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K-shell Radiative Transition Width to Auger Transition Width in Low Z Elements

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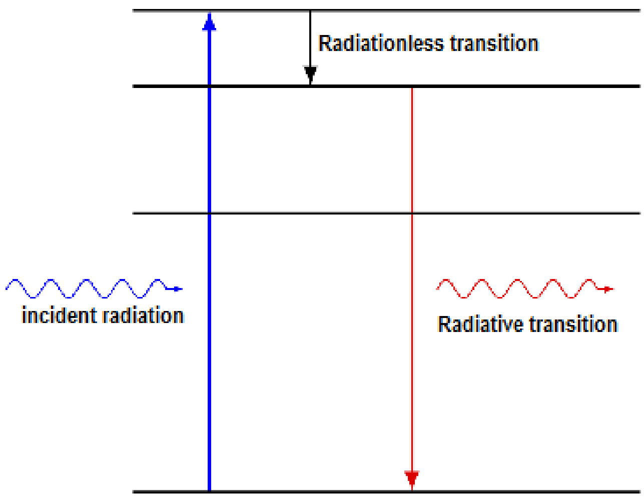
Abstract

The ratio of radiative transition width to Auger transition width in the K-shell for low Z elements is estimated. The ratio of line widths is computed using simple calculations. From the available database, on the K-shell X-ray fluorescence yield, the ratio of radiative transition width to the Auger transition width in the K-shell of low Z elements have been tabulated. The ratios compared for experimental, theoretical and semi-empirical fit values and a linear relation of Z dependence with the ratio of the transition widths is established. The uncertainty in the present work is due to the uncertainty in the values of fluorescence yield for K-shell. Present work focuses on the predominance of Auger process during the electron rearrangement mechanism in the excited atoms in the low Z elements causing decreasing ratios of the line widths.

Keywords: K-shell fluorescence yield, radiative transition and Auger transition

***Graphical Abstract*—**



- Atomic de-excitation leading to radiative and Auger transition in the K-shell of target element.
- Ratio of line widths increase with heavier elements.
- Measurement of line widths is useful in the calculation of K X-ray fluorescence yield in low Z elements.

1. Introduction

Studies on the process of atomic excitation by various techniques viz. photon excitation, secondary excitation, electron capture etc. results in the electron rearrangement in the atomic shells and its subshells. If atomic de-excitation results in X-ray fluorescence (XRF) emission, the X-ray fluorescence parameters like, fluorescence yield, fluorescence cross-section, X-ray intensity ratio, vacancy transfer probability, ratio of radiative to radiationless /non-radiative transition line widths, jump ratio and jump factor measurements helps understand the atomic structure and the electron rearrangement processes respectively. X-Ray fluorescence studies has been around for many years, several researchers have been studying the various X-ray fluorescence parameters in elements, compounds and alloys. K – shell X-ray fluorescence or the emission of characteristic X-rays in pure elements finds application in various fields viz. atomic, molecular spectroscopy, material science, nuclear science etc. In this regard, the knowledge and knowhow of accurate values of XRF parameters are of utmost importance. K-shell XRF parameters like, the K- shell fluorescence yield, fluorescence cross-section, K_β/K_α X-ray intensity ration, K to L shell total vacancy transfer probability, K X-ray line width in pure elements is been exhaustively studied theoretically, experimentally, empirical and using semi-empirical fit methods [1-6]. It is established that the interaction at low energies of the incident gamma radiation or the X-ray photons with energy slightly above the electron binding energy, initiates electron rearrangement in the atomic shells of the target. The probability of electron rearrangement in the atomic shells of the target element is mainly by the process of radiative transition in heavier elements while the electron rearrangement mechanism is chiefly through radiation-less transitions or the Auger electron emission in the low Z elements respectively. Since, a fewer discussion on the ratio of line widths of radiative to non-radiative or radiation-less transition or Auger transition is been reported. Experimental measurement of the line widths of Radiative transition and non-radiative transition [5] involves complicated techniques and radioactive source strength of high order. The dosage of radiation used to study the line widths may be harmful to persons involved in the study. On the other hand, theoretical estimation for the line widths of radiative transition and non-radiative transition gives accurate values of the possible line widths in elements of higher atomic number. But in case of elements in the low atomic number, the line widths of radiative and non-radiative transitions depend on the processes viz. Radiative transfer, Auger emission and Coster-Kronig emissions respectively.

