Finally, although some of the low-energy transitions in Ag<sup>110</sup> observed by Kalinkin et al.<sup>21</sup> may be fitted between some levels seen in the present work, definitive

<sup>21</sup> L. F. Kalinkin, I. V. Estulin, and A. S. Melioranskii, Izv. Akad. Nauk. SSSR, Ser. Fiz. **28**, 227 (1964) [English transl.: Bull. Acad. Sci. USSR, Phys. Ser. **28**, 144 (1965).]

assignments of the low-energy transitions and their placement in the decay scheme must await studies with higher resolution.

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# Internal Conversion Coefficients with Relativistic Hartree-Fock Model for the Deformed Region

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Internal conversion coefficients for E2 transitions in six cases of the deformed nuclear region are presented. New calculations are based upon the relativistic Hartree-Fock potential in the Slater-exchange approximation with the inclusion of only the static finite-nuclear-size effects. For the  $2^+ \rightarrow 0^+$  transitions in Gd<sup>156</sup>, Dy<sup>160</sup>, Er<sup>166</sup>, Yb<sup>170</sup>, Os<sup>186</sup>, and Os<sup>188</sup>, a comparison of present calculations with the weighted mean of all experimental values for  $L_1/L_2$  indicates that the latter are larger by  $(6.2\pm3)\%$ ,  $(5.9\pm4.3)\%$ , (8.4 $\pm 4.4)\%$ ,  $(7.3\pm 3.9)\%$ ,  $(7.5\pm 6.4)\%$ , and  $(2.8\pm 5.6)\%$ , respectively. Corresponding results for  $L_1/L_3$  are  $(5.5\pm 1.8)\%$ ,  $(5.5\pm 2.5)\%$ ,  $(6.3\pm 2.3)\%$ ,  $(5.5\pm 2.4)\%$ ,  $(6.6\pm 4.6)\%$ , and  $(4.3\pm 4.1)\%$ . The uncertainties assigned to the percentage deviations correspond to an estimate of error at approximately 90% confidence level. Deviations of about the same magnitudes were pointed out by several experimentalists in a comparison with the calculations of Sliv and Band and of Rose. Numerical results are also given for the Ksubshell and M subshells in the above cases. It is suggested that M-subshell ratios be measured. A comparison of the experimental M-subshell ratios and K-conversion coefficient (within an accuracy of 2% or so) would provide additional information so that the origin of deviations in L-subshell ratios could be pinpointed. A possible explanation may be the effects of nuclear deformation on the  $L_1$  internal conversion coefficient.

## I. INTRODUCTION

HERE are two extensive calculations of internal conversion coefficients (ICC)-one by Rose and his collaborators<sup>1</sup> and the other by Sliv and Band.<sup>2</sup> These calculations have been used profitably for the last ten years or so; in fact, the contribution of these authors has been, and is, of utmost importance in the assignments of spins and parities in low-lying nuclear states. The common features of these two calculations are the inclusion of finite-nuclear-size effects (static effects) and the atomic screening considered by the statistical model of Thomas, Fermi, and Dirac (TFD). The main difference between the two models is that nuclear currents are taken to be of the form of delta functions at the nuclear surfaces in the model of Sliv and Band, in contrast to that of Rose, wherein no current is considered. It is to be noted that the contribution of the region inside a nucleus to the imaginary part of the conversion matrix element (and therefore to ICC) is different in the two calculations. In most cases of practical interest, such a contribution calculated by either procedures is expected to be much smaller than that from the region outside the nuclear radius. Consequently, one would expect that differences of a few percent in the results of Refs. 1 and 2 should occur. This in fact is true for most of the tabulated

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U. S. Atomic Energy Commission. ‡ Supported, in part, by the National Aeronautics and Space Administration under Grant No. NsG-381. <sup>1</sup> M. E. Rose, Internal Conversion Coefficients (North-Holland

<sup>&</sup>lt;sup>2</sup> L. A. Sliv and I. M. Band, *Coefficients of Internal Conversion of Gamma-Radiation* (USSR Academy of Sciences, Moscow-Leningrad, 1956), Part I and Part II. Also see L. A. Sliv and I. M. Band, in *Alpha-, Beta-, and Gamma-Ray Spectroscopy*, edited by K. Siegbahn (North-Holland Publishing Company, Amsterdam, 1965), Vol. 2.

cases. (However, certain discrepancies do appear in some cases for very low gamma energies; some of these differences are due to interpolation procedures, while others may be due to the computational techniques or errors.) Recently, several investigators<sup>3-9</sup> have reported their measurements on L-subshell ratios on several  $2^+ \rightarrow 0^+$  transitions in the rare-earth region. A summary of the experimental data reported at the International Conference on Internal Conversion Processes held in May 1965 is given by Hamilton.<sup>10</sup> A comparison of the experimental L-subshell ratios with the appropriate interpolated values using existing tables<sup>1,2</sup> indicated a discrepancy for the  $L_1/L_2$  ratio in particular. Two points need to be noted here. First, an energy interpolation relevant to the gamma energies was made which introduced some errors, at times as large as 5%. Secondly, the tables in Refs. 1 and 2 have already been prepared for most Z values by interpolation with respect to atomic number. Furthermore, the experimental data, which indicated a large (15-20%) deviation from the interpolated values, had relatively large assigned experimental errors. Recently, two groups, one at Brookhaven National Laboratory<sup>4</sup> (BNL) and the other at Chalk River Laboratory,3 have made independent and very accurate (within 2%) L-subshell measurements in several cases.

