S$ the second main shell, $n=2$.

So the standard electronic arrangement and orbital diagram for a fluorine atom is:



First Stage

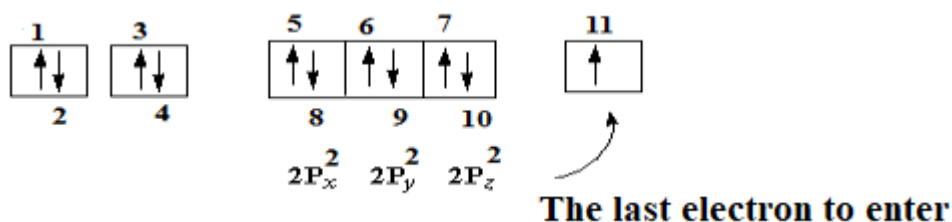


Question: Write the standard electronic arrangement as well as the orbital diagram for an atom of the element neon ${}_{10}^{20}\text{Ne}$?

- Sodium atom ${}_{11}^{23}\text{Na}$

An atom of the metal element sodium (or metal) has eleven electrons. The first ten electrons are arranged in the same way as around the nucleus of neon gas ${}_{10}\text{Ne}$. Because all the orbitals of the first and second shells are filled with electrons, the eleventh electron occupies the lowest (in terms of energy) secondary shell of the $n=3$ shells of the third main shell, which are **3d**, **3P**, **3S**. Yes, **3S** is energetically lower than 3P and 3d.

So the standard electronic arrangement and orbital diagram are as follows:

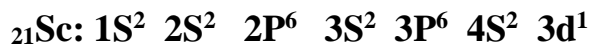


It is noted from the above examples that the electronic arrangement has ended either in an S-type secondary shell or a P-type secondary shell, as is the case for the sodium element and the nitrogen element, respectively. Now we study the method of writing the electronic arrangement of elements whose electronic arrangement ends in the secondary shell of d-type.

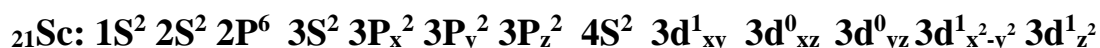
First Stage

- **Atom or metal of Scandium** ${}_{21}^{45}\text{Sc}$

Using the diagonal or diagonal rule, the standard electronic arrangement and orbital diagram are as shown below.



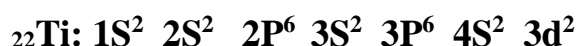
For the purpose of clarifying the distribution of electrons on the variously oriented orbitals of the P and d shells, the above arrangement can be rewritten as follows:



Note: The sign (-) between **x**, **y** in the $3\text{d}_{x^2-y^2}$ orbital symbol is a comma between the **x**, **y** space planes and not a mathematical sign. Note that the electron bearing the number **21** is the last of the electrons to be distributed again, and since the orbitals of the secondary shell, **d**, are equal in energy, there is no difference in the placement of the electron in any one of the five orbitals of equal energy and varying space direction. Chemists have agreed to encode the orbitals belonging to the secondary shells of the type **f**, **d**, **p** according to the alphabetical sequence of space planes or the Cartesian coordinate's **z**, **y**, **x**. It was also agreed to place the first electron in a spin-up form (i.e. \uparrow) in the first orbital. So we must respect this agreement and follow it when writing the standard electronic arrangement or Orbital Diagram.

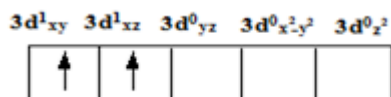
- **Titanium atom** ${}_{22}^{48}\text{Ti}$

It is noted that the above metal atom contains **2S** electrons, that is, only one electron more than the element or scandium atom. The first 21 electrons are distributed in the same way as they were distributed in the element scandium. As for the last electron, or **22**, according to Hund's rule for maximum multiplicity, it occupies the **3d** orbital, which is symbolized by the symbol 3d_{xz} . Below is the electronic arrangement of the titanium atom



In order to shorten the time, we will limit ourselves to writing the orbital diagram for the 3d secondary shell only because what comes before it is identical to what was stated in the arrangement of the electrons of the metal element scandium.

First Stage



If we wanted to describe the 21 and 22 electrons in the titanium atom using the four quantum numbers, the description would be as follows:

| Quantum Numbers No. of electron | n | ℓ | mℓ | m _s |
|------------------------------------|---|---|----|----------------|
| 21 | 3 | 2 | +2 | +1/2 |
| 22 | 3 | 2 | +1 | +1/2 |

It is noted that the four number systems for electrons 21 and 22 are not identical, as they differ in the value of the magnetic quantum number $m\ell$, which indicates the space direction of the orbital. This difference means that the space direction of orbital or electron 21 differs from the space direction of orbital electron 22. This is also clear if we return to the orbital diagram above, where we notice that electron 21 occupies orbital $3d_{xy}$ while electron 22 occupies orbital $3d_{xz}$. The non-identity in the four number systems is consistent with Hund's rule of maximum multiplicity.

Question: (a): Write the four quantum numbers for electrons **19** and **20** in the ${}_{22}\text{Ti}$ atom.

(b): Using symbols for secondary shells and Cartesian coordinates, write the symbols for the orbitals containing electrons **14**, **16**, **19** in the titanium atom.

(c): Calculate the numerical value of the total spin of the titanium atom.

(d): Calculate the maximum multiplicity

✚ Write the electronic arrangement and orbital diagram of the **3d** shell of the metal vanadium atom ${}_{23}^{51}\text{V}$.

First Stage

- **Chromium atom** ${}_{24}^{52}\text{Cr}$

Following the standard electronic arrangement writing method and the advanced orbital diagram above, the electronic arrangement of the chromium atom is as follows:



To shorten the effort and time, we write the orbital diagram for the two secondary shells 3d^4 and 4S^2 above.



Unfortunately, studies have shown that the atomic spectrum is wrong with the electronic arrangement and orbital diagram above. The correct order is:

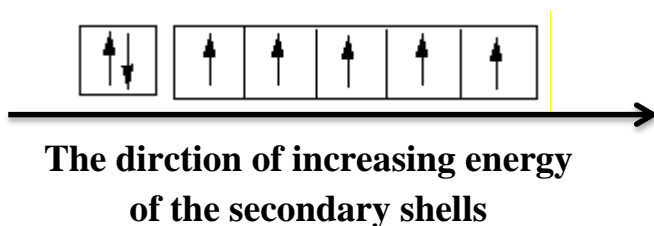


This arrangement is expressed in the half-filled arrangement because each of the last two secondary shells, 3d and 4S , contains half of their maximum carrying capacity, which is 2 and 10 electrons, respectively. It is clear that the distribution of electrons (according to the correct distribution or arrangement) is outside the rules followed in writing the standard electronic arrangement and the orbital diagram, which among them is that the upper secondary shell (4S) be filled before the shell (3d) with electrons. The reason behind this departure from the rules followed in writing the electronic arrangement will be explained later.

- **Manganese atom** ${}_{25}^{55}\text{Mn}$

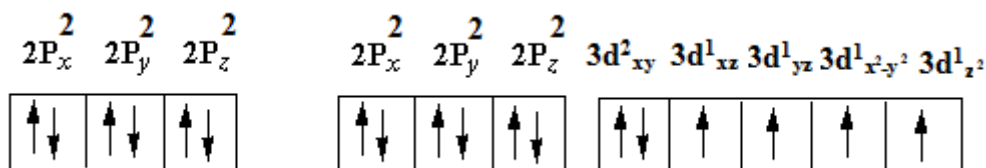
The electron configuration in the manganese atom is within the rules stated previously. As for the 3d and 4S orbitals, the 4S is filled with electrons first, and then the remaining five electrons are distributed individually (that is, according to Hund's rule for maximum multiplicity) to the five orbitals of the 3d secondary shell. Thus, the electronic arrangement and orbital diagram are as follows:

First Stage



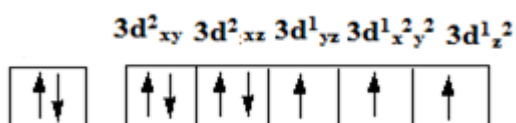
• Iron atom ${}_{26}^{56}\text{Fe}$

The number of electrons in an atom of iron metal is only one more than in an atom of manganese metal ${}_{25}\text{Mn}$. Therefore, the distribution of the first twenty-five electrons in the iron atom is identical to their distribution in the manganese atom. As for the twenty-sixth electron, it forms a double with the twenty-first electron in the work of the 3d_{xy} orbital. This is in accordance with Pauli's exclusion rule.

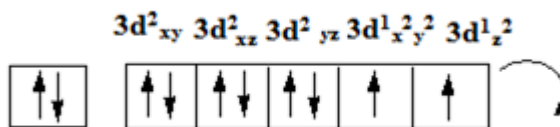


When writing the electronic arrangement and orbital diagram for metal atoms [cobalt] ${}_{27}^{59}\text{Co}$ and [nickel] ${}_{28}^{59}\text{Ni}$

The phenomenon of pairing of electrons will continue. In the cobalt atom, the twenty-seventh electron will participate with the twenty-second electron in using the 3d_{xz} space. In the nickel atom, electrons **27** and **28** will share with electrons **23** and **24** in using orbitals 3d_{yz} and 3d_{xz} , respectively. For further clarification, we present the complete standard electronic arrangement and orbital diagram for the 3d and 4S secondary shells only for the elements cobalt and nickel.

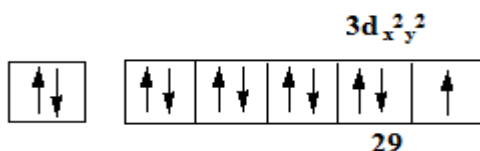


First Stage

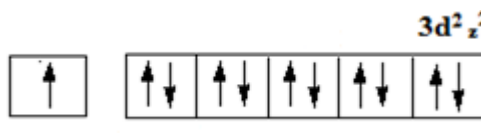
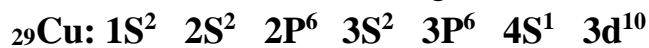


• Copper atom ${}_{29}^{64}\text{Cu}$

If the pairing of electrons continues, the twenty-ninth electron in the copper atom will share the twenty-fourth electron in the orbital, which has the symbol $3d_{x^2-y^2}$. Accordingly, we will get the following arrangement:



Once again, studies of atomic spectrometry have shown that the standard electronic arrangement and orbital diagram expected above are incorrect. The correct arrangement is:



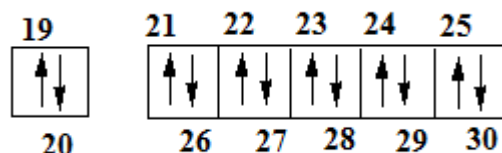
It is clear that the 3d secondary shell was filled with the highest number of electrons before the lower-energy 4S secondary shell. Thus, the electronic arrangement of the copper atom is the second arrangement that deviates from the established rules after the arrangement of the chromium element. This arrangement is called the saturated electronic arrangement because the secondary shell **d** has the highest permitted number of electrons. Completely filled term.

We will discuss later the reasons for the deviation of the electronic arrangement of copper from what is expected.

First Stage

- Zinc atom ${}_{30}^{65}\text{Zn}$

The zinc atom has an electronic arrangement and an orbital diagram that is consistent and identical to what is expected.

Miscellaneous notes:

1. It is noted from the above that the expected electronic arrangement of the atoms of the elements chromium and copper does not agree with what has been reached practically through various studies of the atomic spectra of these elements, which was described above as the correct electronic arrangement. It is worth noting that the phenomenon of departure from the expected electronic arrangement is not limited to the atoms of the two elements above, but rather includes dozens of atoms distributed in different locations in the middle part of the periodic table of atoms of chemical elements. But what draws attention and attention is that all these naughty atoms!! It belongs either to the group of elements called outer transition metal, or to the group of elements called inner transition metal.