1.1 Objective of the Study

To overcome the difficulty in the experimental measurement of radiative transition line width and the radiation-less transition line width using high strength radioactive sources and the detector assembly, further the uncertainty in the theoretical estimation for radiative line widths and non-radiative transition line widths in low Z regime, the present work, suggests a simple hybrid modelling method that involves computational method to compute for radiative transition line width to non-radiative transition line width for a few low Z elements using experimental values and theoretical approach together.

1.2 Organization

The computed values using the simple hybrid modelling method for the ratio of radiative transition width to the non-radiative transition width is in good agreement. were selected for which fewer studies are available and the ratio of radiative transition width to the Auger transition or the radiation-less transition width (Γ_R^K/Γ_A^K) in these few low Z elements is been systematically studied. From the weighted mean of the K-shell fluorescence yield for selected few low Z elements in the range $14 < Z < 30$ available from the compilation work as in [7], the ratio of radiative transition width or the line width to the Auger transition width for these low Z elements using the methods discussed elsewhere in [8-10] is been computed. The computed values for the line widths of both radiative and radiation-less transitions in the K-shell for the elements investigated seems to fit closely with both experimental and theoretical values as in [5] and [1] respectively. It is been found that the ratio Γ_R^K/Γ_A^K is linear for the elements investigated and increases with Z agreeing with the literature [8]. The computed values are in good agreement with the theory of atomic excitation by [1] and [8]. The uncertainty in the calculated values for Γ_R^K/Γ_A^K for low Z elements in the present work is accounted for the uncertainties in the weighted mean value of the K-shell X-ray fluorescence yield of the elements investigated. The present study helps understand the process of electron rearrangement process which seems to be predominantly through the emission of Auger electrons in the region of low Z elements and by radiative decay in the medium and high Z elements. This exhibits that the method used in this work is simple and reliable as well. Further, the study finds scope in comparing the theoretical and experimental values for total transition line widths in low Z elements by determining the widths of radiative transition, line width of Auger transition and probability of line width of Coster-Kronig transitions in medium Z elements. The present study also finds scope in estimating the other X-ray fluorescence parameters viz, K –shell intensity ratio, total K to L vacancy transfer probability, atomic cross section, jump ratio and jump factor in low Z elements where the data seems to be scarce.

2. Related Work

Ratio of radiative transition width to non-radiatve transfer width is been theoretically calculated as in Atomic radiative and radiation-less yields in the K and L shells in [8]. The elements covered include low, medium and high Z range. Experimental measurement for the radiative transition line width and the non-radiative transition width for a few elements is been reported in [5]. The ratio of K-shell radiative transition to Auger transition in a few medium Z elements using a simple 2π-geometry involving a weak radioactive source is reported in [9,10]. In the present study, using hybrid model, the ratio of K-shell radiative transition to the radiation-less transition/Auger transition is studied for a few low Z elements in the range 14 < Z < 30. The findings are presented in section 5 Result and Discussion.

