

Origin of $L\beta_2^0$ Satellite in the L-emission Spectra on the Basis of $(Z+1)$ Approximation

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Abstract— One of the satellite lines accompanying the intense diagram line $L\beta_2$ in the L-emission spectra, is the satellite β_2^0 . It is well known that the satellites occur due to electronic transition in multiply ionized atoms. In the present investigation, we have theoretically investigated the origin of $L\beta_2^0$ satellite in the elements from ${}_{71}\text{Lu}$ to ${}_{84}\text{Po}$, ${}_{88}\text{Ra}$, ${}_{90}\text{Th}$ and ${}_{92}\text{U}$, in which this satellite has been observed. Shahlot and Soni have also theoretically investigated the $L\beta_2^0$ satellite using Hartree-Fock-Slater (HFS) formulae applicable in jj coupling for two hole states. A perusal of their results shows that in some cases the agreement between theoretical and experimental values is not so good. Hence, in the present investigation we have tried alternative calculations for calculating the energy of the satellite using the method of $(Z+1)$ approximation. Our calculations show better agreement with the experimental values than that obtained from the values of Shahlot and Soni. However, in some cases, our calculations also do not yield good results and this has been discussed.

Keywords—L-emission spectra, satellite $L\beta_2^0$, multiple ionization theory, $(Z+1)$ approximation, transition array

I. INTRODUCTION

When X-rays are generated by electron impact, the radiation consists of a continuous spectrum and a superimposed line spectrum characteristic of the target. A typical characteristic X-ray spectrum of a heavy element consists of a number of groups of closely spaced discrete spectral lines. The X-ray emission spectral lines have been classified into two broad groups, namely, diagram lines and non-diagram lines or satellites. The spectral lines resulting from transitions between atomic states, involving single vacancy are called ‘diagram lines’, because energy of such lines can be expressed as the difference of two terms in the ‘single vacancy’ energy level diagram. The diagram lines are found to be accompanied by groups of lines of slightly different energies and usually much smaller (10^{-2} – 10^{-3}) intensities. Such lines have energies, which do not correspond to the energy difference between any two states of the normal single vacancy energy level diagram of the element concerned. These spectral lines are known as ‘non-diagram lines’ or more commonly as ‘X-ray satellite lines’. A survey of the theories reveals that the most widely accepted theory of X-ray satellites is the multiply ionization theory. In a multiple ionized atom, the energy levels of the atom are different than those in a singly ionized atom because the electrostatic

attraction of the nucleus for the remaining electrons is increased by the absence of a second or more electrons. The X-ray satellite emitted due to transition in the multiply ionized atom has a different energy than the parent diagram line emitted by a transition in a singly ionized atom. Several methods have been used to calculate the energy difference between the double vacancy initial and final states, which could explain the origin of X-ray satellites.

The intense diagram line $L\beta_2$ in the L-emission spectra arises because of strong dipole transition L_3-N_5 ($2p_{3/2}-4d_{5/2}$) between singly ionized states. In the elements with $Z \geq 71$, the line $L\beta_2$ is accompanied with its satellites on the higher energy side. One of these satellite lines is the satellite β_2^0 [1]. In the present investigation, we have theoretically investigated the origin of $L\beta_2^0$ satellite in the elements from ${}_{71}\text{Lu}$ to ${}_{84}\text{Po}$, ${}_{88}\text{Ra}$, ${}_{90}\text{Th}$ and ${}_{92}\text{U}$, in which this satellite has been observed. Shahlot and Soni have theoretically investigated the $L\beta_2^0$ satellite and have found all the possible transitions using jj coupling scheme for the transition arrays $L_3N_x-N_xN_5$ ($x = 1 - 5$). They have used Hartree-Fock-Slater (HFS) formulae applicable in jj coupling for two hole states. They have devised a new method to find adiabatic relaxation energy which should be subtracted from the value of energy found by HFS method to arrive at the corrected value of the theoretical energy for a satellite. A perusal of their results shows that in some cases the agreement between theoretical and experimental values is not so good. Hence, in the present investigation we have tried alternative calculations for calculating the energy of the satellite using the method of $(Z+1)$ approximation. The transition array $L_3N_x-N_xN_5$ ($X=1-5$) has also been assumed by us, as the origin of this satellite, as assumed by Shahlot [2] and Soni. The experimental values have been compared with our theoretically calculated values as well as with those of Shahlot and Soni.

