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Origin of $L\beta_2^0$ satellite in higher Z elements

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Abstract. One of the satellite lines accompanied with the intense diagram line $L\beta_2$ (L_3-N_5) on the higher energy side, is the satellite β_2^0 in the elements from $_{71}$Lu to $_{84}$Po, $_{88}$Ra, $_{90}$Th and $_{92}$U. Shahlot and Soni have theoretically investigated this satellite and have found all the possible transitions using jj coupling scheme using Hartree-Fock-Slater formulae. 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 by using the tables of Parente et al. While these calculations are relativistic ab initio calculations, those of Shahlot and Soni are non-relativistic semi-empirical calculations. Considering the same grouping of transition schemes as assigned by Shahlot and Soni, calculations have been done by us using the tables of Parente et al, which gives the values of transition energies only for the 11 elements. The transition energies for intermediate elements have been calculated by us by linear interpolation method. 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.

1. Introduction

The X-ray emission spectra consists of diagram lines and non-diagram lines or satellites. The diagram lines result from transitions between atomic states, involving single vacancy. 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 intensities called satellites. 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. 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. In the present work we have attempted to explain the origin of one of the L-emission 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, in which this satellite has been observed. Shahlot [2] 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 and 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 theoretical transition energies by Parente *et al.* and assuming the same transition array as the origin of this satellite, as assumed by Shahlot and Soni. The experimental values have been compared with our theoretically calculated values as well as with those of Shahlot and Soni.

2. Calculations

In the present investigation, we are concerned with the theoretical investigations of $L\beta_2^0$ satellite in the elements from $_{71}$Lu to $_{84}$Po, $_{86}$Rn, $_{88}$Ra, $_{90}$Th and $_{92}$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 using energies of transitions in the doubly ionized atom as theoretically calculated by Parente *et al.* [3] and given in the form of tables. For our present calculations of the energies of $L\beta_2^0$ satellite, we have assumed the transition arrays responsible for the origin of the satellite $L\beta_2^0$ 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), i.e., the same as assumed by Shahlot and Soni. Our method of calculation is given below**.**

2.1. Method of Calculation of Energies of Satellites using tables of Parente et al.

As pointed out above, the available theoretical calculations by Parente *et al.*, which give energies of transitions in doubly ionized atoms that arise from the presence of one 'spectator hole' in the M- or N-shells of the emitting atom which can be used to explain the origin of L- emission satellites. They have listed for 11 elements, namely , $_{65}$Tb, $_{67}$Ho, $_{70}$Yb, $_{74}$W, $_{78}$Pt, $_{80}$Hg, $_{85}$At, $_{88}$Ra, $_{90}$Th, $_{92}$U, $_{95}$Am, the energies of all electric dipole and electric quadrupole L X-rays for which the final state comprises two vacancies in the M- and N-Shells.

Energies of initial and final atomic states have been computed separately to allow for complete relaxation. With a local approximation to the atomic potential, Dirac-Hartree-Slater (DHS) wave functions have been computed. A vacuum polarization correction has been included by means of first order perturbation according to the method of Huang [4] The self-energy shift has been calculated from Mohr's coulomb shifts [5]. The effect of screening, relaxation and finite nuclear extent on self - energy has been taken into account approximately. The computations have been carried out in j-j coupling appropriate for the high Z-region. The electrostatic interactions between the two inner-shell holes in the initial and final states have been included, but coupling with unfilled sub-shells, if any, has been neglected. No electron-electron coulomb correlation effects have been included.

In these tables have been listed all the X-ray satellite theoretical energies for the selected 11 elements. The tables do not give which observed satellites correspond to which transitions. One has to identify the transitions corresponding to the observed satellites.

In the present investigation, we have used the tables of Parente et al. not only for the 11 elements for which Parente et al have listed the transition energies, but also for nearly all the elements from Z = 60 onwards. This has been done by us using interpolation method. The transition energies for intermediate elements have been calculated by interpolation from transition energies for nearby elements among the 11 elements. Our calculated values for the energies of $L\beta_2^0$ satellite using the tables of Parente et al. are given in table 1 along with the experimental values.

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 1: Theoretical values of energy (in eV) $L\beta_2^0$ satellite and their comparison with experimental values

S. No.	Elements	Present calculated value using tables of Parente *et al.* as mean of transition schemes L_3N_x - N_xN_5 (x = 1-5)	Shilpa Shahlot's theoretical value as corrected value of mean of transition schemes L_3N_x- N_xN_5 (x =1-5)	Experimental value
1.	$_{71}$Lu	9061.88[a]	9064.76[a]	9055.64
2.	$_{72}$Hf	9363.55[a]	9366.85	9354.84
3.	$_{73}$Ta	9665.22[a]	9668.17[a]	9659.39
4.	$_{74}$W	9966.89	9971.14	9969.96
5.	$_{75}$Re	10289.42[a]	10290.12[a]	10282.32
6.	$_{78}$Pt	11257.00	11247.48	11259.18
7.	$_{79}$Au	11612.30[a]	11589.52[a]	11594.71
8.	$_{81}$Tl	12328.22[a]	12273.61[a]	12283.05
9.	$_{82}$Pb	12688.85[a]	12618.72	12632.96
10.	$_{83}$Bi	13049.51[a]	12991.56[a]	12991.09
11.	$_{88}$Ra	14852.60	14871.23	14858.55
12.	$_{90}$Th	15636.90	15623.36[a]	-
13.	$_{92}$U	16443.84	16375.29[a]	16444.34

Note - [a] Denotes interpolated values

2.2 Shilpa Shahlot and Soni's theoretical method of calculation of energies of the satellite $L\beta_2^0$

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 [6] to calculate spin orbit interaction energy, the values of spin orbit constants have been taken from tables of Larkins [7]. 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 [8]. 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 and is taken as the theoretical energy of the $L\beta_2^0$ satellite.

Shirley [9] 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 is named as 'adiabatic relaxation energy' (ARE). The adiabatic relaxation energy (ARE) for a transition can be written as k(initial) - k(final) = Δk and is calculated as the difference between the theoretically calculated transition energies in intermediate

coupling using HFS formulae 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 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 this table that the agreement between the theoretical and experimental values is not good in some of the elements.

3. Results and discussions

The results are given in table 1. It can be seen from the table that 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 and that we have also used the same transitions for our calculations. 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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