3. Theory/Calculation

Interaction of gamma radiation or X-ray photons with matter causes atomic excitation or inoisation in them. If the energy transfer during the interaction emits an electron from the inner shell viz. K shell, the electrons from the higher shell occupies the electron vacancy in the K-shell. This may result in a high rate of radiative transfer as in high Z elements or predominance of Auger emission of electrons in the low Z elements. In addition to these processes Coster-Kronig radiation -less transition from the subshells to the major shell of where the electron vacancy is created is also possible this process is seen in higher shells like the L shells. Hence the natural atomic width is the total widths of radiative, Auger and Coster-Kronig transitions. According to the uncertainty principle the relation between the life-time τ of a single vacancy in a given level to the natural width $\Gamma$of that level is [8],

$$\Gamma\tau = \hbar \tag{1}$$

The K-shell natural level width Γ_K obtained from the K-shell radiative width Γ_R^K and the K-shell fluorescence yield ω_K is,

$$\Gamma_K = \frac{\Gamma_R^K}{\omega_K} \tag{2}$$

As K-shell has a single subshell in the 1s state and assuming the natural line width is due to the sum of radiative transitions and Auger emissions, the ratio of width of radiative transition to the Auger or radiation-less transition for the K-shell is given as,

$$\frac{\Gamma_R^K}{\Gamma_A^K} = \frac{\omega_K}{(1-\omega_K)} \tag{3}$$

4. Experimental Method

Ratio of radiative transfer to Auger transfer for a few low Z elements in the range 14 < Z < 30 is been studied both experimentally and theoretically. Experimental techniques involve complicated assembly both the detector and the usage of high strength radioactive source. whenever a gamma photon of low energy interacts with atoms in the low Z elements, Auger emission of electrons being predominant and the estimation of Auger electrons is studied through Auger spectroscopy. The Auger transition line width can also be computed by measuring the radiative transition width to the total line width. Alternately, In the present work, using a simple hybrid model, the ratio of radiative transition width to Auger transition width is estimated for a few low Z elements in the range 14 < Z < 30. The hybrid method, A spread sheet is created using MS excel available in the Windows 10 software and the data of the K-shell fluorescence yield for the elements under study is taken from the database in [7] and is entered in the spread sheet. The formula as in eqn. 3 is entered in the spread sheet and the ratio for radiative transition width to the Auger transition width is compiled. Similarly, the ratio of radiative width to Auger transition width for all the elements under study is computed. Using the K-shell fluorescence yield for the elements investigated by different researchers as in [3] and [4], the ratio of radiative transition width to the Auger transition width is computed. The data for the ratio of radiative transition width to Auger transition width is transferred from the excel sheet to the Origin workbook and the data is fitted for linearity with the atomic number Z for the low Z elements studied. Using

Origin software, the regression coefficient R value is correlated for the straight line fit of the ratio of the radiative transition width to Auger transition width and the atomic number Z of the elements investigated.

Using the weighted mean of K-shell fluorescence yield for an element under study, the ratio of radiative transition line width to the Auger transition line width for that element is computed. Similarly, the ratio of radiative transition line width to the Auger transition line width in the atomic range 14 < Z < 30 is estimated and tabulated. The weighted mean of K-shell fluorescence yield of an element under study in the range investigated is obtained from [7] and the ratio of the widths of radiative transition to the Auger emission transition is computed using eqn. 3. The uncertainty in the calculation for every target element investigated is been systematically estimated. It reported that the uncertainty is found to arise due to the association of uncertainty with the weighted mean of K-shell fluorescence yield of the element investigated as reported by the researchers in [7].

5. Results and Discussion

Using a simple hybrid model, the ratio of K-shell radiative transition width to Auger transition width in a few low Z elements in the range of 14 < Z < 30 is been calculated. The ratio of radiative transition width to the Auger transition width for the elements investigated is systematically computed using the K-shell fluorescence yield of these elements as measured by different researchers in the study of fluorescence spectroscopy and is available in the updated database of [7]. Γ_R^K/Γ_A^K values for the low Z elements investigated in the present study is tabulated in Table 1. It is found that the values for Radiative transition to Auger transition for the elements investigated is consistent with literature. The probability dependence of Auger emission process in low Z elements is studied and is graphically shown as in Fig.1. The present study helps to understand the electron rearrangement process in low Z elements during atomic excitation or ionization that takes place between a low energy gamma/X-ray photon interaction with matter. The ratio of K-shell radiative transition width

Table 1. Ratio of K-shell radiative transition width to Auger transition width in low Z elements.