It is the purpose of this paper to present new calculations of ICC for these cases for the appropriate gamma energies. The present calculations are for K, L, and Msubshells. The relevance of M-shell ICC to the problem can be understood as follows. Measurements, as yet unavailable, of  $M_1/M_2$  and  $\sum_i M_i/L_3$  could be compared with the new calculations. In the unlikely event that dynamic effects<sup>11</sup> are significant in these transitions, the *M*-subshell ratios should still agree with the theory, in contrast to  $K/L_3$  ratio, which should be most influenced by these effects. This follows from the observation of Church and Weneser.<sup>11</sup>

In contrast to earlier calculations,<sup>1,2</sup> we use the relativistic potential calculated in the Hartree-Fock-

<sup>b</sup> S. E. Karlsson, I. Andersson, O. Nilsson, G. Malmston, and E. Iisonberg, in *Internal Conversion Processes*, edited by J. H. Hamilton (Academic Press Inc., New York, 1966), p. 513.
 <sup>b</sup> R. Stepic, M. Bogdanovic, and M. Mladjenovic, in *Internal Conversion Processes*, edited by J. H. Hamilton (Academic Press Inc., New York, 1966), p. 507.
 <sup>7</sup> T. Novakov and J. M. Hollander (private communication to U. H. Hamilton).

J. H. Hamilton).

<sup>8</sup> W. H. Brantley, S. C. Pancholi, and J. H. Hamilton, in Internal Conversion Processes, edited by J. H. Hamilton (Academic Press Inc., New York, 1966), p. 535. ° C. J. Herrlander and R. L. Graham, Nucl. Phys. 58, 544 (1964).

 (1964).
 <sup>10</sup> J. H. Hamilton, Phys. Letters 20, 32 (1966).
 <sup>11</sup> E. Church and J. Weneser, Phys. Rev. 104, 1382 (1956);
 Ann. Rev. Nucl. Sci. 10, 193 (1960); T. A. Green and M. E. Rose,
 Phys. Rev. 110, 105 (1958); M. E. Voikhansky, M. A. Listengarten, and A. P. Feresin, in *Internal Conversion Processes*, edited by J. H. Hamilton (Academic Press Inc., New York, 1966), p. 581.

Slater (H-F-S) approximation. Using this theoretical model, but with nonrelativistic Hartree-Fock-Slater potential, the author<sup>12</sup> has recently reported ICC calculations for the M4 transition in tellurium. These calculations<sup>12</sup> agree fairly well for all subshells (including M subshells) with the experimental data of Chu et al.13 The relevant procedure is described in detail elsewhere.14

The calculations reported in this paper are an improvement over those in Refs. 1 and 2 because (1) the relativistic Hartree-Fock-Slater treatment represents a better description of an atom than the T-F-D model (reflected in the excellent agreement of the eigenvalues with the experimental electron binding energies), (2) a choice of a fine mesh size in the numerical integration was made possible by larger computer memories available now, and (3) the calculations were done for the appropriate gamma energies (no interpolation uncertainties). The essential points of the present calculation are summarized in the next section. Section III contains the relevant numerical results, followed by a discussion and the conclusions.

#### **II. METHOD OF CALCULATIONS**

The notation in this paper is as follows. The gamma energy is represented by k (mc<sup>2</sup> units) and the nuclear radius is equal to  $1.2A^{1/3}$  F. The fine-structure constant is denoted by  $\alpha (= 1/137.037)$ . The integer values of  $\kappa$ specify the total angular momentum  $(= |\kappa| - \frac{1}{2})$  and the orbital angular momentum  $\{= |\kappa| - \frac{1}{2} + \kappa/(2|\kappa|)\}.$ The calculations were performed by using the surfacecurrent model of Sliv and Band.<sup>2</sup> The internal conversion coefficients were calculated by using the bound-state functions and the appropriate continuum functions. The essential points of these calculations for radial functions are described next.

## A. Self-Consistent Relativistic Hartree-Fock-Slater Wave Functions

Several investigators have previously reported the results of their calculations for the relativistic selfconsistent wave functions. The first such calculation was by Williams<sup>15</sup> for Cu<sup>+1</sup>, followed by Mayers,<sup>16</sup> and Cohen<sup>17</sup>. The exchange contribution was neglected in these works.<sup>15–17</sup> More recently, Liberman, Waber, and Cromer<sup>18</sup> have reported extensive calculations including the exchange contribution in the Slater approximation. The static effects of a finite nucleus were completely

- Hamilton (Academic Fress Inc., New Fork, 2007, p. 119
  Phys. 82, 433 (1966).
  <sup>18</sup> Y. T. Chu, O. C. Kistner, A. C. Li, S. Monaro, and M. L.
  Perlman, Phys. Rev. 133, B1361 (1964).
  <sup>14</sup> C. P. Bhalla, Z. Physik 196, 26 (1966).
  <sup>15</sup> A. O. Williams, Phys. Rev. 58, 723 (1940).
  <sup>16</sup> D. F. Mayers, Proc. Roy. Soc. (London) A241, 93 (1957).
  <sup>17</sup> S. Cohen, Phys. Rev. 118, 489 (1960).
  <sup>18</sup> D. Liberman, J. T. Waber, and Don T. Cromer, Phys. Rev. 137 A27 (1965). 137, A27 (1965).

