Origin of the Lβ2 satellites in the X-ray emission spectra of the middle-Z elements from \(^{40}\)Zr to \(^{52}\)Te

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Abstract. In this communication, the origin of the Lβ\(_2\) satellites Lβ\(_2\)\(_i\), Lβ\(_2\)\(_{ij}\), Lβ\(_2\)\(_{ii}\) and Lβ\(_2\)\(_{iii}\), in the L emission spectra of the middle-Z elements from \(^{40}\)Zr to \(^{52}\)Te, has been explained on the basis of multiple ionization theory. As done in earlier reports, it has been assumed that the various transitions, which may give rise to these satellites, belong to the transition scheme L\(_{ii}\)M\(_{xx}\)N\(_{4,5}\) (where \(x = 1\)-5). The energies and the intensities of the 41 possible transitions corresponding to this transition scheme have been calculated theoretically. The energies have been calculated using the available Hartree-Fock-Slater data on K-LM and L-MN Auger transition energies. The intensities of the various transitions have been estimated by considering cross sections for Coster-Kronig transitions as well as for M-shell shake-off process. Theoretical Lβ\(_2\) satellite spectra have been computed. There are four intense peaks in the theoretical Lβ\(_2\) satellite spectra which have been identified as the four satellites Lβ\(_2\)\(_i\), Lβ\(_2\)\(_{ij}\), Lβ\(_2\)\(_{ii}\) and Lβ\(_2\)\(_{iii}\). Consequently, the satellites have been assigned those intense transitions which have been found to rise to the corresponding four peaks in the theoretical Lβ\(_2\) satellite spectra. The present work is an improvement over the earlier reports.

1. Introduction

In the elements \(^{40}\)Zr to \(^{52}\)Te, the intense diagram line Lβ\(_2\) is accompanied with its satellites on the higher energy side which have been designated as Lβ\(_2\)\(_i\), Lβ\(_2\)\(_{ij}\), Lβ\(_2\)\(_{ii}\) and Lβ\(_2\)\(_{iii}\) [1]. Soni and Poonia [2] have theoretically investigated the origin of these satellites. They have suggested that all these satellites arise mainly due to the transition array 2p\(_{3/2}\)\(_x\)3x\(_i\) - 3x\(_i\)\(_x\)4d\(_{5/2,3/2}\)\(_x\) (\(x = s, p, d\)), i.e., L\(_i\)M\(_x\) - M\(_x\)N\(_{4,5}\) (where \(x = 1\)-5). These authors have calculated relative intensities of the transitions, corresponding to this transition scheme, using McGuire’s tables for Coster-Kronig transition probabilities [3]. McGuire’s tables have been superseded by the tables of Chen et al. [4]. While McGuire’s tables are based on non-relativistic calculations, the tables of Chen et al. are based on relativistic calculations. Hence, we thought it proper to do fresh calculations of intensities of transitions using Chen et al.’s tables. The values of relative intensities calculated in the present work are different than those calculated by Soni and Poonia [2]. The result is that the assignments of transitions to the satellites in the present work are slightly different than those of these authors. Also, Soni and Poonia [2] have studied selected elements only, leaving several elements between. Hence, we thought that it would be proper to study all the elements from \(Z = 40\) to \(52\).

2. Theoretical calculations

2.1 Initial and final states for Lβ\(_2\) satellites

As assumed by Soni and Poonia [2], we also assume that the origin of the Lβ\(_2\) satellites, can be ascribed to the transition scheme 2p\(_{3/2}\)\(_x\)3x\(_i\) - 3x\(_i\)\(_x\)4d\(_{5/2,3/2}\)\(_x\) (\(x = s, p, d\)), i.e., L\(_i\)M\(_x\) - M\(_x\)N\(_{4,5}\), (\(x = 1\)-5).
2.2 Calculation of energies of transitions in doubly ionized atoms

The formula for calculation of transition energy of say, L₁M₆ - M₈N₈, transition, has been written as –

\[
E (L₁M₆ - M₈N₈) = E (Kα₁) + E (L₃ - M₈N₈) - E (K - L₃M₆)
\]

The energy of Kα₁ line, i.e., E (K - L₁) has been taken from the tables of Cauchois and Senemaud [1] instead of the earlier tables of Bearden and Burr [5] used by Soni and Poonia [2]. The energies of the Auger transitions L₃ - M₈N₈ and K - L₁M₆ have been taken from the tables of Larkins [6].

