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Research Paper

Radiative to Auger transition width in few low Z elements ranging 14 to 30

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Abstract— K-shell fluorescence yield for a few low Z elements taken from the database compiled by Kahoul (2012) is studied. Ratio of radiative transition width to radiationless transition width in the atom of the K-shell is estimated. Z dependence of the ratio of the transition widths is tabulated and compared for experimental, theoretical and semi-empirical fit values as reported. The uncertainty in the present work is attributed to the uncertainty in the values of fluorescence yield for K-shell. In the present work we have studied the predominance of Auger process in the electron rearrangement mechanism in the excited atoms in the low Z elements.

Keywords— Radiative transition width, Auger transition width, K-shell fluorescence yield.

1. Introduction

For many years, several researchers have been studying the process of atomic excitation resulting in X-ray fluorescence (XRF) emission. It is been reported XRF spectroscopy particularly 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, 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, Kβ/Kα 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 at low energies of the incident gamma radiation or the X-ray photons with matter the probability of electron rearrangement in the electron orbits due to atomic excitation is mainly by the process of radiative transition in heavier elements while the electron rearrangement mechanism is chiefly through radiationless 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 radiationless transition is been reported. In the present work, we have studied the K-shell ratio of radiative transition width to the Auger transition or the radiationless width (Γ_R^K/Γ_A^K) for a few low Z elements. The weighted mean of K-shell fluorescence yield for a few low Z elements in the range 14 < Z < 30 available from the compilation work of Kahoul et al. [7] for K-shell fluorescence yield and have computed the ratio of radiative transition width to the Auger transition width for these low Z elements using the methods discussed [8 – 10]. It is been found that (Γ_R^K/Γ_A^K) is linear for these elements and increases with Z. The computed values are in good agreement with the theory of atomic excitation. The uncertainty in the calculated values of (Γ_R^K/Γ_A^K) in the present work is due to the uncertainties in the weighted mean value of the K-shell fluorescence yield for these elements. The present study helps understand the process of electron rearrangement is predominantly through the emission of Auger electrons in the region of low Z elements. The study finds scope in experimentally determining the widths of radiative transition, line width of Auger transition and probability of line width of Coster-Kronig transitions and to estimate the total transition line width respectively.

2. Theory

In this Interaction of gamma radiation or X-ray photons with matter causes atomic excitation or ionisation 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 radaitive 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 radiationless 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 Γ of that level is [8],

$$\Gamma\tau = \hbar \qquad (1)$$

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,

$$\Gamma_K = \frac{\Gamma_R^K}{\omega_K} \qquad (2)$$

Since, 1s state has a single subshell in K-shell and for 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 radiationless transition for the K-shell is given as,

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

3. Experimental Method

Auger emission of electrons being predominant whenever a gamma photon of low energy interact with atoms in the low Z elements. The Auger transition line width is studied from the Auger spectroscopy for these elements. Alternately, In the present work, for a few low Z elements, using the weighted mean for their K-shell fluorescence yield, we have estimated the ratio of radiative transition line width to the Auger transition line width in the atomic range $14 < Z < 30$. The weighted mean of K-shell fluorescence yield of an element under study in the range studied is obtained from Kahoul et al. (2012) and the ratio of widths of radiative transition to the Auger emission transition is computed using eqn. 3. The uncertainty in our calculation is been systematically estimated and is found to arise due to the association of uncertainty with the weighted mean of K-shell fluorescence yield of the element investigated. A spread sheet is created using MS excel available in the Windows 10 software and the data of the K-shell fluorescence yield from the database of Kahoul et al. for the elements investigated is entered to compute the ratio of radiative transition width to the Auger transition width. The data for the ratio of radiative transition width to Auger transition width is copied from the excel sheet to the Origin workbook and the data is fitted for linearity with the atomic number Z for the 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.

