Transition probabilities for explaining the origin of L-emission satellite

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Abstract. The X-ray satellites are caused by transitions in atoms which are doubly ionized or multiply ionized. To explain the origin of X-ray satellites, the relative intensities of the various possible transitions between the doubly ionized initial and final states of an atom, have to be calculated. The intensity can be calculated from the probability of creation of the double vacancy states. These probabilities are due to Coster-Kronig and Auger transitions and can be calculated using the tables of McGuire. These tables are based on non-relativistic calculations. The latter calculations of transition probabilities are of Chen et al., who have done relativistic calculations in elements with $18 \leq Z \leq 96$. The aim of the present work is to study the variation with atomic number (Z) of the transition probabilities for the different Coster-Kronig transitions as given in McGuire’s tables and Chen et al’s tables and to discuss the difference between the two calculations. The present study shows that for calculation of the intensity of a satellite, the tables of Chen et al. should be preferred over the tables of McGuire while investigating the origin of L-emission satellites.

1. Introduction

When X-rays are generated by electron impact on a target in an X-ray tube, the radiation consists of both the continuous X-rays and characteristic X-rays. The characteristic X-ray spectrum can be classified into two broad groups, namely, diagram lines and non-diagram lines or satellite lines. The diagram lines are those which can be represented by transitions in the normal energy level diagram of a singly ionized atom. The X-ray satellites are caused by transitions in atoms which are doubly ionized or multiply ionized. Though intensive work on the theories of their origin has been published, the theories regarding their origin do not appear to have as yet reached a final decisive stage. Hence, we have been interested in finding possible explanations of the origin of the satellites in the region of the L-emission spectra, especially because, several new satellites have been reported experimentally from our X-ray laboratory.

Any transition taking place between the energy levels in a multiply ionized atom will be associated with an X-ray emission line of slightly different energy than the corresponding diagram line arising as a result of transition in a singly ionized atom. 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) Auger transition: The process of radiationless reorganization of an atom ionized in an inner shell is known as the Auger effect. After an Auger transition an atom may be left doubly ionized in inner shells.
(ii) Shake-off process: A vacancy in the outer shell of the atom may be created by shake-off process when an electron from the outer shell of the atom may escape out simultaneously to the formation of an inner shell vacancy. Photo ejection of an inner shell electron in an atom results in a sudden change of atomic potential. This sudden change can excite other electron to an unoccupied bound state (electron shake-up) or eject into the continuum (electron shake-off).

2. Calculation of transition energies and transition probabilities in multiply ionized atoms

To investigate the origin of the X-ray satellite lines, the requirements are: (i) identification of the double vacuum initial and final states, (ii) the energy difference between these states and (iii) the relative intensities of the transitions between these states. To calculate the energy of a satellite theoretically, the difference in energies of the double vacancy initial and final states has to be calculated. This simple explanation becomes complicated when one has to take into account the RS or LS, jj or intermediate coupling between the two states which leads to the multiplicity of levels. Since, we have been interested in assigning transitions in doubly ionized atom which give rise to the various L-emission satellites; this can be done by calculating the theoretical X-ray satellite spectrum. To obtain such a spectrum, we require energies of different transitions which are allowed between the initial and final double vacancy states and relative probabilities of such transitions. Ab initio calculation of energies and intensities of various double hole state transitions, considering multiplicity of energy levels, is a difficult and laborious task. It is also not necessary because, alternatively, calculations can be done with the help of several tabulations, in which necessary data are available.

For energy calculations, one can use either the tables of Larkins [1] which contain theoretically calculated Auger-electron energies for a wide range of transition processes in all the elements from Z = 1 to 100 or the tables of Parente et al. [2] which contain the energies of L-series X-ray satellites that arise from the presence of one ‘spectator hole’ in the M-shell or N-shell of the emitting atom, for 11 elements, namely 65Tb, 67Ho, 70Yb, 72W, 75Pt, 80Hg, 85At, 88Ra, 90Th, 92U and 95Am.

For calculations of intensities of satellites, one can use the tables of McGuire [3] which contain non-relativistic calculations for Coster-Kronig transition probabilities for creation of double vacancy states or the tables of Chen et al. [4] which contain relativistic calculations of the rates of all energetically possible radiationless transitions with intensities above $10^5$ milli atomic units with initial K- and L1,2,3 - shell vacancies in elements with $18 \leq Z \leq 96$.

