Influence of Chemical Environment on M1 Internal Conversion Rates and their Connection with the Mössbauer Isomer Shift

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Abstract. By measuring the change in decay rate $\Delta\lambda/\lambda$ for M1 transitions and the corresponding Mössbauer isomer shift it is possible to extract the change of nuclear charge radius $\delta R/R$. Numerical results are given for ^{119}Sn (23.87 KeV), ^{57}Fe (14.4 KeV) and ^{195}Pt (99 KeV).

1. Assumption

It has been shown several times [1], [2], [3] that the internal conversion coefficient α for M1 transitions is approximately proportional to the electron density $|\Psi_i(0)|^2$ at the nucleus, i. e.

$$\alpha_i = \text{const} \, |\Psi_i(0)|^2 \tag{1}$$

where the index i denotes the different shells involved in internal conversion. This statement (1) is not a fundamental law, but an approximate relation holding to an accuracy of about 1% which is adequate for our present purposes.

2. M1 Internal Conversion Transitions

(a) *The calculation of internal conversion coefficients for outer shells*

In the following we shall consider the 14.4 KeV transition of ^{57}Fe and the 1.64 KeV transition of ^{193}Pt. In Table 1 the Ml internal conversion coefficients (ICC) are collected for various subshells of iron together with the corresponding electron densities. We note that for the K, L_I, M_I and N_I shells the α/ϱ ratio is practically a constant, as is expected according to Sliv and Band [4]. We note also that the total conversion coefficient $\alpha_T = 8.57$ agrees very well with the new experimental value $\alpha_T = 8.26 \pm 0.19$

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published recently by Freund and McGeorge [5]. All ICC values except those for the N_I shell were computed directly with the program MONICA [6] by using a relativistic Hartree-Fock-Slater (HFS) potential for the calculations [7]. According to Dragoun et al. [8] the computation of the N_I ICC is achieved by means of the relation

$$\alpha = \alpha_0 \cdot f_{scr} f_n . \tag{2}$$

Here, α_0 denotes the unscreened point nucleus ICC, f_{scr} is the screening correction due to atomic electrons and f_n the correction accounting for the finite nuclear size. Chu and Perlman [9] have recently shown that the simple relation (2) gives reliable results for outer shells by comparing measured and theoretical conversion coefficients.

Table 1

The calculated M1 and E2 ICC values are collected for the different shells of ^{57}Fe. The transition energy is 14.4 KeV. The two last entries give the electron density ϱ of the corresponding shell and the ratio α/ϱ of the ICC α to the density ϱ, respectively.

ICC for the 14.4 KeV transition in Fe^{56}.

Shell	α_{M1}	α_{E2}	$\varrho(3\,d^6\,4\,s^2)$	α_{M1}/ϱ
K_I	7.675	0.3945 $(+\,3)$	0.6673 $(+\,4)$	1.15 $(-\,3)$
L_I	0.7223	0.300 $(+\,2)$	0.6292 $(+\,3)$	1.149 $(-\,3)$
L_{II}	0.438 $(-\,1)$	0.554 $(+\,2)$	0.3400 $(+\,1)$	–
L_{III}	0.1774 $(-\,1)$	0.996 $(+\,2)$	0.1549 $(-\,3)$	–
M_I	0.1064	0.439 $(+\,1)$	0.8659 $(+\,2)$	1.152 $(-\,3)$
M_{II}	0.6107 $(-\,2)$	0.7657 $(+\,1)$	0.4387 (0)	–
M_{III}	0.2447 $(-\,2)$	0.1375 $(+\,2)$	0.2001 $(-\,4)$	–
M_{IV}	–	–	0.4078 $(-\,8)$	–
M_V	–	–	0.7350 $(-\,13)$	–
N_I	0.0049	–	4.321	1.14 $(-\,3)$

A direct calculation of M1 and E2 ICC values has also been performed for the 1.64 KeV transition in ^{193}Pt. The results are given in Table 2. The ICC values denoted by an asterisk are calculated with relation (2), where α_0 had to be extrapolated below the Coulomb threshold. This table also shows that α/ϱ is practically constant for the N_I, O_I and P_I subshells. We note that the α/ϱ ratio is almost constant (within a few percents) also for all other shells characterized by the same Dirac quantum number κ, i.e. $(\alpha/\varrho)_K = $ const.

We should like to point out that we have some doubts on previous experimental work done on the 1.64 KeV ^{193}Pt transition. Firstly, the M1–E2 mixing ratio δ^2 deduced from the N_I/N_{II} subshell intensity is found to be 0.0014%, whereas Marelius [10] found a value of 0.01%. The reason for this discrepancy may be the use of extrapolated ICC values in Ref. [10]. Secondly, the experimental N_I/O_I ratio of 1.5 $\pm$ 0.5 cannot be obtained with our directly calculated conversion coefficients. The E2–M1 mixing ratio deduced from the N_I/N_{II} ratio is then low enough to justify the neglect of E2 admixture. A comparison of M1 γ-transition with the Weisskopf estimate yields a moderate retardation factor of 26.

Table 2

The M1 and E2 ICC for the 1.64 KeV transition of ^{193}Pt are collected. The nomenclature is the same as in Table 1. The values marked with an asterisk are calculated with the help of Ref. [8] and include the screening correction.

ICC for the 1.64 KeV transition in ^{193}Pt.