Element	Z	$\bar{\omega}_K$	$\sigma\bar{\omega}_K$	Γ_R^K/Γ_A^K
Si	14	0.05	--	0.052
S	16	0.0775	0.001	0.084±0.002
Cl	17	0.087	--	0.095
K	19	0.14	--	0.162
Ca	20	0.174	--	0.211
Ti	22	0.2056	0.0225	0.258±0.040
V	23	0.2275	0.0275	0.294±0.050
Cr	24	0.2787	0.0105	0.386±0.021
Mn	25	0.3348	0.0228	0.503±0.050
Fe	26	0.3253	0.0332	0.482±0.070
Co	27	0.3497	0.0424	0.537±0.092
Ni	28	0.3861	0.0529	0.628±0.122
Cu	29	0.4459	0.0249	0.804±0.064
Zn	30	0.4699	0.0200	0.886±0.053

$\bar{\omega}_K$ – weighted mean; $\sigma\bar{\omega}_K$ –weighted uncertainty; --values not available

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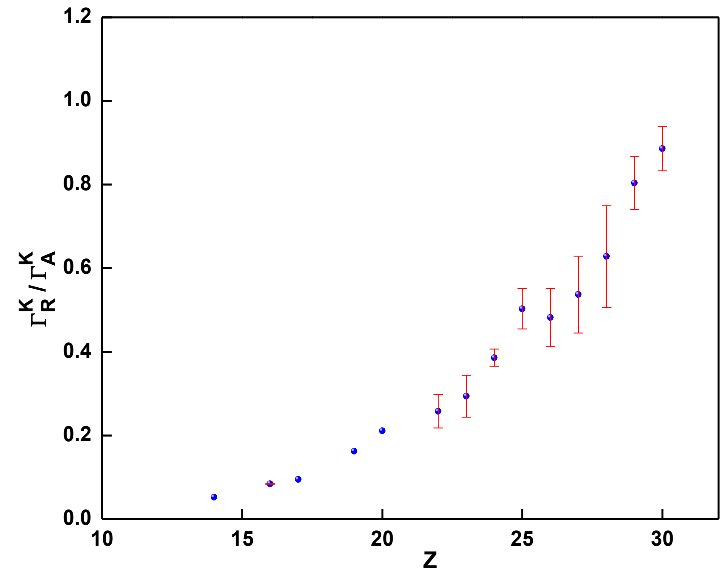

Figure 1. Linearity of Γ_R^K/Γ_A^K with atomic number Z

to Auger transition width is been studied using the K-shell fluorescence yield of the low Z elements in the range 14 < Z < 30 available in the updated database of [7].Γ_R^K/Γ_A^K in the present work is compared with the ratio of K-shell radiative transition width to the Auger transition width for these elements as calculated using the semi-empirical and fitted values for K-shell fluorescence yield of elements in the range 14 < Z < 30 from [3], [8], and [4]. The comparison of the ratios of Radiative transition width to Auger transition width Γ_R^K/Γ_A^K for the elements investigated is tabulated in table 2. A graphical analysis of the ratios of Radiative transition width to Auger transition width Γ_R^K/Γ_A^K for the elements in the range of 14 < Z < 30 is presented in Fig.2.

A good agreement is established between the ratios of Radiative transition width to Auger transition width Γ_R^K/Γ_A^K for all the elements investigated in the present study and the ratios of Radiative transition width to Auger transition width for the elements under study by different methods and theoretical models available. An uncertainty of less than 2% in ratio of Radiative transition width to the Auger transition width is reported for elements of atomic number 15 to 25.

