Calculation of Coster-Kronig energies and transition probabilities by linear interpolation method

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Abstract. The X-ray emission spectrum consists of two types of spectral lines having different origins. The diagram lines originate because of transitions in singly ionized atom, while the non-diagram lines or satellites originate due to transitions in doubly or multiply ionized atom. The X-ray satellite energy is the difference between the energies of initial and final states which are both doubly or multiply ionized. Thus, the satellite has a different energy than the energy of the X-ray diagram line. 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 may get converted through a Coster-Kronig transition to a double hole state. The probability of formation of double hole state via this process is written as \( \sigma \sigma' \), where \( \sigma \) is the probability of creation of single hole state and \( \sigma' \) is the probability of the Coster-Kronig transition. The value of \( \sigma' \) can be taken from the tables of Chen et al. [1], who have presented the calculated values of \( \sigma' \) for almost all possible Coster-Kronig transitions in some elements. The energies of the satellites can be calculated by using the tables of Parente et al. [2]. Both of these tables do not give values for all the elements. The aim of the present work is to show that the values for other elements, for which values are not listed by Chen et al. and Parente et al., can be calculated by linear interpolation method.

1. Introduction

The spectrum of the radiation emitted from an x-ray tube consists of characteristic spectrum of the target superimposed over the continuous spectrum. The spectral lines of the characteristic spectra resulting from transitions between atomic states, involving single vacancy are called diagram lines, because energy of such lines can be expressed as the difference of two terms in the single vacancy energy level diagram. The diagram lines are generally found to be accompanied by groups of lines of slightly different energies and usually smaller intensities. The energies of these lines do not correspond to the energy difference between any two states of the normal single vacancy energy level diagram of the element concerned. These lines are known as X-ray satellite lines or non-diagram lines.

Since the discovery of the X-ray satellites, the problem of finding the origin of these satellites has attracted the attention of many workers and various theories have been put forward from time to time. The most widely accepted theory of X-ray satellites is the multiple ionization theory. The parent diagram line is emitted by a transition in the singly ionized atom. The X-ray satellite line is emitted due to transition in the multiply ionized atom. The X-ray satellite energy is the difference between the energies of initial and
final states which are both doubly or multiply ionized. Thus, the satellite has a different energy than the energy of the X-ray diagram line.

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 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.

Earlier attempts of explaining the origin of X-ray satellites and assigning transitions to them were mainly confined to energy considerations alone. In the recent years, however, intensities of the various transitions have also been considered and attempts have been made to compute theoretical X-ray satellite spectra. This can be done by calculating the theoretical X-ray satellite spectrum. To obtain such a spectrum, the requirements are:

(i) The energies of the different transitions which are allowed between the initial and final double vacancy states,

(ii) The relative probabilities of such transitions.

Ab initio calculations 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. Such tabulations for calculations of energies of doubly ionised atoms are the following tables of Auger-electron energies:

(i) Tables of Larkins [3] The energies have been calculated by means of a general semi empirical method developed within an intermediate coupling framework. He has used the data derived from atomic Hartree-Fock calculations and has combined it with experimental electron subshell binding energies data.

(ii) 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 \( ^{65} \text{Tb}, ^{67} \text{Ho}, ^{70} \text{Yb}, ^{74} \text{W}, ^{78} \text{Pt}, ^{80} \text{Hg}, ^{85} \text{At}, ^{88} \text{Ra}, ^{90} \text{Th}, ^{92} \text{U} \) and \( ^{95} \text{Am} \). The energies of initial and final atomic states have been computed separately to allow for complete relaxation. Dirac-Hartree-Slater (D.H.S.) wave functions have been used with a local approximation to the atomic potential.

Since, the tables of Parente et al. are relativistic calculations and those of Larkins are non relativistic calculations, hence it is preferable that the tables of Parente et al. are used for calculations of the energies of the L emission satellites.

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 \( \sigma \) 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 \( \sigma' \) as given in the following tables Coster-Kronig transition probabilities. After multiplication, one gets the Coster-Kronig transition probability for the creation from the single vacancy state to the double vacancy state, i.e., \( \sigma \cdot \sigma' \).

(i) Tables of McGuire [4] which contain non-relativistic calculations for Coster-Kronig transition probabilities for creation of double vacancy states.

(ii) Tables of Chen et al. [1] 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 L\(_{1,2,3} \) shell vacancies in elements with \( 18 \leq Z \leq 96 \).

Since, the tables of Chen et al. are relativistic calculations and those of McGuire are non relativistic calculations, hence it is preferable that the tables of Chen et al. are used for calculations of the probabilities of creation of two hole-states which are required for the L emission satellites.