The electronic arrangement of the outer transition element group ends in the secondary shell nd , while the electronic arrangement of the inner transition element group ends in the secondary shell $4f$ [n = principal quantum number]. Examples of the atoms of the internally disturbed transition elements!! That is, the correct electronic arrangement is contrary to what is expected: Molybdenum ${}_{42}\text{Mo}$, Silver ${}_{47}\text{Ag}$, Gold ${}_{79}\text{Au}$, Niobium ${}_{41}\text{Nb}$.

The content of the rule or principle that deals with the exit of the chromium atom and the copper atom is: When the expected electronic arrangement ends with $4\text{S}^2 3\text{d}^4$ [as for the chromium atom] or $4\text{S}^2 3\text{d}^9$ [as for the copper atom], the electronic arrangement is rewritten as $4\text{S}^1 3\text{d}^5$ or $4\text{S}^1 3\text{d}^{10}$, respectively. This means transferring or departing only one electron from the lowest-energy secondary shell, 4S , to the higher-energy secondary shell, 3d . This violates the rule of filling the lower-energy

First Stage

secondary shell before the higher-energy secondary shell, which is directly next to it in the order.


But the question remains: What are the reasons or influential factors that led to the unexpected correct electronic arrangement according to Aufbau's rules?

Before answering this question, we must mention that there is more than one explanation, justification, or answer to the above question. This means that there is no definitive and confirmed answer. However, we will present below the most common and accepted explanation.

The answer to the above question can be summarized as follows:

First: It is certain that the difference between the energy of the **4S** secondary shell and the **3d** secondary shell is very small, meaning that the two shells are very close in energy.

Second: A) In the case of the chromium atom ${}_{24}\text{Cr}$, the energy required to pair the two electrons in the **4S** secondary shell and then produce the expected electronic arrangement [**3d⁴ 4S²**] is that the energy of the electronic pairing is much higher than the energy difference between the low-energy **4S** secondary shell and the next secondary shell in Top energy **3d**. This relationship between the two energies leads to the electron entering individually into the **3d** shell and thus producing the correct electronic arrangement that is observed practically or experimentally, which is **3d⁵ 4S¹**.

The energy needed to overcome the forces of repulsion between two electrons and then pair the two electrons in one orbital  is called the electron pairing energy.

It can be expressed by the following relationship:-

$$\textit{Pairing energy} = \textit{Replusion energy} + \textit{Exchange energy}$$

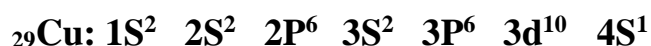
Exchange energy is one of the concepts of quantum mechanics.

(B): As for the correct electronic arrangement of the copper atom ${}_{29}\text{Cu}$, in addition to what was stated first above, and due to the increased influence of the influential nuclear charge Z^* on the electrons of the **3d** and **4S** secondary shells, the energies of the mentioned secondary shells decreased to a point where the energy of the **3d** secondary shell became less than the energy of the secondary shell. Secondary **4S**.

First Stage

Based on the rule that the lowest-energy secondary shell is filled first, the **3d** secondary shell is filled with ten electrons, leaving one electron to occupy the orbital or the **4s** secondary shell, and then the correct electronic arrangement is produced, which is not expected according to the energy arrangement of the secondary shells observed experimentally or practically.

Accordingly, we can express the standard electronic arrangement of the copper metal atom as follows:



Note that this form of arrangement of the secondary shells is more accurate than others.

The electronic arrangement that ends with **3d⁵ 4s¹** or **3d¹⁰ 4s¹** is called half-saturated and saturated, respectively, and their energies are lower than the energy of the **4s² 3d⁴** or **3d⁹ 4s²** arrangement. Atoms containing such low-energy electronic arrangements are also characterized by kinetic stability. Note that there are two types of stability, one of which is called **Dynamic Stability** and **Thermo Stability**.

1. It is clear from the above that the standard, complete, or complete electronic arrangement consists of a series of secondary shells arranged from left to right according to their increasing energy.

Each component (part) of this series consists of three components:

- (a) Secondary cover symbol (f, d, p, s).
- (b) A positive integer placed to the left of the shell symbol. This number is the principal quantum number (**n**) that refers to the main energy shell to which the secondary shell belongs, whose symbol is located to the right of the integer.
- (c) An integer placed in the upper right corner of the symbol for a particular secondary shell. This number symbolizes the number of electrons present that occupy that secondary shell.

As expected, the length of the chain representing the secondary shells increases with the increase in the atomic number (number of electrons) of the atom of the element whose standard or complete electronic arrangement is required to be written.

First Stage

In order to write a useful brief electronic arrangement, the electronic arrangement of the noble gases was used as a basis for the abbreviated notation of atoms of chemical elements. This abbreviated Noble Gas Notation is called the Noble Gas Notation. Before talking about the symbolization of the noble gas, we would like to learn briefly about the group of elements called the noble element group. This group forms the eighteenth column (in some classification and numbering systems, the column designated by the Latin symbol VIIIA) in the periodic table of atoms of chemical elements (see the periodic table to learn about this group).

All of these elements are found in the form of gases. The elements of this group are helium ${}^4_2\text{He}$, neon ${}^{20}_{10}\text{Ne}$, argon ${}^{40}_{18}\text{Ar}$, krypton, ${}^{84}_{36}\text{Kr}$ xenon, ${}^{131}_{54}\text{Xe}$ and radon ${}^{222}_{86}\text{Rn}$.

Its standard electronic arrangement is characterized by being a saturated arrangement, meaning that all secondary shells contain the maximum permissible number of electrons. For example:

Helium; ${}_2\text{He} : 1\text{S}^2$.

Neon; ${}_{10}\text{Ne} : 1\text{S}^2 2\text{S}^2 2\text{P}^6$.

Argon; ${}_{18}\text{Ar} : 1\text{S}^2 2\text{S}^2 2\text{P}^6 3\text{S}^2 3\text{P}^6$.

Krypton; ${}_{36}\text{Kr} : 1\text{S}^2 2\text{S}^2 2\text{P}^6 3\text{S}^2 3\text{P}^6 4\text{S}^2 3\text{d}^{10} 4\text{P}^6$.

We suffice with this number of examples. We return to the noble gas notation. To write the noble gas notation for the electronic arrangement of an atom of an element, we follow the following steps:

(A): Identify the noble gas element that immediately precedes the element whose electronic arrangement is to be written, by its location in the periodic table or by the number of its electrons.

Example: When writing the electronic arrangement of the atom of the element sodium ${}_{11}\text{Na}$, the noble element that immediately precedes it in terms of location in the periodic table or in terms of the number of its electrons is the element neon ${}_{10}\text{Ne}$.

(b): Write the complete or standard electronic arrangement for the required element. We return to the example of the sodium atom ${}_{11}\text{Na}$.

${}_{11}\text{Na} : 1\text{S}^2 2\text{S}^2 2\text{P}^6 3\text{S}^1$.

First Stage

(C) Rewrite the above electronic arrangement after replacing the first three shells that match the electronic arrangement, so the arrangement becomes as follows:



Or

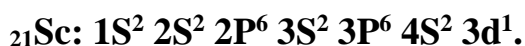


The arrangement containing (**a noble element**) is called the noble gas notation of the electronic arrangement.

Example: $_{21}\text{Sc}$

The element that precedes scandium $_{21}\text{Sc}$ in the periodic table or in terms of number of electrons is the noble element called argon $_{18}\text{Ar}$.

The complete electronic arrangement of scandium is:



The part of the complete electronic arrangement that is underlined matches or is similar to the complete electronic arrangement of the atom of the noble element argon, so we replace it with $[\text{Ar}]$ or $_{18}[\text{Ar}]$ and we obtain:



Exercise: Write the electron configuration called the noble gas notation for the following elements: $_{22}\text{V}$, $_{17}\text{Cl}$, $_{14}\text{Si}$, $_{9}\text{F}$.

It is noted from the above that the standard electronic arrangement consists of two parts, which are the part similar to the electronic arrangement of an atom of a noble gas element. This part is called the **Noble gas core**, or the center or heart of the noble gas, and the remaining part is called the outer shell or the **valence shell**.

The valence shell electrons determine the nature and chemical and physical properties of the element's atom. In contrast, the electrons of the shells, which we call the Noble gas core, do not participate in chemical reactions and do not determine the physical properties. Therefore, these electrons are of secondary importance compared to the electrons of the valence or outer shell.

First Stage

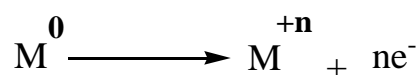
1. One of the benefits of writing or drawing an orbital diagram with the standard or complete electronic arrangement is that it gives us an easy opportunity to describe any electron in an atom or any atomic orbital using atomic quantum numbers.
2. Write the electronic arrangement of the ion.

Writing Electron Configuration for Ions

To express the electronic arrangement of positive ions and negative ions, the same previous methods used to express the electronic arrangement of electrically neutral atoms can be used.

- **Positive ions M^+**

Where **M** refers to the atom of an element and **+n** refers to the number of positive charges.



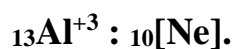
The above chemical equation indicates that an atom of the element **M** lost n-number of electrons and transformed into the ion **M^{+n}** . It is clear that the actual number of electrons remaining in the positive ion is less than the electrons of the electrically neutral atom by the amount **ne-**. [Where **n** is a positive integer, it does not mean the principal quantum number]. Therefore, when writing the electronic arrangement of the positive ion, we must reduce the atomic number (the number of protons = the number of electrons for the neutral atom) by the amount **n** of electrons, which is always equal to the number of positive charges appearing in the upper right corner of the chemical symbol for the ion.

Example: Write the electronic arrangement of the aluminum atom and the aluminum ion ${}_{13}\text{Al}^{+3}$?

• **In terms of the symbology of the noble gas - the aluminum atom.**



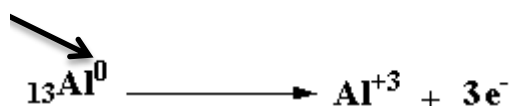
Aluminum ion this means that the electronic arrangement of the **Al^{+3}** ion is similar to the arrangement of the noble gas atom called neon.



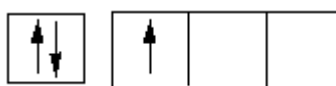
First Stage

When comparing the electronic arrangement of the atom and the aluminum ion, it becomes clear that the three electrons that the aluminum atom lost when it turned into the triple positive aluminum ion are the electrons of the last outer shell or the valence shell electrons, which are distinguished by being farthest from the nucleus and having more energy than the Noble Gas Core electrons.

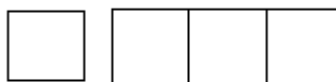
It means electrically neutral



- In terms of the standard or perfect electronic arrangement and the orbital diagram of the aluminum atom:



Note: For brevity, we have contented ourselves with writing the valence shell orbital diagram.



The secondary shell that is farthest from the nucleus or has the most energy is lost first, and after losing all its electrons, the atom is lost from the shell that is immediately next in line and has the lowest energy. Regarding the example of the aluminum ion above, the secondary shell, **3P**, lost first, and then the shell, **4S**, lost its electrons.

Exercise: Write the standard electron order for ${}_{16}\text{S}$, ${}_{16}\text{S}^{+2}$, ${}_{16}\text{S}^{+4}$, ${}_{16}\text{S}^{+6}$?

