PRAMANA
— journal of
physics

Vol. 56, No. 5
May 2001
pp. 697–703

Measurement of K_β/K_α values using proton beam

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MS received 8 June 2000; revised 19 December 2000

Abstract. The K_β/K_α intensity ratios are measured in some $3d$ shell elements by using a 2 MeV proton beam along with a high resolution Si(Li) detector. The present K_β/K_α intensity ratios are in good agreement with Scofield modified theoretical values, thus supporting the basic assumptions in that theory. From the present K_β/K_α intensity ratios, it is evident that due to chemical effects, the experimental K_β/K_α intensity ratios will be increased while they will be decreased due to the presence of simultaneous M-shell vacancies which are produced due to proton excitation.

Keywords. K_β/K_α intensity ratios; 2 MeV proton beam; Si(Li) detector; Scofield modified theory; chemical effects; multiple ionization phenomenon.

PACS Nos 32.30.Rj; 41.75.-i; 41.75.Ak; 32.80.Hd

1. Introduction

Study of the K x-ray intensity ratios is of importance to understand the atomic inner shell ionization process and to test the relevant existing theories. The availability of highly sophisticated x-ray detectors with good energy resolution permits accurate measurement of x-ray intensities. The K-ray intensity ratios have been measured by several authors [1–28].

The K x-ray intensity ratios due to different authors with different excitation modes are summarized in table 1. In the same table, the theoretical K_β/K_α intensity ratios due to Scofield's old [29] and modified [30] theories are also given. From the table, it is observed that the K_β/K_α intensity ratios due to some of the authors [1,5,8,21,34] for some of the elements agree with Scofield's old theoretical values [29] while the K_β/K_α intensity ratios due to some other authors agree with Scofield's modified [30] theoretical values. However, limited experimental data on K_β/K_α intensity ratios with proton excitation is available. Kasagi *et al* [11] have used 3.5 MeV protons as exciting agents and measured the K_β/K_α intensity ratios in the region of the elements $62 \leq Z \leq 82$ and found reasonable agreement with Scofield modified [30] theoretical values. Richard *et al* [32] have used proton beam in the energy range 6 to 10 MeV and studied the dependence of K_β/K_α intensity ratios with projectile energy. The K_β/K_α intensity ratios for Cu element obtained by them is lower than Scofield modified [30] theoretical values.

Benka [10] studied the energy dependence of K_β/K_α intensity ratios in Si element with different proton energies. They have observed that K_β/K_α intensity ratios will depend on proton energy. They have explained this energy dependence as due to the formation of simultaneous $3p$ (M-shell) vacancies in addition to a vacancy in the $1s$ (K-shell) shell (multiple ionization phenomenon). Li *et al* [15] have measured the K_β/K_α intensity ratios in some $3d$ shell elements using charged particle excitation. The K_β/K_α intensity ratios obtained by them due to carbon ions are also given in table 1. Their values due to carbon ions are much higher than Scofield's [29,30] theoretical values and also the experimental values due to other excitation modes.

Brunner *et al* [41], Kucukonder *et al* [34], Tamaki *et al* [36], Mukoyama *et al* [7], Kataria *et al* [35] and Raghaviah *et al* [42] have studied the effect of chemical environment on K_β/K_α intensity ratios in some $3d$ shell elements. They have observed that the K_β/K_α intensity ratios are enhanced by about 4 to 5% due to the chemical effects.

In the present work, the K_β/K_α intensity ratios have been measured in some $3d$ shell elements using 2 MeV proton beam. The motivation of the present work is (1) to verify

Table 1. K_β/K_α intensity ratios obtained in the present work along with those due to earlier authors.

