

Introduction

The science known as spectroscopy is a branch of physics that deals with the study of the radiation absorbed, reflected, emitted, or scattered by a substance. Although, strictly speaking, the term radiation only deals with photons (electromagnetic radiation), spectroscopy also involves the interactions of other types of particles, such as neutrons, and protons, which are used to investigate matter.

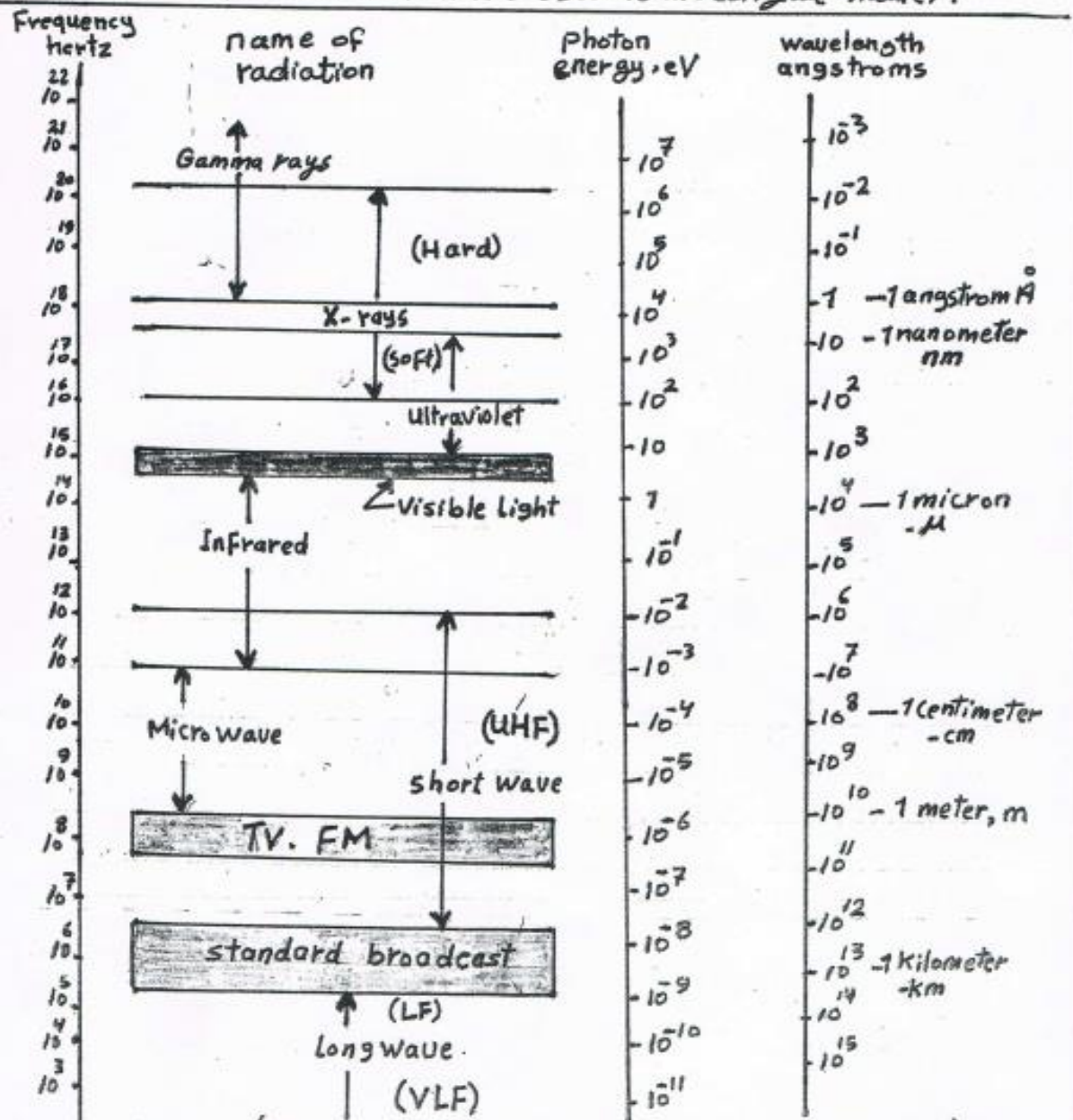
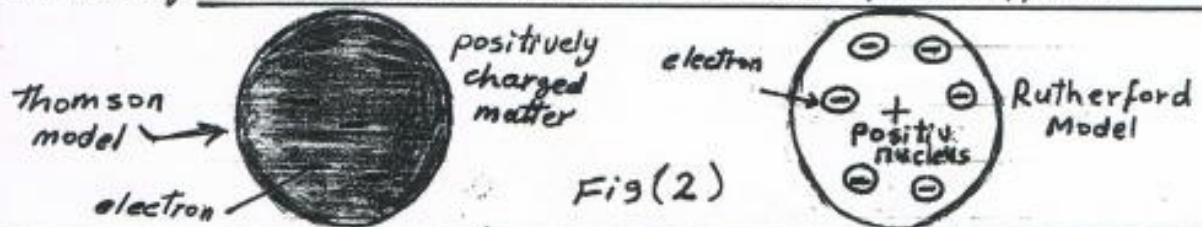


FIG (1) (the spectrum of electromagnetic radiation)

Atomic structure :

In 1898 the British physicist J.J Thomson suggested that the atoms are just positively charged lumps of matter with electrons embedded in them like raisins in fruitcake Fig(2). because Thomson had played an important role in discovering the electron, his idea was taken seriously. but the real atom turned out to be quite different.



