

Notes For Bachelor of Science (TU)



# BSC NOTES PDF COLLECTION



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## X-Rays

(Wilhelm Konrad Rontgen - 1895)

W.K. Rontgen - 1895

(- Bikash Sharma)

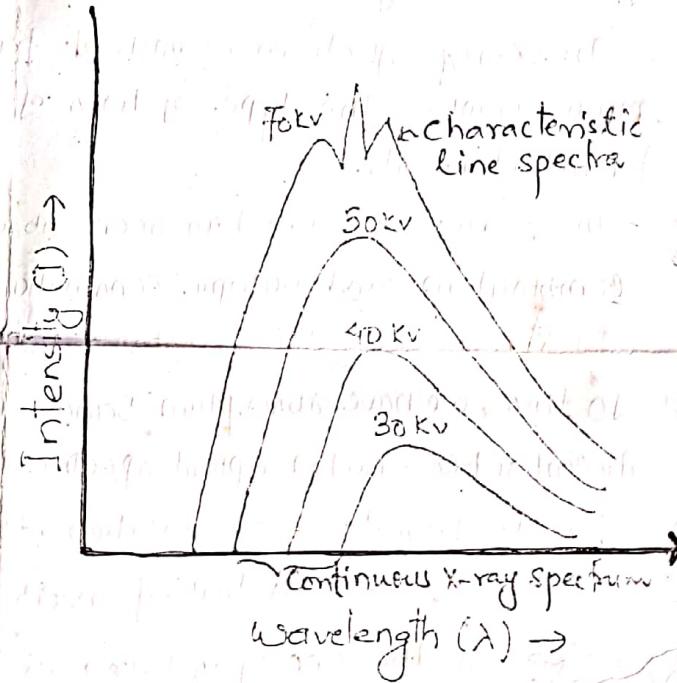
When highly accelerated electrons or cathode rays strike the target material, they lose their kinetic energy. This loss in K.E. is converted to the electromagnetic radiation named as X-rays or X-rays. X-rays have much shorter wavelength (about  $10^{-10}$  m).

The intensity distribution of X-ray beam depends upon the potential difference between cathode and anode of the X-ray tube, as shown below.

From the figure we see that, for a given potential, for the P.D.s 30 kV, 40 kV and 50 kV, intensity versus wavelength curves are smoothly varying.

These smoothly varying curves represent the continuous X-ray spectra.

Spectra: Actually these spectra are white. But for high P.D. i.e. 50 kV, two sharp peaks are observed. The sharp peaks represent the line X-ray spectra. These line spectra are the characteristics of the target material and usually known as characteristic line spectra.



The main difference between the continuous X-ray radiation and characteristic X-ray is that the continuous X-ray rad-

## Difference between Characteristics X-ray and Optical spectra

The following points give the essential difference between X-ray and optical spectra.

- (1) The X-ray spectrum arises due to the transition in the innermost part of atom, while the optical spectrum arises due to transition in the outermost part.
- (2) Since the regions of transition in two cases are different, in X-ray emission spectrum, high frequency radiations are emitted and in optical spectrum low-frequency radiation are observed.
- (3) The X-ray spectral lines occupy a narrow region of spectrum beyond the ultraviolet, while the optical spectrum covers a wide range.
- (4) The spectral lines in the X-ray spectrum are classified into two groups, one of short wavelength region and the other of long wavelength region.
- (5) The X-ray spectrum consists of fewer lines than the optical spectrum. Hence much simpler. The type of lines of a particular series is almost the same for all elements.
- (6) The X-ray spectrum has been observed to be independent of the chemical combination and isotopic constitution of the element approximately.
- (7) In X-ray absorption spectrum there is no selective absorption of spectral lines. In this, we have absorption bands with definite edges and critical absorption discontinuities. But in optical spectrum there is a selective absorption of lines.
- (8) In diagrammatical representation, the zero of the energy in the case of X-ray spectrum is taken as that of neutral atom, while in the case of optical spectrum is zero of the energy is taken as that of ionized atom.

$$E_R \cdot R \alpha = A \delta \cdot A \delta$$

$$m_e^2 = ev = \frac{hc}{\lambda}$$

$$\lambda = \frac{hc}{ev}$$

contain the X-rays of all possible wavelengths above the minimum wavelength limit whereas, characteristic X-ray radiation contain only the X-ray of certain wavelength.

### Origin and feature of continuous X-ray spectrum:

According to electromagnetic theory, when charged particles such as electrons are deaccelerated, they emit electromagnetic radiation of different frequencies in such a way that a part of K.E. is transformed into the energy of emitted radiation.

In the X-ray tube, when the accelerated electrons strike the target, their motion becomes retarded and hence they emit electromagnetic radiation with continuous distribution of wavelength starting from the minimum. The wavelength of emitted radiation depends upon the amount of kinetic energy (eV) transformed into the emitted radiation (X-ray) where V is the potential difference between cathode and anode in the X-ray tube and 'e' be the charge of electron.

When total energy (eV) is transformed into the energy of X-radiation, the frequency of emitted X-radiation is maximum and wavelength is minimum which is given by,

$$eV = h\nu_{\max} \quad \dots \dots (1)$$

and  $\lambda_{\min.} = \frac{hc}{eV} \quad \dots \dots (2)$

where 'h' is Planck's constant

This process of emission of electromagnetic radiation with

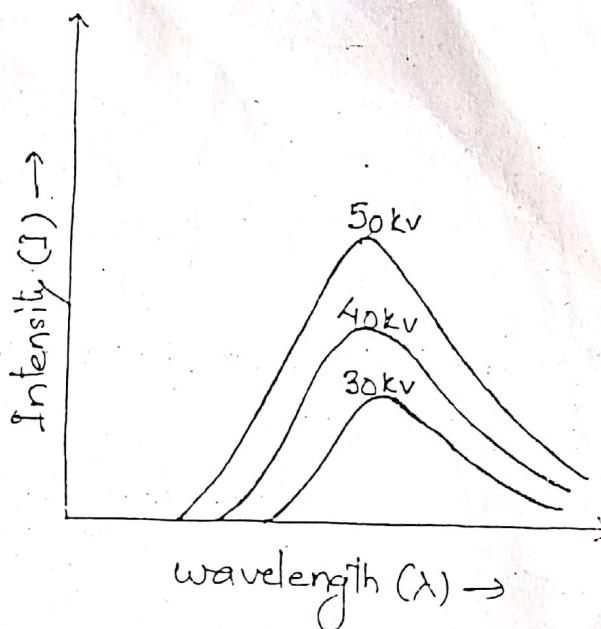
Continuous distribution of wavelengths from the deaccelerated electrons is known as Bremsstrahlung process (brake radiation).