To calculate the probability of creation of the initial double vacancy state by the process of Coster-Kronig transition and/or the process of shake-off, the cross section for creation of single vacancy state has to be first calculated. This can be done by using the formulae given by Moores et al.[5]. This cross section is then multiplied by the transition rates for the Coster-Kronig transition. After multiplication, one gets the Coster-Kronig transition probability for the creation from the single vacancy state to the double vacancy state. 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 is multiplied by the shake-off probability. After multiplication, one gets the shake-off probability for the creation from the single vacancy state to the double vacancy state. 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. From these probabilities of creation of doubly ionized initial states, the probability of transition between doubly ionized initial and final states can be calculated by assuming the cross section for a set of double vacancy levels to be the total probability of all the transitions from this set. This probability can be distributed statistically among all the allowed transitions from this set of levels for relative probabilities of the transitions, taking into consideration all the multiplets of supermultiplet from various $^{(2S+1)}L$ levels of the set.

In the present paper, we are concerned with the calculations of the intensities of L-emission satellites.
For such calculations, one can use the tables of McGuire or the tables of Chen et al. Both of these tables have been used by several authors for explaining the origin of the satellites. Our aim is to compare these tables and to know which table is better to be used for assigning transitions to the satellites. Hence, the details of the tables are first described here in brief.

**Figure 1.** Variation of transition probability of elements (along Y-axis) with increasing atomic number (Z) (along X-axis) as given in the tables of McGuire, for transition arrays $L_2M_x$ (for $X=1\text{-}5$) (left figure) and $L_3M_x$ (for $X=1\text{-}5$) (right figure).

**Figure 2.** Variation of transition probability of elements (along Y-axis) with increasing atomic number (Z) (along X-axis) as given in the tables of Chen et al., for transition arrays $L_2M_x$ (for $X=1\text{-}5$) (left figure) and $L_3M_x$ (for $X=1\text{-}5$) (right figure).
3. Coster-Kronig transition probabilities using McGuire’s and Chen’s tables

McGuire has calculated the probability of creation of double vacancy states due to Auger and Coster-Kronig transitions in j-j coupling scheme and has tabulated the values in the form of tables. The calculations have been done using Harman-Skillman one-electron eigenvalues, radial matrix elements and oscillator strengths. They have tabulated the transition probabilities only for 14 elements, namely, 18Ar, 22Ti, 26Fe, 30Zn, 35Br, 40Zr, 47Ag, 54Xe, 60Nd, 67Ho, 74W, 79Au, 83Bi and 90Th.

The latter calculations of Coster-Kronig transition probabilities are of Chen et al., who have done relativistic calculations of the rates of all energetically possible radiationless transitions with intensities above 10^-2 milli atomic units with initial K- and L1,2,3 - shell vacancies in 25 elements, namely, 18Ar, 20Ca, 25Mn, 30Zn, 35Br, 36Kr, 40Zr, 42Mo, 45Rh, 47Ag, 50Sn, 52Te, 54Xe, 59Ba, 60Nd, 63Eu, 67Ho, 76Yb, 78W, 80Hg, 83Bi, 85Ra, 90Th, 92U and 96Cm. The Auger transition probabilities have been calculated from perturbation theory, in j-j coupling, assuming frozen orbitals. The wave functions were generated according to the Dirac-Hartree-Slater approach for configurations that contain one initial inner-shell vacancy. The continuum wave functions were obtained by solving the Dirac-Slater equations with the same atomic potential as that used for the initial state. With this treatment, the orthogonality of the wave functions is assured, and the approximation is good for all but the lightest elements. A general relativistic Auger program was used to compute the radiationless transition probabilities.

4. Results and discussions

The difference between McGuire’s tables and Chen et al.’s tables is that Chen et al.’s tables are based on relativistic calculations and have been published much after the publication of McGuire’s tables, which are based on non-relativistic calculations. Also, for using McGuire’s tables, one has to use the probabilities of the creation of single hole states in the L1 or L2 or L3 subshell, while for using Chen et al’s tables, one has to use the probabilities of the creation of single hole states in the K-shell.

The main difficulty experienced in the use of both the tables is that both of them give the values of transition probabilities for selected elements. For explaining the origin of satellite in any element, the transition probabilities are required for that element, which may not be available in any of the tables. The only alternative is to estimate the values of that element using linear interpolation method. In the present work, we have explored this possibility by plotting the tabulated values of transition probabilities versus the atomic number Z. The obtained plots of atomic number Z versus the transition probabilities for the different Coster-Kronig transitions as given in McGuire’s tables and Chen et al.’s tables are shown in Figs. 1 and 2 respectively. These figures clearly demonstrate the difference between the two calculations. If one uses the values given in the McGuire’s table for linear interpolation, then one may not get proper values of transition probabilities for intermediate elements, since the curves do not have regular variations. On the other hand, the plots of values of Chen et al.’s tables show regular variation with Z. Hence, if they are used for linear interpolation, one is likely to get the correct values of transition probabilities for intermediate elements. From the present study, it is clear that, since Chen et al.’s tables are based on relative calculations and since the method of linear interpolation can be used for estimating the values of transition probabilities for those elements, for which values are not given in the tables, these tables should be used for calculations of intensities of the satellites and thereby for explaining the origin of the L-emission satellites.

References
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