	K_β/K_α (experimental)		K_β/K_α (theory)	
Element	Present (proton)	Early authors	Scofield [29]	Scofield [30]
Ca	0.131 ± 0.003	0.069 [21] (RD), 0.128 [20] (X), 0.128 [31] (SE), 0.175 [15] (C)	0.106	0.131
Ti	0.134 ± 0.003	0.094 [21] (RD), 0.123 [1] (RD), 0.103 [34] (P), 0.132 [20] (X), 0.133 [1] (X), 0.134 [31] (SE), 0.162 [15] (C)	0.114	0.135
V	0.135 ± 0.003	0.105 [21] (RD), 0.121 [1] (RD), 0.148 [4] (P), 0.134 [1] (X), 0.128 [8] (X), 0.156 [15] (C)	0.116	0.137
Cr	0.136 ± 0.003	0.113 [21] (RD), 0.127 [1] (RD), 0.131 [36] (RD), 0.112 [5] (P), 0.135 [20] (X), 0.134 [1] (X), 0.132 [8] (X), 0.135 [31] (SE), 0.152 [15] (C)	0.115	0.134
Mn	0.136 ± 0.003	0.122 [21] (RD), 0.129 [24] (P), 0.134 [25] (P), 0.115 [5] (P), 0.137 [35] (P), 0.138 [23] (P), 0.135 [7] (X), 0.137 [35] (X), 0.153 [15] (C)	0.119	0.138
Fe	0.135 ± 0.003	0.128 [21] (RD), 0.129 [1] (RD), 0.116 [34] (P), 0.136 [20] (X), 0.135 [1] (X), 0.133 [8] (X), 0.135 [31] (SE), 0.153 [15] (C)	0.121	0.139
Zn	0.139 ± 0.003	0.135 [21] (RD), 0.136 [1] (RD), 0.134 [24] (P), 0.139 [25] (P), 0.137 [1] (X), 0.151 [18] (X), 0.138 [8] (X), 0.133 [33] (E), 0.135 [13] (E), 0.138 [31] (SE), 0.164 [15] (C)	0.124	0.141

RD: radioactive decay; P: photons; X: x-rays; E: electrons; SE: semi-emperical (Salem); C: carbon ions.

Table 2. List of compounds used in the present work.

Element	Compound
Ca	$CaCO_3$
Ti	TiO_2
V	V_2O_5
Cr	$K_2Cr_2O_7$
Mn	$MnSO_4$
Fe	$FeSO_4$
Zn	$ZnSO_4$

which Scofield theoretical values will explain the K_β/K_α intensity ratios due to proton excitation; (2) to observe the possible chemical effects; (3) whether multiple ionization takes place with proton excitation.

2. Experimental details

In the present work, K_β/K_α intensity ratios were measured for elements Ca, Ti, V, Cr, Mn, Fe and Zn using a 2 MeV proton beam. The elements used in the present work are taken in the form of their compounds. The chemical compounds of different elements that are used in the present work are shown in table 2. Targets of different elements are prepared using dipping technique. The thickness of different targets range from 2 mg/cm^2 to 3 mg/cm^2.

The present experiments were carried out using 3 mV tandem pelletron accelerator facility at the Institute of Physics, Bhubaneswar. The collimated beam of protons of diameter 1.5 mm is directed on to the target. The target is kept at an angle of 45° to the beam direction. The emitted K x-rays are passed through a 3.5 mg/cm^2 mylar window, 5 cm air gap and 0.012 mm thick Be window and reach the Si(Li) detector. The Si(Li) detector is kept at an angle of 90° to the beam direction. The resolution of the Si(Li) detector is 160 eV (FWHM) at 5.9 keV photon energy.

The efficiency of the Si(Li) detector at different energies is calculated using ^{241}Am, ^{55}Fe, ^{57}Co and ^{133}Be radio active sources. The efficiency of the detector is also calculated theoretically as described by Padhi *et al* [37]. The following expression is used to calculate the intrinsic efficiency

$$e_d = e^{-(\mu_{Be}X_{Be}+\mu_{Au}X_{Au}+\mu_{Si}\Delta x_{Si})}(1 - e_{Si}^{-\mu}X_{Si}),$$

where μ is the absorption coefficients due to Be window of the detector. The thickness of the Au layer on the Si(Li) crystal at the given energy is X_{Au} and ΔX_{Si} is the thickness of the insensitive region of the Si(Li) crystal. The X's are as per specification of the detector manufacturer and the absorption coefficients are taken from the tables of Hubbell *et al* [38]. The values of X used in the present calculation are given in table 3. The detector efficiency is calibrated at different energies. The resulting efficiency curve as obtained is shown figure 1.