4. Results and Discussion

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 from the K-shell fluorescence yield measured by different researchers in the study of fluorescence spectroscopy that is available in the updated database [7]. Γ_R^K/Γ_A^K values for the low Z elements investigated in the present study is tabulated in Table 1. 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 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 Kahoul et al. 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 Bambynek et al., Krause, and Hubbell et al. The comparison of the ratio Γ_R^K/Γ_A^K is tabulated in table 2. A graphical analysis of the ratios of Γ_R^K/Γ_A^K for the elements in the range $14 < Z < 30$ is presented in Fig.2. A good agreement is established between the Γ_R^K/Γ_A^K values of the present method and different methods and theoretical methods available.

Figures and Tables

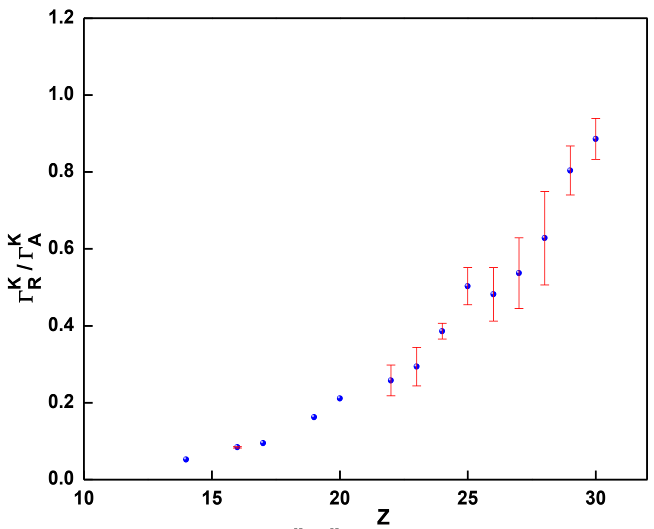

Fig.1. Linearity of Γ_R^K/Γ_A^K with atomic number Z

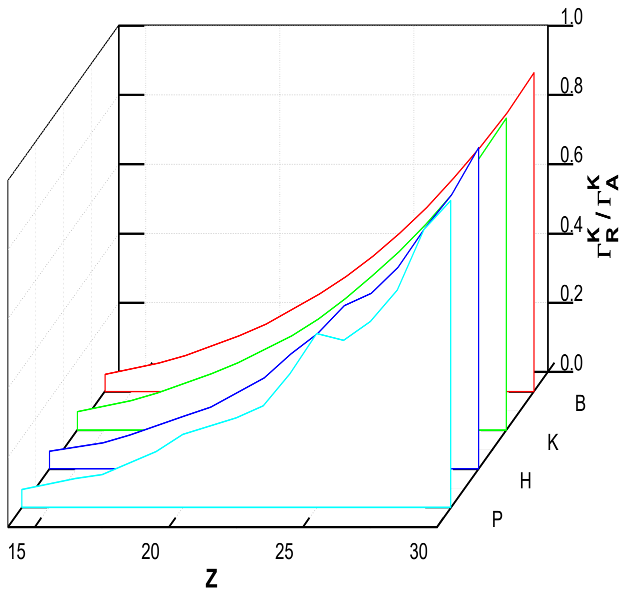

Fig.2. Γ_R^K/Γ_A^K using ω_K from [3], [8],[4] and the present values against Z

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

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

Elements	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.

5. Conclusion and Future Scope

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. The results are in good agreement with the theoretical model and with the empirical and semi-empirical fits. 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, we report that the present study is an alternate method to find the Auger electron count rate in low Z elements.

Data Availability

The data pertaining to the K-shell fluorescence yield of the low Z elements in the present study is available in the data tables of M.O. Krause, Bambynek et al. and Kahoul et al.

Conflict of Interest

There is no conflict of interest, as the data is taken from the published articles and been duly acknowledged.

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Authors' contribution

The present work being studied by single author, the literature survey, data analysis and interpretation is been carried out solely.

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