In 1911 Geiger and Ernest Marsden as the Rutherford suggested, they used the alpha particles emitted by certain radioactive elements. Alpha particles are helium atoms that have lost two electrons leaving them with a charge of $(+2e)$. these particles can travel in air a few centimeters before they are stopped, but in a vacuum they travel long distance without losing energy. Rutherford apparatus is shown in Fig (3)

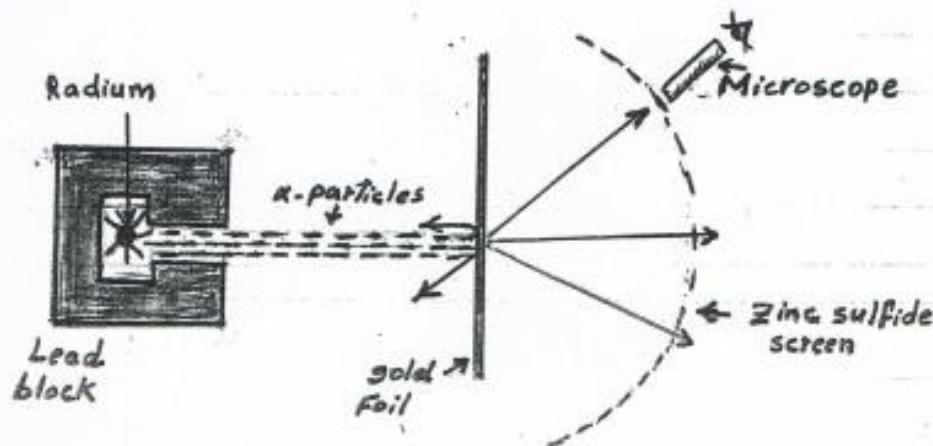


Fig (3)

Radium was placed in a cavity at the end of a narrow tunnel in a lead block. Alpha particles were emitted in random directions by this source and the lead absorbed all except those emitted along the axis of the tunnel. This beam of (α -particles) was directed at a thin gold foil. A zinc sulfide screen, which gives off a visible flash of light when struck by (α -particles), was set on the other side of the foil with a microscope to see the flashes.

According to the Thomson model in which the electric charge inside an atom is assumed to be uniformly spread through its volume, hence it was expected that the α -particles would go right through the foil. But they found that although most of (α -particles) indeed were not deviated by much, but a few were scattered through very large angles, and some were even scattered in the backward direction. Rutherford assumed that the positive, massive part of the atom was concentrated in a very small volume at the center of the atom. This core, now called the nucleus, is surrounded by a cloud of electrons, which makes the entire atom electrically neutral.

Spectral Series :-

A century ago the wavelength in the spectrum of an element were found to fall into sets called a spectral series. The first series was discovered by J.J. Balmer in 1885 of the hydrogen spectrum Fig (4) shows the Balmer series.

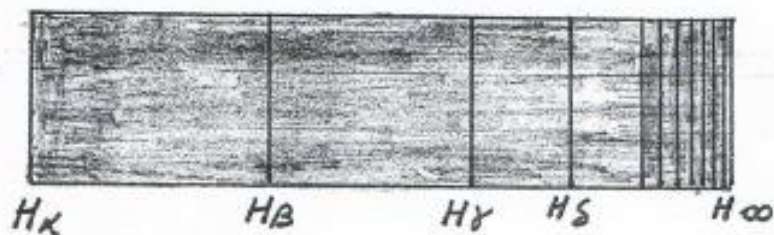


Fig (4)

The line with longest wavelength 6563 \AA is designated (H_{α}) and the next wavelength (4863 \AA) is designated (H_{β}). as the wavelength decreases, the lines are found closer together and weaker in intensity until there are no further separate lines, just continuous spectrum. Balmer formula for the wavelengths which is empirical formula of this series is :-

$$\frac{1}{\lambda} = R \left(\frac{1}{2^2} - \frac{1}{n^2} \right) \quad n = 3, 4, 5, \dots \quad \text{----- (1)}$$

the quantity (R), known as the Rydberg constant has the value

$[R = 1.097 \times 10^7 \text{ m}^{-1} = 1.097 \times 10^2 \text{ nm}^{-1}]$. the H_{α} line corresponds to $n=3$, the H_{β} line to $n=4$ and so on. The Balmer series confined in the visible region of the Hydrogen spectrum. in the ultraviolet and infrared regions fall into several other series. Lyman series in the ultraviolet and those wavelengths are given by the formula.

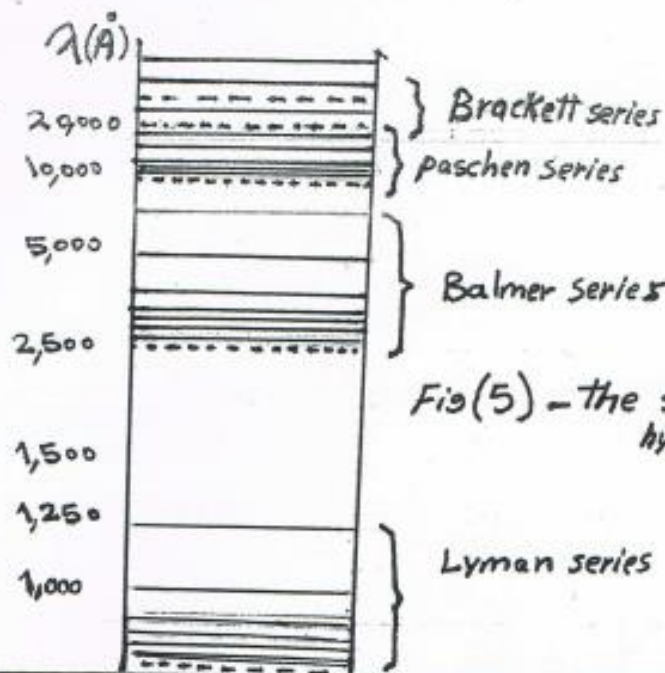
Lyman
$$\frac{1}{\lambda} = R \left(\frac{1}{1^2} - \frac{1}{n^2} \right) \quad n = 2, 3, 4, \dots \quad \text{----- (2)}$$

in the infrared region, three spectral series have been found, and which the wavelengths are given by the formulas.

paschen
$$\frac{1}{\lambda} = R \left(\frac{1}{3^2} - \frac{1}{n^2} \right) \quad n = 4, 5, 6, \dots \quad \text{----- (3)}$$

Brackett
$$\frac{1}{\lambda} = R \left(\frac{1}{4^2} - \frac{1}{n^2} \right) \quad n = 5, 6, 7, \dots \quad \text{----- (4)}$$

pfund
$$\frac{1}{\lambda} = R \left(\frac{1}{5^2} - \frac{1}{n^2} \right) \quad n = 6, 7, \dots \quad \text{----- (5)}$$



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Fig(5) - the spectral series of hydrogen