### Feature:

From the figure, it is seen that

- i) for each potential difference, there is a minimum wavelength limit ( $\lambda_m$ ) below which no radiation is emitted. Above  $\lambda_m$ , the intensity of continuous spectrum increases rapidly with increasing wavelengths and after reaching a maximum value, intensity decreases gradually but it never reaches to zero,

Showing that the spectrum contains all possible wavelengths above the minimum limit ( $\lambda_m$ ).



- ii) The maximum value of intensity of continuous spectrum increases with increasing P.D. For higher value of P.D., the value of  $\lambda_m$  is smaller.

-x-

(3)

## Origin and nature of characteristic X-ray spectra:

The origin of characteristic X-ray spectra can be explained according to Bohr's theory.

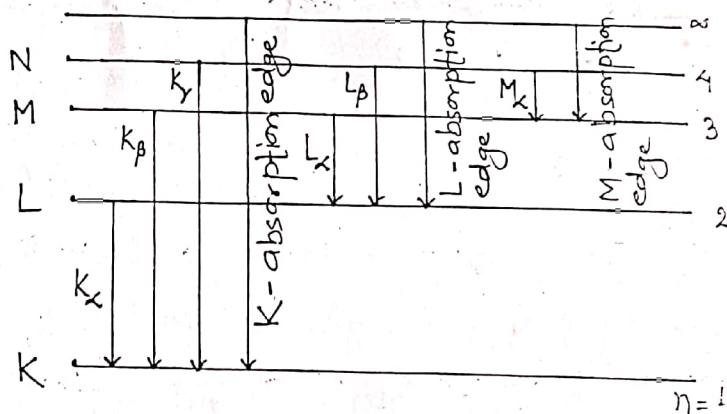
Let us suppose an atom in the target is bombarded by a high speed electron and a K-electron is removed. Then, a vacancy is created in the K-Shell which can be filled up either by an electron from L, M or N shells or by free electron. These possible transitions of electron from L, M or N shells to the K-shell give rise to the radiation which is called characteristic X-ray. Thus characteristic X-ray is observed due to transition of electron in the inner most part of the atom that have been disturbed by the incident electrons.

### Nature (or feature):

The transition of electron from L, M or N shell to K-Shell is respectively denoted by  $K_{\alpha}$ ,  $K_{\beta}$  and  $K_{\gamma}$ . The group of lines  $K_{\alpha}$ ,  $K_{\beta}$  and  $K_{\gamma}$  of shortest wavelength is called K-Series. Usually  $K_{\alpha}$  and  $K_{\beta}$  lines are detected.

Similarly, the transition from M, N shell to L-Shell is respectively denoted by  $L_{\alpha}$  and  $L_{\beta}$  lines which constitute L-Series of longer wavelengths.

For heavy elements, third series called M-Series has been detected.



## Difference between characteristic X-ray Spectra and optical spectra

Refer to G.K.S. book (p.n. 429)

### Emission of characteristic X-ray Spectral Lines from the atom

When an electron accelerated to very high energy in the X-ray tube strikes the target, it may collide inelastically with an inner shell electron (i.e. K-electron) in the target atom due to which this electron may be emitted from the atom. If the kinetic energy of the incident electron is  $eV$ , where  $V$  is the potential difference between anode and cathode within the X-ray tube and the binding energy of the electron in K-shell of the atom is  $E_K$ , then the electron emitted from the atom will have the kinetic energy,

$$\frac{1}{2}mv^2 = eV - E_K \quad \dots \dots (1)$$

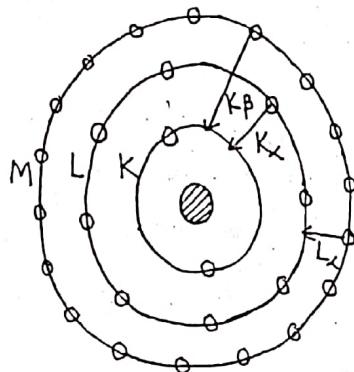
Clearly, to eject out the electron from the K-shell of the atom, the striking electron must have at least the kinetic energy equal to the binding energy of electron in that shell.

When an electron ejects out from the K-shell, a vacancy may be created which can be filled up by the transition of a relatively loose bound electron from an outer shell i.e. L, M, N etc. Due to the transition a photon is emitted which takes the excess energy of the electron which is excited. The energy of the photon depends upon the binding energy of the electron in that shell. These binding energies are the characteristics of the target atom.

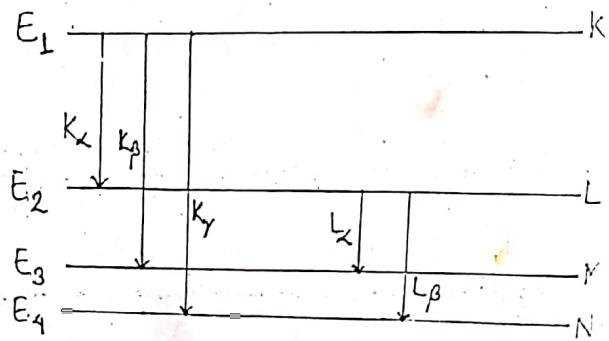
(4)

For the given target atom, more than one X-ray Spectral Lines are observed which have different wavelengths. The X-ray Spectral Lines originating due to the transitions from L, M, N etc shells to the inner most K-shell constitute the K-Series of the Spectrum. Similarly, the X-ray Spectral lines originating due to the transitions from M, N etc shells to L-shell constitute the L-Series of the Spectrum and so on.