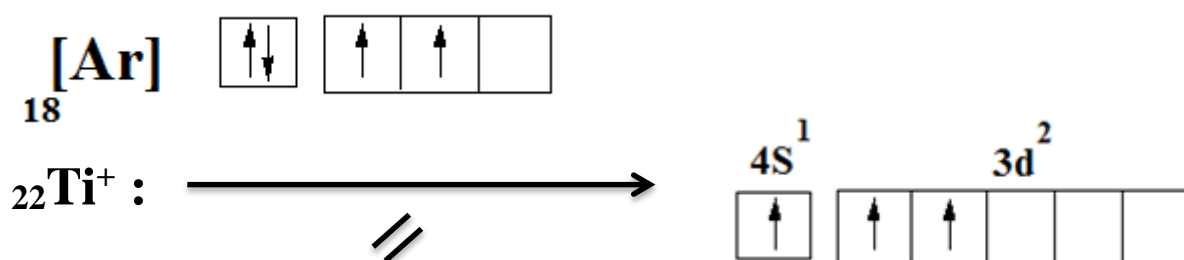
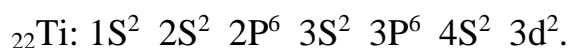
Writing the electronic arrangement of the ions of the external transition elements.

We previously mentioned that the electronic arrangement of the last outer shell (or valence shell) of the atoms of these elements can be expressed in the general formula $\text{ns}^a (\text{n}-1)\text{d}^b$, where **a** is an integer ranging from 2, 1, while **b** takes integer values from 1 to 10. The atoms of

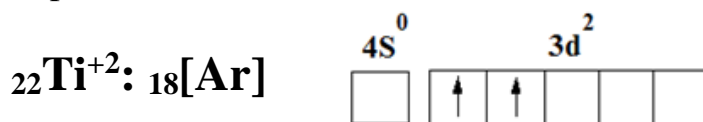
First Stage

these elements tend to lose one or more electrons from the last outer shell and form only positively charged ions. Exclusively and specifically, the $(n-1)d$ secondary shell loses its electrons before the $(n-1)d^b$ secondary shell, and there is no exception.

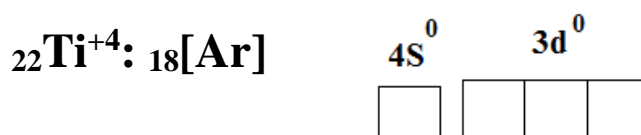
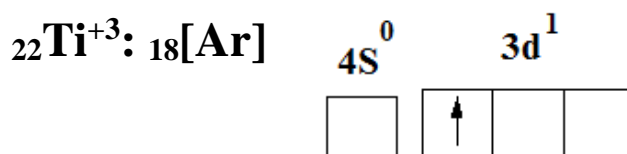
Example: Write the ground state electronic arrangement for ${}_{22}\text{Ti}$, ${}_{22}\text{Ti}^+$, ${}_{22}\text{Ti}^{+2}$, ${}_{22}\text{Ti}^{+3}$, ${}_{22}\text{Ti}^{+4}$.



When comparing the electronic arrangement of the outer shell of the titanium metal atom with its single positive charge ion, we can notice that the $4S$ shell lost one of its electrons during the process of transforming the atom into an ion. Note that we contented ourselves with writing the electronic arrangement of the valence shell only because of its importance.



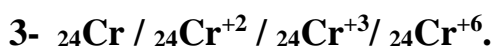
The ionization process from $\text{Ti}^+ \rightarrow \text{Ti}^{+2}$ was accompanied by the loss of the second and last electron to the $4S$ secondary shell. Therefore, any further ionization will lead to the gradual extraction of ions from the $3d$ secondary shell.



First Stage

It is clear that the electronic arrangement of the Ti^{+4} ion is similar to the electronic arrangement of the atom of the noble gas element called argon. Look at the position of $_{18}\text{Ar}$ in the periodic table of atoms of chemical elements, which precedes, as expected, the position of the titanium metal atom in the same table.

Question: Write the standard electronic arrangement and the electronic arrangement in terms of the noble element, as well as the orbital diagram for the following atoms and ions:

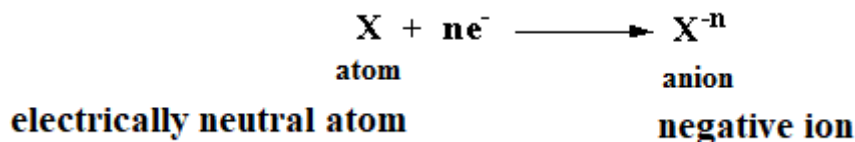


We noticed from the above that when ionized, the atoms of the external transition elements first lose one or more electrons as needed from the **4S** secondary shell and then as needed from the **3d** secondary shell.

Regarding the copper atom $_{29}\text{Cu}$, the above is expected and consistent with the rules of electronic construction because the **4S** secondary shell is higher in energy than the **3d** secondary shell. As for most transition element atoms, the loss of **4S** electrons before the **3d** secondary shell electrons is considered a departure from the rules of electronic structure, because **4S** is lower in energy than **3d**. So, how do we explain or explain this departure from the rules of electronic construction? To clarify this, we mention the following: The loss of one or more electrons from the valence or outer shell of transition element atoms leads to a decrease in the force of electrostatic repulsion between the remaining shell electrons. As a result of this decrease in the strength of repulsion and the fact that the energy difference between **3d** and **4S** is very small, the energy of **3d** becomes lower than the energy of **4S**, and according to the rules of electronic structure, the **3d** secondary shell is filled before the **4d** secondary shell with ions of the external transition elements.

*First Stage***Negative ions X^{-n}**

Where **X** it symbolizes an atom of an element and **n** is an integer that takes values from one and above. A negative ion is formed by adding one or more electrons to an electrically neutral atom of an element.

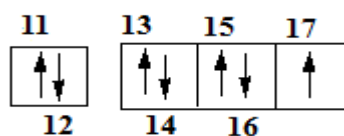
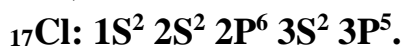


To write the electronic arrangement, one or more electrons are added to the last unfilled subshell, so we start adding from the point where the electronic arrangement of the electrically neutral atom ended.

Below are a number of illustrative examples.

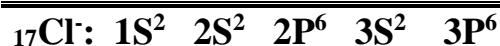
Example: Write the standard electronic arrangement, the orbital diagram, and the arrangement in terms of the atom of the noble gas element for the following atoms and ions:

(a): ${}_{17}\text{Cl}$, ${}_{17}\text{Cl}^-$.

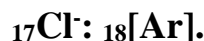


Before writing the electronic arrangement of the chloride ion ${}_{17}\text{Cl}^-$, look at the arrangement of the chlorine atom above, where you will notice the following:

1. The valence shell consists of $3\text{S}^2 3\text{P}^5$. For this reason, put a line under it in order to distinguish it from the rest of the secondary shells.
2. The 3P secondary shell contains room to accommodate only one electron, why only one? Try to know the answer. Therefore, any addition of electrons will start from it, and then we will use the highest energy shells according to their known gradient. Note this when writing the electronic arrangement of the chloride ion, which has a single, negative charge.

First Stage

electron no. 18



From the electronic arrangement of the chloride ion (${}_{17}\text{Cl}^-$), the following can be extracted:

1. The total number of electrons in a negative ion = the atomic number of the atom of that ion + the number of negative charges appearing at the top of the chemical symbol for the ion.

This is why the electronic arrangement of the chloride ion includes a total of 18 electron (1+17).

2. The electronic arrangement of the chloride ion ${}_{17}\text{Cl}^-$ in terms of the number of electrons and their distribution in the secondary shells of varying energy, matches the electronic arrangement of the atom of the noble gas element called Argon, ${}_{18}\text{Ar}$.

Atoms and ions (positive or negative) are expressed by the term **isoelectronic if they have the same number of electrons and the same electronic arrangement**. On this basis, ${}_{17}\text{Cl}^-$, ${}_{18}\text{Ar}$ is isoelectronic.

The following positive and negative ions are described as isoelectronic ${}_{9}\text{F}^-$, ${}_{11}\text{Na}^+$, ${}_{12}\text{Mg}^{+2}$, ${}_{13}\text{Al}^{+3}$. To verify the validity of this claim, write the standard electronic arrangement for these ions and compare among them in terms of the total number of electrons as well as their electronic arrangement.

Exercise: Look at the periodic table of elements and find an atom that forms a pair that can be described as isoelectronic with each of ${}_{3}\text{Li}^+$, ${}_{20}\text{Ca}^{+2}$, ${}_{8}\text{O}^-$, ${}_{8}\text{O}^-$.

Exercise: Write the standard electron arrangement, noble gas element notation, and orbital diagram for ${}_{7}\text{N}^{+5}$, ${}_{15}\text{P}^{+5}$, ${}_{15}\text{P}^{+3}$, ${}_{16}\text{S}^-$, ${}_{7}\text{N}^{-3}$.

First Stage

The Summary of Quantum Mechanical Model

- 1:** Electrons are located in specific Energy Levels.
- 2:** Electrons have no exact path around the nucleus.
- 3:** The model is entirely mathematical, the model is unable to tell exactly where an electron can be found but the model estimates the probability of finding an electron in a certain position at any given time.
(This is in line with Heisenberg's uncertainty principle).
- 4:** The model treated an electron as both particle and wave. This is in line with De Broglie equation.
- 5:** The model uses three quantum number (namely, n , ℓ , and m_ℓ) to describe the atomic orbital of hydrogen atom. In addition, it uses one quantum number (i.e. m_s) to describe the electron's spin within the orbital.
- 5:** In quantum mechanical model the total number of orbitals in each main energy level is equal to n^2 (Where n is the principle quantum number). The model limits the maximum amount of electron in each orbital may be vacant. Occupied with one or two electrons.

Similarities and Differences between Bohr Model and Schrodinger Model

- 1:** Bohr's Model is a physical model of the atom structure that can tell you where an electron can be found; whereas Schrodinger's model (quantum mechanical model) is entirely or completely mathematical, instead of being able to tell exactly where an electron can be found, the model gives the probability of finding an electron in a certain area of the space around the nucleus at any give time.
- 2:** Bohr's model established a certainty that electron can be found at a specific shell or orbit depending on their energy levels. Schrodinger model gives no such guarantee.
- 3:** In Bohr's model an electron moves in a circular path around the nucleus, whereas the Schrodinger model does not identify the exact path that an electron takes around the nucleus.
- 4:** Bohr's model treated an electron as a particle, whereas Schrodinger model treated an electron as both a particle and a wave. This means

First Stage

Bohr's model limited to one dimension, whereas Schrodinger's model account for all three dimension.

5: While Bohr model uses one quantum number (i.e n), Schrodinger's model uses three quantum numbers to describe the electron or orbital of an atom.

6: Similar to Bohr's model. Schrodinger (or the quantum mechanics) model describes the energy of Hydrogenic electron. In both theorier (or models).

- The principal quantum number determine the energy of a given electron,
- The energy levels of Hydrogenic atoms (or atom and ions) are identical.

This means that The Schrodinger's model does not provide more accurate values (energy values) than the Bohr's model did for energy states of Hydrogenic atom and ions.

Electronic Structure and Periodic Table

The periodic table consists of eight main numerical groups (groups, columns) and seven horizontal periods (periods).

1- Short Periods

a- First short periods

This period consists of only **two** elements and this period is filled with only two electrons. It will be discussed in the second semester.

b- Second short periods

This period consists of **eight** elements and is filled with only eight electrons. It will be discussed in the second semester.

c- Third short period

This period is filled with only **8** electrons, which means that it consists of eight elements. It will be discussed in the second semester.

