

Origin of the satellites $L\alpha_6$ and $L\alpha_7$ in the elements $_{40}\text{Zr}$ to $_{50}\text{Sn}$

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Abstract. The origin of the satellites $L\alpha_6$ and $L\alpha_7$ have been explained in the elements from $_{40}\text{Zr}$ to $_{50}\text{Sn}$. The energies and the intensities of the various transitions corresponding to the $L_3M_x - M_xM_{4,5}$ (where $x = 1-5$) transition array, which may give rise to these satellites, have been calculated theoretically. The transition energies have been calculated using the available Hartree-Fock-Slater data for K-LM and L-MM Auger transition energies. The intensities of the various transitions have been estimated by considering cross sections $L_1-L_3M_x$ for Coster-Kronig transitions as well as for M-shell shake-off process occurring simultaneous to a L_3 hole creation. The total cross sections for initial two-hole states have been then distributed statistically amongst various allowed transitions from the initial states L_3M_x to the final states $M_xM_{4,5}$. Each transition has been assumed to give rise to a Gaussian line and then the theoretical satellite spectrum has been computed by summing up these Gaussian lines. The calculated energies have been found to be comparable with the measured energies of the satellites $L\alpha_6$ and $L\alpha_7$. Consequently, the transitions which give rise to these satellites have been identified. The satellite $L\alpha_6$ has been assigned the transition $^3D_2L_3M_3 - ^3F_3M_3M_5$ and the satellite $L\alpha_7$ the transition $^3P_0L_3M_3 - ^3P_1M_3M_5$ in all the elements from $_{40}\text{Zr}$ to $_{50}\text{Sn}$.

1. Introduction

$L\alpha$ satellites $L\alpha_6$ and $L\alpha_7$ have been observed [1] in the elements from $_{40}\text{Zr}$ to $_{50}\text{Sn}$. Poonia and Soni [2] have theoretically studied the $L\alpha$ satellites in these elements but they have not studied $L\alpha_6$ and $L\alpha_7$ satellites. Hence, in the present study, we have theoretically studied these satellites using the multiple ionization theory. The origin of these satellites has been explained by computing the theoretical satellite spectra and then by assigning the transitions to these satellites. Earlier, we have theoretically investigated the satellites $L\alpha_3$, $L\alpha_4$ and $L\alpha_5$ in these elements and have assigned transitions to the satellites [3]. Hence, to complete the investigation of $L\alpha$ satellites in these elements, we have now studied $L\alpha_6$ and $L\alpha_7$ satellites.

2. Theoretical considerations

Poonia and Soni [2] have assigned the origin of $L\alpha$ satellites to the transition array $2p^{-1}3x^{-1} - 3x^{-1}3d_{3/2,5/2}^{-1}$ ($x = s, p, d$). Hence, we have also assumed that the origin of the $L\alpha$ satellites observed near the dipole lines $L\alpha_1(L_3-M_5)$ and $L\alpha_2(L_3-M_4)$ can be ascribed to the transition scheme $2p^{-1}3x^{-1} - 3x^{-1}3d_{3/2,5/2}^{-1}$ ($x = s, p, d$), i.e., $L_3M_x - M_xM_{4,5}$, ($X = 1, \dots, 5$). This means that if an atom happens to be in a doubly ionized state with an electron missing from each of the two states L_3 and M_x , then a similar transition from $M_{4,5}$ to L_3 state will now leave the atom in the doubly ionized state $M_xM_{4,5}$. This hole in M_x subshell remains a spectator and is called spectator vacancy. L_3M_x is initial state and $M_xM_{4,5}$ is



final state. All the possible initial $2p^{-1} 3x^{-1} (L_3M_x)$ states and final $3x^{-1} 3d_{3/2,5/2}^{-1} (M_xM_{4,5})$ states are calculated in LS coupling scheme. Considering the dipole selection rules, 49 transitions have been found out corresponding to the transition scheme $L_3M_x - M_xM_{4,5}$ [3]. In the earlier work [3], the energies and intensities of these 49 transitions have been calculated and then theoretical satellite spectra have been synthesized for all the elements under consideration. In the present investigation, we have utilised the same theoretical calculations and the same theoretical satellite spectra as reported in ref. [3]. However, in the present paper we are reproducing the method of calculations and the spectra, reported in ref. [3], for completeness.

3. Calculations

3.1. Calculation of energies of transitions in doubly ionized atoms

The energy of a satellite has been calculated, on the basis of multiple ionization theory by using the energies of Auger transitions and by taking the energy of the diagram line, to which the satellite belongs. The formula for calculation of transition energy of say, ${}^3D_2L_3M_3 - {}^3F_3M_3M_5$ transition, has been written as

$$E({}^3D_2L_3M_3 - {}^3F_3M_3M_5) = E(K\alpha_1) + E(L_3 - {}^3F_3M_3M_5) - E(K - {}^3D_2L_3M_3)$$

The energy of $K\alpha_1$ line, i.e., $E(K - L_3)$ has been taken from the tables of Cauchois and Senemaud [1]. The energies of the Auger transitions $L_3 - {}^3F_3M_3M_5$ and $K - {}^3D_2L_3M_3$ have been taken from the tables of Larkins [4].