The origin of different X-ray lines are shown below:



Kossel diagram



X-ray energy level diagram

Experimental observations shown that the characteristic X-ray lines are not single, they have their own fine-structure. The fine-structure of X-ray lines can be explained on the basis of vector atom model by considering the quantum numbers  $n$  (p.q.n.),  $l$  (orbital q.n.) and  $j$  (total angular momentum q.n.).

According to Moseley's law, the frequency of emitted X-ray spectral line depends on the atomic number of the target atom by the relation:

$$\omega \propto Z^2 \quad \dots \quad (2)$$

where  $\omega$  is frequency of emitted X-radiation and  $Z$  be the atomic number of the target atom.

~ X ~

## Moseley's law:

The English physicist Moseley found that the frequencies of characteristic X-ray spectral lines vary continuously with the atomic number of the target atom. If the square root of the frequency of given line i.e.  $\sqrt{\nu}$  is plotted against the atomic number ( $Z$ ) of the target atom, then a straight line is obtained showing the following relationship:

$$\text{statement} \quad \sqrt{\nu} \propto Z \quad \dots \dots \dots (1)$$

The frequency of a spectral line in X-ray spectrum varies as the square of the atomic number of the element emitting it i.e.  $\nu$ .

Eq. (1) can also be written as,

$$\nu = a(Z - b)^2 \quad \dots \dots \dots (2)$$

where  $(Z - b)$  is the effective atomic number of the target atom, 'b' is constant for particular line called Screening Constant and 'a' is a general constant.

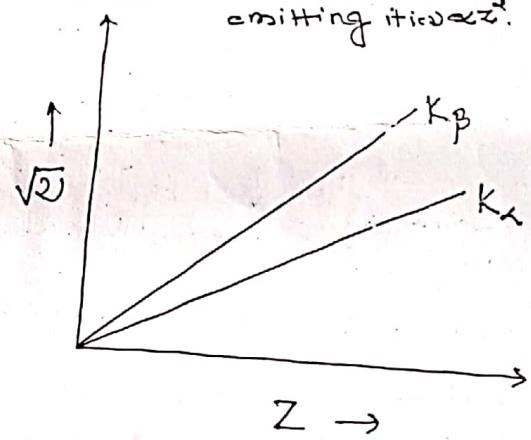
Eqs. (1) or (2) is called Moseley's law.

Moseley's law follows from the origin of X-ray spectra

The origin of characteristic X-ray spectra is the electronic transition in the inner most part of the atom which can be explained by Bohr's theory.

According to Bohr's theory, the energy of an atom revolving in the orbit with principal quantum number  $n_1$  is given by,

$$E_1 = -\frac{2\pi^2 m e^4 z^2}{n_1^2 h^2} \cdot \frac{1}{(4\pi E_0)^2} \quad (\text{in S.I.}) \quad \dots \dots \dots (3)$$



Similarly, the energy of electron revolving in the orbit with  $p_{q,n}$ .  
 $n_2$  is given by,

$$E_2 = -\frac{2\pi^2 me^4 Z^2}{n_2^2 h^2} \cdot \frac{1}{(4\pi\epsilon_0)^2} \quad \dots \dots (4)$$

where 'm' and 'e' are mass and charge of electron, 'Z' is atomic number and 'h' is Planck's constant.

If we take the Screening effect into account, then we have to replace  $Z$  by  $(Z-b)$ , where ' $b$ ' is screening constant.

Then, the energy difference between the two orbits of electron with  $Z = (Z-b)$  can be written as,

$$E_1 - E_2 = \frac{2\pi^2 me^4}{h^2} \cdot \frac{1}{(4\pi\epsilon_0)^2} \left[ \frac{(Z-b_2)^2}{n_2^2} - \frac{(Z-b_1)^2}{n_1^2} \right] \dots \dots (5)$$

For heavy elements i.e. large  $Z$ ,

$$b_1 \approx b_2 \approx b \quad \dots \dots (6)$$

Thus frequency of spectral line corresponding to the transition of electron between two orbital state is given by,

$$\nu = \frac{(E_1 - E_2)}{h} = \frac{2\pi^2 me^4}{h^3} \cdot \frac{1}{(4\pi\epsilon_0)^2} (Z-b)^2 \left[ \frac{1}{n_2^2} - \frac{1}{n_1^2} \right] \dots \dots (7)$$

for  $K_\alpha$  line  $n_1 = 2$  and  $n_2 = 1$ , the frequency is given by,

$$\nu_{K\alpha} = \frac{2\pi^2 me^4}{h^3} \cdot \frac{1}{(4\pi\epsilon_0)^2} (Z-b)^2 \left[ \frac{1}{1^2} - \frac{1}{2^2} \right]$$

$$= \frac{3}{4} \cdot \frac{2\pi^2 me^4}{h^3} \cdot \frac{1}{(4\pi\epsilon_0)^2} (Z-b)^2$$

$$\text{or, } \nu_{K\alpha} = a(Z-b)^2 \quad \dots \dots (8)$$

where  $a = \frac{3}{4} \cdot \frac{2\pi^2 me^4}{h^3} \cdot \frac{1}{(4\pi\epsilon_0)^2} = \frac{3}{4} RC$  = constant. R is Rydberg constant and c is velocity of light.

'Screening effect' which screens the charge on nucleus.

Comparing Eq.(8) with Eq.(2), we can say that Moseley's law follows from the origin of X-ray spectra.