Table 1. Assignments of transitions to the satellites Lβ₂,₅, Lβ₂,₇ and Lβ₂,₉

| S. No. | Atomic number (Z) | Satellite Lβ₂,₅ | Satellite Lβ₂,₇ | Satellite Lβ₂,₉ |
|--------|------------------|-----------------|-----------------|-----------------|
|        | Experimental value of energy [1] (eV) | Theoretical values Energy (eV) Relative intensity | Experimental value of energy [1] (eV) | Theoretical values Energy (eV) Relative intensity |
| 1      | 40               | 2241.3          | -               | 2243.8          | 2248.0          | 289.80          |
| 2      | 41               | 2397.3          | 2396.8          | 31.52           | -               | 2399.0          | 271.20          |
| 3      | 42               | 2543.2          | 2549.2          | 28.6            | 2547.8          | 2552.9          | 265.50          |
| 4      | 43               | -               | 2706.8          | 36.1            | -               | 2710.0          | 279.01          |
| 5      | 44               | 2860.1          | 2866.9          | 34.27           | 2865.3          | 2870.8          | 237.64          |
| 6      | 45               | 3026.6          | 3034.8          | 39.79           | 3030.7          | 3038.8          | 260.92          |
| 7      | 46               | 3197.9          | 3204.6          | 95.54           | 3202.7          | 3208.7          | 227.17          |
| 8      | 47               | 3377.1          | 3381.1          | 88.88           | 3381.7          | 3385.1          | 192.44          |
| 9      | 48               | 3558.1          | 3561.1          | 104.80          | 3562.9          | 3565.9          | 188.40          |
| 10     | 49               | 3744.6          | 3747.1          | 113.68          | 3749.6          | 3753.1          | 179.27          |
| 11     | 50               | 3937.4          | 3938.0          | 35.83           | 3941.7          | 3944.1          | 180.98          |
| 12     | 51               | 4133.9          | 4134.1          | 122.66          | -               | 4141.0          | 175.92          |
| 13     | 52               | 4337.1          | 4335.2          | 125.71          | -               | 4342.0          | 232.99          |

Considering the dipole selection rules, the 41 possible transitions have been found out corresponding to this transition scheme. The energies and intensities of these transitions have been calculated as follows.
2.3 Calculation of intensities of transitions in doubly ionized atoms

The probabilities of creation of a single hole states, $1s^1$ and $2p_{3/2}^{-1}$ ($K^{-1}$ and $L_3^{-1}$), have been calculated by using Moore et al.'s method [7]. Once the singly ionized state has been created, it is the probability of a particular subsequent process that will lead to the formation of two-hole state. The single hole so created may get converted through a Coster-Kronig transition to a double hole state. In the present work, the value of the probabilities of formation of double hole states via this process have been taken from 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. We have determined the shake-off transition probabilities by interpolation method from the values reported by Carlson and Nestor [8].

Finally, the total probability of creation of doubly ionized initial state, say, $L_3M_4$, has been determined by adding both the cross sections calculated above for the two processes, i.e., by Coster-Kronig transition and by shake-off process. For calculating the relative intensities of the transitions of each multiplet, this probability has then been statistically distributed among all the allowed transitions from this set of levels, considering first of all the multiplets of super multiplets from various $^{(2S+1)}L$ levels of the set and then using the tables of White and Eliason as given by Condon and Shortley [9].

2.4 Synthesis of satellite spectra

A composite spectrum formed by spectral lines emitted by the 41 transitions for the elements has been computed by taking each as a Gaussian line. For this we have taken energy on x-axis and intensity on y-axis. The peak height of each line is taken equal to transition probability and peak position on x-axis is taken at the energy of the transition. The theoretical satellite spectrum obtained for the element $^{75}$Sn is given in the figure 1 as a representative spectrum for all these elements under consideration.

3. Results and discussion

The $L\beta_2$ satellite spectra as computed in the present study for the middle-Z elements have four peaks, which have been identified by us as the four observed satellites: $L\beta_2^{(a)}$, $L\beta_2^{(b)}$, $L\beta_2^{(c)}$ and $L\beta_2^{(d)}$. From the analysis of the transitions which give rise to these four peaks, the assignments of the transitions, which can be responsible for the origin of these four satellites, have been made. Table 1 gives the theoretical energies and relative intensities of the satellites along with experimental values of the energy.

3.1 $L\beta_2^1$ satellite

The first peak in the computed spectra has been identified as the $L\beta_2^1$ satellite. Considering the various transitions which give rise to this first peak, we have found that the transitions $^3D_3 - ^3F_4 (3p)$ and $^3D_3 - ^3D_1 (3p)$ are the common transitions in all the elements under consideration. As a result, we have assigned these transitions for the origin of the satellite $L\beta_2^1$ in all the elements. The transition $^3F_4 - ^1F_4$
(3d) has also been found to contribute to the intensity of the satellite \( \text{L}_\beta^2 \) in the elements with \( Z = 46 \) to 52.