II. CALCULATIONS, RESULTS AND DISCUSSION

In the present investigation, we are concerned with the theoretical investigations of $L\beta_2^0$ satellite in the elements from ${}_{71}\text{Lu}$ to ${}_{84}\text{Po}$, ${}_{86}\text{Rn}$, ${}_{88}\text{Ra}$, ${}_{90}\text{Th}$ and ${}_{92}\text{U}$, as in most of these elements, the satellites have been observed. We have tried to assign transitions to the $L\beta_2^0$ satellite, on the basis of the calculations of energies of satellites considering $(Z + 1)$ approximation, i.e, the energy of the second hole in the

doubly ionized atom, both in the initial and final states, is taken as that for $(Z + 1)$ atom. The transition arrays responsible for the origin of the satellite $L\beta_2^0$ has been taken as $2p_{3/2}^{-1}4x - 4x 4d_{5/2}^{-1}(x = s, p, d)$ i.e. $L_3N_x - N_xN_5$ ($x = 1-5$) as also used by Shahlot and Soni. Our method of calculation is given below.

A. Method of Calculation of Energies of Satellites using $(Z+1)$ Approximation

The method of $(Z + 1)$ approximation can be understood by taking an example of say, $L\beta_2^0$ satellite, which appears close to and on the high energy side of the strong dipole line $L\beta_2$, which arises due to L_3-N_5 transition. Following Shahlot and Soni, $L\beta_2^0$ can be ascribed to the transition $L_3N_x - N_xN_5(x=1-5)$. This means that if initially an atom is in the singly ionized state L_3 , then a transition to N_5 state will give rise to the line $L\beta_2$. However, if the atom happens to be in a doubly ionized state with an electron missing from each of the two states L_3 and N_x , then a similar transition from a N_5 to a L_3 state will now leave the atom in the doubly ionized state N_xN_5 and give rise to the satellite $L\beta_2^0$. Let $(E_{L_3N_x})_Z$ be the energy of an atom of atomic number Z from which a L_3 and a N_x electron has been removed, then to a close approximation.

$$(E_{L_3N_x})_Z = (E_{L_3})_Z + (E_{N_x})_{Z+1}$$

since the removal of a L_3 electron is practically equivalent to increasing the pull on the N_x electron by augmenting the nuclear charge one proton unit.

$$\text{Also, } (E_{N_xN_5})_Z = (E_{N_x})_Z + (E_{N_5})_{Z+1}$$

Then, for the satellite $L\beta_2^0$ which has been assigned the transition $L_3N_x - N_xN_5$ we have

$$(E_{L\beta_2^0})_Z = (E_{L_3N_x})_Z - (E_{N_xN_5})_Z = [(E_{L_3})_Z + (E_{N_x})_{Z+1}] - [(E_{N_x})_Z + (E_{N_5})_{Z+1}]$$

For calculations, the energy values can be taken from the tables of Bearden and Burr [3]. Using this $(Z+1)$ approximation we have calculated the values of energies for all the transitions of the array $L_3N_x - N_xN_5(x=1-5)$. The averages of these values of energies have been calculated and are given in Table 1. In this table, the values for elements $_{83}\text{Bi}$ and $_{88}\text{Ra}$ are the values estimated by us by using linear interpolation method. Our theoretically calculated values of energies of $L\beta_2^0$ satellite have been compared with the experimental values, which are also given in Table 1. The agreement is good in most of the elements. However, in some elements, the agreement is not so good. It may be remarked here that $(Z+1)$ approximation method suffers from the defect that it does not take into account the multiplicity of levels in two hole states.

As already pointed out in the introduction, Shahlot and Soni have also theoretically calculated the energies of the satellite $L\beta_2^0$. In order to compare our method with their method of calculation and also to compare our theoretical values with

their theoretical values, their method of calculation and the results obtained by them are described below in brief.