### Importance of Moseley's law:

#### 1) Identification of elements:

By using Moseley's law, we can identify an unknown element by using it as the target. For this, we study the X-ray spectra emitted by the unknown element with the help of X-ray spectrometer and determine the wavelength of corresponding X-ray. Then frequency will be obtained and by using Moseley's Law, we can find the atomic number  $z$  of the unknown element.

For  $K_{\alpha}$  line, Moseley's law gives,

$$2 \propto (z-1)^2 \quad \dots \quad (1)$$

Since  $b=1$  for  $K_{\alpha}$  line.

Eq.(1) gives very useful relation,

$$\frac{2_1}{2_2} = \frac{(z_1-1)^2}{(z_2-1)^2}$$

$$\text{or, } \frac{\lambda_2}{\lambda_1} = \frac{(z_1-1)^2}{(z_2-1)^2} \quad \dots \quad (2)$$

If we know the atomic number of the atom emitting  $K_{\alpha}$  line with known wavelength, then atomic number of an unknown element emitting the same radiation can be determined by using Eq.(2). This method can also be used to check whether the element contains impurities or not.

→ helped to perfect the periodic table ① the discovery of new elements e.g. hafnium (72), technetium (43) etc. and ② the determination of the atomic numbers of rare-earths and fixing their positions in the periodic table.

Correct  
Before  
(Z) had not  
elements in  
increasing  
accord  
disc  
bef

(6)

## Correct placement of the elements in the Periodic table:

Before Moseley's research, the real significance of atomic number ( $Z$ ) had not been realized. Moseley's research shown that the elements in the periodic table should be arranged according to increasing atomic number not according to increasing atomic weight.

Mandeleev had arranged the elements in the periodic table according to increasing atomic weight. In his arrangement some discrepancy were noticed. for example, Mandeleev placed Nickel before Cobalt. Since Nickel has low atomic weight than Cobalt. The chemical properties of these two elements show that Cobalt should be placed before Nickel. Also Moseley's diagram for  $K_{\alpha}$  lines shows that the frequency of  $K_{\alpha}$  line emitted by the Nickel is larger than that emitted by Cobalt. Thus the equation  $\nu_{K_{\alpha}} = \frac{3}{4} R C (Z-1)^2$  suggest that Nickel has larger atomic number than cobalt. This discrepancy is removed by Moseley by placing Cobalt (27) before than Nickel (28). Similarly, he placed  $^{18}\text{A}$  before  $^{19}\text{K}$ .

In this way, Moseley arranged correctly the elements in the periodic table. Furthermore, during the arrangement of elements, Moseley left gap at  $Z=72$  and  $Z=43$  because these elements had not been discovered. But after the discovery of hafnium (72) and technetium (43), these vacancies were fulfilled.

—x—

## Moseley's diagram and its Salient features:

Refer to G. K. S. book (p.n. 422)

?  
 $\rightarrow {}^{27}\text{Co}^{58.9}$   
 $\rightarrow {}^{28}\text{Ni}^{58.7}$   
 $\rightarrow {}^{18}\text{Ar}^{40}$   $\rightarrow {}^{19}\text{K}^{99}$

$$\sqrt{\frac{\nu_1}{\nu_2}} = \frac{Z_1 - b}{Z_2 - b} = \sqrt{\frac{\lambda_2}{\lambda_1}}$$

$$\rightarrow Z_2 = (Z_1 - b) \sqrt{\frac{\lambda_1}{\lambda_2}} + b$$

b = 7.4 K = 1

- (1). When sample of unknown z is used as a target for electron beam in x-ray it emits a series of characteristic spectral lines in which two target wave lengths are  $0.222\text{nm}$  and  $10.192\text{nm}$ . What is element?
- (2). X-ray spectra of an element displays characteristic spectral line at  $0.72\text{nm}$  and at  $0.16\text{nm}$ . What is the element?
- Rept. 2  
(3) X-ray produced from a cobalt target wavelength of  $1.73 \times 10^{-8}\text{m}$  is lines of two impurities present in the target give wavelengths of  $2.285\text{nm}$  and  $1.537\text{nm}$ . Find the impurities present.
- (4) X-ray incident on a rock salt ( $\text{NaCl}$ ) crystal are diffracted in the first order at an angle  $30^\circ$ . It is interatomic distance  $2.82\text{A}^\circ$ . Calculate wavelength of incident rays.
- (5) The wavelength of L $\alpha$  x-ray ~~target~~ lines of Na and Pt are  $4.15\text{ nm}$  and  $1.32\text{A}^\circ$  respectively. A unknown substance emits L $\alpha$  x-ray with wavelength  $0.97\text{nm}$ . Determine atomic no. of unknown substance.
- (6).

longest b = 7.4.

shortest b = 1.

$$MN_2' = \frac{13.99 \times 13.99}{2 \times 13.99 - 41}$$

$$\gamma_{MN_2} = \sqrt{\frac{I_{N_2}}{MN_2}} =$$

## X-ray absorption spectrum:

When a monochromatic beam of X-rays is allowed to pass through the slab of material, the intensity of the emerging beam is found to decrease.

If the monochromatic beam of X-rays having intensity  $I_0$  is allowed to pass through the slab of thickness  $dx$ , then the decrease in intensity of the emerging beam is found to be proportional with emerging intensity and the thickness  $dx$  of the slab i.e.

$$dI \propto I dx$$

$$\text{or, } dI = -\mu I dx \quad \dots \dots (1)$$

Where  $\mu$  is linear absorption coefficient of the material and negative sign shows that intensity decreases for increasing value of thickness of the slab.

Eq.(1) can also be written as,

$$\frac{dI}{I} = -\mu dx \rightarrow \log_e I - \log_e I_0 = -\mu x$$

Integrating both sides, we get

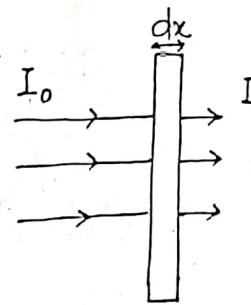
$$I = I_0 e^{-\mu x} \quad \dots \dots (2)$$

where  $I_0$  is the intensity of incident beam.