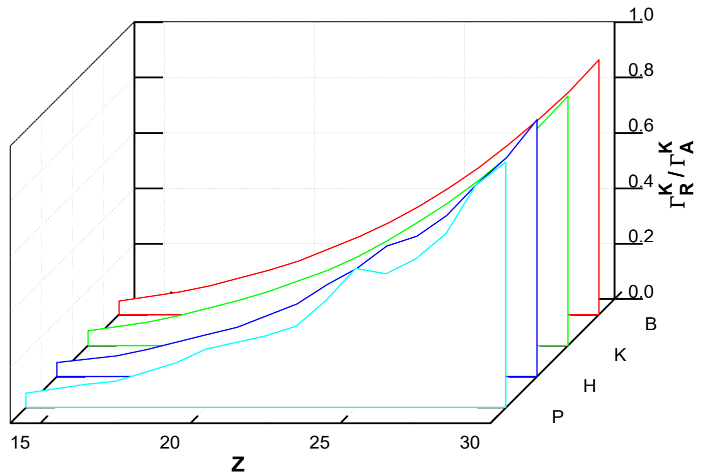

Figure 2. Γ_R^K/Γ_A^K using ω_K from [3], [8],[4] and the present values against Z

Table 2. Calculation and comparison of ratios of Γ_R^K/Γ_A^K

Element	Z	Present work	[3]	[8]	[4]
Si	14	0.052	0.049	0.053	0.050
S	16	0.084	0.082	0.085	0.075
Cl	17	0.095	0.104	0.107	0.098
K	19	0.162	0.160	0.163	0.152
Ca	20	0.211	0.194	0.195	0.178
Ti	22	0.258	0.280	0.272	0.263
V	23	0.294	0.332	0.321	0.332
Cr	24	0.386	0.391	0.379	0.391
Mn	25	0.503	0.458	0.445	0.471
Fe	26	0.482	0.531	0.515	0.506
Co	27	0.537	0.616	0.595	0.582
Ni	28	0.628	0.707	0.684	0.695
Cu	29	0.804	0.805	0.786	0.792
Zn	30	0.886	0.919	0.901	0.927

[3]-Bambynek et al.; [8]- Krause ; [4]- Hubbell et al.

The uncertainty in the computation of the ratio of radiative transition width to the Auger transition width is between 3% to 4% for elements with atomic number between 25 to 29. The difference in the uncertainty in the ratio of radiative transition width to Auger transition is accounted to the weighted uncertainty in the measurement of K-shell X-ray fluorescence yield for the target elements investigated.

6. Conclusion and Future Scope

In the present investigation, the ratio of K-shell radiative transition width to the Auger transition width of a few low Z elements in the atomic range of 14 < Z < 30 is been calculated using the K-shell fluorescence yield of these target elements. The results for the ratio of radiative transition to the Auger transition for the elements investigated in the present work is in good agreement with the theoretical model and with the empirical and semi-empirical fits. As, the experimental measurement for the K – Shell X-ray fluorescence yield for low Z elements is cumbersome because of the need of high-resolution low energy detectors, using the method in the present investigation, the values for the ratio of radiative transition to Auger transition for the elements in the category of low atomic number can be calculated. The method finds a simple technique in estimating the K-shell X-ray fluorescence yield, X-ray fluorescence yield in the subshell of K shell in these target elements as well. Also, measuring the line widths for radiative and radiation less transitions is cumbersome, the method in the present investigation finds an alternative and simple technique in estimating the line widths of radiative and non-radiative transition in low Z regime. It is shown in the literature that by measuring the K-shell X-ray intensity ratios and K-shell X-ray fluorescence yield, the total vacancy transfer probability for an electron that is created during the atomic excitation de-excitation process in the K-shell can be estimated. Since, the ratio of radiative transition width to the Auger transition width in the present work is found to increase proportionally with the atomic number Z, the present study seems to be an alternate method to find the Auger electron count rate in low Z elements. The present study also finds scope in estimating the fluorescence parameters viz, K –shell intensity ratio, total K to L vacancy transfer probability, atomic cross section, jump ratio and jump factor in low Z elements where the data seems to be scarce.

7. Author's statements

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Conflict of Interest- There is no conflict of interest.

Data Availability- The data is available as research article in the references cited herewith.

5. Copyright Notice

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