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PHYSICAL REVIEW C VOLUME 7, NUMBER 6 JUNE 1973

How Good Are the Theoretical Internal-Conversion Coefficients?*

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(Received 12 February 1973)

We have accurately measured the total-conversion coefficient for the 156.0-keV, $M4$ transition in ^{117}Sn as $\alpha_T = 46.40 \pm 0.25$. The Hager and Seltzer theoretical value is 47.8. A comparison between experimental and theoretical α_K and α_T values for 15 $E3$ and $M4$ transitions shows that the theoretical values are *systematically* 2–3% higher.

I. INTRODUCTION

It is generally believed that the theory of internal conversion is in broad agreement with experiment. There exist several tabulations of calculated internal-conversion coefficients. Basically, these calculations require a knowledge of the bound-state and continuum electron wave functions. In the tables of Hager and Seltzer,[1] the wave functions are relativistic Hartree-Fock-Slater solutions to the Dirac equation.

To estimate the uncertainties in any calculation is difficult. It is difficult enough to assess the influence of physically reasonable variations in the assumptions that go into any calculation (what is the correct screening function or nuclear charge distribution? – is a central potential or nonrelativistic treatment adequate? – etc.), not to speak of several "one-percent effects" that are altogether omitted (higher-order terms in the fine-structure constant, static nuclear multipole moments, penetration effects, chemical shifts, electron correlations, etc.). What, in particular, is the combined effect of all these effects? To answer these questions indirectly, we have resorted to the philosophy, "The test of all knowledge is experiment," expressed succinctly by Feynman, Leighton, and Sands.[2]

II. EXPERIMENTAL PROCEDURE AND RESULTS

To test the theory to say 1%, we of course need a conversion-coefficient (α) measurement that we can trust to the same accuracy. When an isomer deexcites via two transitions in cascade, it is possible to deduce the α_T ratio by measuring photon intensities only[3]—a measurement inherently capable of better than 1% accuracy. Consider the case of 14-day ^{117}Sn^m decay shown in Fig. 1. The 156.0-keV (γ_1) transition is known to be $M4$,[4] and the 158.6-keV (γ_2) transition $M1 + <0.05\%$ $E2$.[5] We can write

$$I_{\gamma_1}(1+\alpha_{1T}) = I_{\gamma_2}(1+\alpha_{2T}), \quad \alpha_T = I_{ce}/I_\gamma .$$

If the photon-intensity ratio $I_{\gamma_2}/I_{\gamma_1}$ is measured and if α_{2T} is small (say <0.2) and set equal to the experimental or theoretical value, α_{1T} can be readily obtained. The crucial point is that any percentage uncertainty in α_{2T} is reduced by a factor $\alpha_{2T}/(1+\alpha_{2T})$ in the determination of α_{1T}.

The 156.0–158.6-keV γ-ray doublet, well resolved with a 1.0-cm^3 Ge(Li) x-ray detector, is shown in Fig. 1. The ^{117}Sn^m sources were produced by the ^{118}Sn$(n, 2n)$ reaction with 14-MeV neutrons. 13 spectra were recorded with two different detectors, two analyzers, and two irradiated ^{118}Sn foils (0.51 and 1.52 mm thick).

Bearing in mind that we are interested only in the relative photopeak areas, an iterative self-consistent analysis of each spectrum was carried out with the same shape functions (a smoothed-step function to represent the background continuum + a Gaussian term + a tailing term) employed to represent both peaks. Apart from statistical and curve-fitting uncertainties (typically 0.2–0.3%