Eq.(2) can also be written as

$$I = I_0 e^{\frac{-\mu}{S} Sx}$$

$$\text{or, } I = I_0 e^{-\mu_m m} \quad \dots \dots (3)$$



where  $\mu_m = (\lambda/\beta)$  is the mass absorption coefficient and  $m = (\beta z)$  is the mass per unit area of an absorber.

The decrease in the intensity of a X-ray beam while passing through the matter may be due to several reasons:

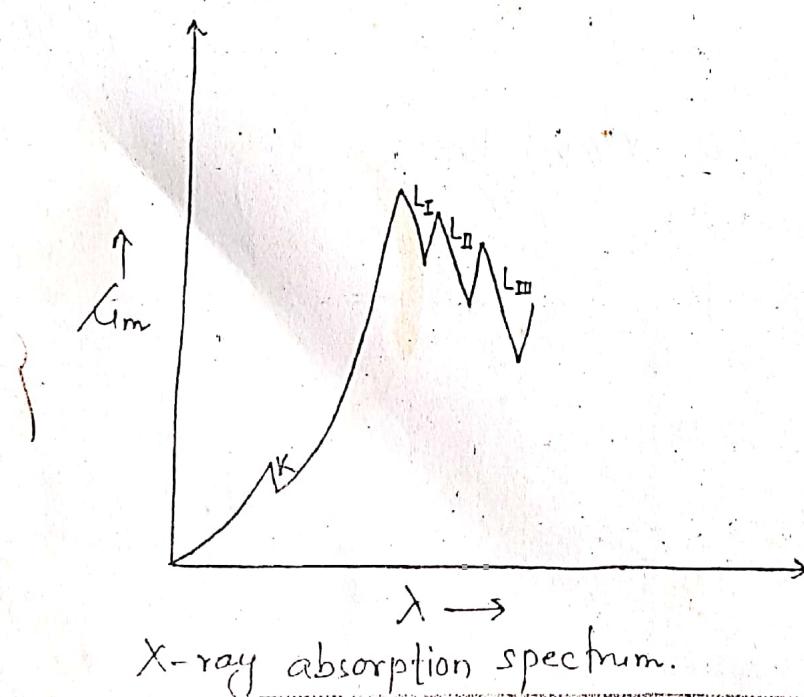
- ① There may be photoelectric absorption of the X-ray photons by the electrons in the inner shell of the atom which are thereby ejected.
- ② There may be scattering of the X-rays by the atomic electrons.
- ③ At higher energies, there may be photonic effect and other effect which causes the decrease in energy of the X-rays beam.

Let us consider the case of photoelectric absorption.

In this case, the mass absorption coefficient ( $\mu_m$ ) varies as the cube of the incident wavelength ( $\lambda^3$ ) and also the atomic number ( $Z^3$ ) of the absorber i.e.

$$\mu_m \propto \lambda^3 Z^3 \dots (4)$$

Thus when  $\lambda$  increases,  $\mu_m$  increases. The variation of  $\mu_m$  with  $\lambda$  is shown below:



## Fine structure of X-ray levels

Experimental observations shown that the X-ray levels are not Singlet, they have their own fine structure. for example, L level has three sublevels, M level has five sublevels etc.

→ To account the fine structure of X-ray level, we consider the effect of electrons which screen the nuclear charge and the effect of spin of electrons spin.

For the L-electrons, which move in approximately Coulomb field, the K-electrons behave as if they have merged into the nucleus and thereby reducing the nuclear charge by two. The reduction of nuclear charge by the <sup>nearby</sup> surrounding electrons is called Screening effect.

If we consider only the Screening effect, then the total energy of System can be taken as like hydrogen atom i.e.

$$T = \frac{R(z-b)^2}{n^2} \quad \dots \dots \quad (1) \quad (z-b) \text{ is effective atomic number of the element}$$

where R is Rydberg Constant ( $= 2\pi^2 me^4 / ch^3$ ), n is principal quantum number, z is atomic number and b is Screening constant which also includes the effect of outer electrons on the inner ones, called external Screening. (z-b) is effective nuclear charge.

[When] an electron moves in an orbit of low quantum number in the field of the nucleus of high atomic number, the velocity of electron is high enough so that the relativistic variation of mass can be taken into account. [With this argument,] Sommerfeld and Wentzel shown that the energy of the system is calculated by,

$$T = \frac{R(z-b)^2}{n^2} + \frac{R\alpha^2}{n^4}(z-d)^4 \left[ \frac{n}{k} - \frac{3}{4} \right] + \frac{R\alpha^2}{n^6}(z-d)^6 \left[ \frac{1}{4} \left( \frac{n}{k} \right)^3 + \frac{3}{4} \left( \frac{n}{k} \right)^2 - \frac{3}{2} \left( \frac{n}{k} \right) + \frac{5}{8} \right] + \frac{R\alpha^2}{n^8}(z-d)^8 \left[ \frac{1}{8} \left( \frac{n}{k} \right)^5 + \frac{3}{8} \left( \frac{n}{k} \right)^4 + \frac{1}{8} \left( \frac{n}{k} \right)^3 - \frac{15}{8} \left( \frac{n}{k} \right)^2 + \frac{15}{8} \left( \frac{n}{k} \right) - \frac{35}{64} \right] \quad \dots \quad (2)$$

where  $\alpha^2 = \frac{4\pi^2 e^4}{c^2 h^2}$  is the fine structure constant,

$k$  is Sommerfeld azimuthal quantum number ( $= 1, 2, 3, \dots$  for s, p, d, f electrons),

$d$  is Sommerfeld Screening Constant.

The Screening Constant ' $b$ ' depends upon the distribution of electrons in the shells both outside and inside the shell containing the considered electron. Whereas the Screening Constant ' $d$ ' depends upon the variation of mass with velocity and spin motion of electron.