Shell	α_{M1}	α_{E2}	$\varrho(5\,d^9\,6\,s^2)$	α_{M1}/ϱ
N_I	0.996 (+ 4)	0.315 (+ 6)	0.6814 (+ 4)	1.46 (0)
N_{II}	0.1045 (+ 4)	0.559 (+ 8)	0.5183 (+ 3)	–
N_{III}	0.1225 (+ 3)	0.763 (+ 8)	0.1910 (− 1)	–
N_{IV}	0.261 (+ 2)	0,122 (+ 7)	0.1526 (− 3)	–
N_V	0.141 (+ 2)	0.113 (+ 7)	0.4312 (− 8)	–
N_{VI}	–	–	0.3229 (− 11)	–
N_{VII}	–	–	0.5618 (− 16)	–
O_I	0.1936 (+ 4)	0.655 (5)	0.13135 (+ 4)	1.47
O_{II}	0.178 (+ 3)	0.919 (+ 7)	0.8634 (+ 2)	–
O_{III}	0.198 (+ 2)	0.123 (+ 8)	0.3015 (− 2)	–
O_{IV}	0.196 (1)*	0.812 (5)*	0.1252 (− 4)	–
O_V	0.98 (0)*	0.825 (5)*	0.3358 (− 9)	–
P_I	0.144 (+ 3)*	–	0.1027 (+ 3)	1.42

(b) *Connection of the Mössbauer isomer shift (IS) with the change in the decay rate $\Delta\lambda/\lambda$.*

The Mössbauer IS connects the difference of the electron density $\Delta\,|\,\Psi(0)\,|^2$ between two chemical states evaluated at the nucleus with the relative change in nuclear charge radius $\delta R/R$:

$$\Delta\delta = \frac{4\,\pi\,e^2\,Z\,R^2\,c}{5\,E_\gamma}\cdot\Delta\,|\,\Psi(0)\,|^2\cdot\frac{\delta R}{R} = c_M\cdot\Delta\,|\,\Psi(0)\,|^2\cdot\frac{\delta R}{R}\,,\qquad(3)$$

where Z is the nuclear charge number, R the nuclear radius and E_γ the transition energy. From equation (1) we obtain the following simple formula for the change of the decay rate λ:

$$\frac{\Delta\lambda}{\lambda} = \frac{\Delta[\lambda_\gamma(1+\alpha)]}{\lambda_\gamma(1+\alpha)} = \frac{\Delta\,\Sigma\,|\,\Psi_i(0)\,|^2}{\Sigma\,|\,\Psi_i(0)\,|^2}\cdot\frac{\alpha}{(1+\alpha)}\,,\qquad(4)$$

where λ_γ is the γ-transition probability of the bare nucleus. In the sum, the index i runs over all electron shells for which the energy conservation allows internal conversion. In some low energy transitions, inner shells are not involved in internal conversion. Hartree-Fock calculations show that the change in the electron density of the inner not converted shells is negligible compared to the changes of the outer shells which are converted. Therefore, we have in practice

$$\Delta\,|\,\Psi(0)\,|^2 = \sum_i \Delta\,|\,\Psi_i(0)\,|^2\,.\qquad(5)$$

A combination of equations (3), (4) and (5) thus gives the following connection between $\Delta\lambda/\lambda$ and $\Delta\delta$:

$$\frac{\Delta\lambda}{\lambda} = \frac{\Delta\delta}{c_M \frac{\delta R}{R} \sum |\Psi_i(0)|^2} \cdot \frac{\alpha}{(1+\alpha)}.$$ (6)

Because the electron density $\sum |\Psi_i(0)|^2$ can easily be calculated with a Hartree-Fock-Slater program, we see that a simultaneous measurement of $\Delta\lambda/\lambda$ and $\Delta\delta$ yields the change of nuclear radius $\delta R/R$. This formula also shows the expected result that $\Delta\lambda/\lambda$ will be large provided only the outer shells are converted.

3. Results and Discussion

The 23.87 KeV transition of ^{119}Sn is an example where both Mössbauer isomer shift and internal conversion measurements exist. Boquet et al. [11] measured the N/O ratio for internal conversion in two different chemical environments. Their final result is

$$\frac{\alpha_{N_I}}{\alpha_O} = 13.6 \pm 0.6 \quad \text{for SnO}_2$$

and

$$\frac{\alpha_{N_I}}{\alpha_{O_I}} = 9.3 \pm 0.3 \quad \text{for white Sn.}$$

The corresponding isomer shift measured by Lees and Flinn [12] was found to be $\delta = 2.48 \pm 0.03$ mm/s. According to chapter 1 the relation $\alpha_{N_I}/\alpha_{O_I} = \varrho_{N_I}/\varrho_{O_I}$ with ϱ_{N_I} and ϱ_{O_I} as the 4 s and 5 s electron densities at the nucleus is a good approximation. It seems worth to note that from the calculated ICC values $\alpha_{N_I} = 0.1455$ and $\alpha_{O_I} = 0.00165$ together with the corresponding HFS electron densities we obtain the ratios $(\alpha/\varrho)_{N_I} = 0.40 \cdot 10^{-3}$ and $(\alpha/\varrho)_{O_I} = 0.44 \cdot 10^{-3}$. We should also mention that the total ICC calculated with the program MONICA [7] yields $\alpha_T = 5.08$ which is in very good agreement with the experimental value of Kostroun and Crasemann [13] who obtained $\alpha_T = 5.13 \pm 0.15$. The total change $\Delta |\Psi(0)|^2$ of the electron density which is measured in Mössbauer isomer shift experiments is practically given by the change of the 5 s electron density, while the 4 s electron density is almost unaffected by different chemical environments. These two statements have been found valid by performing relativistic HFS calculations for various free-ion configurations $5 s^n 5 p^m$ ($n = 0, 1, 2$ and $m = 0, 1, 2$). The results of these calculations are given in Figure 1. Under the above mentioned assumptions we obtain finally for the total change in electron density between white Sn and SnO$_2$