The Bohr Model and Theory of the atom :-

In Bohr's model of the atom an electron of charge (e), mass (m_e) and tangential speed (v) revolves in a circular orbit of radius (r) around a massive nucleus having a positive charge Ze . The centripetal force acting on the orbiting electron is the electrostatic force of attraction of nuclear charge, then

$$F_e = F_c$$

$$F = \frac{1}{4\pi\epsilon_0} \frac{Ze \cdot e}{r^2} = \frac{mev^2}{r} \quad (6)$$

From this equation we find that

$$v^2 = \frac{Ze^2}{4\pi\epsilon_0 m_e r} \quad (7)$$

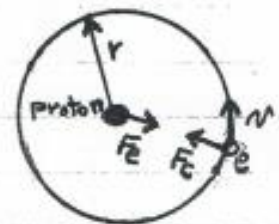


Fig (6)

For the hydrogen atom Bohr introduced a restrictive conditions which is known of Bohr's postulates. The first postulate is that (i) [Only those orbits occur for which the angular momenta of the planetary electron

are integral multiples of $\left(\frac{h}{2\pi}\right)$ that is $\frac{nh}{2\pi}$.], here (n) is any integer, h is plank's constant. the first postulate is

$$m_e v r = n \frac{h}{2\pi} = n\hbar \quad \text{--- (8)}$$

(\hbar) called h -bar, $n = 1, 2, 3, \dots$

after eliminating (v) between eqs (7) (8) we find the permitted orbits in hydrogen atom are only those that have radii

$$r_n = \frac{\epsilon_0 \hbar^2 n^2}{\pi m_e z e^2} \quad \text{--- (9)}$$

with numerical values inserted, this gives $r_n = (5.29 \times 10^{-11}) n^2 \text{ m}$ or $r_n = (0.529) n^2 \text{ \AA}$ where $z=1$ for H-atom, thus the first Bohr has a radius of 0.529 \AA , the second has a radius of 2.116 \AA , etc. the total energy (E) of the electron in H-atom is the sum of its kinetic and potential energies which are.

$$\left(E_K = \frac{1}{2} m_e v^2 = \frac{e^2 z}{8\pi\epsilon_0 r} \right), \left(E_P = \frac{-ze^2}{4\pi\epsilon_0 r} \right) \quad \text{where } z=1 \text{ for H-atom}$$

(the minus sign follows from the choice of $E_P = 0$ at $r = \infty$, that is, when the electron and proton are infinitely far apart.) Hence

$$E = E_K + E_P = \frac{ze^2}{8\pi\epsilon_0 r} - \frac{ze^2}{4\pi\epsilon_0 r}$$

$$\text{then } E = -\frac{ze^2}{8\pi\epsilon_0 r} \quad \text{--- (10)}$$

by using the eq (9) to eliminate the (r) we find that:

$$E_n = -\frac{m_e e^4 Z^2}{8 \epsilon_0^2 h^2 n^2} \quad \text{----- (11)}$$

where $n = 1, 2, 3, \dots$ For the energy states that it is possible for the electron to have. the integer (n) is called the total or principle quantum number, the values of (n) determine the energies of the states. the energy required to remove an electron from a particular state to infinity is called the (Binding energy) of that state, which its numerically equal to E_n .

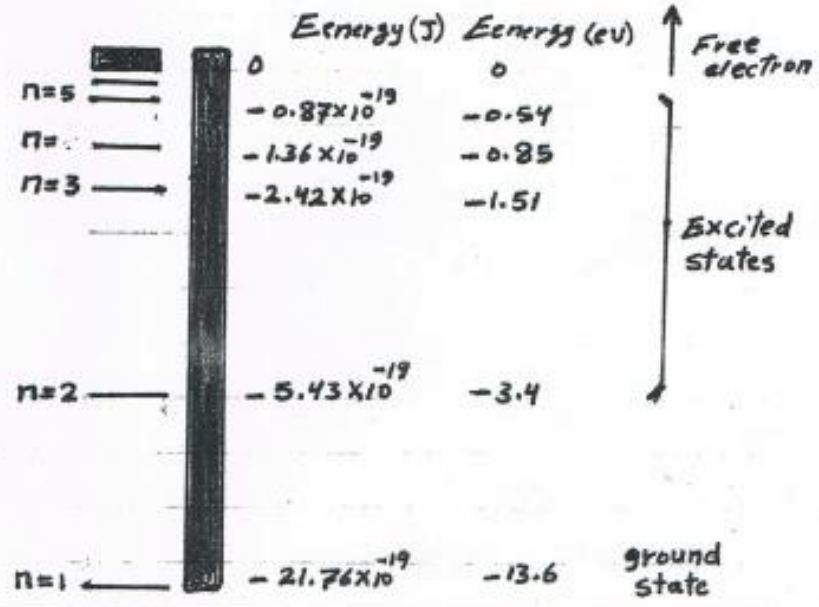


Fig (7)
Energy levels of the (H-atom)

According to classical theory, an orbital electron should radiate energy because of its centripetal acceleration. Bohr had to devise a theory which would violate this classical prediction and its contained in his second postulate (ii) which states that (no electron radiates energy so long as it remains in one of the orbital energy states, and that radiation occurs only when an electron goes from a higher energy state to a lower one, the energy of the quantum of radiation, $h\nu$, being equal to the energy difference of the states.)

let the quantum number of higher energy state is n_2 , and for lower state n_1 , ($n_2 > n_1$), then the second Bohr postulate can be written as

$$h\nu = E_{n_2} - E_{n_1} \quad \text{--- (12)}$$

substituting for the energies from eq (10), we have for the frequency of the emitted radiation.

$$\nu = \frac{me^4 Z^2}{8\epsilon_0^2 h^3} \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \quad \text{--- (13)}$$

in terms of wave number

$$\tilde{\nu} = \frac{1}{\lambda} = \frac{\nu}{c} = \frac{me^4 Z^2}{8\epsilon_0^2 h^3 c} \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \quad \text{--- (14)}$$

comparing eq (14) with any equation of hydrogen spectral series like Balmer, Lyman, Paschen, ... shows that both have the same form, and the constant factor of the Bohr formula is the Rydberg constant. we find that, since $Z=1$ for hydrogen atom

$$R = \frac{me^4}{8\epsilon_0^2 h^3 c} = 1.0973731 \times 10^7 \text{ m}^{-1} \quad \text{--- (15)}$$

