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Calculation of Internal Conversion Coefficients for all Atomic Shells

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Abstract. Today extensive calculations of internal conversion coefficients (ICC), including screening and finite nuclear size effects, are available for the K , L , M and N_1 through N_5 atomic shells. In the present paper conversion coefficients for all atomic shells and various nuclear charge numbers, Z , are calculated with Hartree–Fock–Slater bound state wave functions and compared to approximate calculations and to experimental results. The knowledge of theoretical outer shell conversion coefficients offers the possibility of evaluating the change in total electron density $\Delta|\psi(0)|^2$ at the nucleus for isotopes decaying in two different chemical compounds.

I. Introduction

As is well known, atomic screening plays a very important role in the calculation of internal conversion coefficients (ICC). Today, extensive calculations taking into account screening effects and finite nuclear size are available [1, 2] for the K , L and M shells and also, more recently, for the N_1 through N_5 shells [3] but only for isotopes with high nuclear charge number Z . For outer shells, the point nucleus unscreened coefficients with the appropriate correction for atomic screening and finite nuclear size have been calculated [4]. Conversion coefficients for the N_6 , N_7 , P_1 through P_5 and Q_1 shells can be obtained from relation

$$\alpha = \alpha_0 f_{\text{scr}} f_{\text{fns}} \quad (1)$$

where α_0 is the point nucleus unscreened conversion coefficient, f_{scr} the appropriate screening correction factor and f_{fns} the correction to account for finite nuclear size. For low charge number Z , the ICC for the K , L_1 through L_3 and M_1 shells can be calculated directly with the aid of the program 'MONICA' outlined in Ref. [5]. In this program [5], the bound state problem for the screened Coulomb potential can be solved either with the Thomas Fermi Dirac model or by using extensive tabulations of non-relativistic Hartree–Fock–Slater screening functions.

With the advent of modern computers it has been possible to obtain from SCF calculations for molecular orbitals information about the valence structure of elements in chemical compounds. Apart from these extensive calculations the change in the decay rate λ of highly converted γ -transitions [6] or the measurement of the $K\alpha$ and $K\beta$ X-ray shifts in different chemical compounds [7, 8] also yield information about the

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participation of valence electrons in chemical bonds. In low energy γ -transitions, electrons of outer shells are strongly converted. Measurements of these conversion electrons give accurate experimental binding energies and a comparison of theoretical ICC with experimental ones should also yield information about the valence configurations in chemical bonds. As was already outlined in Ref. [6] a measurement of the relative change in the decay rate yields—in the special case of M1 transitions—the difference in total electron density at the nucleus $\Delta|\psi(0)|^2$ in two different chemical compounds. Connecting $\Delta|\psi(0)|^2$ with the Mössbauer isomer shift it is easy to obtain a reliable value for the change in nuclear charge radius $\delta R/R$.

II. Calculation of Internal Conversion Coefficients

In this section we shall illustrate our calculations of ICC by some examples of converted γ -transitions. All the conversion coefficients were calculated directly with the aid of the program 'MONICA' [5] using a relativistic Hartree–Fock–Slater potential as input. Instead of solving the bound state problem with the method outlined in Ref. [5], the electron wave functions needed for the evaluation of the radial matrix elements are directly taken from the same HFS calculations and interpolated at the required mesh points of the numerical integration. It is worth noting that the conversion coefficients are formed deep inside the atom as was pointed out by Sliv and Band [9], i.e. the radial magnetic and electric integrals reach their asymptotic value at about the radius of the K shell for all electron shells. Results of some calculations are now presented.

In Tables 1, 2 and 3 we collect the theoretical conversion coefficients for all atomic shells of the corresponding isotopes. Table 1 shows the ICC of the 14.4 keV M1 transition of ^{57}Fe and the 1.64 keV M1 transition of ^{193}Pt . We chose these two examples since we had already investigated them in a previous paper [6]. For both isotopes the first entry of the table shows the ICC computed with the program 'MONICA' [5], whereas we collect in the second column the ICC calculated with the same program using, however, directly HFS bound state wave functions for the evaluation of the

Table 1

The 'exact' theoretical ICC of the 14.4 keV M1 transition in ^{57}Fe and the 1.64 keV M1 transition in ^{193}Pt are compared with the conversion coefficients calculated with Ref. [5]. Those marked by an asterisk are calculated by means of relation (1).