$$\Delta |\Psi(0)|^2 = \varrho_{O_I} (\text{white Sn}) - \varrho_{O_I} (\text{SnO}_2) = \varrho_{N_I}\left(\frac{1}{9.3} - \frac{1}{13.6}\right).$$

Together with the Hartree-Fock results for the 4 s electron density, $\varrho_{N_I} = 734$ a.u., (1 atomic unit is equal to inverse cube of the Bohr radius, 1 a.u. $= 0.675 \cdot 10^{25}$ cm^{-3}),
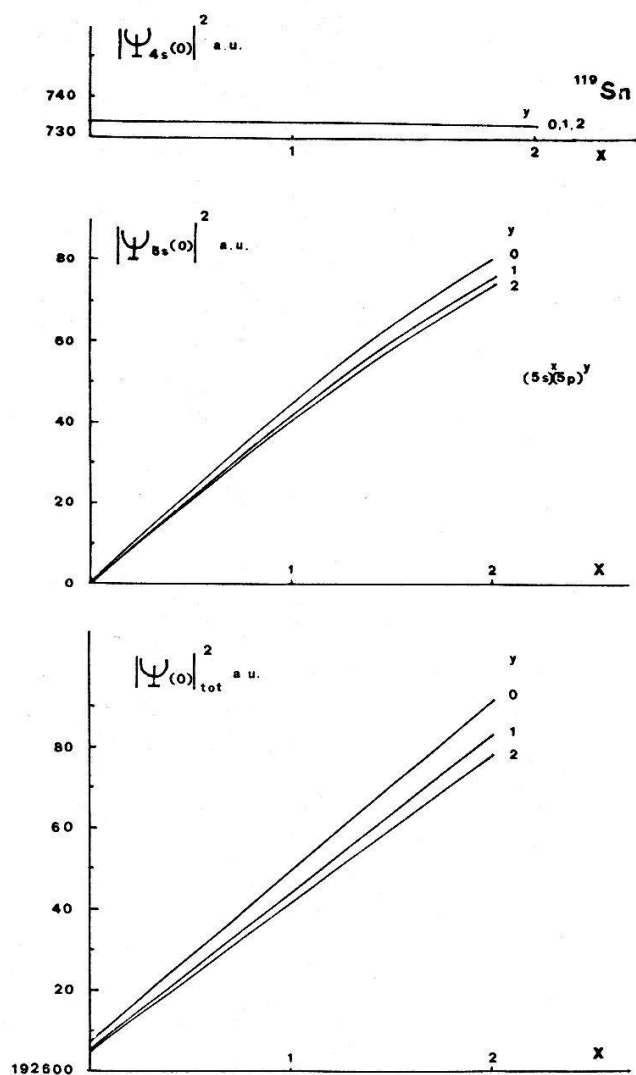
Figure 1
The total electron density and partial density of the N_I (4 s) and O_I (5 s) shell at the nucleus is shown as a function of the occupation number of the O_I shell for various occupations of the O_{II} (5 $p_{1/2}$) shell.

we obtain the following numerical value $\Delta \mid \Psi(0) \mid^2 = 23.5$ a. u. From this result and from the corresponding isomer shift $= 2.48$ mm/s we obtain the relative change of the nuclear radius $\delta R/R = 2.05 \cdot 10^{-4}$. This result differs only slightly from the value $\delta R/R = 1.84 \cdot 10^{-4}$ obtained by Emery and Perlman [14] by a somewhat different approach.

The next example to be considered is the 14.4 KeV transition of ^{57}Fe. According to equation (6) it is possible to extract the unknown electron factor $\Delta \mid \Psi(0) \mid^2$ from a measurement of $\Delta\lambda/\lambda$ and to decide between the rather different values of $\delta R/R$ given by Walker [15] and Šimánek [16]. In order to obtain some reliable information on the expected magnitude of the effect, we made relativistic HFS calculations for various configurations of free ^{57}Fe ions. The computed wave functions were used to evaluate the valence and core electron densities at the nucleus for all interesting states of ionicity. Starting from the free atom configuration $(3 d)^6 (4 s)^2$, we assumed the configuration $(3 d)^y (4 s)^x$ to be relevant for the description of the various chemical iron compounds. Since there is some interest in knowing more about the nature of chemical bonds, we introduced the parameter $I = 8 - y - x$ which describes the ionicity of iron in different chemical compounds.