3.2. Calculation of intensities of transitions in doubly ionized atoms

After the creation of a single-hole state, it is the probability of a particular subsequent process that leads to the formation of initial two-hole state, required for the emission of a satellite. The single-hole state can get converted into the two-hole states by two processes, i.e., Auger transition and shake-off process. To calculate the probability of creation of the initial double vacancy state by the process of Coster-Kronig transition, the cross section for creation of single vacancy state is first calculated by the formulae given by Moores *et al.* [5] and then this cross section is multiplied by the transition rates for the Coster-Kronig transition as given in the tables of Chen *et al.* [6]. The singly ionized state may get converted to doubly ionized state also by an associated shake-off of an electron. Hence, to calculate the probability of creation of the initial double vacancy state by the shake-off process, the cross section for creation of single vacancy state, as calculated above, is multiplied by the shake-off probability as calculated from the reports of Carlson *et al.* [7, 8] and Slater [9]. Finally, the total probability of creation of doubly ionized initial state can be determined by adding both the cross sections calculated above, i.e., by Coster-Kronig transition and by shake-off process. This probability can then be distributed statistically among all the allowed transitions using the tables of White and Eliason as given by Condon and Shortley [10]. In this method, all the multiplets of supermultiplets from various levels of the set are considered.

3.3. Synthesis of satellite spectra

A composite spectrum formed by spectral lines emitted by the 49 transitions has been computed by taking each as a Gaussian line. For this we have taken energy on X-axis and transition probability on Y-axis. The peak height of each line has been taken equal to transition probability and peak position has been taken at the energy of transition. The widths of all the lines in one element have been assumed equal. A representative theoretical satellite spectrum for the element ${}_{48}\text{Cd}$ is shown in Fig. 1 (reproduced from ref. [3]). The two satellites under investigations, i.e., $L\alpha_6$ and $L\alpha_7$ along with the transitions giving rise to them are clearly visible in this figure. The observed and theoretical positions are also marked in the figure. The theoretical spectra have been compared with the available experimental results for energies of the satellites. The intense peaks have been identified as the observed satellite lines and the transition assignment to the satellites, based on the identification of the peaks to the particular transitions, has then been done.

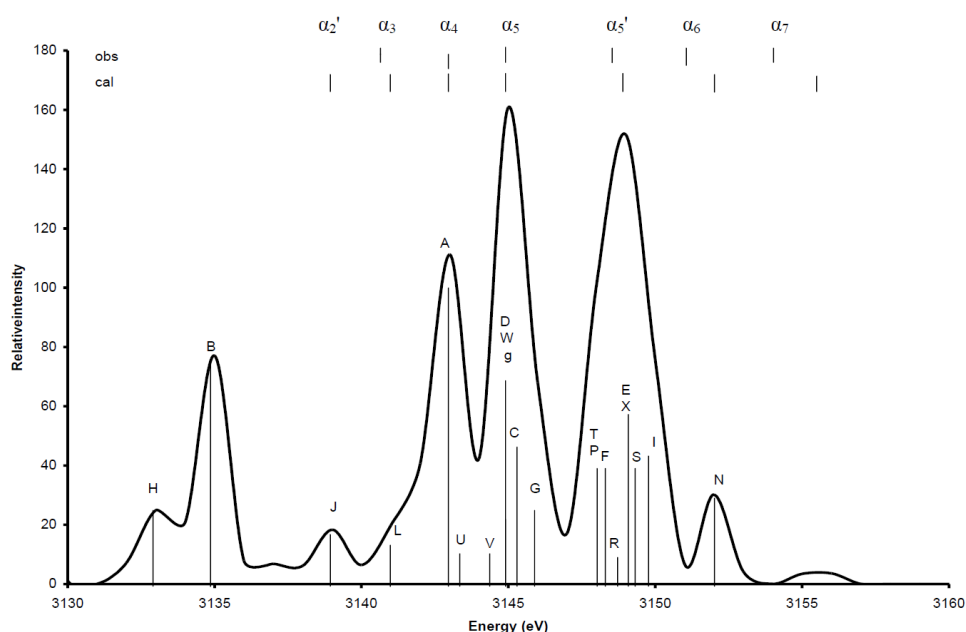


Fig.1 The computed $2p_{3/2}^{-1} 3x^{-1} - 3x^{-1} 3d^{-1} (L_3 M_x - M_x M_{4,5})$ spectrum of ^{48}Cd . The satellite positions experimentally observed and theoretically calculated in the region of La satellites are shown at the top (reproduced from ref. [3]).

Table 1 Assignments of transitions to La satellites La_6 and La_7 in the elements from ^{40}Zr to ^{50}Sn .