Equation (14) states that the radiation emitted by excited (H-atoms) where ($Z=1$) should contain certain wavelengths only. These wavelengths furthermore, fall into definite sequences that depend upon the quantum number n_f (F-Final) of the Final energy level of the electron, here (n_f) will be equal to (n_1) in the equation (14), i.e. ($n_f = n_1$), Fig (8), then the calculated Formulas for the First Five series are:

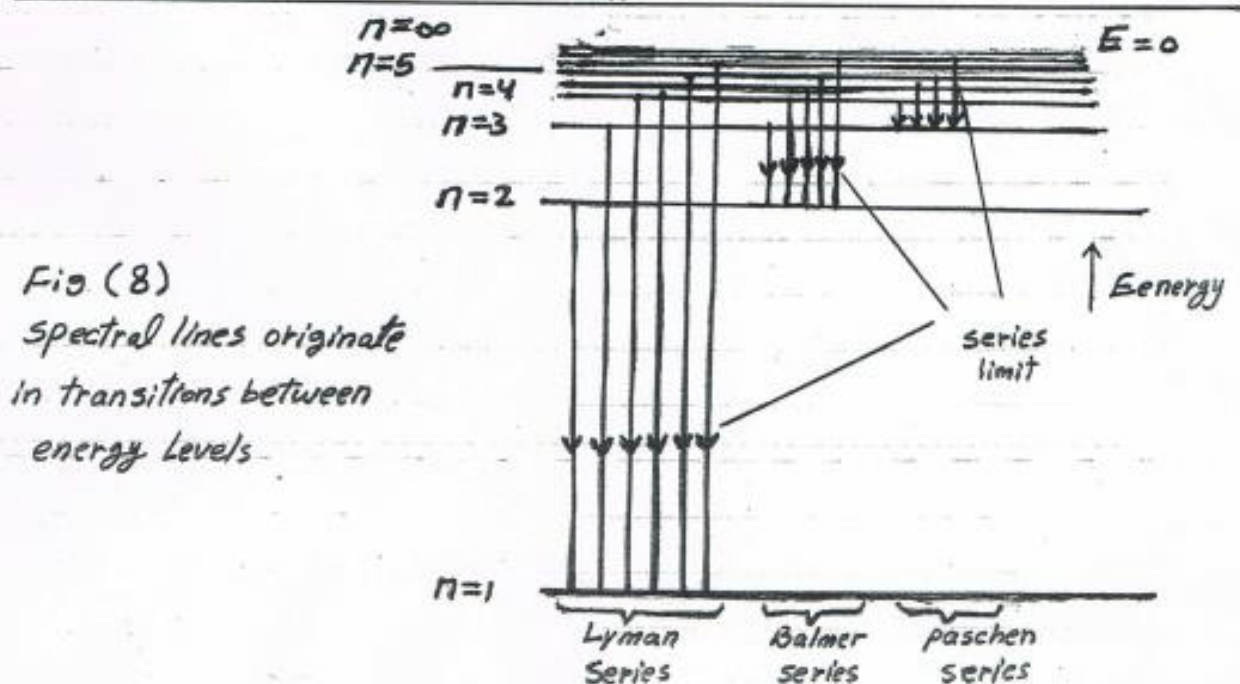
$$\text{Lyman } n_f = n_1 = 1 : \frac{1}{\lambda} = -\frac{E_1}{hc} \left(\frac{1}{1^2} - \frac{1}{n^2} \right) \quad n=2,3,\dots$$

$$\text{Balmer } n_f = n_1 = 2 : \frac{1}{\lambda} = -\frac{E_1}{hc} \left(\frac{1}{2^2} - \frac{1}{n^2} \right) \quad n=3,4,\dots$$

$$\text{Paschen } n_f = n_1 = 3 : \frac{1}{\lambda} = -\frac{E_1}{hc} \left(\frac{1}{3^2} - \frac{1}{n^2} \right) \quad n=4,5,\dots$$

$$\text{Brackett } n_f = n_1 = 4 : \frac{1}{\lambda} = -\frac{E_1}{hc} \left(\frac{1}{4^2} - \frac{1}{n^2} \right) \quad n=5,6,\dots$$

$$\text{Pfund } n_f = n_1 = 5 : \frac{1}{\lambda} = -\frac{E_1}{hc} \left(\frac{1}{5^2} - \frac{1}{n^2} \right) \quad n=6,7,\dots$$



Schrodinger's Equation For The Hydrogen Atom :

A hydrogen atom consists of a proton, a particle of electric charge $+e$ and an electron, a particle of charge $-e$ which is 1836 times lighter than the proton. Schrodinger's equation for the electron in three dimensions, which is what we must use for the H-atom is

$$\frac{-\hbar^2}{2m} \left(\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right) + V \Psi = E \Psi \quad \text{--- (1)}$$

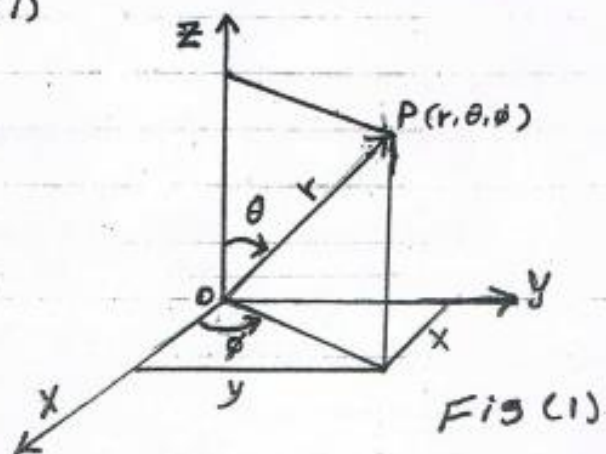
$$\text{and } \frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} + \frac{2m}{\hbar^2} (E - V) \Psi = 0 \quad \text{--- (2)}$$

The potential energy $V(r)$ here is the electric potential energy of a charge $(-e)$ when it is the distance (r) from another charge $(+e)$.