The effect of Screening Constant ' $b$ ' is to break each energy level into  $n$  sublevels and the corresponding terms are called reduced terms. If we add the effect of Second Screening Constant ' $d$ ' to this effect, then each sublevel splits into two levels except the ground level.

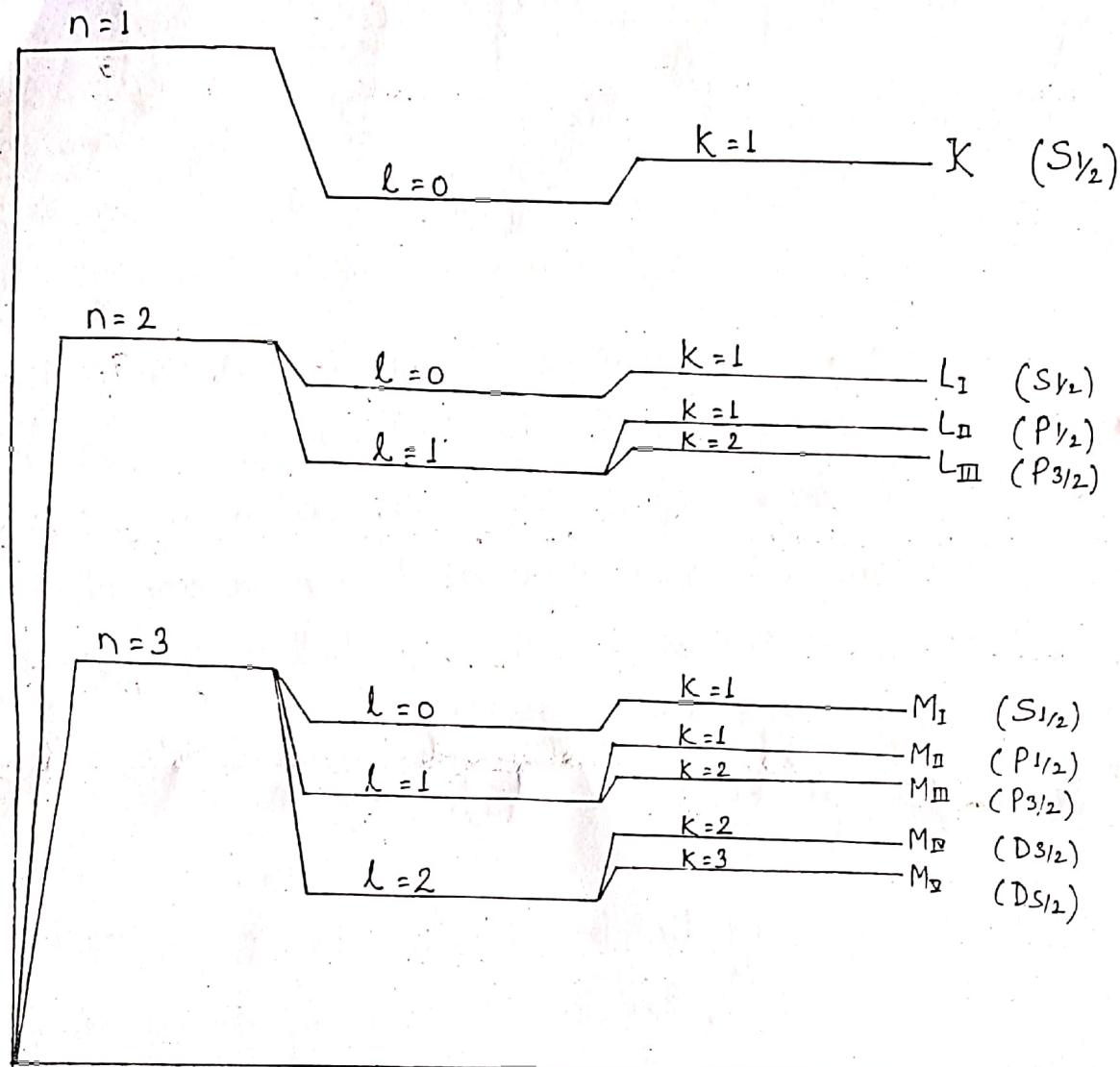
[\*]  $b$  is due to Screening effect and  $d$  is due to spin-orbit interaction and relativity.

(g)

Hydrogen like  
terms

Reduced terms

Observed terms ✓



$$\frac{Rz^2}{n^2}$$

$$\frac{R(z-b)^2}{n^2}$$

normal state

Fine structure of X-ray levels.

## Fine Structure of X-ray Spectral Lines:

In X-ray Spectra, K, L, M, N etc shells or levels are associated with the principal quantum number  $n = 1, 2, 3, 4$  etc. The zero of the energy level is taken as that of normal state of neutral atom.

Let us suppose that a neutral atom is ionized by removing a single electron from K-shell i.e. the atom is in K-energy state.

Let  $E_1$  be the amount of workdone required to remove one electron from K-shell, and  $E_2$  be that required to remove one electron from L-shell. Then, if an electron goes from L-shell to K-shell, the frequency of emitted radiation will be,

$$\nu = \left( \frac{E_1 - E_2}{h} \right) \dots \dots \dots (1)$$

and the corresponding line is called  $K_{\alpha}$  line. If an electron goes from M-shell to K-shell, then the frequency of emitted radiation will be,

$$\nu = \left( \frac{E_1 - E_3}{h} \right) \dots \dots \dots (2)$$

and the corresponding line is called  $K_{\beta}$  line, where  $E_3$  is the amount of workdone required to remove one electron from M-shell. Similarly, when electron jumps from N, O etc shells to K-shell, the different X-ray lines  $K_{\gamma}, K_{\delta}$  etc are obtained.

[From observation] it is found that the transition of electron from L-shell to K-shell is most probable than the transition from M, N etc shells to K-shell. Therefore,  $K_{\alpha}$  line is most strong and  $K_{\delta}$  is faint.