There is a strong screening influence of the 3 d valence electrons on the valence s-states which is shown in Figure 2. In any compound involving d-electrons, a large

change in the density $\mid \Psi_{4s}(0) \mid^2$ (up to a factor 2.5) can be achieved. Comparing e.g. metallic iron to different ^{57}Fe compounds it is simple to see that for ^{57}Fe complex salts $\Delta \mid \Psi_{4s}(0) \mid^2 = [\mid \Psi_{4s}(0) \mid^2$ (Fe metal) $- \mid \Psi_{4s}(0) \mid^2$ (Fe complexes)] < 0, yielding a negative isomer shift, whereas $\Delta \mid \Psi_{4s}(0) \mid^2$ is positive for FeII and FeIII salts.
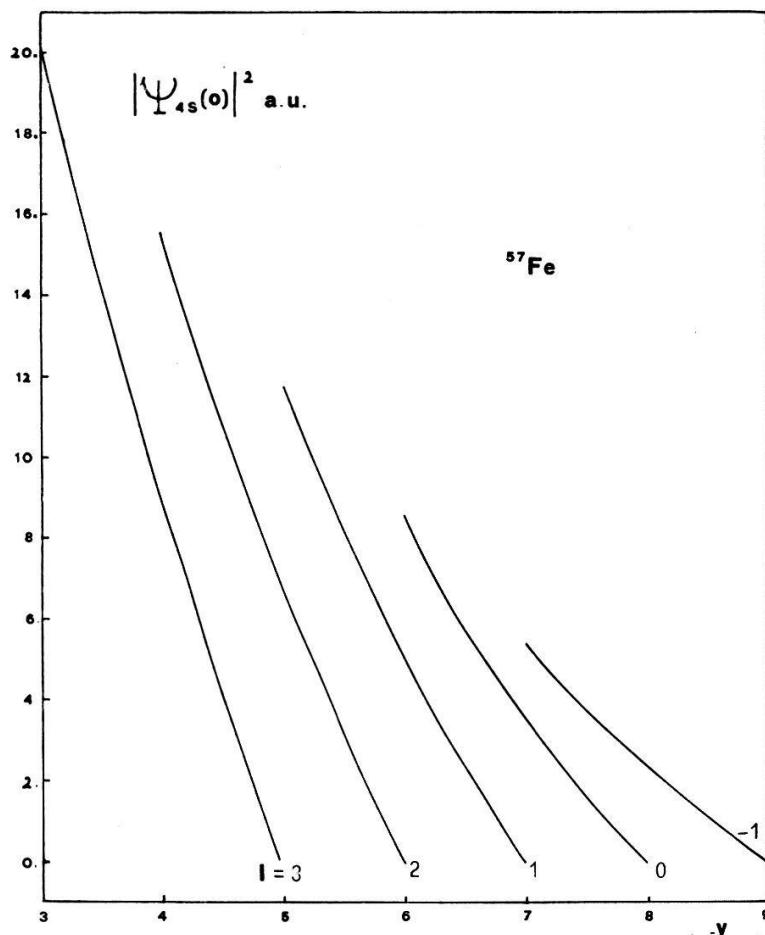

Figure 2
The 4 s electron density is shown as a function of the 3 d occupation number. Each line coresponds to a configuration with constant ionicity.

Since the 3 d valence electrons are strongly involved in chemical bonding, they screen not only the valence electrons but also to a certain amount the core electrons. This is illustrated in Figure 3, where this change is plotted as a function of the 3 d occupation numbers. The relative change of the decay rate $\Delta\lambda/\lambda = [\lambda(Fe\ metal) - \lambda(Fe\ compound)]/\lambda$ depends therefore not only on the 4 s occupation but also on the ionicity. In Figure 4 $\Delta\lambda/\lambda$ is shown for various values of x as a function of the change in ionicity. As expected $\Delta\lambda/\lambda$ is mainly positive for $x \simeq 0$, while $\Delta\lambda/\lambda$ is negative for $x \simeq 1$ (Fe complexes). The detailed participation of core and valence electrons to the change in the decay rate is shown explicitly in Figure 5 for $x = 0.125$. We note that here the core contribution is rather important. Since the relative change of the decay rate $\Delta\lambda/\lambda$ is simply related to the measured Mössbauer IS (see equation (6)) we show in Figure 6 $\Delta\lambda/\lambda$ for various $\delta R/R$ values as a function of the measured isomer shifts δ. It is evident from this picture that even a rather crude experimental value of $\Delta\lambda/\lambda$ could decide between the different proposed values of $\delta R/R$.