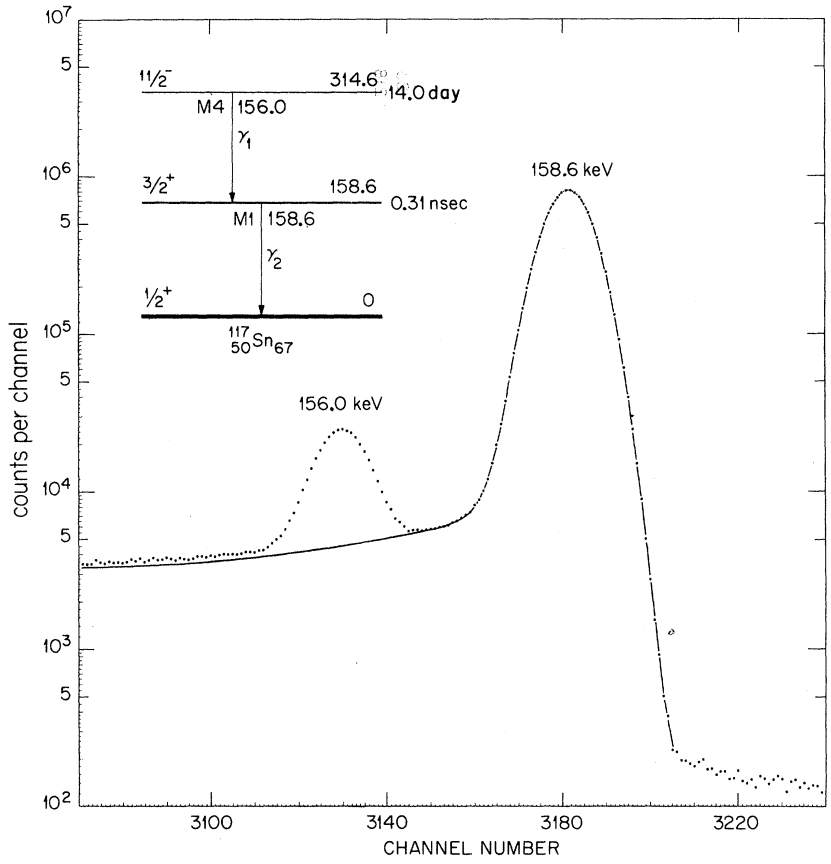

FIG. 1. Selected portion of γ-ray spectrum from $^{117}Sn^m$ obtained with a Ge(Li) x-ray detector. The solid line shows the line shape obtained with the 159.0-keV γ ray from $^{123}Te^m$. The inset shows the 14-day $^{117}Sn^m$ decay scheme (Refs. 4 and 5).

for γ_1), uncertainties in the detector efficiencies (γ_1 is detected with 3.7 ± 0.3% greater efficiency by detector 2), and source self-absorption (γ_1 is attenuated 0.33 ± 0.03% more in the 0.51-mm source), all of which have been taken into account, the factor limiting the accuracy was our ability to determine the shape of the spectrum beneath the 156-keV peak. The good resolution and our detailed studies of detector responses to monoenergetic γ rays helped in this respect. We found, for instance, that in order to obtain correctly the single line shape employing the 159.0-keV transition from $^{123}Te^m$, it was imperative to sandwich the $^{123}Te^m$ source (liquid evaporated to dryness on 0.026-mm-thick Mylar film) between tin foils such that the effective masses of the $^{123}Te^m$ and $^{117}Sn^m$ sources were the same. The measured intensity ratios are given in Table I. We obtained $I(158.6\gamma)/I(156.0\gamma) = 40.88 \pm 0.12$ where the uncertainty represents the external error.

TABLE I. Measured $I(158.6\gamma)/I(156.0\gamma)$ values.

Detector 1 Analyzer 1 1.52-mm foil	Detector 2 Analyzer 2 0.51-mm foil
	40.39 ± 0.20
	40.65 ± 0.23
	40.88 ± 0.21
40.43 ± 0.21	40.91 ± 0.23
40.58 ± 0.25	41.01 ± 0.21
40.67 ± 0.20	41.03 ± 0.21
41.16 ± 0.21	41.09 ± 0.20
	41.11 ± 0.22
	41.53 ± 0.20
40.72 ± 0.17 [a]	40.96 ± 0.11 [a]

40.88 ± 0.12 [a] Adopted value

[a] Weighted average. The uncertainties are external errors which were ≈30% larger than the internal errors.

For the total-conversion coefficient α_{2T} for the 158.6-keV transition, we employed the measured[4] α_K and L/K values and the theoretical[1,6] MNO/K value. With $\alpha_{2T} = 0.1594 \pm 0.0050$ and our measured intensity ratio, we deduced[7] $\alpha_T(156.0\gamma) = 46.40$