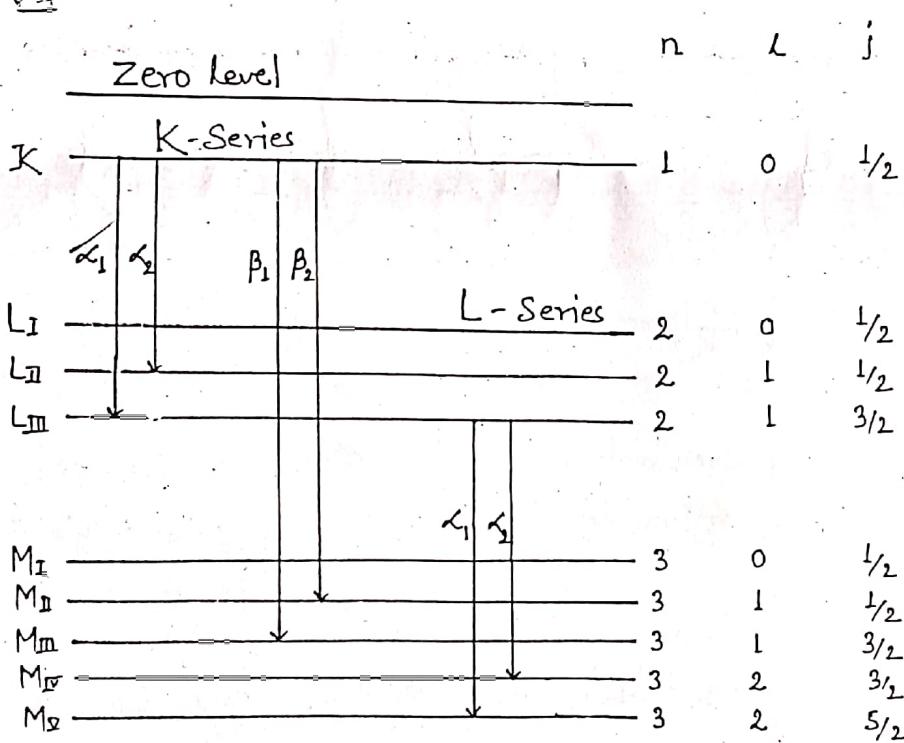
(10)

Similarly, other L, M, N series are obtained when an atom is in L, M, N-energy states respectively.

### Fine structure:

Due to Spin motion of electron, L, M, N - states are not Singlet, although K-state is singlet. L-state splits into three sublevels  $L_I$ ,  $L_{II}$  and  $L_{III}$ , M-state splits into five sublevels  $M_I$ ,  $M_{II}$ ,  $M_{III}$ ,  $M_{IV}$  and  $M_V$  and so on. The lines originating by the transitions from different L sublevels to K-state give  $K_{\alpha_1}$ ,  $K_{\alpha_2}$  lines. Similarly, the lines originating by the transitions from different M sublevels to K-state give  $K_{\beta_1}$ ,  $K_{\beta_2}$  lines as shown below:

QMP



(Selection rules:  $\Delta l = \pm 1$ , and  $\Delta j = 0, \pm 1$ )

TU.0059  
→ What are the spin and screening doublets in  $\gamma$ -ray spectrum.  
Explains their origin.

### Regular doublet (or spin relativity doublet) Law:

$L \Delta j$

by Narayan Jha

In general, the term spin relativity doublet refers to the pair of energy levels which have same  $n$  and  $l$  values but different  $j$  values. In X-ray energy levels,  $L_{II} - L_{III}$ ,  $M_{II} - M_{III}$  and  $M_{IV} - M_{V}$  have same  $n$  and  $l$  values but different  $j$  values, so these pairs are also called regular doublets.

As we know that the relativistic formula for the total energy is

$$T = \frac{R(z-b)^2}{n^2} + \frac{R\alpha^2}{n^4} (z-d)^4 \left[ \frac{n}{K} - \frac{3}{4} \right] + \frac{R\alpha^4}{n^6} (z-d)^6 \left[ \frac{1}{4} \left( \frac{n}{K} \right)^3 + \frac{3}{4} \left( \frac{n}{K} \right)^2 - \frac{3}{2} \left( \frac{n}{K} \right) + \frac{5}{8} \right] + \frac{R\alpha^6}{n^8} (z-d)^8 \left[ \frac{1}{8} \left( \frac{n}{K} \right)^5 + \frac{3}{8} \left( \frac{n}{K} \right)^4 + \frac{1}{8} \left( \frac{n}{K} \right)^3 - \frac{15}{8} \left( \frac{n}{K} \right)^2 + \frac{15}{8} \left( \frac{n}{K} \right) - \frac{35}{64} \right] \quad \dots \dots \quad (1)$$

where  $R$  is Rydberg constant,  $\alpha$  is fine-structure constant,  $K$  is Sommerfeld azimuthal quantum number and  $d$  is Sommerfeld Screening Constant.

$$K = l \pm 1 \neq 0$$

For the  $L$  doublet ( $L_{II} - L_{III}$ ),  $n=2$  and  $K=1$  for  $L_{II}$ , and we have

$$\begin{aligned} T_{L_{II}} &= \frac{R(z-b)^2}{2^2} + \frac{R\alpha^2}{2^4} (z-d)^4 \left[ \frac{5}{4} + \frac{(z-d)^2}{2^2} \times \frac{21}{8} \right] + \frac{(z-d)^4}{2^4} \left[ -\frac{15}{2} + \frac{15}{4} - \frac{35}{64} \right] \\ &= \frac{R(z-b)^2}{2^2} + \frac{R\alpha^2}{2^4} (z-d)^4 \left[ \frac{5}{4} + \frac{(z-d)^2}{2^2} \times \frac{21}{8} + \frac{(z-d)^4}{2^4} \times \frac{429}{64} \right] \\ &\quad \dots \dots \quad (2) \end{aligned}$$

