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HIGH-ENERGY K-CONVERSION COEFFICIENTS FOR ^{114}Cd and ^{150}Sm

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Abstract: High-energy K-conversion coefficients are calculated using relativistic Hartree-Fock-Slater wave functions for ^{114}Cd and ^{150}Sm, multipolarities E1, E2 and M1 and for gamma-ray transition energies from 1 MeV to 17 MeV (existing tabulations do not exceed 2.5 MeV). All the available data for the elements in this energy region are compared, and the serious disagreements are examined. It is concluded that the present results are correct, and that the present theory is valid in this energy domain.

1. Introduction

Conflicting experimental [1,3]) and theoretical [4,5]) results have been reported for high-energy K-shell internal conversion coefficients (ICC) for ^{114}Cd. In addition, there also appears to be a discrepancy between experiment [2]) and the theoretical results presented here for ^{150}Sm.

Smither *et al.* [1,2]) have investigated K-shell ICC for ^{114}Cd and ^{150}Sm, multipolarities E1 and M1 and transition energies from 1 to 9 MeV. In general their work indicates the likelihood that there is a marked difference between predictions from theory and experiment in this energy domain. They show that the experimental E1 and M1 ICC do not cross even at 9 MeV contrary to the *suggestion* from *extrapolation* of the theoretical low-energy values. However, the E1 and M1 ICC do approach each other as the energy is increased as is to be expected from the theoretical considerations of Carroll and O'Connell [6]).

In a recent brief communication [4]), we pointed out that our theoretical results for high-energy K-shell ICC for Cd disagreed seriously with the experimental results of Smither [1]). The approximate theoretical results of Church and Weneser [5]) are also in disagreement with Smither's results. In an attempt to resolve this discrepancy, Moragues *et al.* [3]) remeasured the ICC reported on by Smither. They found their results to be in good agreement with the estimates of Church and Weneser. In addition, our results seem to be in good agreement with the results of Moragues *et al.* as well as those of Church and Weneser as will be discussed below.

The purpose of this communication is (i) to present ICC values, calculated as accurately as possible within the framework of existing theory, for gamma-ray transition energies from 1–7 MeV and multipolarities E1, E2 and M1 for ^{114}Cd and ^{150}Sm; (ii) to compare the available results for ^{114}Cd and ^{150}Sm; (iii) to point out that linear extrapolation from lower-energy results may be quite misleading due to the fact that, in the high-energy domain, the ICC versus energy curve plotted on a log-log scale is *not* linear.

2. Model and calculation details

Our calculation of ICC is based on the use of relativistic Hartree-Fock-Slater wave functions † for both the bound and continuum state electrons. The effect of finite nuclear size are included and the no-penetration model of Rose is used [12]). The experimental electron binding energies tabulated by Bearden and Burr [8]) have been used to compute the energy of the continuum electron. We have used a ninth-order Adams-Moulton method to integrate the Dirac equation for both the bound and continuum wave functions. The radial integrals were evaluated by use of an 11th order closed-type Newton-Cotes formula ††. All calculations were performed on an IBM S/360 in extended precision, and the various parameters were adjusted such that an accuracy of 0.1 % or better was obtained. More complete details concerning the computation will be published elsewhere.

3. Comparison of results

Our results for ^{114}Cd are presented in fig. 1, while those for ^{150}Sm are given in fig. 2. We would like to emphasize that our low-energy results (up to 2.5 MeV) for both ^{114}Cd and ^{150}Sm are in excellent agreement both with the theoretical results of Sliv and Band [10]) and Hager and Seltzer [11]) and, for ^{114}Cd, with the experimental results [1,3]) – this augments our confidence in the correctness (within the framework of existing theory) of our high-energy values.

For ^{114}Cd, the following points are worthy of note:

(i) At 9 MeV, the M1/E1 ratio of the present work is 1.16, Smither obtains 1.7, while both Church and Weneser as well as Moragues *et al.* obtain approximately 1.2.

(ii) The present E2 and M1 theoretical values are in agreement with Church and Weneser and cross at about 3 MeV in contrast to the experimental values of Smither, which do not cross below 4 MeV.

(iii) Using the low-energy results for energies up to 2.5 MeV and extrapolating to higher energies leads to the erroneous conclusion that the E1 and M1 ICC values cross[1]) at 8 or 9 MeV (our theoretical results show that they do not cross even for energies as high as 17 MeV). Thus linear extrapolation is a dangerous procedure in this energy range, the reason being (as is clear from our graphs) that the ICC curves

† The improved version due to Kohn and Sham[7]) was used instead of the original Slater prescription.
†† See ref. [9]) for details concerning the accuracy.