ICC of the 14.4 keV M1 transition of ^{57}Fe			ICC of the 1.64 keV M1 transition of ^{193}Pt		
Shell	α	α	Shell	α	α
K	7.675	7.709	N_1	.9960(+4)	.9428(+4)
L_1	0.7223	.7219	N_2	.1045(+4)	.1018(+4)
L_2	.438(−1)	.438(−1)	N_3	.1225(+3)	.1181(+3)
L_3	.1774(−1)	.1774(−1)	N_4	.261(+2)	.255(+2)
M_1	.1064(0)	.1050(0)	N_5	.141(+2)	.143(+2)
M_2	.6107(−2)	.596(−2)	O_1	.1936(+4)	.1810(+4)
M_3	.2447(−2)	.238(−2)	O_2	.178(+3)	.1694(+3)
M_4	—	.235(−4)	O_3	.198(+2)	.185(+2)
M_5	—	.1883(−4)	O_4	.196(+1)*	.203(+1)
N_1	0.0049*	.650(−2)	O_5	.98(0)*	.108(+1)
			P_1	.144(+3)*	.142(+3)

matrix elements. Especially good agreement with the approximately calculated conversion coefficients is found, except for the N_1 ICC of ^{57}Fe . One should, however, note that in this latter case the nuclear charge number Z is very low and that relation (1) may not be sufficiently reliable for the calculation of such conversion coefficients. A comparison with calculations of Ref. [5] shows at most 6% deviation from the ICC computed with HFS wave functions for the low energy M1 transition of ^{193}Pt . This is not surprising, since one knows that for such a low energy transition mainly outer shell electrons are converted and that the theoretical ICC values are very sensitive to small changes of the bound state wave functions.

In Table 2 we show for the purpose of comparison the ICC of the 65 keV M4 transition of ^{119}Sn computed in different ways. The ICC of the first entry were calculated with the program 'MONICA' [5] using a relativistic HFS screening function for the calculation of the bound state wave function and those marked by an asterisk with relation (1). The second entry shows the ICC calculated with HFS bound state wave

Table 2

The conversion coefficients of the 65 keV M4 transition in ^{119}Sn are collected. The first entry (α^1) shows the ICC calculated with Ref. [5] and those marked by an asterisk with Ref. [4]. The second and third column (α^2 and α^3) show the ICC calculated with HFS and experimental binding energies respectively using HFS bound state wave functions.

ICC of the 65 keV M4 transition of ^{119}Sn

Shell	α^1	α^2	α^3
K	1670	1660	1650
L_1	821.1	814.7	816.7
L_2	179.5	178.4	179
L_3	1840	1823	1826
M_1	187.6	186.4	186.6
M_2	40.2	39.9	39.98
M_3	429.2	424.9	425
M_4	6.7	6.58	6.58
M_5	12.9	12.6	12.6
N_1	39.3	36.2	36.1
N_2	7.6	6.83	6.80
N_3	80.7	72.46	72.30
N_4	0.92*	0.84	0.84
N_5	1.85*	1.61	1.64
O_1	5.45*	3.76	3.88
O_2	0.55*	0.35	0.37
O_3	6.60*	3.48	3.58

functions which were directly inserted in the radial matrix elements. The binding energies were taken from the same HFS calculation. The last entry gives the ICC calculated with experimental electron binding energies taken from Bearden [10]. The excellent agreement between the ICC calculated with the Hartree-Fock binding energies and those calculated with experimental ones is noteworthy. The deviation of the approximate from the 'exact'²⁾ conversion coefficients for the outer shells N_4 , N_5 and O_1 through O_3 is appreciably larger but the relatively simple 'approximate'

²⁾ We shall refer to 'exact' conversion coefficients in the following when they are calculated with the program of Ref. [5] but using directly relativistic Hartree-Fock-Slater bound state wave functions for the evaluation of the radial matrix elements.

Table 3

The ICC calculated for the 42.9 keV transition in ^{246}Cm are shown in the third column ($\alpha_{\text{theor.}}^{(1)}$). The first column ($\alpha_{\text{exp.}}^{(1)}$) gives the experimental ICC as quoted by Chu and Perlman [11], the second column ($\alpha_{\text{theor.}}^{\text{HS}}$) shows the theoretical ICC taken from Ref. [1], whereas those marked by an asterisk are calculated by means of relation (1). The last entry ($\alpha_{\text{exp.}}^*$) shows the experimental conversion coefficients, where the line intensities are given relative to our calculated L_3 ICC.

