INTERNAL CONVERSION COEFFICIENTS FOR THE M SHELL OF THE ATOM

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Numerical values are presented for the internal conversion coefficients of the M_I, M_{II}, and M_{III} atomic subshells for M1, M2, E1, and E2 nuclear transitions. They are obtained by numerical integration of the set of Dirac differential equations, taking into account the effect of the finite size of the nuclei and screening by the Thomas-Fermi-Dirac (Z = 81) and Hartree (Z = 80) methods.

THE first tables of theoretical internal conversion coefficients (referred to below as ICC) for the K and L shells were obtained by Rose and his coworkers[1] under the assumption of a point nucleus. Calculations of ICC with account of both the static and dynamic effects of the finite size of the nuclei were first carried out by Sliv and coworkers.[2-4] Both effects are allowed for in the ICC tables of Sliv and Band (for the K and L shells)[3-4] on the basis of an equivalent uniform charge distribution over a volume of a spherical nucleus with radius

$$R = 1.20 \cdot 10^{-13} A^{1/3} \text{ cm} \quad (1)$$

and surface transition currents (Sliv's model). The radial electron functions used in the calculations by Sliv and Band were obtained by them by numerical integration of the set of Dirac differential equations with account for screening by the Thomas-Fermi-Dirac (TFD) method. The same numerical integration and assumption about the distribution of nuclear charge, but without account of the dynamic effect, were utilized (Rose's "unpenetrable" model) in the second calculation of the ICC for the K and L shells by Rose.[5]

Thus the most precise calculations of the ICC for higher shells (i.e., for the M, N, O, and P shells) have not yet been carried out. True, Rose's book[5] contains tables of ICC for the M shell, calculated without account of screening and the finite dimensions of the nucleus, but the results of a comparison of these tables with the experimental ICC is unsatisfactory (the difference is more than 100 percent).

In this paper we present the results of calculations of ICC for the M_I, M_{II}, and M_{III} subshells (see Table I) with account of screening according to TFD (Z = 81)[6,7] and Hartree (Z = 80).[8] The ICC in Table I were obtained with account of only the static effects of the finite dimensions of the nuclei on the basis of an equivalent uniform charge distribution of a spherical nucleus with radius

$$R = \{1.123A^{1/3} + 2.352A^{-1/3} - 2,070A^{-1}\} \cdot 10^{-13} \text{cm}, \quad (2)$$

since this expression for R which takes into account the effect of the surface layer on the equivalent dimensions of the nucleus is according to Elton[9] in better agreement with experiment for atomic weights A > 16 than (1).

If we consider the Z dependence of the ICC for the L and M shells equal, then an investigation on the basis of Table I and the corresponding tables of Sliv and Band[4] indicates that the values of the ICC with account of screening according to Hartree (Z = 80) differ from those with account of screening according to TFD (Z = 81) somewhat more than they should on account of the increase of Z.[1)]

The corrections to the ICC for the dynamic effect are investigated for Z = 80 on the basis of Sliv's model with the aid of analytic formulas obtained by the author,[10] the coefficients a_K and a_{K_0} entering into these formulas being obtained by numerical integration of the set of Dirac differential equations with a Hartree potential. It turned out that the corrections change somewhat (by 1—10 percent) the ICC for the M_I and M_{II} subshells, the corrections being larger for magnetic than for electric transitions.[2)]

[1)]Reduced to the same Z, the first set of ICC is commonly 1 – 10 percent smaller than the second set. This conclusion must be considered preliminary. It may be refined by calculating the ICC with allowance for screening according to TFD or Hartree (or Hartree-Fock) for the same value of Z (or for several sufficiently close values of Z).

[2)]Sliv's corrections to the ICC for the M_{III} subshell are vanishingly small.

Table I*

Z	k	M_I				M_{II}	
		$\alpha^{(1)}$	$\alpha^{(2)}$	$\beta^{(1)}$	$\beta^{(2)}$	$\alpha^{(1)}$	$\alpha^{(2)}$
80	0.1	3.82 (—2)	2.63 (—1)	1.70 (0)	5.82 (1)	2.42 (—2)	1.16 (1)
	0.2	7.83 (—3)	2.69 (—2)	2.24 (—1)	3.06 (0)	3.05 (—3)	4.58 (—1)
	0.5	9.05 (—4)	2.94 (—3)	1.67 (—2)	8.92 (—2)	2.01 (—4)	8.12 (—3)
	1	2.05 (—4)	6.17 (—4)	2.54 (—3)	8.45 (—3)	2.72 (—5)	5.00 (—4)
	2	5.54 (—5)	1.50 (—4)	4.28 (—4)	1.06 (—3)	4.36 (—6)	4.13 (—5)
81	0.1	4.04 (—2)	3.17 (—1)	1.94 (0)	6.78 (1)	2.52 (—2)	1.34 (1)
	0.2	8.60 (—3)	2.97 (—2)	2.56 (—1)	3.49 (0)	3.35 (—3)	5.28 (—1)
	0.5	1.01 (—3)	3.15 (—3)	1.88 (—2)	1.01 (—1)	2.23 (—4)	9.35 (—3)
	1	2.23 (—4)	7.03 (—4)	2.77 (—3)	9.55 (—3)	3.19 (—5)	5.76 (—4)
	2	5.75 (—5)	1.68 (—4)	4.83 (—4)	1.18 (—3)	4.80 (—6)	4.80 (—5)