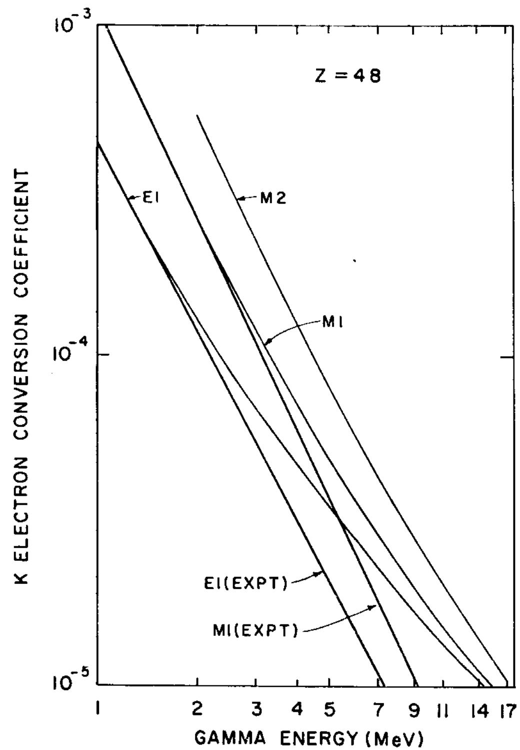

Fig. 1. Theoretical values for K-conversion coefficients for ^{114}Cd, gamma-ray transition energies 1–17 MeV and multipolarities E1, M1 and M2.

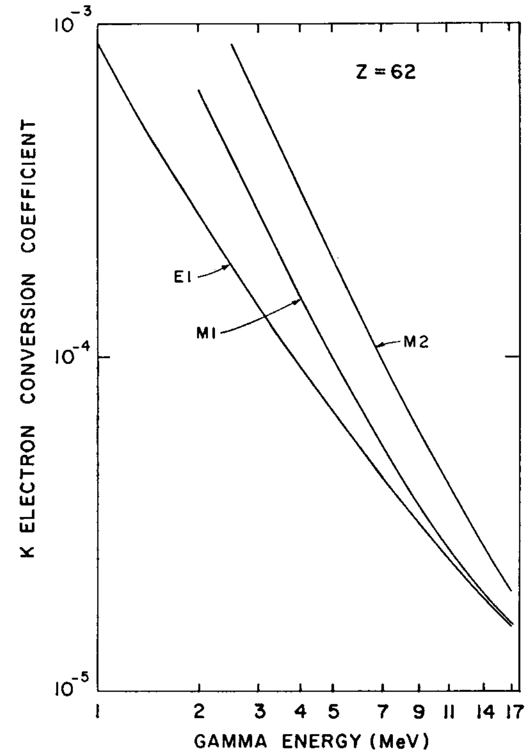

Fig. 2. Theoretical values for K-conversion coefficients for ^{160}Sm, gamma-ray transition energies 1–17 MeV and multipolarities E1, M1 and M2.

themselves are not linear. In other words, the theoretical ICC results *cannot* be represented by a curve of the form ω^{-a} (ω is the transition energy and a some positive constant) in contrast to the experimental data of Smither [1,2]. It should also be mentioned that the theoretical results of Sliv and Band and those of Hager and Seltzer (which do not go above 2.5 MeV) show clearly that the ICC curve is non-linear even in the neighborhood of 2.5 MeV. In fact, a linear least-squares fit to the last 4, 3 and 2 values from both tables results in straight lines of decreasing negative slope. This in fact is the type of curve one obtains for energies as high as 17 MeV (see figs. 1 and 2).

We note from fig. 2 that the ICC for ^{150}Sm exhibit the same general behavior as those for ^{114}Cd. Smither [2] obtains a M1/E1 ratio for ^{150}Sm at 7 MeV of 2, while the result of the present work is 1.24. Although this indicates serious disagreement for ^{150}Sm the lack of experimental data makes further comparison impossible.

4. Summary and conclusions

We have calculated ICC for ^{114}Cd and ^{150}Sm for the K-shell from 1 to 17 MeV. Our results for ^{114}Cd are in good agreement with an approximate calculation [5]) and with one experiment [3]) but in serious disagreement with another experiment [1,2]). (The experimental results of Smither *et al.*[2]) also disagree with our theoretical results for ^{150}Sm.) Because of the possibility of systematic error in the latter experiment [1,2]) and because of the good agreement between the other experimental results and both theoretical results, it is felt that the present theoretical results are correct, and that the theory is valid in this energy region.

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