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Abstract. The origin of the $\text{La}_3$, $\text{La}_4$ and $\text{La}_5$ satellites have been explained in the elements from $^{40}\text{Zr}$ to $^{50}\text{Sn}$, on the basis of multiple ionization theory. The energies and intensities of the various transitions corresponding to the $\text{L}_x\text{M}_x - \text{M}_x\text{M}_4,5$ (where $x = 1-5$) transition array, which may give rise to these satellites, have been calculated theoretically. The energies of the transitions have been calculated using the available Hartree-Fock-Slater data for the energies of K-LM and L-MM Auger transitions. The intensities of the various transitions have been estimated by considering cross sections for $\text{L}_1\text{L}_3\text{M}_x\text{Coster-Kronig}$ transitions as well as for M-shell shake-off process occurring simultaneous to a $\text{L}_3$ hole creation. The total cross sections for initial two-hole states $\text{L}_3\text{M}_x$ have then been distributed statistically amongst the various allowed transitions from these initial states to the final states $\text{M}_x\text{M}_4,5$. By assuming each transition as a Gaussian line, theoretical satellite spectrum has been computed as the sum of these Gaussian curves. The energies of the satellites, as obtained from the theoretical spectrum, have been found to be comparable with the measured energies of the satellites $\text{La}_3$, $\text{La}_4$ and $\text{La}_5$. Consequently, these satellites have been assigned the transitions.

1. Introduction

$\text{La}$ satellites $\text{La}_3$ (or $\text{La}'$), $\text{La}_4$ (or $\text{La}''$) and $\text{La}_5$ (or $\text{La}'''$) have been observed [1] in the elements from $^{40}\text{Zr}$ to $^{50}\text{Sn}$. Poonia and Soni [2] have studied theoretically the $\text{La}$ satellites in some of these elements. In their calculations they have used the Coster-Kronig transition probabilities from the tables of McGuire [3] based on non-relativistic calculations. The tables of McGuire were superseded by the tables of Chen et al. [4], who have done relativistic calculations. Hence, we thought it proper to do fresh calculations using the tables of Chen et al. and to make a comparison of the present calculations with those of Poonia and Soni. Also, we have tried to explain the origin of the satellites in all the elements in which it has been observed.

2. Theoretical considerations

2.1. Initial and final states for the $\text{La}$ satellites

Poonia and Soni have assigned the origin of $\text{La}$ satellites to the transition array $2p^{1}3s^{1}x^{-1} - 3x^{-1}3d_{3/2,5/2}^{-1}$ ($x = s, p, d$). Hence, we have also assumed that the origin of the $\text{La}$ satellites observed near the dipole lines $\text{La}_i(L_{3d}M_4)$ and $\text{La}_j(L_{3d}M_3)$ can be ascribed to the transition scheme $2p^{1}3s^{1}x^{-1} - 3x^{-1}3d_{3/2,5/2}^{-1}$ ($x = s,
2.2. Calculation of energies of transitions in doubly ionized atoms

The formula for calculation of transition energy of say, $^1P_1L_3M_1 - ^3P_0M_3M_5$ transition, has been written as

$$E (^1P_1L_3M_1 - ^3P_0M_3M_5) = E(K\alpha) + E(L_3 - ^3P_0M_3M_5) - E(K - ^1P_1L_2M_1)$$

The energy of $K\alpha$ line, i.e., $E(K - L_3)$ has been taken from the tables of Cauchois and Senemaud [1]. The energies of the Auger transitions $L_3 - ^3P_0M_3M_5$ and $K - ^3D_2L_3M_3$ have been taken from the tables of Larkins [5].

2.3. 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. [6] 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. [4] 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]. 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 [8]. In this method, all the multiplets of supermultiplets from various levels of the set are considered.

2.4. 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. A representative theoretical satellite spectrum for the element $^{116}$Cd is shown in Fig. 1. The three satellites under investigations, i.e., $L\alpha_1$, $L\alpha_2$ and $L\alpha_5$ 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.