(11)

For  $L_{\text{III}}$ ,  $n=2$  and  $k=2$ , and we have

$$T_{L_{\text{III}}} = \frac{R(z-d)^2}{2^2} + \frac{R\alpha^2}{2^4}(z-d)^4 \left[ \frac{1}{4} + \frac{(z-d)^2}{2^2} \times \frac{1}{8} + \frac{(z-d)^4}{2^4} \times \frac{5}{64} \right] \\ \dots \dots \dots (3)$$

Then doublet separation in wave number will be

$$\Delta v = T_{L_{\text{II}}} - T_{L_{\text{III}}} \\ = \frac{R\alpha^2}{2^4}(z-d)^4 \left[ 1 + \frac{(z-d)^2}{2^2} \cdot \frac{5}{2} + \frac{(z-d)^4}{2^4} \cdot \frac{424}{64} \right]$$

Neglecting higher terms, we get

$$\Delta v = \frac{R\alpha^2}{2^4}(z-d)^4$$

doublet separation in wave number.

$$\text{or, } \Delta v \propto (z-d)^4 \quad \dots \dots \dots (4)$$

effective nuclear charge

Equation (4) is the Regular doublet's law, which states that, The doublet separation in wavenumber is approximately proportional to the fourth power of effective nuclear charge  $(z-d)$ .

Sommerfeld's modified

Energy of the system:

$$T = \frac{R(z-d)^2}{n^2} + \frac{R\alpha^2}{n^4}(z-d)^4 \left[ \left\{ \frac{n}{k} - \frac{3}{4} \right\} + \frac{(z-d)^2}{n^2} \left\{ \frac{1}{4} \left( \frac{n}{k} \right)^3 + \frac{1}{4} \left( \frac{n}{k} \right)^4 \times 3 + \frac{1}{4} \left( \frac{n}{k} \right) (-c) + \frac{1}{4} \times \frac{5}{2} \right\} \right. \\ \left. + \frac{(z-d)^4}{n^4} \left\{ \frac{1}{8} \left( \frac{n}{k} \right)^5 + \frac{1}{8} \left( \frac{n}{k} \right)^4 \times 5 + \frac{1}{8} \left( \frac{n}{k} \right)^3 + \frac{1}{8} \left( \frac{n}{k} \right)^2 \epsilon_0 \times \frac{5}{2} + \frac{1}{8} \left( \frac{n}{k} \right) \times 6 \times \frac{5}{2} + \frac{1}{8} \left[ \frac{25}{2} \right] \right\} \right]$$

with all terms having their usual meaning

✓

## Screening doublet (or irregular doublet) law:

In general, the term Screening doublet refers to the pair of energy levels which have same  $n$  and  $j$  values but different  $l$  values. In X-ray energy levels, the pairs ( $L_I - L_{II}$ ), ( $M_I - M_{II}$ ), ( $M_{III} - M_{IV}$ ) have same  $n$  and  $j$  values but different  $l$  values, so these are called Screening doublets.

Taking only the Screening effect into account, we have the total energy formula as,

$$T = \frac{R(z-b)^2}{n^2}$$

$$\text{or, } \left(\frac{T}{R}\right)^{\frac{1}{2}} = \frac{(z-b)}{n} \quad \dots \dots (1)$$

Considering the doublet ( $L_I - L_{II}$ ). for  $L_I$ , we have  $n=2$ , and so

$$\left(\frac{T}{R}\right)_{L_I}^{\frac{1}{2}} = \frac{z-b_1}{2} \quad \dots \dots (2)$$

for  $L_{II}$ ; we have  $n=2$ , and so

$$\left(\frac{T}{R}\right)_{L_{II}}^{\frac{1}{2}} = \frac{z-b_2}{2} \quad \dots \dots (3)$$

Now difference between the square root of term values will be,

$$\begin{aligned} \left(\frac{T}{R}\right)_{L_I}^{\frac{1}{2}} - \left(\frac{T}{R}\right)_{L_{II}}^{\frac{1}{2}} &= \frac{z}{2} - \frac{b_1}{2} - \frac{z}{2} + \frac{b_2}{2} \\ &= \left(\frac{b_2 - b_1}{2}\right) \\ &= \frac{\Delta b}{2} \quad \dots \dots (4) \end{aligned}$$

where  $\Delta b$  is constant.

37  
4

Equation (4) is irregular doublet law, which states that, the difference between the square root of term values for the given <sup>irregular</sup> doublet is constant and is independent to the atomic number ( $Z$ ).

### X-ray Satellites:

The intense X-ray spectral lines are due to transition of electron between the states of singly ionized atom. And these lines + first order lines can be easily fitted on an energy level diagram. Therefore, these lines are known as first order lines or diagram lines.

However, with the instrument having high resolving power, many lines in the X-ray spectral lines are observed which could not be fitted on an energy level diagram. These new lines are known as second order or non diagram lines or satellites. The majority of such lines are faint and are found close to the short wavelength side of more intense diagram lines. It is observed that most of the first order lines are accompanied by the satellite lines.

Satellite lines have following properties:

- i) The excitation potential of certain satellites is greater than that of corresponding parent lines.
- ii) The number of satellites increases as the ionization of atom increases.
- iii) The intensity of K-Satellite lines is found to decrease in a continuous manner with increasing atomic number of radiating atom.
- iv) If, there is no multiple ionization, then the satellites are found to be absent.

The origin of Satellites can be explained on the basis of principle of multiple ionization of inner electrons.

In case of K-satellites, it is found that the energy of excitation is equal to the energy required to eject a K electron plus the L electron from the atom. That means the initial state for the emission of K satellites is a state of double ionization. In this case, the atom has an electronic vacancy in both K and L shell.

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"BEST OF LUCK"

- Bikash Sharma

TU-2159

Q. Discuss the characteristic features of x-ray spectrum from a metal. How is the emission of K and L spectral lines explained?