We have been interested in the study of origin of L emission satellites in the \( \text{L}_\gamma \) and \( \text{L}_\alpha \). For this, both the energies and intensities of the various transitions which can give rise to a particular satellite in doubly ionised atom have to be calculated and then the theoretical satellite spectrum has to be synthesised. By comparing the theoretical spectrum with the experimental spectral energies it is possible to assign the transition to a particular satellite accurately. Since we want to find the origin of the satellites in all the
elements, we require energies and transition probabilities of all the elements which are not available in the tables of Parente et al. and Chen et al. respectively. In the present paper we have shown that these values can be obtained from the tables mentioned above by linear interpolation method.

2. Method of calculation

2.1 Calculation of energies

Chen et al.[1] have given in their tables probabilities of Coster-Kronig transitions for elements $^{70}$Yb, $^{74}$W, $^{80}$Hg, $^{83}$Bi, and $^{88}$Ra. In the present work, the values for other elements have been obtained by linear interpolation method. The justification for linear interpolation can be seen from a sample graphs presented in figs. 1(a) and 1(b) for K-L$^{1}$M$_{1}$, K-L$^{1}$M$_{2}$, K-L$^{1}$M$_{3}$, K-L$^{1}$M$_{4}$ and K-L$_{1}$M$_{5}$ Auger transitions. In this figure the values of transition probabilities of elements given by Chen et al. have been plotted against Z values. The graphs are found to be linear in small regions, justifying the use of linear interpolation method for finding transition probabilities for intermediate elements.

Fig. 1(a) Variation of K-shell Auger transition probabilities (from tables of Chen et al.) with Z. This graph shows that linear interpolation can be used to find values for intermediate elements.

Fig. 1(b) Variation of K-shell Auger transition probabilities (from tables of Chen et al.) with Z. This graph shows that linear interpolation can be used to find values for intermediate elements.

Fig. 2 Variation of energy of L$_{1}$M$_{1}$$^{4}$S$_{0}$-M$_{2}$$^{4}$P$_{1}$ transition (from tables of Parente et al.) with Z. This graph shows that linear interpolation can be used to find values for intermediate elements.
2.2 Calculation of relative intensities of transitions

The relative intensities of the transitions can be 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\textsubscript{1}M\textsubscript{x} through Coster-Kronig transition (K - L\textsubscript{1}M\textsubscript{x}) the tables of Chen et al. have to be used as mentioned above. The second method of calculation used in the present work is by employing the tables of Parente et al. As also pointed out above, Parente et al. have tabulated energies of all the possible transitions which can be assigned to L-emission satellites. However, they have tabulated the energies only for 11 elements namely, \textsubscript{161}Tb, \textsubscript{165}Ho, \textsubscript{170}Yb, \textsubscript{174}W, \textsubscript{180}Hg, \textsubscript{185}At, \textsubscript{188}Ra, \textsubscript{190}Th, \textsubscript{192}U and \textsubscript{195}Am. The transitions included in this table are for all the electric dipole and electric quadrupole L X-ray transitions for which the final state comprises the vacancies in the M and N shells. The probabilities of the transitions are mentioned in the table for all the elements in general and not for individual elements. Hence, we have proposed that by linear interpolation the energies of all the possible transitions of the transition schemes L\textsubscript{1}M\textsubscript{x} - M\textsubscript{x}L\textsubscript{2,3} (x = 1-5) can be obtained for all the elements from the tables of Parente et al. The justification for using linear interpolation method for finding energies for different elements not mentioned in these tables can be seen from a sample graph reproduced in fig. 2 for a sample transition L\textsubscript{1}M\textsubscript{1}\textsubscript{1}S\textsubscript{0} - M\textsubscript{1}N\textsubscript{2}\textsubscript{3}P\textsubscript{1}. In this figure the values of energies of this particular transition is plotted against Z values for the 11 elements for which Parente et al. have reported the energy values. The graph is linear, specially in small regions, justifying the use of linear interpolation method.

3. Results and discussions

For calculating the theoretical X-ray satellite spectrum, the energies and the relative probabilities of the different transitions which are allowed between the initial and final double vacancy states are required. The transition probabilities can be taken from the tables of Chen et al. [1], who have presented the calculated values for almost all possible Coster-Kronig transitions in some elements. The energies of the satellites can be calculated by employing the tables of Parente et al. [2]. Both of these tables do not give values for all the elements. In the present work we have shown that the values for other elements, for which values are not listed by Chen et al. and Parente et al., can be calculated by linear interpolation method.

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