3. Result and discussion

In the middle-Z elements from $^{40}$Zr to $^{50}$Sn, the theoretical spectra of La satellites may have at least 8 peaks in each of these elements under consideration, In $^{50}$Sn the number of peaks is as large as 13. Some peaks are strong and should correspond to the observed satellites. Table 1 gives the theoretical energies and relative intensities of the satellites along with experimental values of the energy.
3.1. Satellite $L\alpha$' (or $L\alpha_3$)
In the present study, the second strong peak in the computed spectra has been identified as the $L\alpha$' (or $L\alpha_3$) satellite which has been reported in almost all the elements. The transition which gives rise to this peak and hence to the satellite $L\alpha$' (or $L\alpha_3$) is A, i.e., $^3F_4 - ^3P_4$ (3d). Transition U, i.e., $^3P_1 - ^3P_0$ (3d) also contributes to the intensity of the satellite.

3.2. Satellite $L\alpha''$ (or $L\alpha_4$)
In the present study, the third peak in the computed $L\alpha$ satellite spectra has been identified as the $L\alpha''$ (or $L\alpha_4$) satellite. Considering the various transitions which give rise to this peak, we have found that the transitions D, V, C, W, G, g, i, u, i.e., $^3P_2 - ^3F_2$ (3d), $^1P_1 - ^3P_1$ (3d), $^3P_2 - ^3D_2$ (3s), $^3P_1 - ^3D_2$ (3p), $^1P_1 - ^3D_2$ (3s), $^3D_2 - ^3P_1$ (3p), $^1P_1 - ^3D_2$ (3s) and $^3P_1 - ^3D_2$ (3s) transitions are responsible for the origin of the satellite $L\alpha''$ (or $L\alpha_4$) in all the elements with $Z = 40$ to 50.

It may be remarked here that in the elements $\alpha_2$Zr, $\alpha_3$Nb, the satellite $L\alpha''$ (or $L\alpha_4$) appears as a clear peak, while the satellite $L\alpha'$ (or $L\alpha_3$) appears as a shoulder on the lower energy side of this clear peak. On the contrary, in the elements $\alpha_2$Mo, $\alpha_3$Tc and $\alpha_4$Ru, the satellite $L\alpha'$ (or $L\alpha_3$) appears as a clear peak, while the satellite $L\alpha''$ (or $L\alpha_4$) appears as a shoulder on the higher energy side of this clear peak. This is an important result of the present study.

Table 1(a) Assignments of transitions to $L\alpha$ satellites $L\alpha_1$ and $L\alpha_2$ in the elements from $\alpha_2$Zr to $\alpha_5$Sn.

| S. No | Z    | Theoretically computed data for satellite $L\alpha_1$ | Theoretically computed data for satellite $L\alpha_2$ |
|-------|------|-----------------------------------------------------|-----------------------------------------------------|
|       |      | Present work Transitions A,U                        | Present work Transitions D,V,C,W,G,i,u                |
|       |      | Energy (eV) Normalized relative intensity | Energy (eV) Relative intensity | Energy (eV) Normalized relative intensity | Energy (eV) Normalized relative intensity |
| 1     | 40   | 2048.8, 115.50                                     | 2048.6, 311.15                                      | 2048.9                                      | 2049.2, 142.57                                  |
| 2     | 41   | 2172.9, 137.83                                     | -                                                    | 2172.4, 84.10                              | -                                                    |
| 3     | 42   | 2300.1, 124.80                                     | 2300.1, 194.52                                      | 2301.4, 78.61                              | 2301.2, 112.41                                  |
| 4     | 43   | 2432.9, 136.36                                     | -                                                    | 2434.4, 99.9                               | -                                                    |
| 5     | 44   | 2566.1, 142.40                                     | 2566.3, 153.30                                      | 2568.1, 100                               | 2567.4, 94.95                                  |
| 6     | 45   | 2705.1, 131.50                                     | -                                                    | 2706.9, 113.81                            | -                                                    |
| 7     | 46   | 2847.1, 137.20                                     | 2847.0, 112.83                                      | 2848.9, 136.1                             | 2848.4, 74.99                                  |
| 8     | 47   | 2993.1, 112.50                                     | -                                                    | 2995.9, 134.66                            | -                                                    |
| 9     | 48   | 3143.0, 114.31                                     | -                                                    | 3144.9, 160.83                            | 3144.9, 9.95                                   |
| 10    | 49   | 3296.2, 107.56                                     | -                                                    | 3298.8, 145.84                            | -                                                    |
| 11    | 50   | 3454.1, 108.20                                     | -                                                    | 3456.1, 134.01                            | -                                                    |

