Origin of the satellite observed on the high energy side of $L\gamma_{2,3}$ diagram lines

Rajeev Trivedi¹, Uma Shrivastava² and B. D. Shrivastava²
¹Alpine Institute of Technology, Ujjain - 456010. India
²School of Studies in Physics, Vikram University, Ujjain - 456010. India

Email: rajeevtrivedi80@gmail.com

Abstract. On the high energy side of the unresolved doublet $L\gamma_{2,3}$ in the L spectra of some elements, a satellite $L\gamma_{2,3}'$ has been reported in literature, which has been ascribed to the transition $L_1M_x$ - $M_xN_{2,3}$, on the basis of energy considerations alone, by earlier workers. In the present work, apart from energy, calculations have also been done for the intensity of the probable transitions which may give rise to the satellite in the elements from $^{40}$Zr to $^{47}$Ag and from $^{57}$La to $^{63}$Eu. Firstly, the probability of creation of a single hole K state has been calculated. Double hole state $L_1M_x$ is created by Coster-Kronig transitions (K - $L_1M_x$) as well as by shake off process. The probabilities of these two processes have been calculated. The total probability of creation of the double hole state thus obtained has been statistically distributed among the 24 allowed transitions from the set of $L_1M_x$ levels. By taking each of the transitions as a Gaussian line, a composite spectrum has been computed. This theoretical spectrum has been compared with the available satellite energy data. The transitions which give rise to this satellite have thus been identified in the elements studied.

1. Introduction
The wavelength tables of Cauchois and Senemaud [1] show that $L\gamma_{2,3}'$ satellite has been observed on the high energy side of the unresolved doublet $L\gamma_{2,3}$ and has been reported in $^{40}$Zr, $^{41}$Nb, $^{48}$Mo, $^{49}$Rh and $^{47}$Ag. In 1986 this satellite has been reported by Shrivastava et al. [2] on the high-energy side of $L\gamma_2$ line in the elements $^{57}$La, $^{59}$Pr, $^{60}$Nd, $^{62}$Sm and $^{63}$Eu. Soni [3] has assigned the transition schemes $L_1M_x$ - $M_xN_{2,3}$ to the satellite $L\gamma_{2,3}'$. Shrivastava et al. [2] have also tried to explain the origin of this satellite. Both Shrivastava et al. and Soni’s assignments are based on energy considerations alone.

In the present work, we have calculated both energy and intensity of the various transitions belonging to the transition scheme $2s_{\epsilon/2}^{-1}3x^{-1}3x^{-2}4p^{-1}$, i.e., $L_1M_x$ - $M_xN_{2,3}$ and have assigned transitions to the satellites. There are 24 transitions which are allowed by selection rules. All these transitions have been taken into consideration in the present study.
2. Method of calculation

2.1. Creation of two hole states
Any two hole state, e.g. one useful as initial state for the emission of \(L_{\gamma^{2,3}}\) satellite can be created by two processes: (a) K-L \(M_x\) Coster - Kronig transition, i.e., conversion of one hole state \(L_{1}\) to a two hole state \(L_{1}M_x(x = 1 - 5)\) through the Auger transition \(K - L_{1}M_x\) and (b) by shake-off process, i.e., an electron from M-shell of the atom may escape out simultaneous to the formation of \(L_{1}\) vacancy.

2.2. Calculation of energies
We have calculated the energies of the transitions using the equation
\[
E(L_{1}M_x - M_xN_{2,3}) = E(K_{\alpha}) + E(L_3 - M_xN_{2,3}) - E(K - L_{1}M_x) \ldots (1)
\]
The energy of \(K_{\alpha}\) line has been taken from the tables of Cauchois and Senemaud [1] and energies of Auger transitions \(L_3 - M_xN_{2,3}\) and \(K - L_{1}M_x\) have been taken from the tables of Larkins [4].