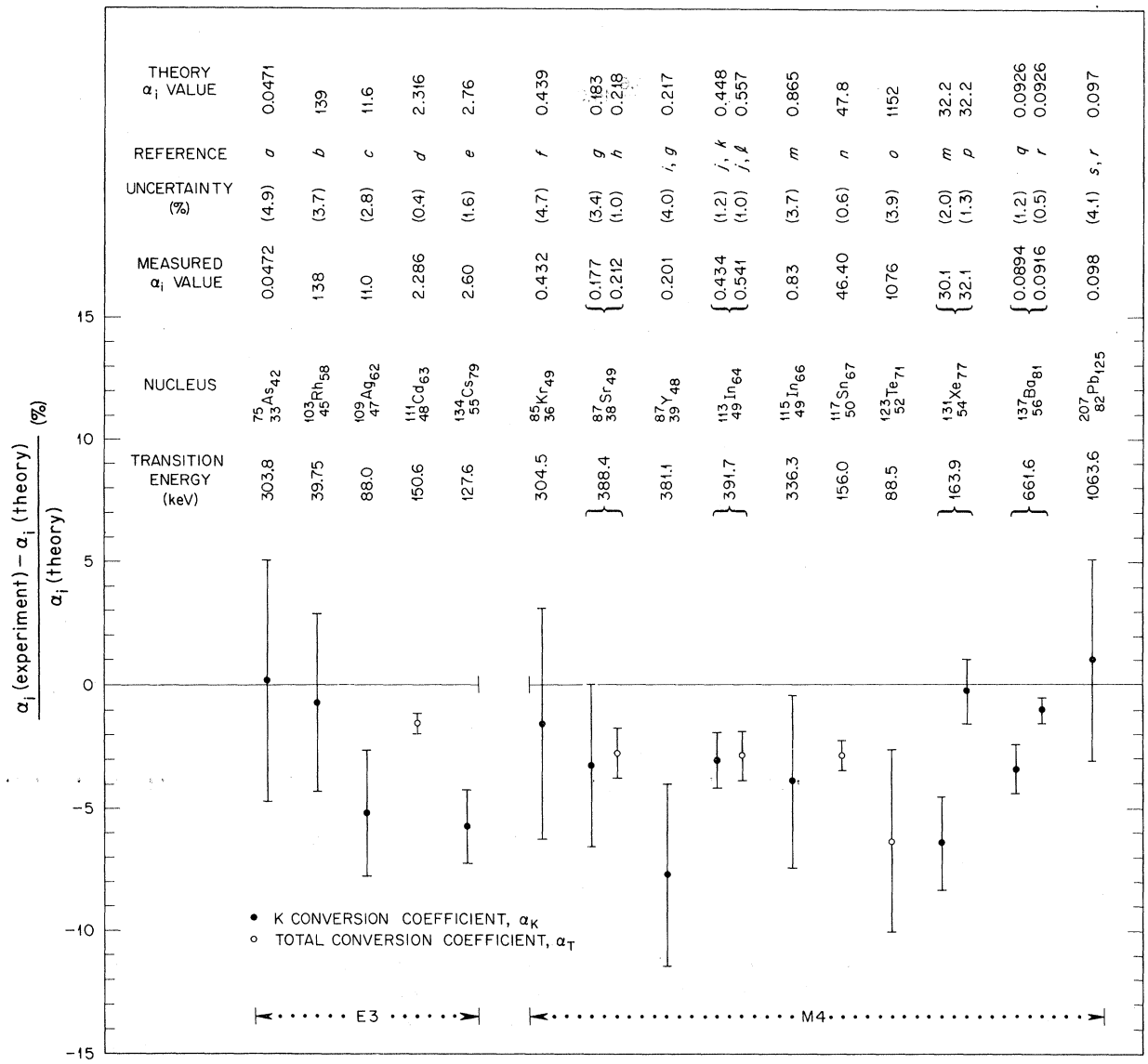

FIG. 2. Comparison between precisely measured (quoted uncertainty <5%) $E3$ and $M4$ conversion coefficients and theoretical values. The theoretical α_K, α_L, and α_M values were obtained from Hager and Seltzer (Ref. 1) and the $(N+O+\ldots)/M$ values from Dragoun, Plajner, and Schmutzler (Ref. 6). The experimental values were obtained from the following references: (a) Th. Paradellis and S. Hontzeas, Can. J. Phys. 48, 2254 (1970); (b) E. B. Nieschmidt and D. A. Pearson, Idaho Nuclear Corporation Report No. IN-1317, 1970 (unpublished), p. 122; (c) H. Leutz, K. Schneckenberger, and H. Wenninger, Nucl. Phys. 63, 263 (1965); (d) D. C. Lu, Phys. Rev. 119, 286 (1960); (e) B. Keisch and E. A. C. Yates, J. Inorg. Nucl. Chem. 17, 183 (1961); (f) F. K. Wohn, W. L. Talbert, Jr., and J. K. Halbig, Nucl. Phys. A152, 561 (1970); (g) J. Legrand, F. Lagoutine, and J. P. Brethon, Int. J. Appl. Radiat. Isot. 21, 139 (1970); (h) I. W. Goodier, F. H. Hughes, and M. J. Woods, Int. J. Appl. Radiat. Isot. 19, 795 (1970); (i) M. Sakai, T. Yamazaki, and J. M. Hollander, University of California, Lawrence Radiation Laboratory Report No. UCRL-16580, 1966, (unpublished), p. 92; (j) H. H. Hansen *et al.*, Int. J. Appl. Radiat. Isot. 22, 1 (1971); (k) S. K. Sen and I. O. Durosinmi-Etti, Phys. Lett. 18, 144 (1965); (l) I. W. Goodier, F. H. Hughes, and M. J. Woods, Int. J. Appl. Radiat. Isot. 21, 678 (1970); (m) S. C. Misra, J. S. Merrit, and J. G. V. Taylor, quoted by J. S. Geiger, in *Proceedings of the International Conference on Internal Conversion Processes, Nashville* (1965), edited by J. H. Hamilton (Academic, New York, 1966), p. 379; (n) present results; (o) Ref. 3; (p) K. Knauf, H. Sommer, and H. Klewe-Nebenius, Z. Phys. 197, 101 (1966); (q) J. S. Merritt and J. G. V. Taylor, Anal. Chem. 37, 351 (1965); (r) H. H. Hansen *et al.*, Z. Phys. 218, 25 (1969); and (s) G. Hedin and A. Backlin, Ark. Fys. 38, 593 (1969).

TABLE II. Theoretical conversion coefficients with different bound-state electron wave functions.

Nucleus	Transition (keV)	Type	Quantity	Theoretical value: Hager and Seltzer (Ref. 1)	Theoretical value: ORNL (Refs. 10 and 12)	Theoretical value: Herman and Skillman (Refs. 10 and 11)
^{111}Cd	150.6	$E3$	α_T	2.316	2.318	2.336
^{134}Cs	127.6	$E3$	α_K	2.76	2.72	2.73