ICC of the 42.5 keV E2 transition of ^{246}Cm

Shell	$\alpha_{\text{exp.}}^{(1)}$	$\alpha_{\text{theor.}}^{\text{HS}}$	$\alpha_{\text{theor.}}^{(1)}$	$\alpha_{\text{exp.}}^*$
L_1	13.5 ± 1.5	15.7	15.8	13.2 ± 1.5
L_2	451 ± 14	421	408	441 ± 14
L_3	(349)	349	341	(341)
M_1	—	4.8	4.90	—
M_2	109 ± 3	113	111.4	106.4 ± 3
M_3	104 ± 3	100	98.14	—
M_4	—	1.62	1.59	—
M_5	—	0.92	0.90	—
N_1	—	1.59	1.46	—
N_2	32 ± 1.2	35.2	30.84	31.2 ± 1.2
N_3	32 ± 1.2	30.4	27.35	31.2 ± 1.2
O_1	—	0.47*	0.38	—
O_2	9.2 ± 1	7.69*	7.65	9 ± 1
O_3	9.2 ± 1	7.49*	6.57	9 ± 1
O_4	—	0.115*	0.097	—
O_5	—	0.054*	0.051	—
P_1	—	0.091*	0.077	—
P_2	$\left. \begin{array}{l} \\ \end{array} \right\} 3.9 \pm 1$	1.23*	1.24	3.8 ± 1
P_3		1.22*	0.93	3.8 ± 1
Q_1	—	0.0088*	0.0038	—

calculation by means of relation (1) gives, however, reliable values of the ICC for outer atomic shells.

Recently Chu and Perlman [11] compared measured and theoretical conversion coefficients for inner and outer shells in ^{246}Cm . The experiments and calculations were investigated for the 42.852 keV pure E2 transition of this isotope. Our theoretical values are found to be in very good agreement with those interpolated from Hager and Seltzer's calculations [1]. Comparing, therefore, the experimental with our 'exact' conversion coefficients we find, especially for the inner shells, i.e. L_1 through N_3 , no notable discrepancies. Apart from the known experimental errors it is necessary to point out that there are still uncertainties in the ICC values of the innermost shells which are not exactly known [12]; higher order effects may in this case play a certain role. On the other hand it is very interesting to note that the theoretical 'exact' ICC for the outer shells, i.e. O_1 through Q_1 show surprisingly good agreement with those calculated by means of relation (1). This gives great confidence in the approximate calculation of outer shell conversion coefficients as outlined by Dragoun et al. [4]. Considering all the results obtained, we expect the agreement between the approximate ICC and our 'exact' ones to be especially good for high nuclear charge number Z , whereas for low charge number Z the approximate values represent rather good estimates. A weak dependence of the screening correction f_{scr} on the multipolarity λ is to be expected. However, more refined experiments should certainly be made to decide if our calculations are relevant for practical cases.

III. Influence of Chemical Environment on Highly Converted γ -Transitions

The knowledge of outer shell conversion coefficients allows in some special cases new experiments concerning the change of the decay rate of isotopes in different chemical environments. Recently, the change in transition probability of highly converted M1 transitions was investigated for some elements in different chemical compounds [6]. From the measurement of the relative change of the decay rate $\Delta\lambda/\lambda$ the difference of the total electron densities taken at the nucleus $\Delta|\psi(0)|^2$ in two compounds can easily be extracted. According to Sliv and Band [9] the relation

$$\frac{\alpha_1}{\alpha_2} \simeq \frac{|\psi_1(0)|^2}{|\psi_2(0)|^2}, \quad (2)$$

where α_1 and α_2 denote the ICC in two different chemical compounds for a fixed shell, holds very well for M1 transitions where mainly s-electrons are converted. However, relation (2) should also be valid for the other electric and magnetic multipolarities. Following Ref. [9] we show in Figure 1 the rapid increase of the conversion coefficients as a function of the upper limit of the radial integrals for the 65 keV M4 transition of ^{119}Sn . Even in this case the function $f(r) = \alpha(r)/\alpha$ reaches unity for all shells almost in the region of the K shell radius. We thus expect relation (2) to hold also for M4 transitions to a certain accuracy. In fact, the ratio $\{\alpha/|\psi(0)|^2\}$ was found to be approximately ($\pm 7\%$) a constant for all atomic shells with the same Dirac quantum number κ .

The measurement of $\Delta\lambda/\lambda$ for different stannous and stannic compounds should give some information about the electron type involved in these chemical bonds.