2.3. Calculation of relative intensities of transitions
The relative intensities of the transitions have been calculated by first calculating the probability of initial single hole creation in the K shell by following the method of Moores et al. [5]. For calculating the probability of conversion of single hole K state to double hole state \(L_{1}M_x\) through Coster - Kronig transition (K - \(L_{1}M_x\) the tables of Chen et al. [6] have been used. The probability of conversion of double hole state \(L_{1}M_x\) through shake-off process has been calculated from the work of Carlson and Nestor [7]. The total probability of creation of \(L_{1}M_x\) double hole state has been found out by taking the sum of Coster-Kronig probability and shake-off probability. The cross section for a set of \(L_{1}M_x\) levels, with \(x\) denoting any one sub-shell of M shell, so calculated, has been assumed as the total probability of all the transitions from this set. This has 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 [8] for relative probabilities of the transition of each multiplet.

2.4. Computation of the theoretical spectrum
A composite spectrum formed by spectral lines emitted by the 24 transitions has been computed by taking each as a Gaussian line. Theoretical spectrum is thus obtained and compared with the available satellite energy data. The theoretical spectra for elements \(^{40}\text{Zr}\) and \(^{60}\text{Nd}\) are reproduced in figs.1 and 2 as representative spectra.

3. Results and discussions

3.1. \(L_{\gamma^{2,3}}\) satellite in elements \(^{40}\text{Zr}\) to \(^{47}\text{Ag}\).
Neither Soni’s [3] nor Shrivastava et al. [2] transition assignments for \(L_{\gamma^{2,3}}\) satellite seem to be correct. According to the present work \(^{3}D_2-^{3}P_2(A), \, ^{3}D_2-^{3}D_3(C), \, ^{3}D_2-^{3}F_3(D)\), \(^{3}D_2-^{3}F_2(E), \, ^{3}D_3-^{3}P_2(F), \, ^{3}D_2-^{3}P_2(H),\)
\(^{3}P_2-^{3}D_3(I)\) and \(^{3}P_2-^{3}P_2(K)\) are mainly and collectively responsible for giving rise to the \(L_{\gamma^{2,3}}\) satellite in the elements \(^{40}\text{Zr}\) to \(^{47}\text{Ag}\) (the abbreviations A, B, C, D .... have been given to the transitions so that they may be marked on the figs. 1 and 2). There are some minor contributor and some negligible contributor transitions, which also add up to give rise to the spectral line of \(L_{\gamma^{2,3}}\) satellite.
3.2. \( L_{\gamma 2,3}' \) satellite in the elements \( 55\text{Cs} \) to \( 63\text{Eu} \)

Shrivastava et al.'s [2] transition assignments for \( L_{\gamma 2,3}' \) satellite seem to be incorrect. The present assignments based on both energy and intensity calculations appear to be more plausible. Thus, satellite \( L_{\gamma 2,3}' \) should arise mainly because of \( ^3P_2-^3D_3 \)(I), \( ^3P_2-^3P_2 \)(K), \( ^3P_0-^3D_1 \)(S) and \( ^3P_1-^3P_2 \)(U) transitions, while \( ^3D_3-^3F_4 \)(A), \( ^1D_2-^1F_3 \)(B), \( ^3D_3-^3D_3 \)(C) and \( ^3P_1-^3P_2 \)(U) contribute to it as minor contributors. Also negligible contributor transitions \( ^3D_3-^3D_3 \)(O), \( ^3D_3-^3D_3 \)(Q) and \( ^3D_1-^3D_2 \)(R) make very small contribution to the intensity of \( L_{\gamma 2,3}' \) satellite. Thus, these 11 transitions are responsible for the occurrence of \( L_{\gamma 2,3}' \) satellite in \( 55\text{Cs} \) to \( 63\text{Eu} \).

Figure 1. The computed \( 2s_{1/2}^13x_{-1}^1-3x_{-1}^14p_{-1}^1 \)(L\( _1^1\)Mc - M\( _1^1\)N\( _2,3^3 \)) spectrum of \( 40\text{Zr} \). The experimentally observed \( L_{\gamma 2,3}' \) satellite positions and theoretically calculated positions are shown at the tops.

