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On the widths of K levels of heavy elements

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Abstract. The ratios of the widths of K levels of heavy elements with atomic number 70 to 92 have been calculated with relativistic wave functions, retardation, screening and field theoretical corrections to relativistic energy. The calculated values have been compared with the available observed data and good agreement has been obtained.

Keywords. Width of lines; K lines of heavy elements; field theoretical corrections; retardation effect; transition probabilities; radiative width.

1. Introduction

The ratios of the widths of K levels for elements of atomic number 70 to 92 have been calculated as a test for the correctness of the one-electron model to explain the widths of x-ray lines.

The computation of the widths of lines is a complicated problem. Several factors contribute to the width of spectral lines, the major ones being those due to Doppler broadening, which is temperature dependent, the influence of hyperfine structure, external effects due to the neighbouring atoms, etc. (Blokhin 1957). However, in the x-ray region, the natural width is so large that the other effects are quite small in comparison. Relativistic radiative decay rates, calculated by Scofield (1969, 1974) and Rosner and Bhalla (1970 *a*, *b*) and non-radiative transition rates by Ramsdale and Bhalla (1970) and other work (Gokhale 1950, Kostroun *et al* 1971, Chen *et al* 1971, Mc Crary *et al* 1971, Bambyneck *et al* 1972) have shown that the non-radiative transition rates to the K levels of the heavy elements are very small when compared to the radiative transition rates. In the case of the higher levels, while the non-radiative widths are comparable to the radiative widths, the radiative widths are themselves very small when compared to the radiative width of the K level.

Nelson *et al* (1969, 1970) have recently determined the widths of K_{α_1} and K_{α_2} lines for a number of elements and compared them with the values obtained from Scofield's (1969) calculations, corrected for non-radiative widths by taking into account the fluorescence yield given by Wapstra *et al* (1959). They observed that the instrumental width for the heavy elements was more or less constant and their experimental values of the width of K_{α_1}, and K_{α_2} lines agreed with the theoretical values of Scofield.

2. Calculations

To reduce the uncertainties in determining the width of lines, the ratio of the width of the K_α line of a given element to that of the K_α line of tungsten has been taken by us for comparison with the experimental values of Nelson *et al* (1969, 1970). For simplicity of calculations, we have assumed that the width of the K_α lines is mainly due to the radiative width of the K level for heavy elements.

In fact, we have taken only the width of K level into consideration. In addition, we have taken the transition probabilities of only the prominent lines, *viz.* K_{α_1}, K_{α_2}, K_{β_1}, K_{β_2}, $K\beta'_2$, and $K\beta''_2$ lines, to calulate the width of K level.

To check the correctness of these assumptions, we have compared the ratio of the widths, using Scofield's (1969) data, both with and without these assumptions. The results are given in table 1. In this table, the first column gives the ratio of the widths calculated according to the method of Nelson *et al* (1969) by taking fluorescence yield into consideration, the second column gives the ratios calculated with only the radiative transition rates and the third column with all the assumptions made by us. Column 4 of the table shows the ratio of the width of K level of the given element to that of tungsten, with the data from Scofield's later paper where Scofield (1974) has also taken exchange corrections into account. A comparison of columns 3 and 4 shows that the exchange corrections alter the width of K levels only to a slight extent. Even for uranium, the value changes only from 2·431 to 2·445, with the inclusion of exchange corrections. For lighter elements, the change is much less. A comprison of the first and second column shows that radiative transitions being comparatively much larger than non-radiative transitions for heavy elements, the results are not very much affected whether fluorescence yield is taken as in column 1 or neglected as in column 2.

Table 1. Comparison of the ratio of the widths of K_α lines of the different elements to the width of the K_α line of tungsten ($Z = 74$), with fluorescence yield (col. 1) radiative transitons alone (col. 2) and taking only the width of K level (col. 3). Column 4 is the same as in col. 3 but with exchange corrections included.