Recently, Pleiter and Kolk [17] obtained a new value for the change in the nuclear charge radius of Fe. Their value $\delta R/R = - (0.45 \pm 0.15) \cdot 10^{-3}$ derived from a measurement of the ratio $\alpha_{N_I}/\alpha_{M_I}$ is in agreement with the value obtained by Šimánek
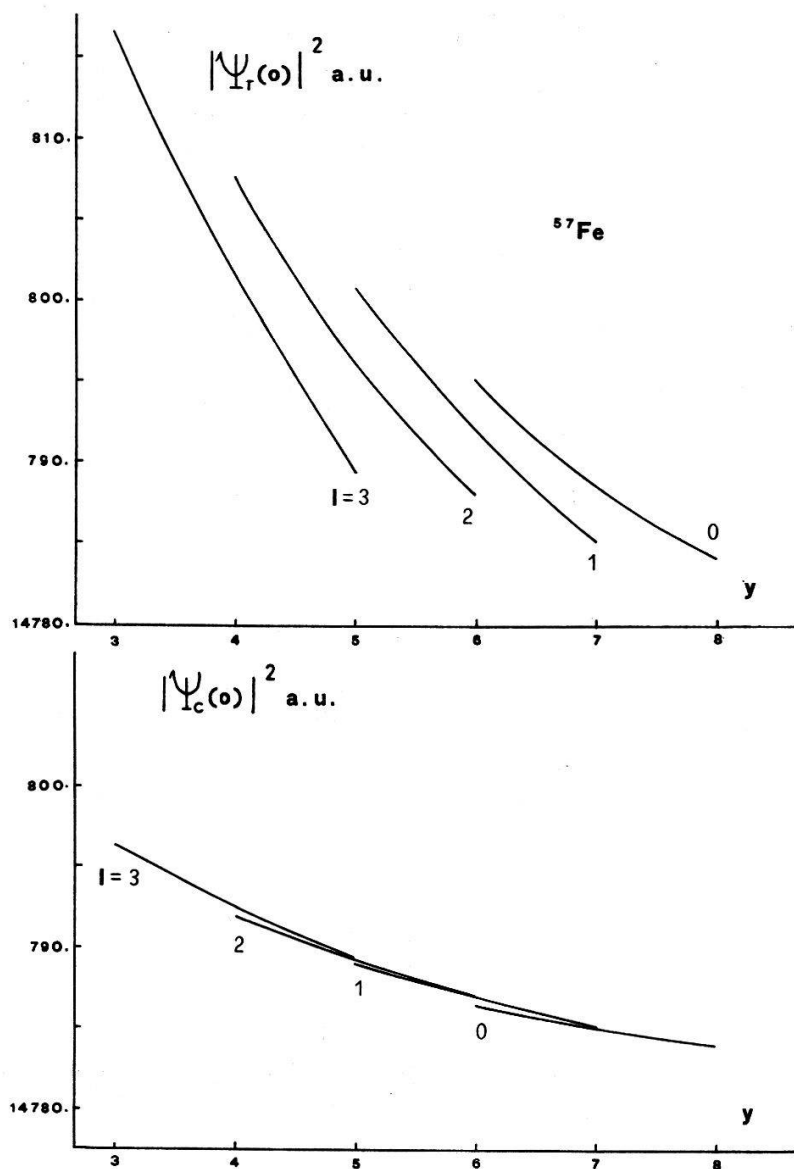
Figure 3

The upper part shows the total electron density at the nucleus versus the number of 3 d electrons. Again, the different lines correspond to configurations with constant ionicity. The lower part shows the change in core electron density versus 3 d occupation number.

by means of high pressure IS measurements. In addition to the assumption of chapter 1 they explicitly assumed that $\varrho_{3s}(0)$ is constant for all investigated chemical environments and that the change in $\varrho_{4s}(0)$ is equal to the total change in electron density at the nucleus. Our HFS values for $\varrho_{3s}(0)$ show a variation from 179.3 a.u. for the $d^4 s^2$ configuration to 169.8 a.u. for the $d^8 s^0$ configuration. However, these configurations are rather extreme and it is believed that the actual change is somewhat smaller and of the order of 2 a.u. The second assumption $\Delta\varrho_{4s}(0) = \Delta\varrho_{tot}(0)$ seems also to be violated because of large core contributions due to the screening of the 3 d electrons. The error introduced by this second assumption cannot be estimated without using a special model of the electron configurations involved which is, of course, rather ambiguous. Taking again the Fe configurations $(3\ d)^8\ (4\ s)^0$ and $(3\ d)^4\ (4\ s)^2$ the change of the 4 s electron density $\Delta\varrho_{4s} = 9.5$ a.u. is accompanied by a change of the core electron
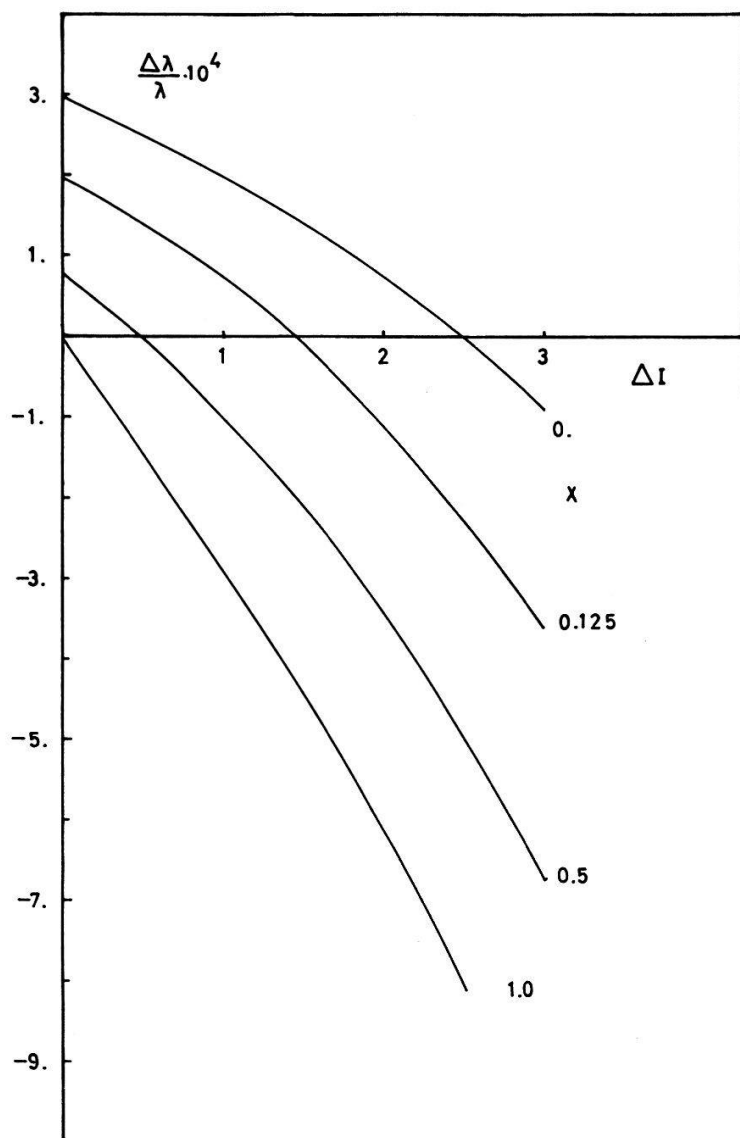
Figure 4
The relative change in decay rate
$\Delta\lambda/\lambda$ is shown for various constant
$4\,s$ occupation values x as function
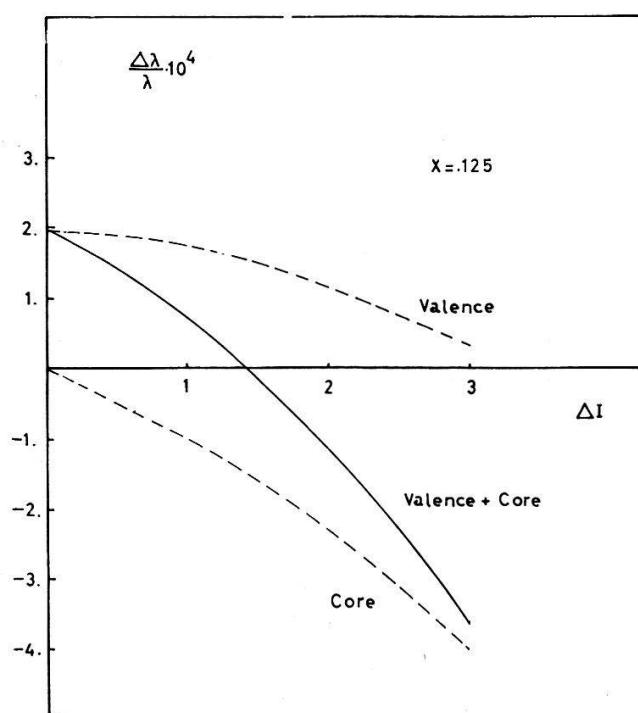of a change of the ionicity ΔI.