$$V = \frac{-e^2}{4\pi\epsilon_0 r} \quad \text{--- (3)}$$

Since V is a function of (r) rather than x, y, z , we cannot substitute eq (3) directly into eq (2), and one can express V in terms of the cartesian coordinates x, y, z by replacing (r) by $\sqrt{x^2 + y^2 + z^2}$ or another one can express schrodinger's equation in terms of the spherical polar coordinates (r, θ, ϕ) as defined in Fig (1)

$$\begin{aligned} x &= r \sin \theta \cos \phi \\ y &= r \sin \theta \sin \phi \\ z &= r \cos \theta \end{aligned}$$



The spherical polar coordinates r, θ, ϕ of the point (P) shown in Fig (1) have the following interpretations :

r = length of radius vector From origin (O) to point (P) .

$$r = \sqrt{x^2 + y^2 + z^2}$$

θ = angle between radius vector and +z axis (zenith angle) .

$$\theta = \cos^{-1} \frac{z}{\sqrt{x^2 + y^2 + z^2}} = \cos^{-1} \frac{z}{r}$$

ϕ = angle between the projection of the radius vector in the (xy) plane and the (+x-axis) measured in the direction shown (azimuth angle)

$$\phi = \tan^{-1} \frac{y}{x}$$

In spherical polar coordinates schrodinger's equation is written

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} + \frac{2m}{\hbar^2} (E - V) \psi = 0$$

----- (4)

substituting eq(3) and multiplying the entire equation by $r^2 \sin^2 \theta$ we obtain

$$\sin^2 \theta \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) + \sin \theta \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{\partial^2 \psi}{\partial \phi^2} + \frac{2mr^2 \sin^2 \theta}{\hbar^2}$$

$$\left(\frac{e^2}{4\pi\epsilon_0 r} + E \right) \psi = 0 \quad \text{----- (5)}$$

Equation (5) is the partial differential equation for the wave function ψ of the electron in (H-atom), which it obeys the conditions of the wave

Function such as that Ψ be normalizable and its derivatives be continuous, single valued at each point (r, θ, ϕ) .

Separation of Variables .

The advantage of writing Schrodinger's equation in spherical polar coordinates for (H-atom) in this form eq(4) and eq(5) is that it can be separated into three independent equations, each involving only a single coordinate. and this separation is possible because the wave function $\Psi(r, \theta, \phi)$ has the form of a product of three different functions as following .

$$\Psi(r, \theta, \phi) = R(r) \Theta(\theta) \Phi(\phi) \quad \text{--- (6)}$$

$R(r)$ describes the Ψ of electron varies along a radius vector (r) with θ and ϕ constant and $\Theta(\theta)$, $\Phi(\phi)$ describe how Ψ varies with the $(\theta$ and $\phi)$ respectively with another variables which are constant like r, ϕ for the function (Θ) and r, θ for the function (Φ) .

then we see that

$$\begin{aligned} \frac{\partial \Psi}{\partial r} &= \Theta \Phi \frac{\partial R}{\partial r} = \Theta \Phi \frac{dR}{dr} \\ \frac{\partial \Psi}{\partial \theta} &= R \Phi \frac{\partial \Theta}{\partial \theta} = R \Phi \frac{d\Theta}{d\theta} \\ \frac{\partial \Psi}{\partial \phi} &= R \Theta \frac{\partial \Phi}{\partial \phi} = R \Theta \frac{d\Phi}{d\phi} = R \Theta \frac{d^2 \Phi}{d\phi^2} \end{aligned} \quad \text{--- (7)}$$

When we substitute $R \Theta \Phi$ for Ψ in Schrodinger's eq(5) and divide the entire equation by $R \Theta \Phi$ we find that

$$\frac{\sin^2 \theta}{R} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{\sin \theta}{\Theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + \frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} + \frac{2mr^2 \sin^2 \theta}{\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0 r} + E \right) = 0 \quad \text{--- (8)}$$

The third term of eq(8) is a function of angle ϕ whereas the other terms are functions of $(r$ and $\theta)$ only. Let us rearrange eq(8) to read

$$\frac{\sin^2 \theta}{R(r)} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{\sin \theta}{\Theta(\theta)} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta(\theta)}{d\theta} \right) + \frac{2mr^2 \sin^2 \theta}{\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0 r} + E \right) = - \frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} \quad (9)$$

This equation can be correct only if both sides of it are equal to the same constant and since they are functions of different variables, then it's convenient to call this constant (m_l^2) . therefore the differential equation for the function Φ is

$$\boxed{- \frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} = m_l^2} \quad (10)$$

Next we substitute m_l^2 for the right-hand side of eq(9) and divide the entire equation by $\sin^2 \theta$ we get

$$\frac{1}{R(r)} \frac{d}{dr} \left(r^2 \frac{dR(r)}{dr} \right) + \frac{1}{\Theta(\theta) \sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta(\theta)}{d\theta} \right) + \frac{2mr^2}{\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0 r} + E \right) = \frac{m_l^2}{\sin^2 \theta} \quad (11)$$

and

$$\frac{1}{R} \frac{d}{dr} \left(r^2 \frac{dR(r)}{dr} \right) + \frac{2mr^2}{\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0 r} + E \right) = \frac{m_l^2}{\sin^2 \theta} - \frac{1}{\Theta \sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta(\theta)}{d\theta} \right) \quad (12)$$

Again we have an equation in which different variables appear on each side, requiring that both sides be equal to the same constant, this constant is called $l(l+1)$, therefore the eq(12) will be

$$\frac{m_e}{\sin^2 \theta} - \frac{1}{\theta \sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta(\theta)}{d\theta} \right) = l(l+1) \quad \text{--- (13)}$$

$$\frac{1}{R(r)} \frac{d}{dr} \left(r^2 \frac{dR(r)}{dr} \right) + \frac{2m_e r^2}{\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0 r} + E \right) = l(l+1) \quad \text{--- (14)}$$

where $l = 0, 1, 2, 3, \dots$

Eqs (10)(13)(14) are usually written

equation for Φ
$$\frac{d^2 \Phi_{(r)} + m_e^2 \Phi_{(r)} = 0 \quad \text{--- (15)}$$

equation for Θ
$$\frac{1}{\sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta(\theta)}{d\theta} \right) + \left[l(l+1) - \frac{m_l^2}{\sin^2 \theta} \right] \Theta(\theta) = 0 \quad \text{--- (16)}$$