^{87}Sr	388.4	$M4$	α_T	0.215	0.216	0.216
^{113}In	391.7	$M4$	α_K	0.448	0.448	0.450
^{117}Sn	156.0	$M4$	α_T	47.8	47.7	48.2
^{131}Xe	163.9	$M4$	α_K	32.2	31.8	32.1
^{137}Ba	661.6	$M4$	α_K	0.0926	0.0923	0.0927

± 0.25. The theoretical value[1,6] is 47.8. The discrepancy from the theoretical value is $-2.9 \pm 0.6\%$. The measured L/K and MNO/K values[4] for the 156.0γ are in good agreement with theory.

III. DISCUSSION

This discrepancy prompted us to examine the literature for all $E3$ and $M4$ conversion coefficients experimentally determined to better than 5% accuracy. Penetration effects should be insignificant (certainly <1% change in α) for these transitions which are at the same time believed to be essentially of pure multipole order from half-life considerations and, in most cases, from subshell ratios. The results of our survey are shown in Fig. 2. It is truly impressive that experimental conversion coefficients as small as 0.0472 and as large as 1076 are predicted by theory. The agreement between theory and experiment could be considered satisfactory were it not for the fact that the theoretical values are systematically 2–3% larger than measured values. The number of precisely known cases is insufficient to decide whether or not the discrepancy is a function of Z or of the energy of the transition. Finally, we note that neither the $E2$ conversion coefficients[8] nor the L-subshell ratios[9] apparently exhibit any such systematic discrepancy.

In an attempt to understand possible reasons for the discrepancy, we have calculated α_K and α_T values with screening functions different from those employed by Hager and Seltzer.[1] For these calculations, we employed the Pauli[10] computer program which accepts different bound-state electron wave functions as inputs. We employed the nonrelativistic Herman and Skillman[11] and the relativistic Oak Ridge National Laboratory (ORNL) wave functions[12] which have been generated by self-consistent Hartree-Fock-Slater-type calculations with the full[13] Slater exchange term. For those cases where the conversion coefficients are experimentally measured to better than 2% accuracy, the results of our calculations[14] are shown in Table II. Our values agree well with the Hager and Seltzer values. Therefore, we do not have a simple explanation for the observed discrepancy.