Figure 5
For the special value $x = 0.125$
of the 4 s occupation the contri-
bution of the valence states and of
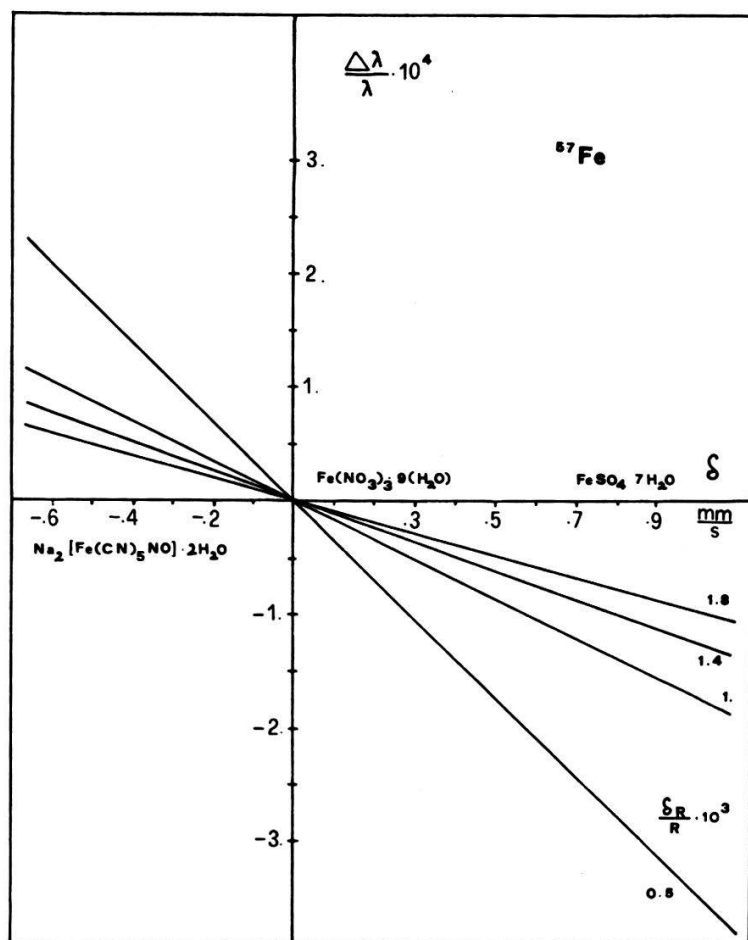the core is exhibited explicitly.

Figure 6
The relative change in decay rate $\Delta\lambda/\lambda$ is shown versus the isomer shift δ for various changes of nuclear radius $\delta R/R$.

density of $\Delta\varrho_{core} = 2.5$ a.u. (see Figures 2 and 3). Similar corrections should also be applied for other Fe configurations.