Z	k	M_{II}		M_{III}			
		$\beta^{(1)}$	$\beta^{(2)}$	$\alpha^{(1)}$	$\alpha^{(2)}$	$\beta^{(1)}$	$\beta^{(2)}$
80	0.1	1.87 (—1)	5.45 (0)	2.85 (—2)	1.20 (1)	1.78 (—2)	2.45 (1)
	0.2	2.49 (—2)	3.82 (—1)	3.20 (—3)	3.86 (—1)	2.21 (—3)	7.99 (—1)
	0.5	1.82 (—3)	1.34 (—2)	1.73 (—4)	4.64 (—3)	1.48 (—4)	7.97 (—3)
	1	2.55 (—4)	1.25 (—3)	2.15 (—5)	1.60 (—4)	2.04 (—5)	3.51 (—4)
	2	3.86 (—5)	1.35 (—4)	3.38 (—6)	1.24 (—5)	3.22 (—6)	2.03 (—5)
81	0.1	2.18 (—1)	6.80 (0)	3.09 (—2)	1.59 (1)	2.00 (—2)	3.14 (1)
	0.2	2.88 (—2)	4.46 (—1)	3.54 (—3)	4.40 (—1)	2.48 (—3)	9.46 (—1)
	0.5	2.14 (—3)	1.59 (—2)	1.94 (—4)	5.23 (—3)	1.57 (—4)	1.07 (—2)
	1	3.03 (—4)	1.71 (—3)	2.31 (—5)	1.24 (—3)	2.29 (—5)	4.03 (—4)
	2	4.57 (—5)	1.57 (—4)	3.74 (—6)	1.38 (—5)	4.06 (—6)	1.96 (—5)

*Both in this and in the other tables the numbers in parentheses indicate the power of ten by which the number in front of the parentheses is to be multiplied.

In the general case the structural corrections to the ICC are expressed in terms of the nuclear parameters u_ν.[10,11] For large values of u_ν, as can occur for strongly forbidden gamma transitions, the contribution of the structural corrections can become appreciable. Thus, for example, the corrections to $\beta^{(1)}_{M_I}$, can even for u(m) = 5[3], k = 0.5 and Z = 80, also calculated by means of the analytic formulas,[10] change the value of $\beta^{(1)}_{M_I}$ by 30 percent.

The use of the above-mentioned analytic formulas makes it possible to investigate the dependence of the corrections on the effect of the surface layer and the deformation of the nucleus upon the electron wave functions. For Sliv's model this dependence is weak but nevertheless noticeable, and allowance for it can bring the theoretical ICC somewhat closer to the experimental values.[4] For sufficiently large values of the nuclear parameters it becomes much more appreciable, and for a more precise comparison of the theoretical results with experiment[5] it must be taken into account.

A comparison of the ICC of Table I with the corresponding values from Rose's tables[5] indicates that on the whole the latter exceed the former by about a factor of one and one half. The ratios of the corresponding ICC from Table I and from Rose's tables depend weakly on k and L. The changes of these ratios exceed somewhat the error limits of the calculations[6] only in several instances.

Table II gives the results of the comparison of the theoretical relative ICC for the M shell for Z = 80 with the experimental values[14-16] (the absolute values of the ICC for the M shell for Z = 80 have so far not been measured). The theoretical values of the relative ICC in the fourth column of Table II were obtained from the corresponding tabulated values of the ICC without account of screening.[5]

From Table II it can be seen that the theoretical relative ICC with account of screening are in better agreement with experiment[7] than the corre-

[3] The values of u(m) of this and higher order of magnitude, determined experimentally from the e–γ angular correlation, are cited, for example, in the work of Yamazaki.[12] We note that for Sliv's model u(m) = 1.

