

## Quadrant II – Transcript and Related Materials

**Programme:** Bachelor of Science (Third Year)

**Subject** : Physics

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**Course Title** : DSC: Atomic and Molecular Physics

**Unit** : X-ray spectra

**Module Name:** Explanation on the basis of quantum mechanics, Energy levels and characteristic X-ray lines

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**Notes** :

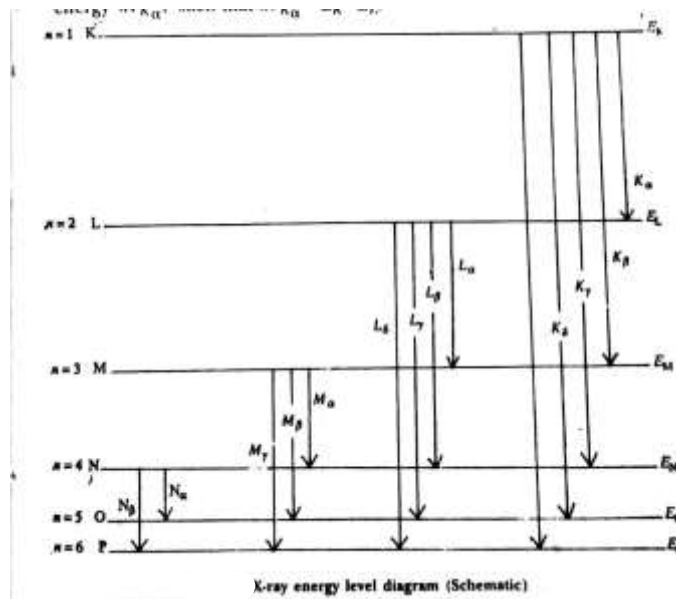
### Explanation on the basis of quantum mechanics, Energy levels

In heavy atoms, the binding energy of the K or L shell electrons is of order of a few keV. Hence in order to remove an electron from the K or L shell, the incident particles, photons or electrons must have sufficiently high energy of the order of a few keV, so that the K or L shell electron is removed to continuum. The requirement that the K shell electron be removed to continuum is because all other higher levels L, M, N etc., are filled in the case of electrons in heavy atoms. Also for the ionization to occur, the incident particle, i.e., the photon or the electron must come sufficiently close to the K shell electron so that it is removed from the atom. The probability that K shell electron is removed is much higher than the probability that a L shell shell electron is removed. Also the probability that a L shell electron is removed is much higher than the probability that a M shell shell electron is removed and so on. The reason for this is as follows.

The K shell electrons are found in a small volume and are more likely to encounter the incident particle than the L shell or M shell electrons which are spread over a larger volume.

Let the binding energy of the K shell electron be  $E_K$  and of those in the L, M, N shells

be  $E_L$ ,  $E_M$ ,  $E_N$  respectively. Suppose that we supply energy  $E_K$  to a K electron so that it is removed, then the atom has an excess energy  $E_K$ . Hence an electron from the L shell may jump to occupy the vacancy in the K shell. Now, the K shell electron is more tightly bound to the nucleus than the L shell electron, and hence the excess energy is given out in the form of a photon of energy  $h\nu_{K\alpha}$  such that  $h\nu_{K\alpha} = E_K - E_L$



Above figure shows the schematic X-ray energy level diagram in the case of an element of high atomic number. The vacancy in the K shell may be filled by the M, N or O electron, and this gives rise to the K series which consists of the following transitions:

$$h\nu_{K\alpha} = E_K - E_L$$

$$h\nu_{K\beta} = E_K - E_M$$

$$h\nu_{K\gamma} = E_K - E_N$$

Similarly if the electron from the L shell is knocked off by the incident photon or electron, the vacancy created in the L shell may be filled by the M, N or O electron giving rise to the series which consists of the following transitions:

$$h\nu_{L\alpha} = E_L - E_M$$

$$h\nu_{L\beta} = E_L - E_N$$

$$h\nu_{L\gamma} = E_L - E_O$$

As the binding energies of the electrons in the K, L, M shells are of the order of a few keV, the characteristic X-ray transitions have energies of the order of few keV. Transitions of electrons from one state to another must obey the following selection rules:

$$\Delta l = \pm 1, \quad \Delta j = 0, \pm 1$$

There is no restriction placed on the change in the value of the principal quantum number  $n$ . The transitions with  $\Delta n = 0$  are very weak and rare, and hence not observed. (These transitions arise as L and M have subshells.)

### characteristic X-ray lines

For every filled shell and a subshell, the resultant from a closed subshell, the allowed values of the orbital, spin and total angular momenta for the remaining electrons in the subshell will be the same as those for the missing electron which would complete the subshell. Hence  $n, l$  and  $j$  for a subshell with one electron missing are the same as for the electron which would complete the subshell. Thus if an electron is missing from the K shell, then the  $n, l$  and  $j$  values will be  $n=1, l=0$  and

$$j = \frac{1}{2}.$$

For the L shell,  $n=2, l=1,0$  and  $j = (\frac{3}{2}, \frac{1}{2}), \frac{1}{2}$ . For the M shell,  $n=3, l=2,1,0$  and

$j = (\frac{5}{2}, \frac{3}{2}), (\frac{3}{2}, \frac{1}{2}), \frac{1}{2}$ . And so on. Hence, one would expect three lines associated with transition of electrons from L shell to K shell, five lines associated with transitions from M shell to K shell and so on. But a detailed study of X-ray spectra shows that there are only two lines corresponding to L to K transitions and M to K transitions. The reason for this are the selection rules which are to be satisfied. These are

$\Delta l = \pm 1$  and  $\Delta j = 0, \pm 1$ . It is found that the transitions for which  $\Delta n = 0$ , rarely occur, which is quite common in optical spectroscopy. The selection rules for  $l$  and  $j$  arise naturally as a result of the quantum mechanical calculation of the probability of an electric dipole transition between the states considered.