From the relation (1) Pleiter and Kolk [17] derived that the conduction electron density at the nucleus is threetimes higher in metallic iron than in the neutral atom. This result must be doubted because the theoretical evaluation of the electron density at the Fe nucleus is quite complicated for the different Pt(^{57}Fe) alloys used in the experiment. Usually, it is assumed that metallic iron has a $(3\,d)^7\ (4\,s)^1$ configuration with a $(3\,d)^7$ core and one conduction electron. Batterman [18] determines the number of $(3\,d)$ electrons to be $n_d = 6.3 \pm 1$, so that it is as well possible to assume the configuration $(3\,d)^6\ (4\,s)^2$. For the Pt (^{57}Fe) alloy the situation is somewhat more obscure. According to Pauling [19], Fe and Pt belong both to the socalled 'buffer' elements. Consequently, it is not possible to obtain any reliable information about the configuration of Fe in Pt (^{57}Fe) alloy by means of Pauling's simple picture. However, adapting Raynor's point of view of a possible transfer of one or two electrons to the transition metal iron [20], it seems possible to interpret the 4 s electron density determined by means of α_{NI}/α_{MI} measurements. The transfer of less than one electron to the transition metal may also be possible as was pointed out by Brack and Taylor [20]. For the sake of simplicity we shall assume here a simple picture of a Fe$^-$ ion in platinium. Pleiter and Kolk determined the ratio ξ of s-conduction electron density to free atom electron density $\xi = |\ \Psi_{4s}^C(0)\ |^2\ /\ |\ \Psi_{4s}^A(0)\ |^2$ to be $\xi = 3$ which should be compared with the theoretical value $\xi = 1.5$ by Ingalls [21]. We may, however, turn the argument around and use Ingalls' ξ value and the HFS calculations which yield a total 4 s

density of $|\Psi_{4s}(0)|^2 = 10.8$ a. u. for the above mentioned iron configuration $(3\ d)^7$ $(4\ s)^2$. From Figure 2 one obtains for the Fe^- ion $(3\ d)^7\ (4\ s)^2$ a value $|\Psi_{4s}(0)|^2$ (Fe^-) $= 6.6$ a. u. The change in the 4 s electron density would then be $\Delta\ |\Psi_{4s}(0)|^2 = 4.2$ a. u. which is in agreement with the result $\Delta\ |\Psi_{4s}(0)|^2 = 4.75$ a. u. obtained from the experimental data of Pleiter and Kolk using our calculated electron densities.

For the evaluation of the relative change $\delta R/R$ it is also necessary to account for changes in density of inner shells. For our above discussed example the change in the 3 s electron density becomes $\Delta\ |\Psi_{3s}(0)|^2 = 1.9$ a. u. This would finally lead to a somewhat smaller change in the nuclear charge radius, i. e. $\delta R/R = -0.32 \cdot 10^{-3}$.

The conclusion that can be drawn from the above discussion is that the only relevant method of determining $\delta R/R$ consists in measuring the relative change of the decay rate $\Delta\lambda/\lambda$. This method yields especially the important quantity $\Delta\ |\Psi(0)|^2$ without any assumption based on a special model for the different chemical bonds.

Finally, we want to discuss the 99 KeV M1 transition of the Mössbauer isotope ^{195}Pt where IS measurements have been carried out recently by Rüegg [22]. The change in decay rate $\Delta\lambda/\lambda$ measured by Marelius [10] for the 1.64 KeV M1 transition of ^{193}Pt would give the possibility of determining the change in electron density $\Delta\ |\Psi(0)|^2$ at the Pt nucleus. Marelius' experiment yields $\lambda(Pt) - \lambda(PtCl_{x \geqslant 1})$ $= (4 \pm 2) \cdot 10^{-2}$. From HFS calculations for the total electron density one thus extracts easily $\Delta\ |\Psi(0)|^2 = 703$ a. u. Some of the results of the computed densities are collected in Table 3. While the density of the N_1 shell remains constant by changing the degree of ionicity, the 6 s valence electron density is strongly affected by the changing number of 5 d electrons and should thus, apart from a slight correction due to the O_1 shell, account for the observed effect. Assuming e. g. the simple picture of a Pt^{4+} ion configuration $5\ d^6\ 6\ s^0$ in the $PtCl_{x \geqslant 1}$ compound one obtains $\Delta\ |\Psi(0)|^2$ $= 48$ a. u. and with a Pt^{2+} $(5\ d^8\ 6\ s^0)$ ion $\Delta\ |\Psi(0)|^2 = 92$ a. u. The conclusion is that the experimentally determined difference of electron density seems to be unreasonably high. The value $\Delta\ |\Psi(0)|^2 = 703$ a. u., as measured by Marelius [10], cannot be obtained by Hartree-Fock calculations even if one assumes drastically different free ion configurations.

Finally, we want to estimate the electron difference $\Delta\ |\Psi(0)|^2$ in the case of the IS measurements made by Rüegg [22]. We use the model of electron transfer to the transition metal because Pt doted iron was used for the IS experiments. With $\Delta\ |\Psi(0)|^2 = |\Psi(0)|^2(Fe[Pt]) - |\Psi(0)|^2(Pt) = 30$ a. u. we obtain the value $\delta R/R = 2.3 \times 10^{-4}$ which is in the order of magnitude of the most calculated $\delta R/R$

Table 3

The electron density $|\Psi_{ns}(0)|^2$ of the N_I, O_I and P_I shells is given for the 1.64 KeV transition of ^{193}Pt.