2- long periods

a- first long period

This period consists of **18** components. It will be discussed in the second semester.

b- Second long period or fifth period

This period consists of **18** components. It will be discussed in the second semester.

First Stage

c- Third long period or sixth period

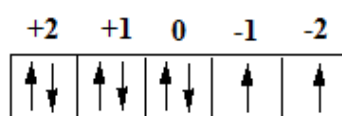
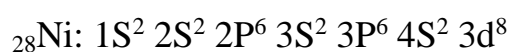
This period consists of **32** components. It will be discussed in the second semester.

d- Forth long period or 7th period

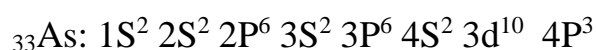
This period consists of **32** components. It will be discussed in the second semester.

Example: Write the electron configuration or. The electronic structure of the following element: **Ni⁺²**, **As**, **₁₀₂No**, **₁₀₃Lw** and determine the four quantum number of the last electron of each element?

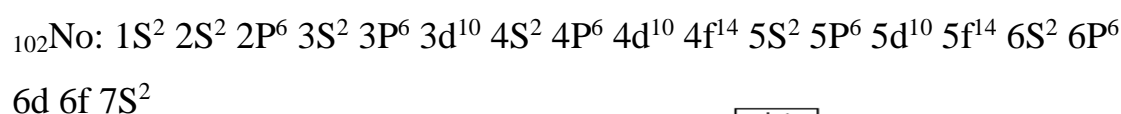
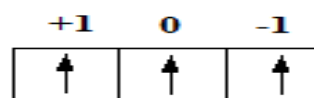
Solution:



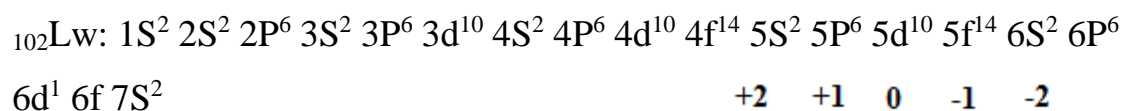
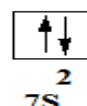
$n=3, \quad \ell=2, \quad m\ell=0, \quad m_s=-1/2$



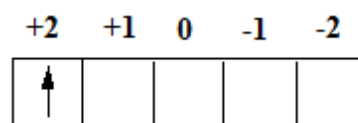
$n=4, \quad \ell=1, \quad m\ell=-1, \quad m_s=+1/2$



$n=7, \quad \ell=0, \quad m\ell=0, \quad m_s=-1/2$



$n=7, \quad \ell=2, \quad m\ell=+2, \quad m_s=+1/2$



"Main group elements" (group and columns)

The periodic table groups are divided into eight main groups, and at the same time they are divided into two secondary groups or two secondary categories, called group **A** and group **B**. The elements in the periodic table are divided into:

1- Noble gases VIII

2- Presentative elements

These elements are divided into two groups: [Noble gas] nS^{1-2} .

A- Alkali metals (elements)

First Stage**B- Alkali earth elements**

As for the third group **B**, it begins with the element boron and ends with the element thallium.

As for the fourth group **B**, it begins with carbon and ends with lead.

As for the fifth group **B**, it begins with the element nitrogen and ends with the element bismuth.

3- Main Transition Elements

These elements are divided into:

A- First transition elements series.

B- Second transition elements series.

C- Third transition elements series.

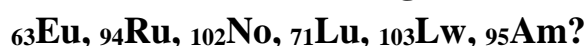
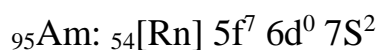
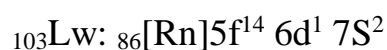
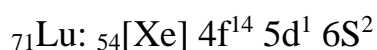
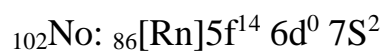
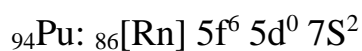
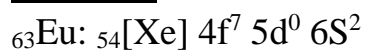
A- First transition elements series

Example: write the electronic structure of the following elements ${}_{40}\text{Zr}$, ${}_{72}\text{Hf}$?

*Inner Transition Elements*

The internal transition elements are called f-block elements, and their outer shell contains sublevels of the type f, d, s (ns , $(n-1)d$, $(n-2)f$) and the f orbitals are not filled. It consists of two families or classes: the lanthanides and actinides.

Example: Write the electronic structure of the following elements:

**Solution:**

Many of these elements have radioactive isotopes such as uranium ${}_{92}\text{U}$, plutonium ${}_{94}\text{Pu}$, and thorium ${}_{90}\text{Th}$.

First Stage

^{2S+1}L_J Term-Symbols "Russell-Sanders"

Previously, we were able to determine the energy of a single electron in an atom in a stable state by knowing the four quantum numbers. The location of the electron determined by or during the orbital angular momentum of the movement of this electron in the orbital within the secondary level ℓ located in the main shell n was also known. The direction of the momentum was also known. The orbital angle in terms of $m\ell$ and knowing the direction of the Permian angular momentum in terms of m_s was related to the electron in the atom.

But if we wanted to determine the energy of the multi-electron atom with all of these electrons it contains, then in this case, whether in the stable or excited state, it was possible to find a relationship to the energy of the atom by finding a relationship between the resultant orbital angular momentum of all electrons in terms of $m\ell$ and the resultant of the bermian angular momentum also for all electrons In terms of m_s .

$$L = m\ell_1 + m\ell_2 + m\ell_3 \text{-----} \quad L = \text{Restant orbital momentum}$$

Orbital Angular Momentum

$$S = ms_1 + ms_2 + ms_3$$

Spin Angular Momentum

when μ_1 The total angular momentum of the atom

$$\mu\ell = \sqrt{\ell(\ell + 1)} \frac{h}{2\pi}$$

$$\mu\ell = \sqrt{S(S + 1)} \frac{h}{2\pi}$$

In an atom in which the number of electrons is 30 or less, the overlap in the L-orbital motions and the S-periodic motions of the electrons is less than the overlap of the orbital motions alone or Permian motions alone, and to determine the energy of such atoms, the resultant orbital angular momentum and Permian angular momentum are linked by the **Russell-sandres rule**, where the value of J=

$$J = /L+S/, /L+S-1/, /L+S-2/ \text{----} /L-S/$$

J= Restant angular momentum of orbital and spin momentum of atom.

Therefore, the values of angular momentum can be calculated in terms of **J** as well, and are equal to:

$$\mu\ell = \sqrt{J(J + 1)} \frac{h}{2\pi}$$

First Stage**Notes on term symbols:-**

1. For the values of **L**, symbols are used in letters corresponding to the spectral letters that were used in the secondary levels, but in capital letters.

| | | | | | | | | | |
|----------|---|---|---|---|---|---|---|---|-------|
| $\ell =$ | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | ----- |
| | S | p | d | f | g | h | i | j | |

| | | | | | | | | | |
|-------|---|---|---|---|---|---|---|---|-------|
| $L =$ | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | ----- |
| | S | P | D | F | G | H | I | J | ----- |

2. To give the atomic state symbol **L** the appropriate letter for the element, you must first determine the value of **L**. This is done by writing the electronic arrangement of the element and knowing its atomic number, taking into account that the value of **L** is equal to **zero** if the element is at rest, saturated or semi-saturated, depending on the outer shell of the atom.
3. After that, the resultant of the spinous motions, **S**, is found and calculated to obtain the multiples of the spin multiblicity from the following ideal equation: **2S+1**. The value of **2S+1** is placed to the top left of the letter that represents the atomic state symbol. After that, the value of **J** is calculated for the state of the atom in all States and **J** values are indicated at the bottom right of the atomic state letter or symbol.
4. **J** takes only positive values, as well as zero, and the numbers do not necessarily have to be integers, unlike the values of **L**, because the values of **J** depend on the values of **S**, which sometimes take fractional numbers. The values of **J** are chosen for the most stable state of the atom.
 - a- When the outer shell (is less than half saturated, the lowest energy level of the atom is when the value of **J** is the lowest possible).
 - b- When the outer shell (is more than half saturated, the lowest energy [lowest energy level] of the atom is when the value of **J** is the highest possible).
 - c- When the outer shell is saturated or semi-saturated, there is one value for **J=S**.
5. With regard to the values of **2S+1**, the state of the atom is considered more stable (when **L** is constant) when the value of **2S+1** is as high as possible because this indicates an increase in

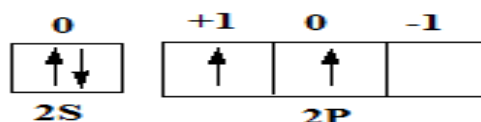
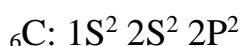
First Stage

individual electrons, meaning that the electronic distribution of the atom depends on Hund's rule.

6. With regard to the values of **L**, the stability of the atom increases with the increase in the value of **L** if the **J** and **2S+1** are constant.

When performing calculations for the values of **J**, **S**, **L**, the electronic distribution of the element within its period is written, meaning what corresponds to the internal electronic distribution that is similar to or contains one of the distributions of the noble elements, in which **L**, **S = 0** because they are saturated elements. Then the values of **J**, **S** are calculated from the stable external distribution.

Example: What is the atomic state symbol for carbon atom ${}_6\text{C}$ in its stable state?



$$L = m\ell_1 + m\ell_2 + m\ell_3 + m\ell_4$$

$$= 0 + 0 + 1 + 0 = 1 \rightarrow P$$

$$S = m_s_1 + m_s_2 + m_s_3 + m_s_4$$

$$= \cancel{1/2} - \cancel{1/2} + 1/2 + 1/2 = 1$$

$$2S+1 = 2 \times 1 + 1 = 3$$

$$J = /L+S/, /L+S-1/, \dots, /L-S/$$

$$= /1+1/, /1+1-1/, /1+1-2/, /1-1/$$

$$0 \quad 1 \quad 0 \quad 0$$

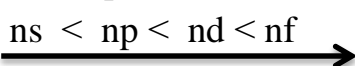
${}^3\text{P}_2 \quad {}^3\text{P}_1 \quad {}^3\text{P}_0$ because it is less than half saturated

Example: Write the term symbols or ${}^{2S+1}\text{L}_J$ of the following atoms and ions and give the more probable state symbol?

N, O, Fe, Cu, Ni, Zn⁺², Cr, Cr⁺³, Cr⁺⁶, Co⁺², Al⁺³

Penetration

The presence of an electron inside shell of other electrons is called penetration. As a result of the penetration the order of energy levels in the same quantum shell (n) of many electrons atom is typically.



Energy increases →

First Stage**Shielding or Screening**

If Bohr's laws were reviewed in calculating the speed of the electron.

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

$$v = \frac{nh}{2\pi mr}$$

(The energy of the electron in the orbit) $E_n = \frac{2\pi^2 me^4 Z^2}{n^2 h^2}$

$$\Delta E = \frac{2\pi^2 me^4 Z^2}{h^2} (1/n_1^2 - 1/n_2^2)$$

$$n_2 > n_1$$

But if we assume that the electron completely left the atom, then $n_2 = \infty$ and ΔE in this case corresponds to the ionization energy.

Ionization energy: It is the least energy required to completely displace or remove an electron from an atom and convert it into a positive ion. This energy is measured in energy units K J mole^{-1} , K cal mole^{-1} .

$$1\text{ev} = 23.6 \text{ K cal.mole}^{-1} = 96.49 \text{ K J mole}^{-1}$$

In the hydrogen atom, the value of $n = 1$, and thus the numerical value of the ionization potential of the hydrogen atom can be found according to the same law.