equation for R
$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR(r)}{dr} \right) + \left[\frac{2m_e}{\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0 r} + E \right) - \frac{l(l+1)}{r^2} \right] R(r) = 0 \quad \text{--- (17)}$$

each of these is an ordinary differential equation for a single function of a single variable. when the equations (15)(16)(17) are solved, it turns out that three quantum numbers are required to describe the electron in (H-atom) in place of the single quantum number of Bohr theory. Hence we may tabulate the three quantum numbers (n, l and m) together with their permissible values as follows:

principal quantum number $n = 1, 2, 3, \dots$

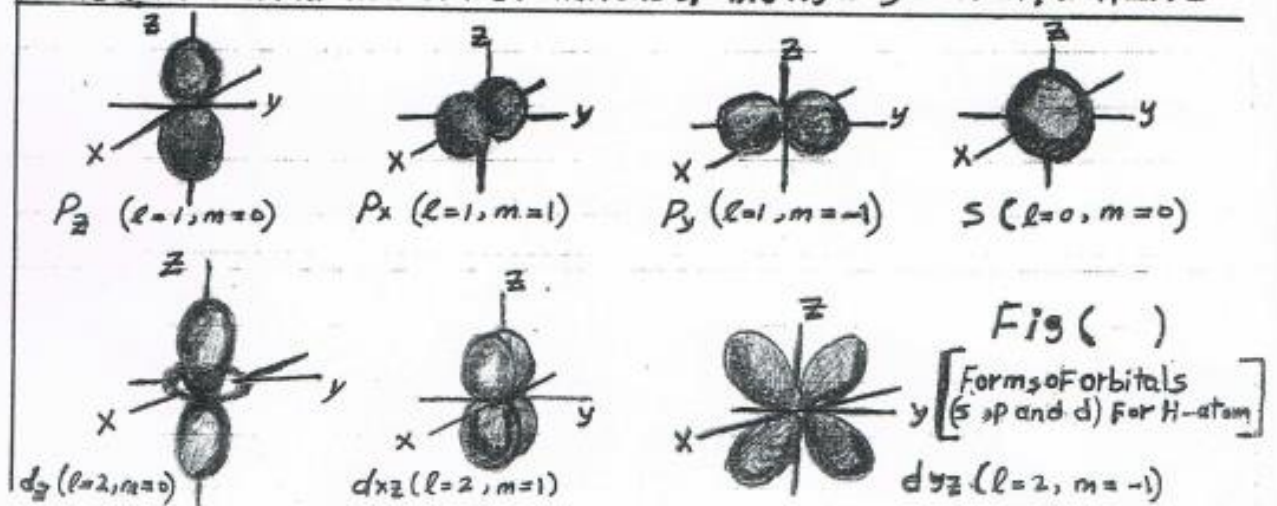
orbital quantum number $l = 0, 1, 2, \dots (n-1)$

magnetic quantum number $m_l = 0, \pm 1, \pm 2, \dots \pm l$

the wave functions R, θ, Φ together with Ψ are given in Table (1) For $n=1, 2$

n	l	m_l	$\Phi(\phi)$	$\theta(\theta)$	$R(r)$	$\Psi(r, \theta, \phi)$
1	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{2}{a_0^{3/2}} e^{-r/a_0}$	$\frac{1}{\sqrt{\pi}} a_0^{-3/2} e^{-r/a_0}$
2	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{2\sqrt{2} a_0^{3/2}} (2 - \frac{r}{a_0}) e^{-r/2a_0}$	$\frac{1}{4\sqrt{2\pi}} a_0^{-3/2} (2 - \frac{r}{a_0}) e^{-r/2a_0}$
2	1	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{6}}{2} \cos\theta$	$\frac{1}{2\sqrt{6} a_0^{3/2}} \frac{r}{a_0} e^{-r/2a_0}$	$\frac{1}{4\sqrt{2\pi}} a_0^{-3/2} \frac{r}{a_0} e^{-r/2a_0} \cos\theta$
2	1	± 1	$\frac{1}{\sqrt{2\pi}} e^{\pm i\phi}$	$\frac{\sqrt{3}}{2} \sin\theta$	$\frac{1}{2\sqrt{6} a_0^{3/2}} \frac{r}{a_0} e^{-r/2a_0}$	$\frac{1}{8\sqrt{\pi}} a_0^{-3/2} \frac{r}{a_0} e^{-r/2a_0} \sin\theta e^{\pm i\phi}$

Table (1) Normalized wave Functions of the Hydrogen atom For $n=1, 2$



Quantum Numbers :

If we return to the equations (15)(16)(17) which every equation is depend on one variable, we see the equation (15) is readily solved and the result is

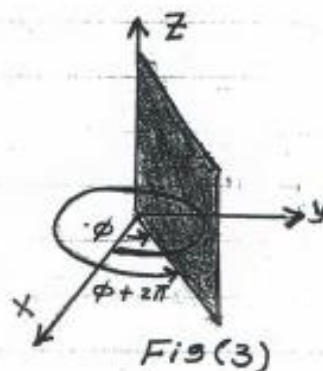
$$\Phi(\phi) = A e^{im_l \phi} \quad \text{--- (18)}$$

As we know, one of the conditions that a wavefunction and hence Φ , which is a component of the Ψ , have a single value at a given point in space, but from the Fig (3) it is clear that ϕ and $\phi + 2\pi$ identify the same meridian plane, it mean.

$$\Phi(\phi) = \Phi(\phi + 2\pi) \quad \text{--- (19)}$$

$$A e^{im_l \phi} = A e^{im_l(\phi + 2\pi)} \quad \text{--- (20)}$$

$$A e^{im_l \phi} = A e^{im_l \phi} \cdot e^{im_l 2\pi} \quad \text{--- (21)}$$



and from the boundary conditions and according to the eq (20) it must be

$$e^{im_l 2\pi} = 1 \quad \text{--- (22)}$$

hence the m_l must be an integer and equal to

$$m_l = 0, \pm 1, \pm 2, \pm 3, \dots \quad \text{--- (23)}$$

The constant m_l is known as the magnetic quantum number of (H-atom) which is determine the component of the angular momentum along z-axis (L_z) or in the magnetic field direction if an external magnetic field (B) was applied in parallel to z direction.

$$\boxed{L_z = m_l \hbar} \quad \text{--- (24)} \quad m_l = 0, \pm 1, \pm 2, \dots \pm l$$

The possible values of m_l for a given value of l , range from $+l$ through (0) to $-l$, so that the number of possible orientations of the angular momentum vector \vec{L} in a magnetic field is $(2l+1)$. when $l=0$, L_z can have only the single value of (0) , when $l=1$, L_z may be $\hbar, 0, -\hbar$; when $l=2$, L_z may be $2\hbar, \hbar, 0, \hbar, -\hbar, -2\hbar$.