S.No	Z	Theoretically computed data for satellite La_6 Transition $^3\text{D}_2 - ^3\text{F}_3 (3p)$		Measured energy (eV)	Theoretically computed data for satellite La_7 Transition $^3\text{P}_0 - ^3\text{P}_1 (3p)$		Measured energy (eV)
		Energy (eV)	Normalized relative intensity		Energy (eV)	Normalized relative intensity	
1	40	2057.9	30.61	2056.6	2058.4	7.32	2059.2
2	41	2181.8	22.40	2181.3	2182.7	5.21	2183.3
3	42	2309.1	27.77	2303.5	2310.5	5.10	2307.1
4	43	2441.8	28.01	-	2443.4	5.23	-
5	44	2575.0	27.07	2575.1	2576.9	5.24	2578.7
6	45	2713.9	26.99	2713.8	2716.0	5.24	2717.9
7	46	2856.1	32.57	2856.7	2858.4	5.29	2861.4
8.	47	3002.2	29.00	3003.3	3004.9	4.68	3008.7
9	48	3152.0	30.13	3153.9	3155.5	5.80	3158.0
10	49	3306.5	31.50	3308.7	3308.1	5.36	3315.2
11	50	3463.0	34.30	3469.4	3466.0	6.34	3473.7

Measured energies are from Cauchois and Senemaud [1].

4. Results and discussions

4.1. Assignments of transitions to satellite $L\alpha_6$

$L\alpha_6$ satellite has been observed in most of the elements from $_{40}\text{Zr}$ to $_{50}\text{Sn}$. The peak corresponding to this satellite should occur at the higher energy side of the $L\alpha_5'$ satellite and very near to it, according to the value of its energy. In our theoretical $L\alpha$ satellite spectra of the elements with $Z = 40$ to 50 , there appears a peak on the higher energy side of $L\alpha_5'$ satellite and we have designated it as $L\alpha_6$ satellite. This peak arises due to transition $^3D_2 - ^3F_3$ (3p). The computed energy of this peak is in agreement with the energy of $L\alpha_6$ satellite in all the elements from $_{40}\text{Zr}$ to $_{50}\text{Sn}$, except for $_{42}\text{Mo}$, $_{49}\text{In}$ and $_{50}\text{Sn}$. On the basis of the present study, it is suggested that in $_{42}\text{Mo}$ the $L\alpha_6$ satellite reported in the tables [1] at 2303.54 eV should be redesignated as $L\alpha_5'$ satellite and the satellite observed at 2307.1 eV and designated as $L\alpha_7$ satellite should be redesignated as $L\alpha_6$ satellite. Similarly, in $_{49}\text{In}$ the satellite reported at 3308.69 eV and designated as $L\alpha_6$ satellite in the table [1] should be redesignated as $L\alpha_7$ satellite. Further, we suggest that $L\alpha_6$ satellite has not been observed in $_{49}\text{In}$. In $_{50}\text{Sn}$ the satellite observed at 3464.43 eV and designated as $L\alpha_5'$ in the table [1] should be redesignated as $L\alpha_6$ satellite. After doing the redesignations as suggested above in the elements $_{42}\text{Mo}$, $_{49}\text{In}$ and $_{50}\text{Sn}$ and also after accepting that $L\alpha_6$ satellite has not been observed in $_{49}\text{In}$, the situation regarding $L\alpha_6$ satellite becomes clear that it arises due to the transition $^3D_2 - ^3F_3$ (3p) in all the elements from $_{40}\text{Zr}$ to $_{50}\text{Sn}$. The table [1] gives the energies and intensities of the peaks identified as the two satellites $L\alpha_6$ and $L\alpha_7$. The measured energies [1] are also given in this table. It can be seen that the theoretical and measured energies agree well with each other.

4.2. Assignments of transitions to satellite $L\alpha_7$

This satellite has been reported [1] in all the elements from $_{40}\text{Zr}$ to $_{50}\text{Sn}$. In our theoretical $L\alpha$ satellite spectra there is a very weak peak on the higher energy side of $L\alpha_6$ satellite. This weak peak is the seventh peak in our theoretical satellite spectra and arises out of the transition $^3P_0 - ^3P_1$ (3p), which has a small relative intensity. The energy of this peak agrees fairly well with the energy of the satellite $L\alpha_7$ in the elements from $_{40}\text{Zr}$ to $_{50}\text{Sn}$, in which it has been observed. Thus, as a result of the present study, the $L\alpha_7$ satellite arises due to transition $^3P_0 - ^3P_1$ (3p) in the middle-Z elements from $_{40}\text{Zr}$ to $_{50}\text{Sn}$.

5. Conclusions

As a result of the present study, it has been found that the satellite $L\alpha_6$ arises due to the transition $^3D_2L_3M_3 - ^3F_3M_3M_5$ and the $L\alpha_7$ satellite arises due to transition $^3P_0L_3M_3 - ^3P_1M_3M_5$ in all the elements from $_{40}\text{Zr}$ to $_{50}\text{Sn}$.

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