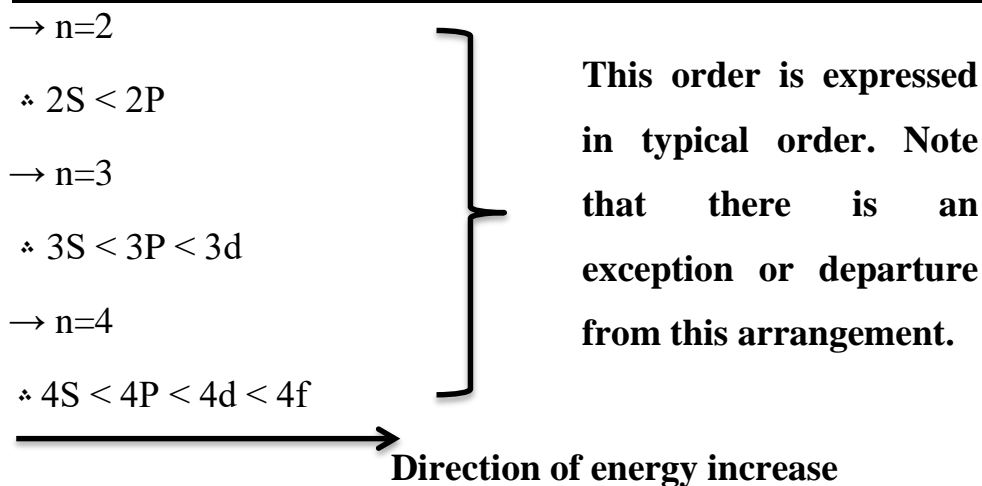


$$\text{IpH} = 13.6 \text{ ev}$$

$$\text{IP} = \frac{2\pi^2 (1.6 \times 10^{-19})^4 \times 9.11 \times 10^{-31} (1)^2}{(1)^2 (6.626 \times 10^{-34})^2}$$

$$\text{IpLi} = \text{IpH} * Z^{*2} / n^2$$

Shielding: The reduction of true nuclear charge (Z) by inner electron or orbitals to the effective nuclear charge (Z^*) that experiences by outer electrons or orbitals is called Shielding or Screening. For a given principle quantum number (n), S orbital is least screened or shielded and has the lowest energy; P, d, and f orbitals have successively higher energy.

First Stage

It was stated above indicates the diversity of the energies of the secondary shells of a particular primary shell in the multi-electron atom [such as ${}_6\text{C}$, ${}_7\text{N}$, ${}_8\text{O}$]. There is no variation in the energies of the secondary shells of excited atoms and hydrogen ions due to the complete lack of blocking in single-electron systems.

*Many Electrons Atoms and Ions**Important Terms*

It is an atom or ion with more than one electron. For example, ${}_2\text{He}$ and ${}_3\text{Li}$ and ${}_3\text{Li}^+$ are many electrons atoms and ion.

The Orbital Approximation

It is not possible to solve the Schrodinger equation, or it is not possible to obtain accurate, precise, or reliable solutions to the Schrodinger equation in the case of multi-electron atoms or ions. Therefore, in order to obtain the method in which the electrons are distributed in such atoms or ions, reliance was placed on the concept or idea of the orbital approximation. Which includes expressing the wave functions of the electrons of an atom or a multi-electron ion with their corresponding wave functions of a hydrogen atom or hydrogen-like ions. According to this concept, the electron of the helium atom, ${}_2\text{He}$, or the single positively charged lithium ion, ${}_3\text{Li}^+$, occupy an atomic orbital that has the same shape as the atomic orbital or wave function of the electron of the hydrogen atom. In any case, this concept is unable to give an idea about the size and energy of the atomic orbital of a multi-electron atom compared to its counterpart of a hydrogen atom.

Shielding Constant $Z^* = Z - S$

In general, the ionization potential of the second atom is higher than the ionization potential of the first atom, and the ionization potential of the third atom is higher than the ionization potential of the second atom, but it has been found in practice that the ionization potential of **Li** is **5.7 eV**, i.e. much lower than the ionization potential of hydrogen, and it is the correct value for the following reasons:

- 1- That the last electron of lithium is located in the **2S** orbital or **n = 2**, and this means that it is farther from the nucleus than the electrons located in the **1S** orbital or **n = 1**, which are closest to the nucleus, so the attraction of the nucleus on the ions of the outer shell located in **2S** is weaker than the attraction of the hydrogen atom. For the outer electron located in **1S**, that is, the energy required to lift the electron is less than the energy required to remove an electron in the hydrogen atom.
- 2- The nucleus of the lithium atom, which is **Z=3**, is surrounded by two **1S²** electrons revolving around the nucleus, which leads to blocking the charge of the nucleus from the third electron located in **2S¹**, meaning that the effect of the charge of the nucleus on the last electron is less than it is with **2S¹** electrons, so the nucleus' attraction to this electron is less. The energy required to remove the electron becomes low, and S orbital electrons are generally considered to be the most sensitive to the charge of the nucleus, or in other words more capable of blocking the charge of the nucleus than the rest of the other electrons. Also, the blocking of **1S** electrons is higher than the blocking of **2S** electrons.

← Increase of shielding

$$S > P > d > f$$

- 1- Increase of sensitivity towards nuclear charge.
- 2- Increase of attraction toward nuclear charge.
- 3- Increase of shielding or screening.

This means that what affects the electrons as their atomic number increases is not the total charge of the nucleus (**Z**), which represents the atomic number, but rather the amount of this charge that reaches the electron and is called the effective charge. We call it Effective nuclear

First Stage

charge, which is the charge that reaches. The electron after some or a percentage of it is blocked by the electrons in the inner shells, that is, after blocking. The effective charge can be calculated from the scientist Slater's equation:

$$Z^* = Z - S$$

Where :

$$Z^* = Z - S.$$

Z^* = effective nuclear charge.

Z = Total nuclear charge (atomic no.)

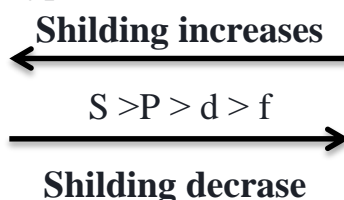
S = Shielding or Screening constant.

The Effective Nuclear Charge (Z^)*

H is the actual nuclear charge that a particular electron experiences. Effective nuclear charge depends on the numerical values of (n) and (ℓ) of the electron of interest, because electrons in different shells and subshells approach the nucleus to different extents. The effective nuclear charge is sometimes expressed in terms of the true nuclear charge (Z) and an empirical shielding constant ;by the writing:

$$Z^* = Z - S$$

Note that the experimental blocking constant varies depending on the secondary shell or the type of orbital.



It can be said that the closer the electron is to the nucleus, the relatively high the effective or actual nuclear charge it senses. The reason for this is due to the diversity of the distances between the various electrons and the nucleus, as well as to blocking by the electrons themselves.

For the purpose of understanding many topics related to the blocking constant, such as atomic size, electronegativity, and ionization energy, the scientist Slater developed a set of preliminary rules to estimate the extent of the approximate blocking of electrons. These rules can be summarized in the following points:

First Stage

To calculate the blocking constant **S** for an electron located in the ns or np secondary level, we follow the following steps:

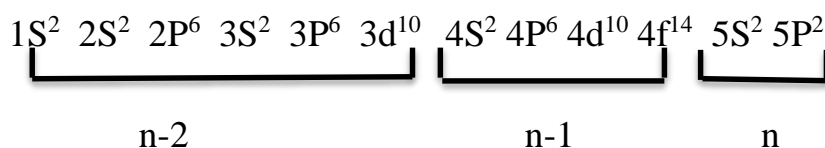
1. The electron configuration of the element is written from left to right according to the following order. This order is called the Slater order.
 2. If the electrons that belong to any group are located to the right of the electron for which the blocking constant is to be calculated, they do not contribute to the value of the blocking constant, or in other words, the value of the blocking constant has = **zero**.
 3. The electron belongs to the same main shell of the **ns** or np type to block the electron for which the blocking constant is to be calculated as **0.35**.
 4. Every electron belonging to the **n-1** main shell blocks the electron for which the blocking constant is to be calculated, with an amount of **0.85**.
 5. Every electron belonging to the main shell of type **n-2** or less is completely blocked, that is, by an amount = **1**.
- a- To calculate the blocking constant for an electron located in the secondary level of the **nd** or **nf** type, all electrons that are located to its left are completely blocked, that is, by one amount, and that are located within the same level. The level is blocked by **0.35**, or in other words, to calculate the blocking constant for an electron located in the secondary level of the nd or nf type, we use all the previous points except points **4.5**, which become as follows:

All electrons located in the groups to the left of the **nd** or **nf** group block the orbital with its blocking constant by an amount equal to **1**, that is, they are completely blocked.

Example: Calculate the effective nuclear charge for the nuclear charge for the electron no. 64 for the Ac element.

Solution

${}_{89}\text{Ac}: 1\text{S}^2 2\text{S}^2 2\text{P}^6 3\text{S}^2 3\text{P}^6 3\text{d}^{10} 4\text{S}^2 4\text{P}^6 4\text{d}^{10} 4\text{f}^{14} 5\text{S}^2 5\text{P}^6 5\text{d}^{10} 5\text{f}^0 6\text{S}^2 6\text{P}^6 6\text{d}^1 6\text{f}^0 7\text{S}^2$.



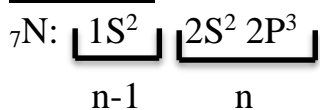
$$S = 3 \times 0.35 + 32 \times 0.85 + 28 \times 1 = 44.35$$

$$Z^* = 89 - 44.35 = 44.65$$

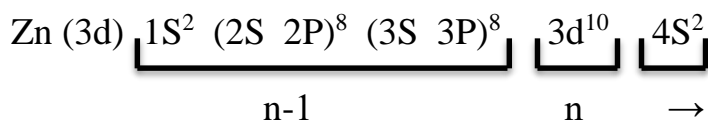
First Stage

Example: Find the effective nuclear charge on the last electron in the following elements and ions, ${}_{7}\text{N}$, ${}_{30}\text{Zn}$, ${}_{51}\text{Sb}$, ${}_{26}\text{Fe}^{+2}$, ${}_{22}\text{Ti}^{+2}$, ${}_{29}\text{Cu}$.