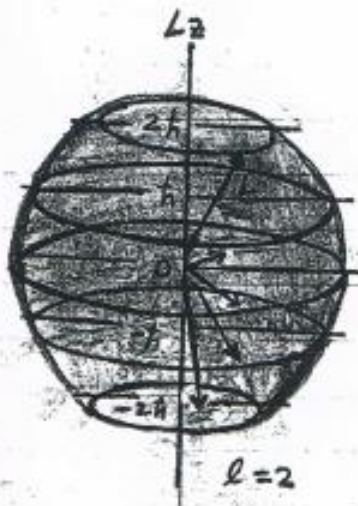


Fig (5) The angular momentum vector \vec{L} precesses constantly about the z -axis.

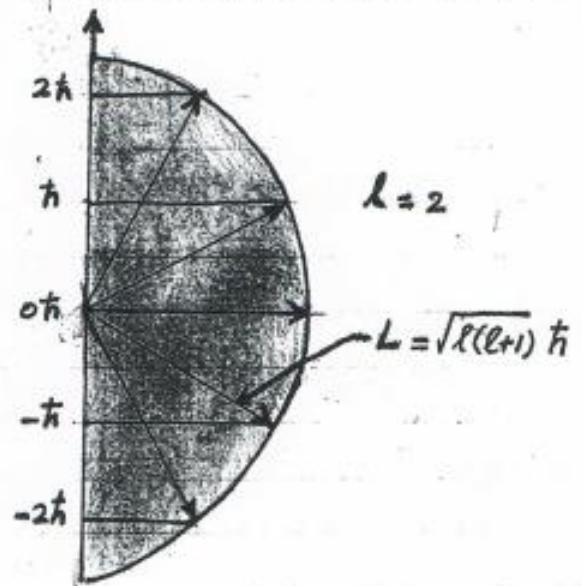


Fig (4) space quantization of orbital angular momentum each value of m_l corresponding to a different orientation relative to the z -axis.

The quantum number l ; this quantum number determines the magnitude of the electron's angular momentum (L)

$$L = \sqrt{l(l+1)} \hbar \quad (25)$$

it is customary to specify electron angular momentum states by a letter, with s corresponding to $l=0$, p to $l=1$ and so on.

$$l = 0, 1, 2, 3, 4, 5, 6$$

$$s, p, d, f, g, h, i$$

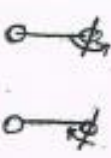


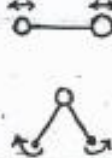



the solution of the equation (17) for the radial part $R(r)$ of the hydrogen atom wave function Ψ also requires that a certain condition be fulfilled. This condition is that (E) be positive or have one of the negative values E_n (signifying that the electron is bound to the atom) specified by

$$E_n = - \frac{m e^4}{32 \pi^2 \epsilon_0^2 \hbar^2} \left(\frac{1}{n^2} \right) = \frac{-13.6}{n^2} \text{ eV} \quad \text{---(26)}$$

we recognize that this is precisely the same formula for the energy levels of the hydrogen atom that Bohr obtained. Another condition that must be obeyed in order to solve equation (17) is that (n) , known as the principal quantum number, must be equal to or greater than $(\ell+1)$. This requirement may be expressed as a condition on ℓ in the form.

$$\ell = 0, 1, 2, 3, \dots, (n-1)$$

Regions of the spectrum

n.m.r	e.s.r	Microwave	Infra-red	Visible and Ultra-violet	X-ray	γ-ray	
							
10^2	1	100	10^4	cm^{-1}	10^6 (Wavenumber)	10^8 (V)	
10m	100cm	1cm	100 μm	1 μm	10nm (wavelength)	100pm (λ)	
3×10^6	3×10^8	3×10^{10}	3×10^{12}	3×10^{14}	Hz	3×10^{16} (Frequency)	3×10^{18} (V)
10^3	10^1	10	10^3	10^5 Joules/mole	10^7 (energy)	10^9 (E)	

Fig(1) the regions of the electromagnetic spectrum.

1. Radio Frequency region, $3 \times 10^6 - 3 \times 10^{10}$ Hz ; 10m - 1cm wavelength, Nuclear magnetic resonance (n.m.r) and electron spin resonance (e.s.r).
2. Microwave region, $3 \times 10^{10} - 3 \times 10^{12}$ Hz ; 1cm - 100 μm wavelength, Rotational spectroscopy. a molecule such as HCl in which H-atom carries a permanent net positive charge and the other a net negative charge is said to have a permanent electric dipole moment. if its consider the rotation of HCl then we see that the plus and minus charges change places periodically and the component dipole moment in a given direction fluctuates regularly Fig (2-a). this fluctuation is plotted in Fig (2-b) and its seen to be exactly similar in form to the fluctuating electric field of radiation, thus interaction can occur, energy can be absorbed or emitted and the rotation gives rise to a spectrum. (All molecules having a permanent moment are said to be "microwave active" if there is no dipole as in H₂ or Cl₂, no interaction can take place and the molecule is "microwave inactive").