3.2 \( \text{L}_\beta^2 \) satellite

The second peak in the computed spectra has been identified as the \( \text{L}_\beta^2 \) satellite. We have found that the intense transitions \( ^3 \text{F}_4 - ^3 \text{G}_4 \) (3d) and \( ^3 \text{F}_4 - ^3 \text{D}_1 \) (3d) along with the weak transitions \( ^1 \text{D}_2 - ^1 \text{F}_2 \) (3d), \( ^1 \text{D}_2 - ^1 \text{P}_1 \) (3d), \( ^3 \text{F}_4 - ^3 \text{G}_4 \) (3d) and \( ^3 \text{P}_2 - ^3 \text{D}_1 \) (3s), i.e., \( ^1 \text{D}_2 - ^3 \text{F}_2 \) (3p) and \( ^3 \text{D}_1 - ^3 \text{D}_1 \) (3p) are the common transitions in all the elements under consideration, which give rise to this peak. Hence, the \( \text{L}_\beta^2 \) satellite has been assigned mainly to these two intense transitions and the six weak transitions in all the elements. The transition \( ^3 \text{F}_4 - ^3 \text{F}_4 \) (3d) has also been found to contribute to the intensity of the satellite \( \text{L}_\beta^2 \) in the elements with \( Z = 40 \) to 45.

Transition \( ^3 \text{F}_4 - ^3 \text{F}_4 \) (3d) deserves special mention because it contributes to the intensity of the satellite \( \text{L}_\beta^2 \) in the elements from \( Z = 40 \) to 45, but in the elements with \( Z > 45 \), it contributes to the intensity of the satellite \( \text{L}_\beta^2 \).

3.3 \( \text{L}_\beta^3 \) satellite

The third peak in the computed spectra has been identified as the \( \text{L}_\beta^3 \) satellite. Considering the various transitions which give rise to this third peak, we have found that the transitions \( ^3 \text{D}_1 - ^3 \text{F}_2 \) (3d), \( ^3 \text{D}_1 - ^3 \text{P}_1 \) (3d) and \( ^3 \text{D}_2 - ^3 \text{F}_1 \) (3d) with the weak transitions \( ^3 \text{D}_2 - ^3 \text{D}_1 \) (3d), \( ^3 \text{D}_2 - ^3 \text{D}_1 \) (3d) and \( ^3 \text{D}_2 - ^3 \text{F}_2 \) (3d) are the common transitions for all the elements which give rise to this peak. Thus, according to the present study, these three intense transitions are responsible for the origin of \( \text{L}_\beta^3 \) satellite along with the three weak transitions.

3.4 \( \text{L}_\beta^4 \) satellite

The fourth peak in the computed spectra has been identified as the \( \text{L}_\beta^4 \) satellite. Considering the various transitions which give rise to this fourth peak, we have found that the intense transitions \( ^1 \text{F}_3 - ^1 \text{G}_4 \) (3d) and \( ^1 \text{F}_3 - ^1 \text{D}_2 \) (3d) along with weak transitions transitions \( ^3 \text{P}_1 - ^3 \text{D}_1 \) (3d), \( ^3 \text{P}_1 - ^3 \text{P}_1 \) (3d), \( ^3 \text{P}_1 - ^3 \text{S}_1 \) (3d), \( ^3 \text{P}_1 - ^3 \text{P}_0 \) (3d) and \( ^3 \text{P}_1 - ^3 \text{D}_1 \) (3d) can be attributed to the origin of the \( \text{L}_\beta^4 \) satellite in all the elements under consideration with \( Z = 40 \) to 52.

Finally, whereas, Soni and Poonia [2] have studied selected elements only, leaving several elements between, we have studied all the elements from \( Z = 40 \) to 52.

4. Conclusions

The \( \text{L}_\beta \) theoretical satellite spectra have been computed for the middle-\( Z \) elements from \( \text{Zr} \) to \( \text{Te} \).

The theoretical spectra show four peaks which have been identified as the four satellites \( \text{L}_\beta^1, \text{L}_\beta^2, \text{L}_\beta^3, \text{L}_\beta^4 \). From the analysis of the transitions which give rise to these four peaks the assignments of the transitions to these four satellites have been done. Our assignments are slightly different than those reported by Soni and Poonia [2].

5. References

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