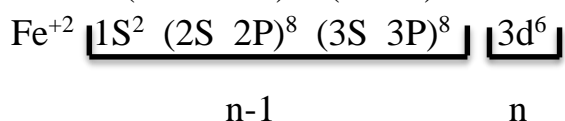
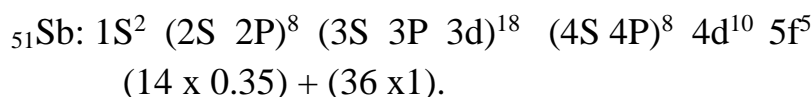
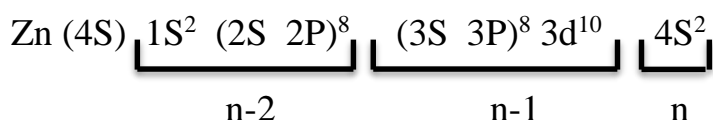
Solution:



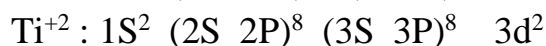
$$4 \times 0.35 + 2 \times 0.85$$



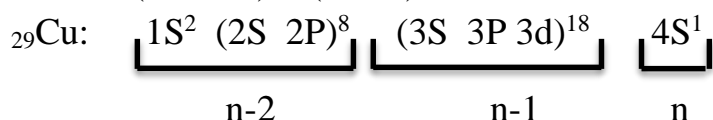
$$Z^* = 30 - 21.15 = 8.85$$



$$(5 \times 0.35) + (18 \times 1)$$

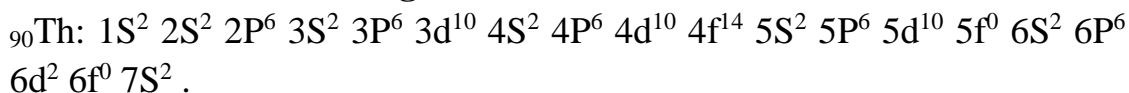


$$(1 \times 0.35) + (18 \times 1)$$



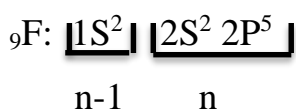
$$(0 \times 0.35) + (18 \times 0.85) + (10 \times 1)$$

Find Z^* for the following elements?



$$S = 9 \times 0.35 + 78 \times 1 = 81.15$$

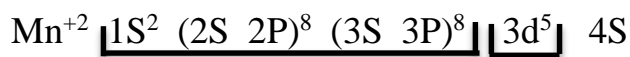
$$Z^* = Z - S = 90 - 81.15 = 8.85.$$



$$S = 6 \times 0.35 + 2 \times 0.85 = 3.8$$

First Stage

$$Z^* = Z - S = 9 - 3.8 = 5.2.$$



$$n-1 \qquad \qquad \qquad n$$

$$S = 4 \times 0.35 + 18 \times 1 = 19.4$$

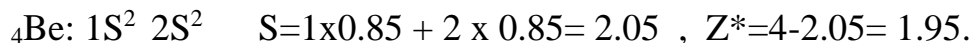
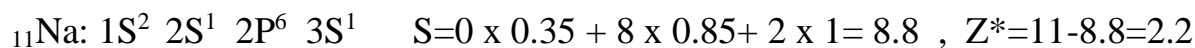
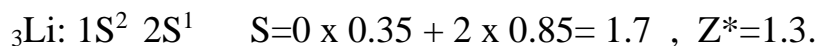
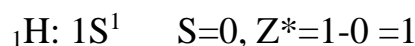
$$Z^* = Z - S = 25 - 19.4 = 5.6$$



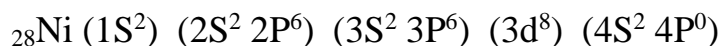
$$n-1 \qquad n$$

$$S = 5 \times 0.35 + 2 \times 0.85 = 3.45$$

$$Z^* = Z - S = 8 - 3.45 = 4.55$$



Example: Calculate the effective nuclear charge Z^* felt by one of the 3d electrons in the nickel atom ${}_{28}\text{Ni}$?



When calculating the total blocking constant, the $4S^2$ electrons are not included in the calculation because they are located in the **3d** plane with respect to the atomic nucleus.

$$S = (18 \times 1.00) + (7 \times 0.35)$$

(18) is the number of electrons present in the levels or orbitals $1S^2 \ 2S^2 \ 2P^6 \ 3S^2 \ 3P^6$, i.e. n-1 orbitals for 3d.

(7) The number of 3d electrons minus the electron to determine the nuclear charge that it senses.

$$= 18 + 2.45$$

$$= 20.45$$

$$Z^* = Z_{\text{True}} - S$$

$$= 28 - 20.45$$

$$= 7.55$$

Exercise (1): Find or calculate Z^* for an electron in 4S of a nickel atom ${}_{28}\text{Ni}$?

First Stage

Exercise (2): Calculate Z^* for an electron in (a) 5S, (b) 5P, and 5d (c) for the tin atom ${}_{50}\text{Sn}$?

✚ Which of the following pairs has the highest I_p and why?

a- Li or Cs

b- Li or F

c- Cs or F

Solution:

$${}_{3}\text{Li}: 1S^2 2S^1 \quad S=2 \times 0.85 = 1.7$$

$$Z^* = Z - S = 3 - 1.7 = 1.3$$

$$I_{p\text{Li}} = I_{p\text{H}} \times (Z^*)^2/n^2 = 13.6 \times (1.3)^2 / (2)^2$$

$$= 5.7118 \text{ eV.}$$

$${}_{55}\text{Cs}: 1S^2 2S^2 2P^6 3S^2 3P^6 3d^{10} 4S^2 4P^6 4d^{10} 5S^2 5P^6 6S^1$$

$$S = 0 \times 0.35 + 8 \times 0.85 + 46 \times 1 = 52.3$$

$$Z^* = Z - S = 55 - 52.3 = 2.7$$

$$I_{p\text{Cs}} = I_{p\text{H}} \times (Z^*)^2/n^2 = 13.6 \times (2.7)^2 / (6)^2$$

$$= 2.754 \text{ eV.}$$

Polarization:

Polarization: is the mutual distortion that occurs to the double ion A+B-. The scientist Fajan's assumed that the polarization that occurs to the negative ion results from the attraction between the electron cloud in it and the field of the positive ion, as well as from the repulsion of the positive ion with the nucleus of the negative ion. A similar polarization may occur for the positive ion. When the negative ion is large in size, the positive ion is able to polarize more easily, that is, the electronic cloud of both ions interferes with each other, and by increasing this interference to the final limit, the formation of a covalent bond occurs. The more polar the ion, the less polar the molecule.

Polarization can also be defined as the appearance of covalent properties in ionic compounds.

The scientist Fajan's has developed rules to determine the factors affecting polarity:

1. Polarization increases when the charge of the positive or negative ion is high.

The repulsion caused by a single-charged negative ion has fewer electrons than a double-charged negative ion. Also, a double-charged

First Stage

or triple-charged positive ion attracts electrons more strongly than a single-charged ion.

- Polarization increases when the size of the positive ion is small and the size of the negative ion is large due to the concentration of the positive charge on a small area due to the small size of the positive ion. The negative ion has a high polarizability. The larger the size of the negative ion, the greater the polarity, that is, the appearance of the covalent character of the bond increases, and thus the degree of melting decreases, since as the polarity increases in compounds, the degree of melting decreases.

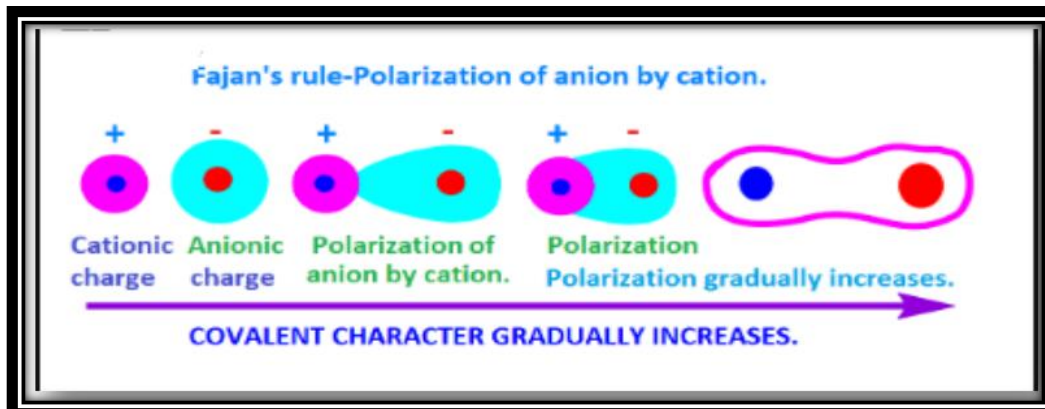


Table: Shows the decrease in melting points with Increase the polarization of the negative ion.

| Compound. | Negative ion | Melting point (Kelvin) |
|-------------------|-----------------|------------------------|
| CaF ₂ | F ⁻ | 1665 |
| CaCl ₂ | Cl ⁻ | 1009 |
| CaBr ₂ | Br ⁻ | 1003 |
| CaI ₂ | I ⁻ | 848 |

First Stage

Table: Shows the decrease in melting point with increase Polarization is the result of an increase in positive charge.

| Compound. | Positive ion | radius | Melting point (Kelvin) |
|-------------------|------------------|--------|------------------------|
| NaCl | Na ⁺¹ | 102 | 1073 |
| MgCl ₂ | Mg ⁺² | 72 | 985 |
| AlCl ₃ | Al ⁺³ | 53 | 453 |

Whereas **F < Cl < Br < I** are from one group, which is the group of halogens, the most polarized of which is iodine **I**, while the least polarized is fluorine **F**. The polarity increases for the following compounds:-



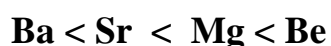
Polarization increases

We note that the positive ion is itself calcium, while the negative ion represents the group of halogens, where it represents the compound

CaF is a compound with **low polarity**, meaning it has an ionic character and a high melting point.

CaI is a **highly polar** compound, that is, it has a covalent nature and a low melting point.

In one group, the polarization of the positive ions increases from bottom to top (that is, as the radius decreases and the charge of the nucleus increases).

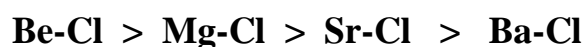


Polarization increases

The beryllium ion **Be** is the smallest in size (less radius), meaning it is more polarized.

As for the barium ion **Ba** it is the largest in size (largest radius), meaning it is less polarized.

So-:



Beryllium chloride is more covalent than the rest of its group members, while barium chloride is less covalent than the rest of its group

First Stage

members, according to the following table, where we notice that the melting points decrease as the covalent character increases.

Table: Shows Melting points of chloride compounds the second group

| Compound. | Positive ion | Melting point (Kelvin) |
|-------------------------|------------------------|------------------------|
| BeCl₂ | Be⁺² | 678 |
| MgCl₂ | Mg⁺² | 985 |
| SrCl₂ | Sr⁺² | 1145 |
| BaCl₂ | Ba⁺² | 1233 |

3. The polarization increases when the electronic arrangement of the positive ion is different from that of the noble gases.

Example:

AuCl, AgCl, CuCl.

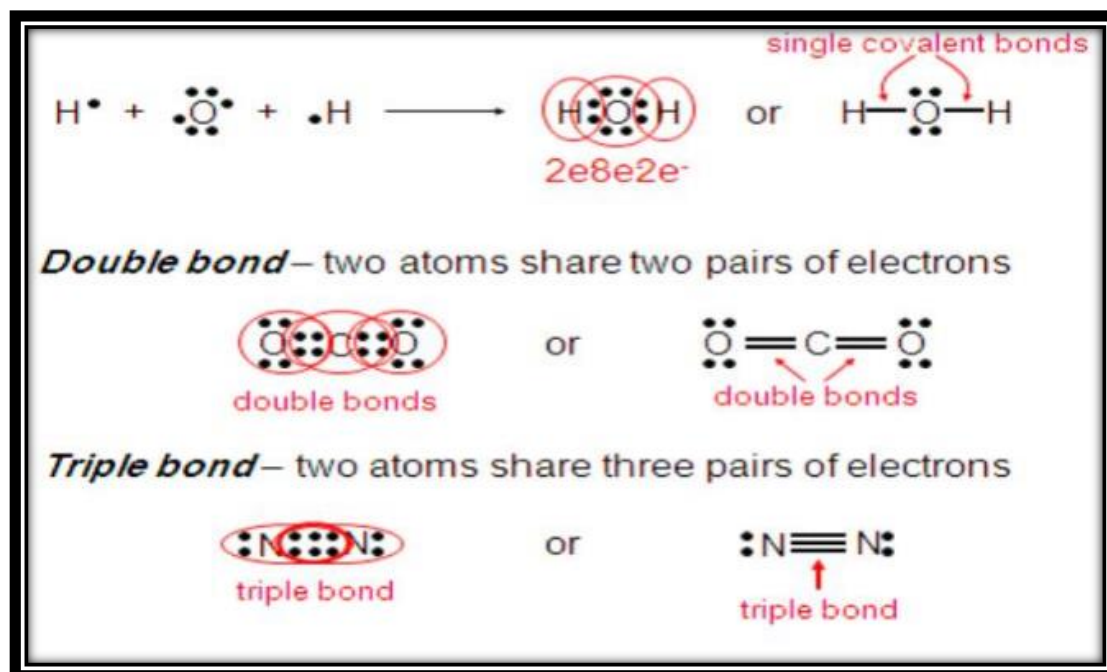
All of them carry a charge of +1 (they do not have an electronic arrangement for the noble gases) that is, they have a greater polarization than the positive ions that have the arrangement of the noble gases, that is, they have lower melting points and less solubility. Either **RbCl, NaCl, KCl**, and they all carry a charge of +1 (have an electronic arrangement similar to the noble gases). That is, it has less polarization and higher melting points than the above ions, in addition to a higher solubility than those that have an electronic arrangement that is not similar to that of the noble gases, according to the table below:

Table: Shows Comparison of the melting points of positive ions that have the noble gas arrangement and ions that do not have the order of the noble gases.

| Compound. | Melting point | Water solubility gm/100 ml |
|-------------|---------------|--------------------------------------|
| NaCl | 1073 | 36 |
| KCl | 1044 | 24 |
| RbCl | 995 | 91 |
| CuCl | 965 | 1.52 |
| AgCl | 728 | 1.5 x 10⁻⁴ |
| AuCl | 443 | It does not dissolve in water |

First Stage**Covalent Bond**

The covalent bond is the bond that is formed as a result of the sharing of two atoms bonded to one or more pairs of electrons, so that each atom contributes half of the number of these bonding electrons.