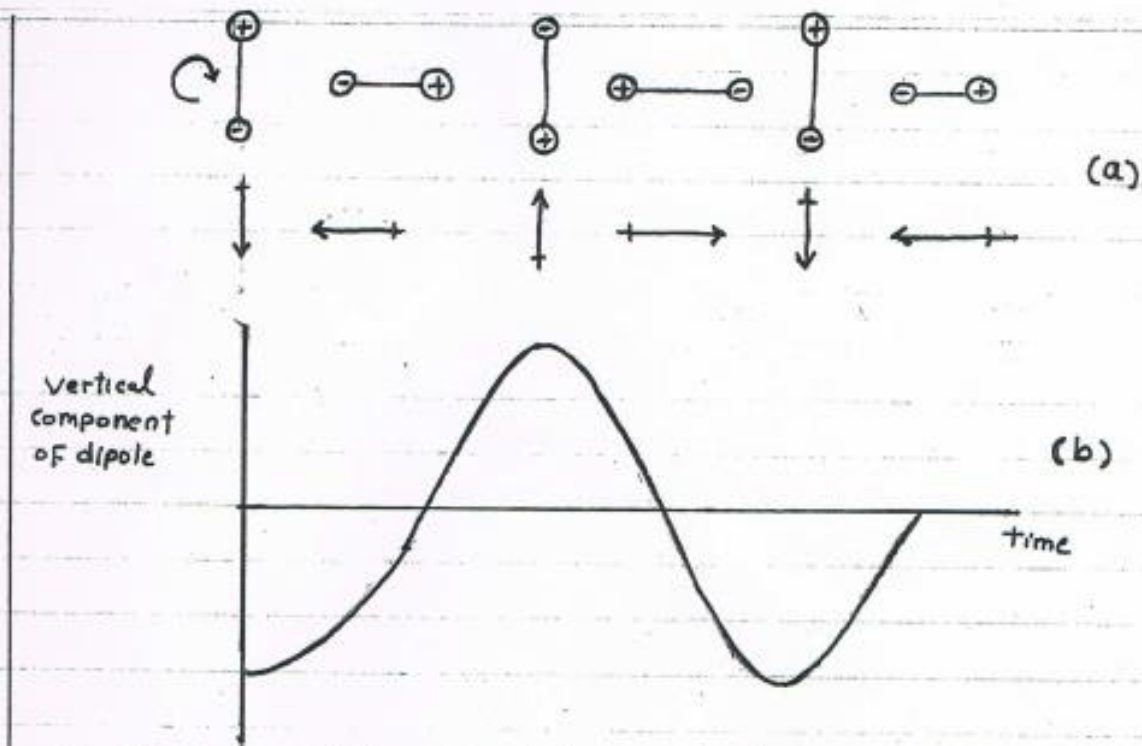
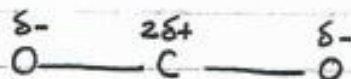
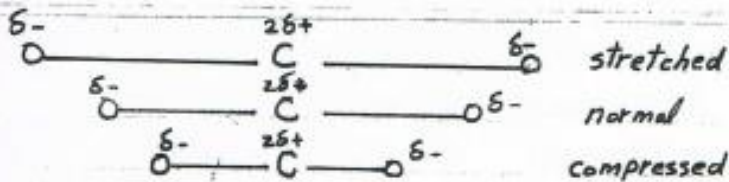


Fig (2) the rotation of a diatomic molecule, HCl, showing the fluctuation in the dipole moment measured in a particular direction.

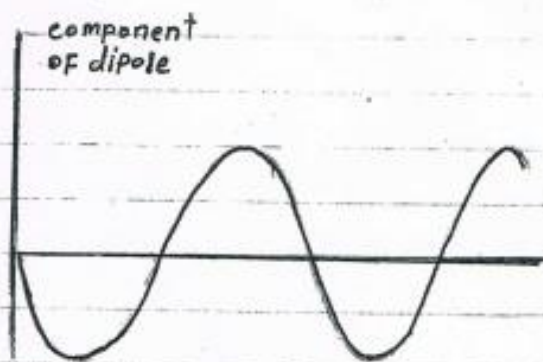
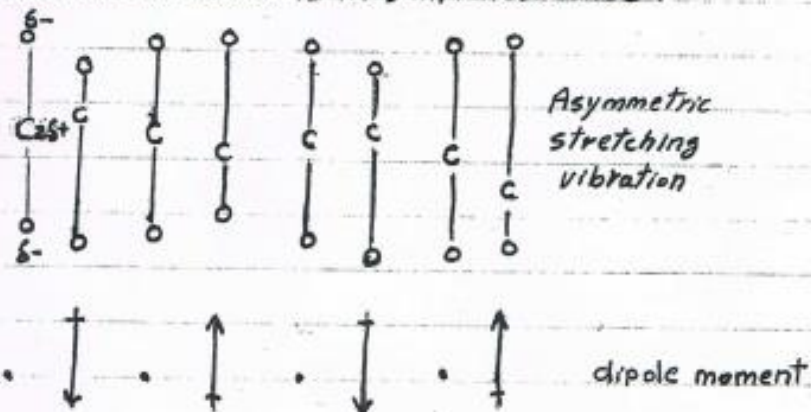
3- Infra-red region $3 \times 10^{12} - 3 \times 10^{14}$ Hz; $100 \mu\text{m} - 1 \mu\text{m}$ wavelength vibrational spectroscopy. here in this region it is vibration rather than rotation which must give rise to a dipole change; for example carbon dioxide molecule in which three atoms are arranged linearly with a small net positive charge on the carbon and small negative on oxygens.



this mode of vibration known as the symmetric stretch i.e. molecule is stretched and compressed alternately and both C-O bonds changing simultaneously as shown in Fig (3) and plainly the dipole moment is zero throughout the whole of this motion thus is called infra-red inactive.



Fig(3) the symmetric stretching vibration of the carbon dioxide molecule
 However there is another stretching vibration called the antisymmetrical stretch Fig(4), here one bond stretches while the other is compressed as be shown in the Fig(4) thus there is a periodic alteration in the dipole moment and the vibration is thus infrared active.



Fig(4)

4- Visible and ultra-violet regions ; $3 \times 10^{14} - 3 \times 10^{16}$ Hz ; $1 \mu\text{m} - 10 \text{nm}$ wavelength , Electronic spectroscopy

5- X-ray region ; $3 \times 10^{16} - 3 \times 10^{18}$ Hz ; $10 \text{nm} - 100 \text{pm}$, wavelength , Energy change involving the inner electrons of an atom or a molecule

6- γ -ray region ; $3 \times 10^{18} - 3 \times 10^{20}$ Hz ; $100 \text{pm} - 1 \text{pm}$, wavelength . Energy changes involve the rearrangement of nuclear particles