TABLE I
THEORETICAL VALUES OF ENERGY (in eV) $L\beta_2^0$ SATELLITES AND THEIR COMPARISON WITH EXPERIMENTAL VALUES

S. No.	Element	Present Calculated value using $(Z+1)$ approximation as mean of transition schemes $L_3N_x - N_xN_5$ ($x = 1-5$)	ShilpaShahlot's theoretical as corrected Value of mean of transition schemes $L_3N_x - N_xN_5$ ($x = 1-5$)	Experimental value
1.	$_{71}\text{Lu}$	9054.1	9064.76*	9055.64
2.	$_{72}\text{Hf}$	9353.9	9366.85	9354.84
3.	$_{73}\text{Ta}$	9657.8	9668.17*	9659.39
4.	$_{74}\text{W}$	9967.5	9971.14	9969.96
5.	$_{75}\text{Re}$	10284.4	10290.12*	10282.32
6.	$_{78}\text{Pt}$	11257.7	11247.48	11259.18
7.	$_{79}\text{Au}$	11589.5	11589.52*	11594.71
8.	$_{81}\text{Tl}$	12280.9	12273.61*	12283.05
9.	$_{82}\text{Pb}$	12630.6	12618.72	12632.96
10.	$_{83}\text{Bi}$	12985.0*	12991.56*	12991.09
11.	$_{88}\text{Ra}$	14877.8*	14871.23	14858.55
12.	$_{90}\text{Th}$	15641.9	15623.36*	-
13.	$_{92}\text{U}$	16439.2	16375.29*	16444.34

Note - * Denotes interpolated values.

B. Shilpa Shahlot and Soni's Theoretical Method of Calculation of Energies of the Satellites $L\beta_2^0$

Shahlot and Soni have calculated $L_3N_x - N_xN_5$ transition energies in elements with $Z \geq 72$ in which jj - coupling approximation is most suitable. The HFS formulas for the energies of two hole states like, L_3N_x and N_xN_5 (for $X = 1-5$) have been established. Each formula shows that the energy of any two hole state is given as the sum of three types of energies. The major part of this energy is due to sum of the energy of single hole states, the second major part is the spin orbit interaction energy between two holes, and the third contribution is due to weak electrostatic interaction energy between two holes. To calculate the total energy for a particular state, the energy of single hole states like L_3 , N_x and N_5 have been taken from the tables of Bearden and Burr to calculate spin orbit interaction energy, the values of spin orbit constants have been taken from tables of Larkins [4]. To calculate the values of electrostatic energies, the values of all Slater integrals F 's and G 's have been taken from the tables of Mann [5]. In these tables the values of Slater integrals are given in atomic units, therefore, all these values have been changed to eV by multiplying the values of integrals by 13.6. The energies for all possible J values for each two hole configuration, under study have been calculated.

Using the energies of two hole states, the energies of various transitions of arrays $L_3N_x - N_xN_5$ have been calculated. Only those transitions have been considered which are allowed according to the dipole selection rules applicable for transitions in two electron system.

The averages of five arrays $L_3N_x - N_xN_5$ have been calculated. Energies of all the five arrays $L_3N_x - N_xN_5$ ($x = 1$ to 5) are mutually very much close with one another and hence simple averages of transitions have been calculated. Their overall average has then been calculated. The $L\beta_2^0$ satellite has been associated with these five arrays.

Shirley [6] in 1973 had suggested that when two electrons are removed from the atom, the orbits of the atom relax and adjust to the new potential field and this relation modifies the energy of the two hole states. This modification in the energy remains within the atom and hence it was named "adiabatic relaxation energy" (ARE). According to Shirley, it is possible to use the intermediate coupling formulae with the values of Slater integrals and of spin orbit parameter, which are applicable for neutral atom, but small correction term for adiabatic relaxation energy (ARE) had to be applied in the end of the formula. The adiabatic relaxation energy (ARE) for a transition can be written as $k(\text{initial}) - k(\text{final}) = \Delta k$. Δk is calculated as the difference between the theoretically calculated transition energies in intermediate coupling using HFS formulas with the experimentally measured energies of satellites. The difference for each transition and satellite energy is found to be nearly constant and an average of the difference is used as the correction term Δk . Using this method Shahlot and Soni have assigned the transition scheme $L_3N_x - N_xN_5$ ($x=1-5$) to the satellite $L\beta_2^0$. The theoretical

values of the energy of the satellite $L\beta_2$ as reported by Shahlot and Soni are given in Table 1. These authors have calculated the theoretical energies for elements with $Z= 72, 74, 78, 82, 88$. The values given in Table 1 for other elements are the values estimated by us by using linear interpolation method. It is seen from the Table 1 that the agreement between the theoretical and experimental values from our calculations is better than from the calculations of Shahlot and Soni. Also, the agreement is not good in some of the elements in the case of Shahlot and Soni's calculations.

III. CONCLUSIONS

Our calculations show better agreement with the experimental values than that obtained from the values of Shahlot and Soni. However, in some cases, our calculations also do not yield good results. The reason for this may be that the procedure used for grouping of the transition schemes, as devised by Shahlot and Soni, may not be the correct procedure. The best alternative is to obtain theoretical satellite spectra. But this is not possible at the moment, because relative intensities of many transitions are not available in literature.

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