**The modern definition of covalent bond**

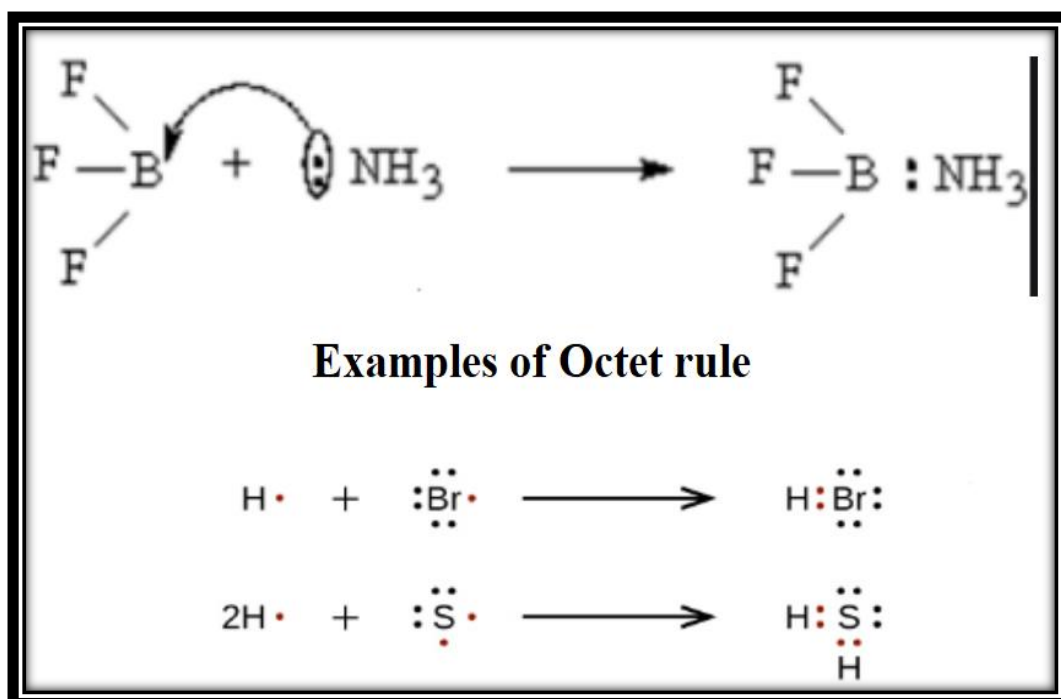
It is the amount of changes that occur or occur in energy when two atoms approach each other, so that the energy of the system becomes the least possible when the distance between the two atoms reaches a distance called the equilibrium distance. The length of the covalent bond is measured using X-ray diffraction.

Important rules for forming covalent bonds

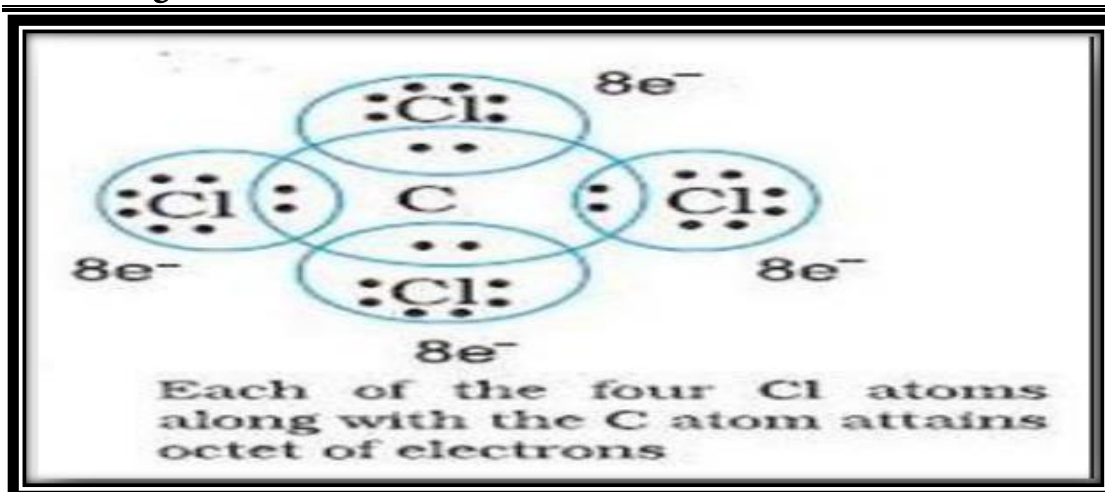
1. In order for a covalent bond to be formed, ionic bonding must not be possible, meaning that the energy of the electron of atom **A** is equal to or close to the energy of the electron of atom **B** for the union of the two atoms and the formation of the covalent bond.
2. The covalent bond results from the sharing of two electrons of close energy, and this means the necessity of double-spinning of these two electrons when forming the bond in application of the Pauli Exclusion Principle.

First Stage

3. The overlap of the orbitals of the two atoms that make up the covalent bond, and this overlap fills the space between the two atoms as a condition for bonding to occur.
4. When covalent bonds are formed between atoms whose orbitals are **S** and **P**, the maximum number of electrons is equal to **8** in the outer shell of each atom, and it is called the octet rule. This is called the Lewis octet structure, so the total sum of electrons for each atom is = 8 in the outer shell. Lewis theory proves that the formation of a stable compound requires that the atoms reach the noble gas arrangement, such as F_2 , NH_3 , and CF_4 . This is for elements whose number of electrons in the outer shell is not less than four. However, when the number of electrons in its outer shell is less than **4**, the octet rule does not apply to it. For example, in the compound BF_3 , the hydrogen atoms need only two electrons to satisfy their S-type outer shell, and the boron atom (**B**) does not have an electronic arrangement that reaches the noble gas because it contains **3** electrons. Only in the outer shell, boron compounds are called electron deficient covalent compounds. Therefore, they can interact with compounds in which an element or central atom has an electron pair that is not covalent.



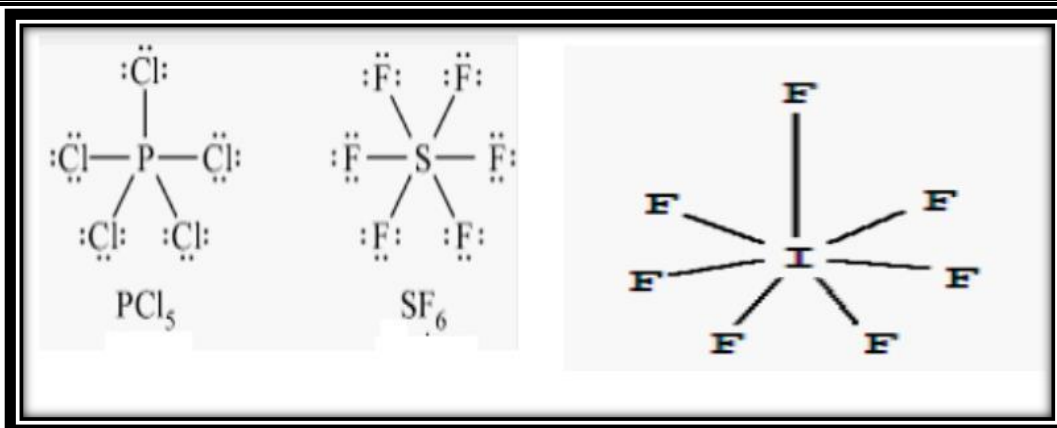
First Stage



| Element | Electron config. | Electron dot symbol |
|---------|-------------------------------------|---------------------|
| Li | [He]2s ¹ | Li [•] |
| Be | [He]2s ² | •Be• |
| B | [He]2s ² 2p ¹ | •B• |
| C | [He]2s ² 2p ² | •C• |
| N | [He]2s ² 2p ³ | •N• |
| O | [He]2s ² 2p ⁴ | •O• |
| F | [He]2s ² 2p ⁵ | •F• |
| Ne | [He]2s ² 2p ⁶ | •Ne• |

5. For the elements that have a **d** shell, their valence shell goes beyond the Lewis octet structure, as the third period has many elements with high valence numbers for metals and transition elements, and the number of outer shell electrons is what determines the covalent bonds and can be **5, 6, 7, 8** such as-:

First Stage

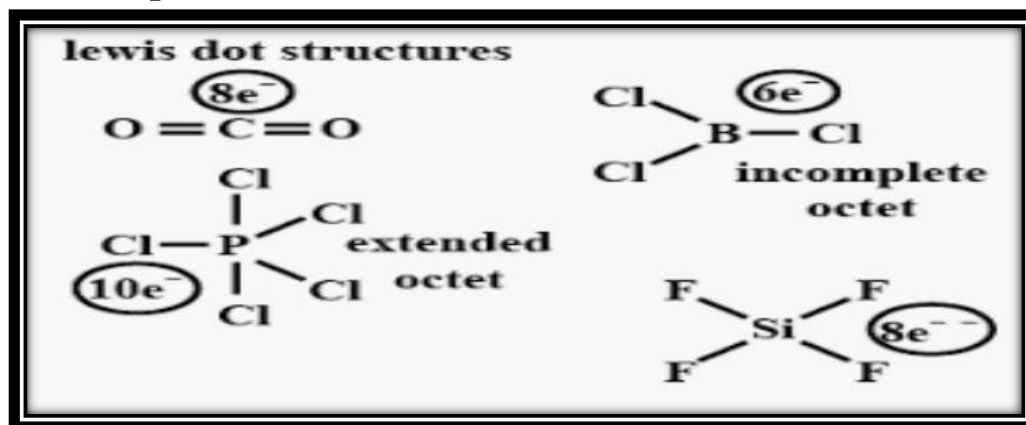


The exceptions to the eight octet rule can be summarized in the points below:

Exceptions to the Octet Rule:

- There are three types of ions or molecules that do not follow the octet rule:
 - Ions or molecules with an odd number of electrons 1 or 3.
 - Ions or molecules with less than an octet.
 - Ions or molecules with more than eight valence electrons (an expanded octet).

Ex: Phosphorus.