Each target is exposed to proton beam and K x-rays spectrum is collected for sufficient long time. The time of collection is such that the uncertainty in counting statistic is less than 1%. The K x-ray spectrum of Fe element recorded with proton beam in shown in figure 2.

Table 3. X-values used in the efficiency equation of the detector.

X_{Be}	0.002253 gm/cm^2
X_{Au}	0.000038622 gm/cm^2
ΔX_{Si}	0.000023212 gm/cm^2
X_{Si}	0.69636 gm/cm^2

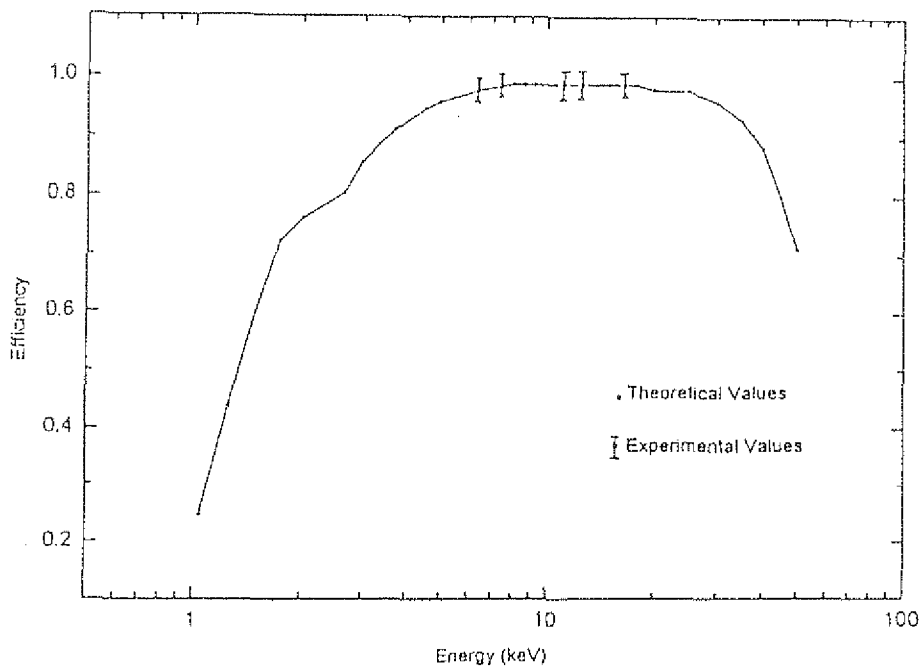

Figure 1. The efficiency curve of the Si(Li) detector.

3. Data analysis

The areas under the K_α and K_β x-ray components are calculated for each element by using the 'analytical x-ray analysis by iterative least square' (AXIL) software program. Using the detector efficiency values, the areas under the K_α and K_β x-ray components are converted to the respective intensities using the relation

$$I_{K_\beta}/I_{K_\alpha} = (A_{K_\beta}/A_{K_\alpha})/(\varepsilon_{K_\beta}/\varepsilon_{K_\alpha}),$$

where I_{K_α} and I_{K_β} are the intensities of K_α and K_β x-ray components. A_{K_α} and A_{K_β} are the areas under K_α and K_β x-ray components, ε_{K_α} and $\varepsilon_{K\beta}$ represent the efficiency values corresponding to K_α and K_β x-ray energies. The efficiency values are taken from figure 1. The K_α and K_β intensity values thus obtained are without self-absorption correction. The intensities are corrected for self-absorption using the formula