In conclusion, there are over 20 favorable cases including several $M4$-$M1$ cascades where conversion coefficients can be measured with good accuracies with our approach. If the Hager and Seltzer $E3$ and $M4$ conversion coefficients are lowered by 2–3%, they are in excellent agreement with the existing measurements. It is quite common to find estimated uncertainties in the 5–10% range quoted in the literature for these theoretical conversion coefficients. In fact, they may be more accurate than generally believed.

ACKNOWLEDGMENTS

One of us (S.R.) would like to thank Dr. M. J. Martin and Dr. M. Schmorak for helpful discussions.

*Research sponsored by the U.S. Atomic Energy Commission under contract with the Union Carbide Corporation and with the University of California.

†Summer research participant from Edinboro State College, Edinboro, Pa., supported by Oak Ridge Associated Universities.

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PHYSICAL REVIEW C VOLUME 7, NUMBER 6 JUNE 1973

Decay Energies of Gaseous Fission Products and their Daughters for $A = 88$ to 93

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(Received 10 January 1973)

A systematic study of β-decay energies has been made for mass-separated activities of Kr gaseous fission products and their daughters at the TRISTAN on-line separator facility at the Ames Laboratory research reactor. A well-type plastic scintillator was used in coincidence with a Ge(Li) γ detector to determine β-group end-point energies and deduce Q values. The following β-decay energies have been determined: ^{88}Kr, 2.93 ± 0.03 MeV; ^{88}Rb, 5.30 ± 0.06 MeV; ^{89}Kr, 4.93 ± 0.06 MeV; ^{90}Kr, 4.35 ± 0.05 MeV; ^{90}Rb, 6.32 ± 0.07 MeV; ^{91}Kr, 6.12 ± 0.07 MeV; ^{91}Rb, 5.68 ± 0.04 MeV; ^{92}Kr, 5.97 ± 0.08 MeV; ^{92}Rb, 7.58 ± 0.15 MeV; ^{92}Sr, 1.93 ± 0.03 MeV; ^{93}Kr, 8.3 ± 0.5 MeV; and ^{93}Rb, 7.23 ± 0.10 MeV. The decay energies are compared with previous measurements, systematics predictions, and two currently accepted mass relations. The energies are used to predict the β-decay energies for 13 additional nuclei by means of systematics.

I. INTRODUCTION

In recent years the study of nuclear masses has been of interest for element-genesis theories in astrophysics and for predictions of decay properties of nuclei far from the line of β stability. This work is concerned with the latter interest and attempts to extend our knowledge of the changes in the nuclear mass surface, as determined from β-decay Q values, for several nuclei far from the line of β stability. The area of particular interest in this work is the neutron-rich region around the mass $A = 90$.

The β-decay energies of short-lived nuclei have been predicted through mass relations that have parameters determined by using mass values for nuclei near the line of stability. Stimulated by an investigation of the astrophysical r process (rapid neutron-capture process), Seeger[1] modified the von Weizsacker liquid-drop model[2] by inclusion of shell-model effects and pairing terms, and created one of the more accurate models currently being used. Seeger used this mass formula to calculate the solar-system isotopic abundances of certain neutron-rich stable isotopes that resulted from the decay of extremely neutron-rich nuclides (20 to 40 units from the line of β stability) formed in conjectured astrophysical environments.

Another highly regarded approach to the prediction of decay energies is that developed by Garvey *et al.*[3] This mass relation is based on the single-particle model of the nucleus and utilizes symmetries implicit in isospin formalism. Relationships between nuclidic masses that are independent of the variation of mass with atomic number and charge are used to formulate a simple mass relation, which is then fitted to known data.

Though there are several other widely used mass formulas, those by Seeger and Garvey *et al.* are considered here to be the most acceptable since they have rather small deviations from experimentally determined masses. Furthermore, they are unique among the available formulas in their accuracy far from stability for neutron-rich nuclei since their predictions for the occurrence of delayed neutron precursors are in agreement with experimental observations.[4,5] These mass formulas have not, however, been subjected to a systematic test using mass differences experimentally determined for nuclei far from stability. This