$^{78}Pt\ |\Psi_{ns}(0)|^2$ of converted shells.

Configuration		N_I	O_I	P_I
5 d^9	6 s^1	6814.2	1313.5	102.8
d^8	s^1	6814.0	1318.7	127.9
d^7	s^1	6814.0	1326.5	151.9
d^6	s^1	6814.2	1336.4	173.5
d^8	s^0	6814.2	1318.2	0
d^6	s^0	6814.4	1338.0	0

values for the various Mössbauer isotopes. With the IS $\delta = 2.8$ mm/s for the 130 KeV transition of ^{195}Pt one would obtain $(\delta R/R)_{130 \text{ KeV}} = 4.5 \times 10^{-4}$.

To conclude, we give an approximate simple formula for the evaluation of the relative change of the decay rate

$$\frac{\Delta \lambda}{\lambda} = \frac{2.92 \cdot 10^3 (\Delta \delta)_{\text{mm/s}} \, E_\gamma(\text{KeV}) \, \alpha \, n^3}{\left(\dfrac{\delta R}{R}\right) Z^2 \, A^{2/3} \, S(Z) \, (1 + \alpha) \, 2 \, c_T (Z - \sigma_i)^2} \, . \tag{7}$$

Here, the IS $\Delta \delta$ has to be inserted in mm/s and the transition energy E_γ in KeV. Z is the nuclear charge number, A the mass number, α the total ICC, $\delta R/R$ the change in nuclear charge radius in units of 10^{-4}, n the principal quantum number of the first shell converted and σ_i the screening numbers for the corresponding shell given by Slater [23]. The factor $S(Z)$ accounts for relativistic effects (tabulated by Shirley [24]) and C_T is a factor for obtaining approximately the total density of the converted shells. The factor C_T is given as a function of Z for the K, L_I and M_I shells in Figure 7. Since HFS calculations are easily available [25] the relation (7) reduces simply to

$$\frac{\Delta \lambda}{\lambda} = \frac{0.93 \cdot 10^3 \, (\Delta \delta)_{\text{mm/s}} \, E_\gamma(\text{KeV}) \, \alpha}{\left(\dfrac{\delta R}{R}\right) Z \, A^{2/3} \, (1 + \alpha) \, | \, \Psi_T(0) \, |^2} \, , \tag{8}$$

where $| \, \Psi_T(0) \, |^2$ is the total relativistic electron density evaluated at the nucleus for the converted shells, In table 4, standard $\Delta \lambda/\lambda$ values calculated with relation (7) are given for different Mössbauer isotopes for $\Delta \delta = 1$ mm/s and $\delta R/R = 1 \cdot 10^{-4}$. These values should give an idea of the order of magnitude to be expected for the relative change of the decay rate.
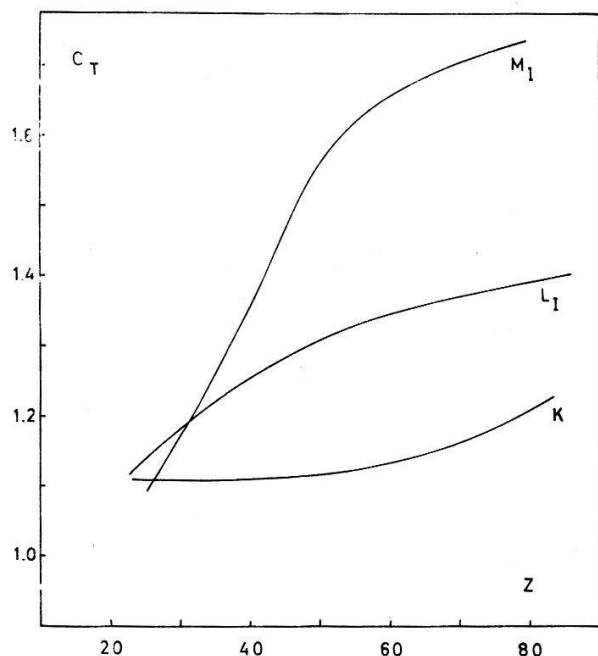

Figure 7
The constant C_T extracted from Hartree-Fock calculations (see equation 7) is shown as a function of the nuclear charge number Z for the K, L_I and M_I shells.

Acknowledgement

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Table 4

The relative change of the decay rate $\Delta\lambda/\lambda$ calculated by relation (7), assuming $\delta R/R = 10^{-4}$ and $\delta = 1$ mm/s, is tabulated for some Mössbauer isotopes. The corresponding transition energy is E_γ (KeV). The total ICC is denoted by α. The last entry gives the lowest shell that can be converted.

Element	Z	E_γ (KeV)	$(\Delta\lambda/\lambda_{St} \times 10^4$	α	Converted shell
^{101}Ru	44	127	1.84	0.16	K
^{197}Au	79	77.3	0.64	3.7	L
^{119}Sn	50	23.87	6.0	5.08	L
^{121}Sb	51	37.2	1.08	10.6	K
^{151}Eu	63	21.6	1.43	29	L
^{169}Tm	69	8.41	1.2	325	M
^{145}Nd	60	72.5	0.62	4	K
^{83}Kr	36	9.3	22.1	10	L
^{137}La	57	10	1.42	140	L
^{237}Np	93	33.2	0.7	240	L

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