Except for the prominent transitions, any other transition is specified by giving the initial and the final atomic level. The general rule, however, is as follows: First series is specified, depending on the value of  $n$ , e.g.  $\alpha, \beta, \gamma, \delta, \epsilon, \zeta, \eta, \theta, \iota, \kappa, \lambda, \mu, \nu, \xi, \omicron, \pi, \rho, \sigma, \tau, \upsilon, \phi, \chi, \psi, \omega, \alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5, \alpha_6, \alpha_7, \alpha_8, \alpha_9, \alpha_{10}, \alpha_{11}, \alpha_{12}, \alpha_{13}, \alpha_{14}, \alpha_{15}, \alpha_{16}, \alpha_{17}, \alpha_{18}, \alpha_{19}, \alpha_{20}, \alpha_{21}, \alpha_{22}, \alpha_{23}, \alpha_{24}, \alpha_{25}, \alpha_{26}, \alpha_{27}, \alpha_{28}, \alpha_{29}, \alpha_{30}, \alpha_{31}, \alpha_{32}, \alpha_{33}, \alpha_{34}, \alpha_{35}, \alpha_{36}, \alpha_{37}, \alpha_{38}, \alpha_{39}, \alpha_{40}, \alpha_{41}, \alpha_{42}, \alpha_{43}, \alpha_{44}, \alpha_{45}, \alpha_{46}, \alpha_{47}, \alpha_{48}, \alpha_{49}, \alpha_{50}, \alpha_{51}, \alpha_{52}, \alpha_{53}, \alpha_{54}, \alpha_{55}, \alpha_{56}, \alpha_{57}, \alpha_{58}, \alpha_{59}, \alpha_{60}, \alpha_{61}, \alpha_{62}, \alpha_{63}, \alpha_{64}, \alpha_{65}, \alpha_{66}, \alpha_{67}, \alpha_{68}, \alpha_{69}, \alpha_{70}, \alpha_{71}, \alpha_{72}, \alpha_{73}, \alpha_{74}, \alpha_{75}, \alpha_{76}, \alpha_{77}, \alpha_{78}, \alpha_{79}, \alpha_{80}, \alpha_{81}, \alpha_{82}, \alpha_{83}, \alpha_{84}, \alpha_{85}, \alpha_{86}, \alpha_{87}, \alpha_{88}, \alpha_{89}, \alpha_{90}, \alpha_{91}, \alpha_{92}, \alpha_{93}, \alpha_{94}, \alpha_{95}, \alpha_{96}, \alpha_{97}, \alpha_{98}, \alpha_{99}, \alpha_{100}$ . The most prominent transition (hence the strongest line) that is observed even with an instrument of low resolving power is called  $\alpha$ , the next strongest  $\beta$  and so on. When observed with an instrument of high resolving power, it is found that  $\alpha$  line is generally doublet. Here the more intense line is called  $\alpha_1$  and the weaker line is called  $\alpha_2$ .

In the L series  $\beta_1$  line is the next strongest line. The other weaker lines in this series are called  $\beta_2, \beta_3, \dots$  etc. The same procedure is used to designate Y lines. For the lines which are less prominent, the method of numbering is not unique as a numbering system which seems logical for one element appears totally chaotic for an element with a different atomic number.

When an electron from a  $L_{III}$  level ( $n = 2, l = 1$  and  $j = \frac{3}{2}$ ) jumps to fill the vacancy in the K shell,  $K_{\alpha 1}$  line results.  $K_{\alpha 2}$  line results due to the transition a  $L_{II}$  level ( $n = 2, l = 1$  and  $j = \frac{1}{2}$ ) to the K shell. The number of electrons in  $L_{III}$  is four ( $2j+1 = 2 \times \frac{3}{2} + 1$ ) and in  $L_{II}$ , it is two ( $2j+1 = 2 \times \frac{1}{2} + 1$ ). Hence the  $K_{\alpha 1}$  line should be twice as intense as the  $K_{\alpha 2}$  line. This has been observed experimentally. Also the  $K_{\beta 1}$  line arising from the transition from a  $M_{III}$  level ( $n = 3, l = 1, j = \frac{3}{2}$ ) is twice as intense as the  $K_{\beta 2}$  line which arises from the transition from a  $M_{II}$  level to the K shell. Here again the ratio of the values of ( $2j + 1$ ) is 4:2. But as seen earlier, this kind of simple proportionality exists only for the intensities of two lines with almost the same frequency. Thus  $K_{\alpha 1}$  is much more intense than  $K_{\beta 2}$  even though both have  $2j+1$  equal to four. This is because the probability that an L electron will fill a K vacancy is much greater than that of an M electron filling it.