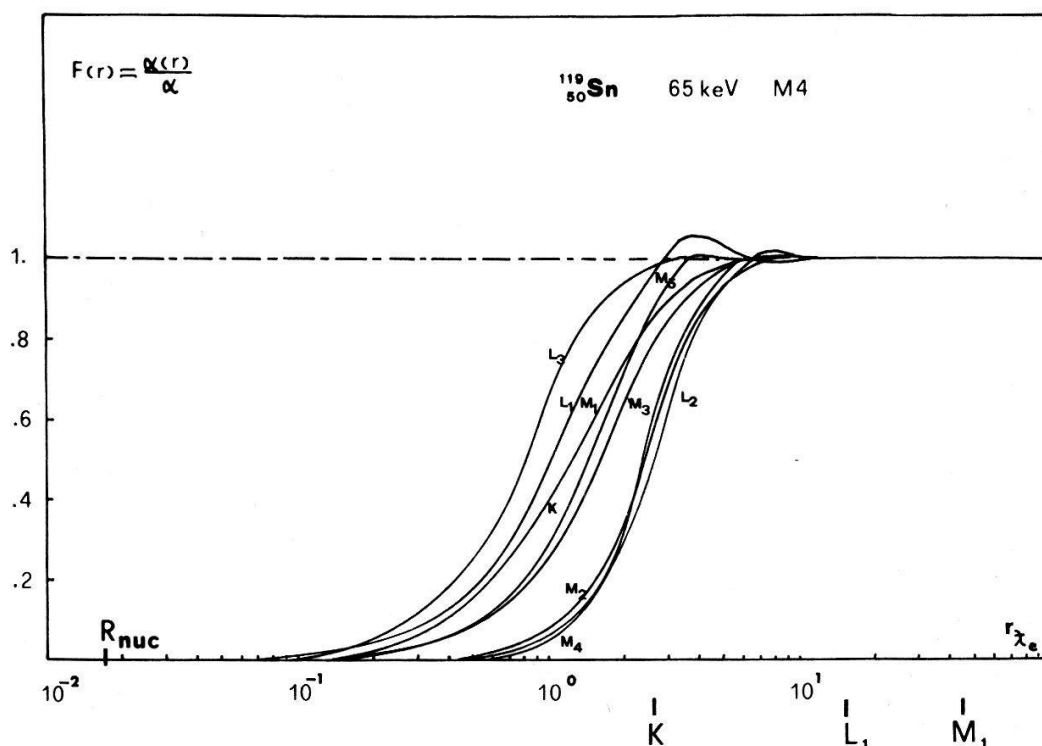


Figure 1

The function $f(r) = \alpha(r)/\alpha$ where $\alpha(r)$ denotes the ICC as a function of the upper limit of the radial magnetic matrix element, is plotted versus the radial distance r . The nuclear radius R_{nuc} , the K, L and the M shell radius are specified in the lower part of the figure. Note that the scale is logarithmic.

Using relation (2) and the fact that for highly converted γ -transitions $\Delta\lambda/\lambda = \Delta\alpha/\alpha$ we obtain

$$\frac{1}{\alpha} \sum_i \alpha_i \frac{\Delta|\psi_i(0)|^2}{|\psi_i(0)|^2} = \frac{\Delta\lambda}{\lambda} \quad (3)$$

From Table 2 one sees that a change in the decay rate can be achieved through $5s_{1/2}$ (O_1 shell) and $5p_{3/2}$ (O_3 shell) valence electrons. The contribution from the $5p_{1/2}$ (O_2 shell) electrons can be neglected. From a chemical point of view all $5s$ and $5p$ valence states are involved in the stannic compound SnO_2 and only the $5p$ in the stannous SnO . The measurement of the ratio $\Delta\lambda/\lambda$ which is given by

$$\frac{\Delta\lambda}{\lambda} = \frac{\lambda(\text{SnO}_2) - \lambda(\text{SnO})}{\lambda(\text{SnO})}$$

would yield the possibility of determining the difference of total electron density $\Delta|\psi(0)|^2$ between the two compounds. Since $|\Delta\psi_{5s}(0)|^2 \simeq \Delta|\psi(0)|^2$ where $\Delta|\psi(0)|^2$ is the change in total electron density (see Ref. 6) we obtain with relation (3)

$$\Delta|\psi(0)|^2 = |\psi_{5s}(0)|^2 \cdot \frac{\Delta\lambda}{\lambda} \cdot \frac{\alpha}{\alpha_{5s}} \quad (4)$$

where α denotes the total conversion coefficient and α_{5s} the ICC of the O_1 shell. The ICC α and α_{5s} can be calculated directly by the method outlined previously, while $|\psi_{5s}(0)|^2$ must be taken from a relativistic Hartree-Fock calculation. The greatest uncertainty comes from the evaluation of the $5s$ electron density at the nucleus where an error of 10% is certainly to be accepted. Assuming Sn to be in ionic configurations in SnO and SnO_2 , i.e. $5s^25p^0$ and $5s^05p^0$ respectively, we expect the magnitude of the decay rate to be $\Delta\lambda/\lambda = 7 \cdot 10^{-4}$ which is qualitatively in agreement with the magnitude of the effect measured for the M4 transition in ^{125}Te [13]. The total change in electron density at the nucleus obtained this way then allows the determination of the change in nuclear charge radius $\delta R/R$ in the Mössbauer isomer shift. Various measurements of $\Delta\lambda/\lambda$ for different chemical tin compounds should thus yield also some accurate information about the electronic structure of the bonds.

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