Z	1	2	3	4
70	0·800	0·790	0·794	0·794
73	..	0·943	0·945	0·945
74+	1·000	1·000	1·000	1·000
78	1·237	1·250	1·242	1·243
79	..	1·318	1·309	1·310
80	1·369	1·389	1·379	1·380
81	..	1·463	1·451	1·453
82	1·515	1·542	1·526	1·528
90	2·206	2·274	2·226	2·237
92	2·409	2·489	2·431	2·445

Values are from Scofield's data (1969, 1974) and those given by Nelson *et al* (1969).

The width of K_{α_1} line is the sum of the widths of K and L_{III} levels and that of K_{α_1} is the sum of K and L_{II} levels. The average of K_{α_1} and K_{α_2} calculated in this manner is taken in the first two columns. However, it is assumed that K level is mainly responsible for the width of K lines and that the width due to L levels can be neglected. These results are given in column 3. This assumption does not introduce any substantial difference as given by a comparison of columns 2 and 3. A comparison of first, second and third column shows that nonradiative transitions can be neglected for the heavy elements, the width is mainly due to K level and one treats the width of the line as due to K level alone, in these approximate calculations, the values are not materially affected. Hence the assumptions made are not unjustified. In our computations of transition probabilities, Slater screening constants were used with relativistic Dirac wave functions. The frequency factor used was according to Bethe and Salpeter (1957) and retardation effect as given by Babushkin's formula (Babushkin 1964, 1965, 1967). Relativistic energies of the different transitions were evaluated with the Modified Sommerfeld-Dirac Energy Formula (Krishnan and Nigam 1973) with Sommerfeld screening constants σ_1 and σ_2 (Sommerfeld 1934). The second and fourth order field theoretical corections such as radiative, relativistic, magnetic moment, vacuum polarisation, finite mass and finite nuclear size corrections (Series 1957, Harriman 1956) were included in the energy computations. The results obtained for energy as well as intensity ratios were compared with the observed values available (Bearden 1967, Sandsträm 1957) and the details are given elsewhere (Krishnan 1971). [A more refined calculation will be to make use of Erickson's formula (Erickson 1969, 1971; Erickson and Yennie 1965) for the calculation of field theoretical corrections].

3. Results

The results of the present calculations are given in table 2 for elements of atomic number 70 to 92. Comparison has been made with the observed values of Nelson *et al* (1969, 1970). As K_{α_1} and K_{α_2} have not been separately taken for comparison in the present calculations, the mean of the K_{α_1} and K_{α_2} widths of Nelson *et al* have been taken.

Even though the one-electron model is insufficient to explain phenomena such as the extended fine-structure of the absorption edges, which involve the effect of the neighbouring atoms, yet for a satisfactory explanation of the binding energies of the inner electrons, the intensity ratios and the width of x-ray lines, a logical extension of the one-electron model with the application of the field theoretical corrections seems to be adequate. However, as in any accurate calculations of the width of lines, all the factors that influence the width have to be considered and the present computation is more an estimate of the order of the ratios rather than an accurate calculation of the width of the line itself.

These computations were carried out with a CDC 3600 computer.

Table 2. Comparison of the ratios of widths of K_α lines of different elements to the width of K_α line of tungsten ($Z = 74$)

Z	1 Calc.	2 Obs.	Z	1 Calc.	2 Obs.
70	0·762	0·835	82	1·677	1·620
71	0·816	1·013	83	1·785	1·813
72	0·874	0·957	84	1·900	..
73	0·935	0·923	85	2·021	..
74^{++}	1·000	1·000	86	2·149	..
75	1·069	1·121	87	2·285	..
76	1·141	1·188	88	2·428	..
77	1·218	1·155	89	2·580	..
78	1·300	1·364	90	2·740	2·045
79	1·386	1·247	91	2·910	..
80	1·478	1·480	92	3·089	2·303
81	1·574	1·707	..	..	..

Col. 1 Ratio of the widths obtained from the present calculations.

Col. 2. Ratio of the widths from experimental values of Nelson *et al* (1969, 1970). The error of the ratios of widths is about 11% for observed values.

$^{++}$ Standard.

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