3.3. Satellite $L\alpha'''$ (or $L\alpha_5$)
The fourth peak on the higher energy side of $L\alpha''$ (or $L\alpha_4$) satellite and well separated from it, has been identified as the satellite $L\alpha'''$ (or $L\alpha_5$) in the theoretical $L\alpha$ satellite spectra. The transitions which give rise to this peak and hence to the satellite $L\alpha'''$ (or $L\alpha_5$) are E, F, S and T, i.e., transitions $^5D_3 - ^3F_4$ (3d), $^5D_2 - ^3F_3$ (3d), $^1F_3 - ^3D_2$ (3d) and $^1P_1 - ^3D_2$ (3d) along with some weak transitions. Poonia and Soni and Poonia have also assigned the same transitions to this satellite.
Table 1(b) Assignments of transitions to L\(\alpha\) satellite L\(\alpha\)_5 in the elements from \(\alpha\_Zr\) to \(\alpha\_Sn\).

| S. No | Z  | Present work Transitions E, F, S, T | Energy (eV) | Normalized relative intensity | Poonia's work | Energy (eV) | Relative intensity | Measured energy (eV) |
|-------|----|--------------------------------------|-------------|-------------------------------|---------------|-------------|-------------------|---------------------|
| 1     | 40 |                                      | 2052.3      | 188.03                        |               | 2052.1      | 309.74            | 2053.0              |
| 2     | 41 |                                      | 2176.3      | 152.42                        |               |             |                   |                     |
| 3     | 42 |                                      | 2304.0      | 147.26                        |               | 2304.2      | 201.53            | 2302.0              |
| 4     | 43 |                                      | 2436.9      | 159.48                        |               |             |                   |                     |
| 5     | 44 |                                      | 2570.9      | 164.4                         |               | 2570.9      | 164.4            | 2570.5              |
| 6     | 45 |                                      | 2710.0      | 150.59                        |               |             |                   |                     |
| 7     | 46 |                                      | 2852.1      | 136.21                        |               | 2852.2      | 122.75            | 2852.1              |
| 8     | 47 |                                      | 2999.1      | 101.52                        |               |             |                   |                     |
| 9     | 48 |                                      | 3148.9      | 151.6                         |               | 3148.9      | 151.6            | 3148.5              |
| 10    | 49 |                                      | 3303.2      | 138.26                        |               |             |                   |                     |
| 11    | 50 |                                      | 3460.1      | 109.04                        |               |             |                   |                     |

Measured energies are from Cauchois and Senemaud [1].

4. Conclusion

In the present study, the origin of the L\(\alpha\) satellites L\(\alpha\)_3 (or L\(\alpha\)'), L\(\alpha\)_4 (or L\(\alpha\") and L\(\alpha\)_5 (or L\(\alpha\"')) have been explained in the elements from \(\alpha\_Zr\) to \(\alpha\_Sn\), i.e., in all the elements in which they have been observed. The present assignment of the transitions to these satellites is different from those of Poonia and Soni [2]. This is because, the present assignments are based on relativistic calculations while those of Poonia and Soni are based on non-relativistic calculations.

Reference

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