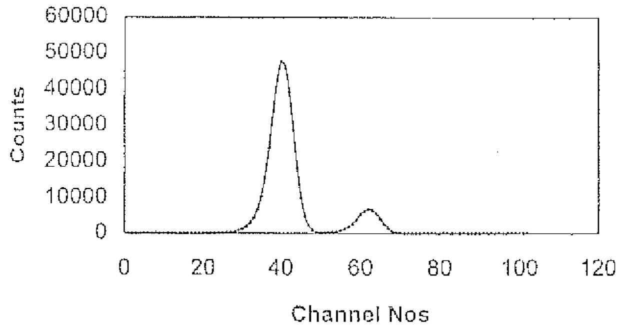

Figure 2. K x-ray spectrum of Fe due to proton beam.

$$I = I_0[1 - e^{-\mu t}].$$

Here I_0 represents the intensity of x-rays after absorption correction, t represents the thickness of the target and μ represents the attenuation coefficient. These attenuation coefficients are calculated using the total cross sections given in the tables of Storm and Israel [39]. In the present work, since compounds are used, the attenuation coefficient corresponding to the respective compound is evaluated using 'sum rule' [40].

4. Results and discussion

The K_β/K_α values obtained in the present work with 2 MeV proton beam for different elements are given in table 1. The present experimental values are associated with an overall uncertainty of about 2.2% which is contributed cumulatively by individual uncertainty due to detector efficiency, counting statistics and self-absorption correction.

From table 1, it is observed that the K_β/K_α values obtained in the present work did not support Scofield theoretical calculations [29] while they support Scofield modified theoretical values [30]. In Scofield modified version [30], the radial wave functions of all the single particle states of a given sub-shell are assumed to be identical. He has included the exchange correction in the calculation of decay rates. In modified version, a separate relativistic HF calculation is considered for the initial state with a vacancy in the $1s$ sub-shell and for final state with a vacancy in a p sub-shell.

The effect of chemical environment on K_β/K_α has been studied by several authors [1,5,8,21,34] in $3d$-shell elements. Their results indicated that the K_β/K_α intensity ratios of the elements when they are in compound form are 4–5% higher than those for pure elements as well as Scofield modified theoretical values [30]. In the present work, the elements are taken in the compound form and due to chemical effects, it is expected that the present K_β/K_α intensity ratios may be higher than Scofield theoretical values and other earlier data by about 4 to 5%. But, the present experimental values are in close agreement with Scofield theoretical values [30]. This may be due to the multiple ionization taking place in the target atoms while using protons as exciting agents.

Benka [10] has explained the variation of K_β/K_α intensity ratios with proton energy as due to the formation of simultaneous M-shell vacancies in addition to a K-shell vacancy.

Li *et al* [15] calculated the functional dependence of K_β/K_α intensity ratios on the initial inner shell vacancy configuration. From their calculations, it is noticed that the K_β/K_α intensity ratio is a strongly increasing function of the simultaneous L-shell vacancies and a smoothly decreasing function of simultaneous M-shell vacancies. In the present work, since protons are used as projectiles, as mentioned by Benka [10] simultaneous M-shell vacancies may be produced and according to Li *et al* [15], these simultaneous M-shell vacancies will reduce the experimental K_β/K_α intensity ratios.

In the present work, since compounds are used, due to chemical effects, the experimental K_β/K_α intensity ratios may be higher than the normal values, while the experimental K_β/K_α intensity ratios may simultaneously be reduced due to multiple ionization effects. Hence, the present K_β/K_α intensity ratios may be expected to be in agreement with Scofield theoretical values as well as earlier experimental values which is evident from table 1.

5. Conclusion

In the present work, the K_β/K_α intensity ratios are measured in some $3d$ shell elements by using a 2 MeV proton beam. From the present results, the following are the conclusions:

1. The present K_β/K_α intensity ratios are in good agreement with Scofield modified theoretical values thus supporting the basic assumptions of that theory.
2. From the present K_β/K_α intensity ratios, it is evident that due to chemical effects, the experimental K_β/K_α intensity ratios may be increased while they may be decreased simultaneously due to the presence of simultaneous M-shell vacancies that are produced due to proton excitation.

Acknowledgements

One of the authors S Bhuloka Reddy acknowledges the authorities of Andhra University for sanctioning him a minor research project to carry out the present investigaions.

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