Figure 2. The computed \( 2s_{1/2}^13x_{-1}^1-3x_{-1}^14p_{-1}^1 \)(L\( _1^1\)Mc - M\( _1^1\)N\( _2,3^3 \)) spectrum of \( 60\text{Nd} \). The experimentally observed \( L_{\gamma 2,3}' \) satellite positions and theoretically calculated positions are shown at the tops.
Table 1. Theoretical and experimental energies (in eV) for the Lγ₂,₃′ satellite in the elements ⁴₀Zr to ⁴₇Ag

| S.No. | Elements | Present calculated value | Additional higher energy peak | Experimental value\(^1\) | Soni's calculated value\(^3\) | Shrivastava et al. calculated value\(^2\) |
|-------|----------|--------------------------|-------------------------------|--------------------------|-------------------------------|-----------------------------------|
| 1     | ⁴⁰Zr     | 2525.2                   | 2527.9                        | 2527.21                  | 2527.0                        | 2525.2                            |
| 2     | ⁴¹Nb     | 2684.4                   | 2690.7                        | 2690.6                   | 2690.8                        | 2687.5                            |
| 3     | ⁴²Mo     | 2855.7                   | 2859.0\(^*\)                 | 2860.8                   | 2861.3                        | 2855.3                            |
| 4     | ⁴³Mo     | 3034.8                   | 3038.3                        | -                        | -                             | -                                 |
| 5     | ⁴⁴Mo     | 3214.0                   | 3217.5                        | -                        | -                             | -                                 |
| 6     | ⁴⁵Rh     | 3393.0                   | 3396.7                        | 3392.2                   | 3392.4                        | 3392.1                            |
| 7     | ⁴⁶Rh     | 3584.0                   | 3587.1                        | -                        | -                             | -                                 |
| 8     | ⁴⁷Ag     | 3781.2                   | 3784.5                        | 3783.4                   | 3783.5                        | 3777.5                            |

Table 2. Theoretical and experimental energies (in eV) for the Lγ₂,₃′ satellite in the elements ⁵⁵Cs to ⁶₃Eu.

| S. No. | Elements | Calculated value\(^*\) | Experimental value\(^1,2\) | Shrivastava et al.'s calculated value\(^5\) |
|--------|----------|--------------------------|-----------------------------|-----------------------------------------------|
|        |          | Present value             | Present value               |                                               |
| 1      | ⁵⁵Cs     | 5577.2                   | 5594.7                       | -                                             |
| 2      | ⁵⁶Ba     | 5838.2                   | 5847.5                       | 5854.4                                        | 5844.7                            |
| 3      | ⁵⁷La     | 6105.0                   | 6114.1                       | 6118.7                                        | 6110.3                            |
| 4      | ⁵⁸Ce     | 6371.4                   | 6287.3                       | -                                             | -                                |
| 5      | ⁵⁹Pr     | 6649.0                   | 6659.2                       | 6664.0                                        | 6652.9                            |
| 6      | ⁶⁰Nd     | 6933.8                   | 6944.0                       | 6945.5                                        | 6937.7                            |
| 7      | ⁶¹Pm     | 7223.8                   | 7239.5                       | -                                             | -                                |
| 8      | ⁶²Sm     | 7523.6                   | 7534.2                       | 7535.7                                        | 7528.3                            |
| 9      | ⁶³Eu     | 7829.4                   | 7841.2                       | 7851.1                                        | 7831.3                            |

References

[1] Cauchois Y and Senemaud C 1978 *Wavelengths of X-ray emission lines and absorption edges* (Pergamon, Oxford)
[2] Shrivastava B D, Jain R K, Mishra A and Singh D 1986 *J. Phys. B* 19 3839
[3] Soni S N 1980 *J. Phys. B* 13 2859
[4] Larkins F P 1977 *Atom. Data Nucl. Data Tables* 20 311
[5] Moores D L, Golden L B and Sampson D H 1980 *J. Phys. B* 13 385
[6] Chen M H, Crasemann B and Mark H 1979 *At. Data. Nucl. Data Tables* 24 13
[7] Carlson T A and Nestor Jr C W 1973 *Phys. Rev. A* 8 2887.
[8] Condon E U and Shortley G H 1967 *The theory of atomic spectra* (Cambridge Univ. Press) pp 241