6. The repulsion between non-covalent electrons and covalent electrons must be as little as possible. As the number of non-covalent electrons increases, the energy of breaking the covalent bond decreases.



First Stage

In the F_2 molecule, there are non-allergic doublets that repel the allosteric electrons, causing the atoms to push. As a result, the bond length increases and its breaking energy decreases.

7. Covalent molecules have low melting points because they are electrically neutral, and the most common thing that links them is Van der Waals forces. They are characterized by their poor ability to conduct electrical current due to the lack of electrostatic forces.

| Physical properties of some selected compounds | | | |
|---|------------------------|-------------------------------|-------------------------------|
| Compound. | Type of Bonding | Melting temperature °C | Boiling temperature °C |
| F_2 | Nonpolar covalent | -220 | -188 |
| CH_4 | Nonpolar covalent | -183 | -162 |
| NH_3 | Polar covalent | -78 | 33 |
| CH_3Cl | Polar covalent | -64 | 61 |
| KBr | ionic | 730 | 1435 |
| Cr_2O_3 | ionic | ? | 4000 |

There are two theories to explain the formation of the covalent bond:

1. Valance bond theory.
2. Molecular orbital theory.

Ionic bond

An ionic bond is a type of chemical bond in which there is an electrostatic attraction between ions of opposite charge. That is, the positively charged ion forms a bond with the negatively charged ion, and transfers electrons from one atom to another. This type of chemical bond occurs when valence electrons are permanently transferred from one atom to another atom. An atom that loses electrons becomes a cation (positively charged), and an atom that gains electrons becomes an anion (negatively charged).

The concept of ionic bonding

An ionic bond is the bond through which electrically charged particles, called ions, interact to form ionic solids and liquids. This bond is the product of electrostatic interactions between hundreds of millions of ions, and is not limited to just a couple; That is, it bypasses the attraction between the positive charges towards the negative charge. Consider, for example, the ionic compound sodium chloride $NaCl$, better

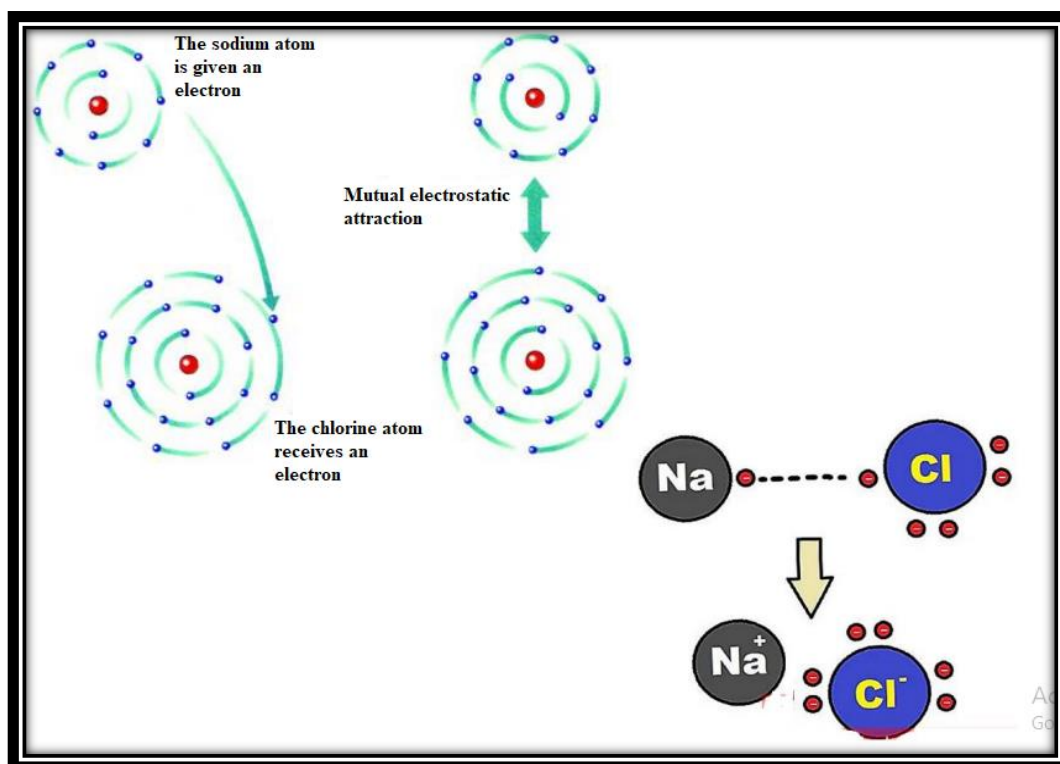
First Stage

known as table salt. In sodium chloride, the ionic bond predominates, so it consists of sodium ions Na^+ which is the positive ion or cation, and the chloride ion Cl^- which is the negative ion or anion.

Also known as an electrovalent bond or electrovalency, it is a type of bond that results from the electrostatic attraction between ions of opposite charge to each other in a chemical compound. This bond is created when the valence electrons move permanently from one atom to another atom. Atoms that lose electrons become positive ions (cations), while atoms that gain electrons become negative ions (anions). Ionic bonds are found in compounds known as ionic or electrovalent compounds, which can be simplified by the compounds that result from the interaction of nonmetals with alkali or alkaline earth metals. In such compounds, each positive ion is surrounded by negative ions, and each negative ion is surrounded by with positive ions.

Ionic bonding consists of three steps:

1. The active metal (metal) loses the electron furthest from the nucleus, and becomes positively charged.
2. The non-metal (non-metal) gains this electron, and becomes negatively charged.
3. An electrostatic attraction occurs between the positive and negative ions.



First Stage

For the formation of an ionic bond, the following conditions must be met:

1. There should be an active metal capable of losing one or more electrons with the lowest amount of energy, i.e. the smallest ionization potential of the metal atom (metal), and the elements to which the first condition applies are the first and second groups, which are the alkaline elements and the alkaline-earth elements, respectively.
2. That there is an active non-metal capable of gaining one or more electrons without the need for significant energy, i.e. a high electronic affinity for the metal (non-metal). The elements to which the second condition applies are the elements of the seventh and sixth groups.
3. The energy of crystal bonding and the energy of electrostatic attraction between ions are large.

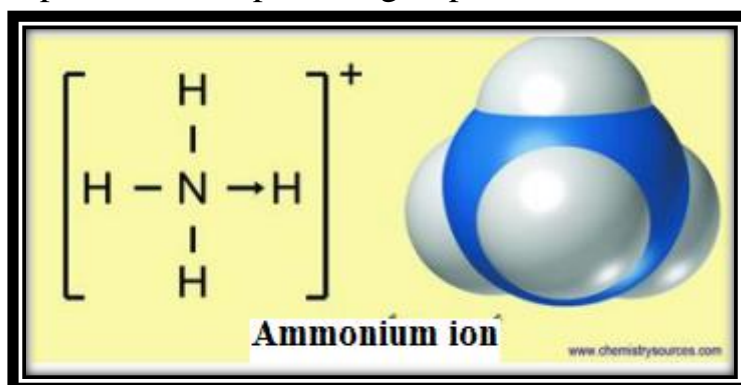
The ionization energy of metals is low, which makes them tend to lose electrons and form positive ions.

Nonmetals are distinguished by their high electrical affinity, and thus their eagerness to gain electrons and form negative ions.

When a non-metal atom approaches a metal atom, it tends to attract the valence electrons of the metal atom, so the positive and negative ions are formed, and as a result, an electrical attraction occurs between them, which leads to the release of a large amount of energy due to this attraction, so the energy of the resulting compound decreases.

The energy resulting from the attraction of negative and positive ions is known as the energy of the crystal lattice and is defined as the amount of energy resulting from the attraction of positive and negative ions to form one mole of crystals of a solid.

An ionic bond can arise between atomic groups such as the negative nitrate group NO_3^- with a positive group ion such as the ammonium group.



*First Stage**Examples of ionic bonds*

The element chlorine reacts with the element sodium to form the compound substance sodium chloride (sodium salt).

The atomic number of sodium is **(11)**, so its electronic structure is (2,8,1).

The atomic number of chlorine is **(17)**, and therefore its electronic composition is (2,7,8).

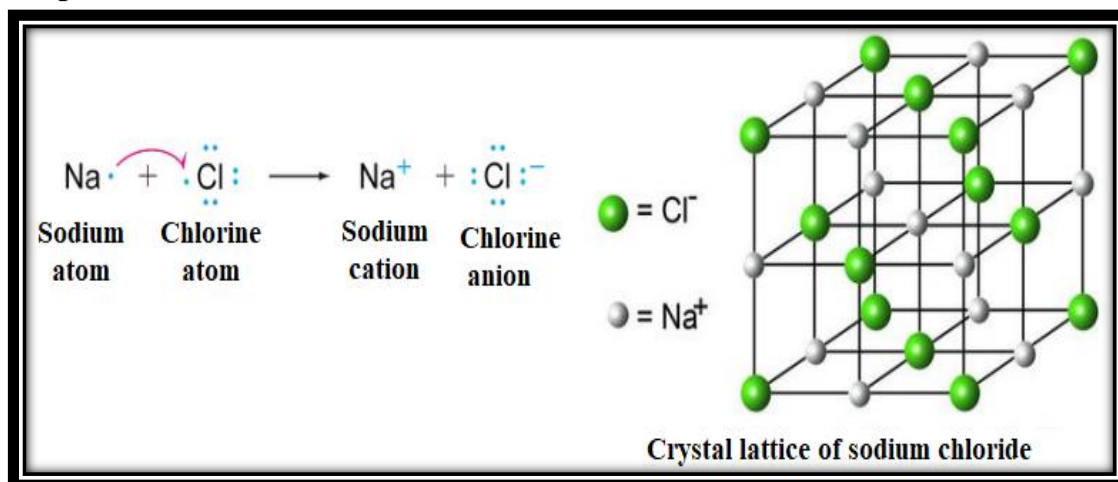
One electron moves from the outer shell of the sodium atom to the outer shell of the chlorine atom, thus forming a chloride ion, whose electronic structure is similar to neon.

The chlorine ion carries a negative electrical charge because the number of electrons in the orbitals has become eighteen **(18)**, while the number of protons in the nucleus is **(17)**.

Sodium ion carries a positive electric charge because the number of electrons in orbitals is **(10)**.

While the number of protons in the nucleus did not change **(11)**.

There is an electrostatic force of attraction between these two ions that keeps them in contact with each other.



Ionic compounds are formed when strongly electropositive atoms and strongly electronegative compounds interact with each other. Ions in a crystal of an ionic substance hold together through attractive forces between opposite charges. An ionic bond is not a bond in the real sense at all, as the ions attract each other just as the poles of a magnet attract each other. When an ionic substance is dissolved in water, the ions separate from each other and are able to move freely in the solution.

First Stage

General Properties of Ionic Compounds

Ionic compounds are characterized by the following:

1. It is distinguished from other solid materials in that it is brittle and cannot be malleable or ductile. The fragility of these materials is due to the fact that any attempt to compress the crystals leads to severe repulsion and the crystal shatters.
2. Its melts and solutions are characterized by good conduction of electrical current, due to the disintegration into positive and negative ions, and these ions conduct electricity.
3. It is characterized by high melting and boiling points, and the reason is due to the increased forces of attraction between the positive and negative ions, which act as double electrodes with a certain torque that results in the ions coming together.
4. It does not dissolve in organic solvents, but rather it dissolves in polar solvents such as water. The reason for the dissolution of ionic substances in polar solvents is due to the formation of a type of bond between the ion and the polar solvent molecules.
5. The reaction is fast and complete, because the reaction occurs once the ions collide.