[4] Thus, for instance, $\alpha_K^{(2)}$ for the Gd^{152} 345-keV transition is according to the tables of Sliv and Band 0.0278; $\alpha_K^{(2)}$ calculated with allowance for the effect of the surface layer and nuclear deformation on the structural corrections is 0.0281, while the experimental value is 0.0283 ± 0.0008.[13]

[5] It should be noted here that the effect of the surface layer and nuclear deformation on the basic radial integrals of the ICC is very small and can (as is commonly done) be neglected.

[6] If we take into account that in dividing the first ICC by the second the errors incurred in their calculation add.

[7] If in the case of the transition E_γ = 158 keV we consider the results of de Vries et al. more accurate than those of Van Heerden et al.[15]

Table II

Isotope	E_γ, keV	Transition	Relative ICC	Theory: without account of screening	Theory: with account of screening	experiment
Hg^{199}	50	$M1$	$M_{II} : M_I$	1.07 (—1)	1.10 (—1)	1.24 (—1) [14]
			$M_{III} : M_I$	9.7 (—3)	1.05 (—2)	<2.5 (—2) [14]
Hg^{197}	134	$E2$	$M_I : M_{II} : M_{III}$	0.124 : 1.27 : 1	0.157 : 1.34 : 1	(0.29±0.06) : (1.49±0.9) : : (1.00±0.10) [15]
Hg^{199}	158	$E2$	$M_I : M_{III}$	0.24	0.20	0.166 [14], 0.28±0.5 [16]
			$M_{II} : M_{III}$	1.47	1.42	1.33 [14], 1.40±0.10 [16]

Table III

Z	Sub-shell	Binding energy of electrons: experiment	Binding energy of electrons: theory	$g(R)\,R$	$f(R)\,R$
80	M_I	0.0069748	0.0067463	0.0065397	—0.0015885
	M_{II}	0.0064229	0.0062330	—0.00048471	+0.0018985
	M_{III}	0.0055736	0.0053892	+0.00073475	—0.000099542
81	M_I	0.0072546	0.0075750	0.0069477	—0.0017104
	M_{II}	0.0066910	0.0070814	—0.00053374	0.0020640
	M_{III}	0.0057908	0.0061432	+0.00079009	—0.00010842

sponding ICC without account of screening. An exception is the value 0.20 in the sixth column. It differs from the experimental result (column 7) by at least 13 percent. If we take into account that the ICC of Table I are calculated with some error (cf. Appendix), then this difference may become smaller. Table II also shows that the effect of screening on the relative ICC is incomparably weaker than its effect on the absolute values.

APPENDIX

The basic radial integrals, in terms of which the ICC are expressed, were calculated by integration by parts. The basic radial integrals here are[10]

$$R^{(1)}_{\varkappa,\varkappa_0}(m) = (R_1 + R_2)_{\varkappa,\varkappa_0} \tag{3}$$

for magnetic ICC, and

$$R^{(1)}_{\varkappa,\varkappa_0}(e) = (\varkappa_0 - \varkappa)\,(R_5 + R_6)_{\varkappa,\varkappa_0} + L(R_6 - R_5 + R_3 + R_4)_{\varkappa,\varkappa_0} \tag{4}$$

for electric ICC; the right-hand sides of (3) and (4) are in the standard notation. Each basic radial integral was calculated within the limits from R to ∞ with the aid of the radial functions of the electron obtained by numerical integration of the system of Dirac differential equations using the Thomas-Fermi-Dirac (Z = 81) and Hartree (Z = 80) potentials. The intranuclear part of each basic radial integral was calculated from formulas derived on the basis of[10].

The normalized coefficients of the electron radial functions, obtained by the above numerical integration, were used as a_κ and a_{κ_0} which enter in these formulas; thus both parts of each basic integral were calculated with the same accuracy.

The radial functions for the continuous energy spectrum were obtained in precisely the same way as described by Sliv and Band.[4] The radial functions for the bound states of the electron were found following Rose.[5] In Table III we present the values of these functions on the boundary of the nucleus, and also the theoretical and experimental electron binding energies on the M_{I-III} atomic subshells. The table indicates that the theoretical values of the binding energy obtained with allowance for screening by the Hartree method are in better agreement with experiment than those obtained with the TFD potential. Numerical integration was carried out over the variable ρ, related to r by the relation

$$\rho = {}^1/_{137} r + \ln r, \tag{5}$$

where r is in relativistic units. The basic radial integrals were calculated with an accuracy of 1—3 percent. In view of the fact that they enter in the ICC as squares, the ICC were obtained with an accuracy of 2—6 per cent.

The problem of the usefulness of ICC calculations on the upper shells of the atom with allowance for screening according to TFD and Hartree was discussed by B. S. Dzhelepov and V. A. Krutov for which the author is much indebted.

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