<sup>&</sup>lt;sup>8</sup> W. Gelletly, J. S. Geiger, and R. L. Graham, Bull. Am. Phys. Soc. 11, 352 (1966); this issue, Phys. Rev. 156, 1043 (1967). <sup>4</sup> P. Erman, G. T. Emery, and M. L. Perlman, Phys. Rev. 147, 579 (1997).

<sup>858 (1966)</sup> 

<sup>&</sup>lt;sup>5</sup> S. E. Karlsson, I. Andersson, O. Nilsson, G. Malmston, and

<sup>&</sup>lt;sup>12</sup> C. P. Bhalla, in Internal Conversion Processes, edited by J. H. Hamilton (Académic Press Inc., New York, 1966), p. 373; Nucl.

ignored in the previous work, probably because calculations were primarily to be used in atomic-physics problems.

In the present work,<sup>19,20</sup> finite-nuclear-size effects are included because of the importance of such effects on the small component. The contribution of the Breit interaction and other similar higher-order corrections is neglected in the present work, as was done in all the previous calculations.

The essential technique of the relativistic Hartree-Fock-Slater method is to obtain the radial functions from a central potential V(r) so that the potential computed using these radial functions is essentially the same as V(r) for all values of r. This necessarily involves an iterative procedure so that the self-consistent wave function can be obtained. In contrast to the nonrelativistic H-F-S method,<sup>21</sup> where a Schrödinger equation is used, the Dirac equation is used for the relativistic H-F-S method. The exchange contribution is approximated by the Slater's method, which assumes the validity of the plane-wave approximation in calculating the exchange integral.

We use relativistic units:  $\hbar = m = c = 1$ . For a centralfield potential, the wave function for the Dirac equation can be written as

$$\psi_{\kappa}^{\mu} = \begin{pmatrix} -if_{\kappa}\chi_{-\kappa}^{\mu} \\ g_{\kappa}\chi_{\kappa}^{\mu} \end{pmatrix},$$

where  $f_{\kappa}$  and  $g_{\kappa}$  are the radial functions and are real. The radial functions obey the first-order coupled differential equations (where F = rf and G = rg)

$$dF/dr = (\kappa/r)F - (W - 1 - V)G, \qquad (1a)$$

$$dG/dr = (W+1-V)F - (\kappa/r)G.$$
 (1b)

The total energy W is less than 1 for a bound state.  $\chi_{\kappa^{\mu}}$  is the spin-angular-momentum function. The static effects of finite nuclear size (for a uniformly charged sphere) are considered by taking

$$V(\mathbf{r}) = -\left(\alpha Z/2\rho\right) \left[3 - (\mathbf{r}/\rho)^2\right]$$

for  $r \leq \rho$ . The nuclear radius is denoted by  $\rho$ , and Z is the atomic number. In the first iteration, we take V(r)outside the nuclear radius to be equal to the nonrelativistic H-F-S potential<sup>21</sup>  $V_1(r)$ . The coupled differential equations were numerically integrated for all the orbitals in an atom by the Runge-Kutta method.

The standard procedure of matching F/G at a match point (usually near the classical shell radius) is described in detail by Rose.<sup>1</sup> Iterations were continued until

$$\chi(W) = \left| \frac{y_R - y_L}{y_L} \right| \le 10^{-6}.$$

<sup>19</sup> C. L. Tolliver, C. P. Bhalla, and W. R. Garrett, Bull. Am. Phys. Soc. 11, 512 (1966). <sup>20</sup> C. P. Bhalla (to be published). This paper contains extensive

TABLE 1. COMDANSON OF CHERRY CIPCHVALUES IOF THE INTYUDE	TABL	εI.	Com	parison	of	energy	eigenval	ues	for	Hg	in	rvdberg
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Shell	j	Present work <sup>b</sup> (finite nuclear size)	Present work°	Liberman et al. <sup>d</sup>	Cohen®	Expt. x-ray levels <sup>f</sup>
1.5	1/2	6126.32	6130.19	6130.18	6145.7	6108.3
2S	1/2	1089.73	1090.30	1090.31	1081.8	1091.2
2P	1/2	1047.74	1047.74	1047.75	1041.7	1044.4
	3/2	903.04	903.04	903.03	897.9	902.91
<b>3</b> S	1/2	260.01	260.14	260.14	255.7	261.8
3P	1/2	240.69	240.69	240.68	236.1	241.1
	3/2	208.51	208.51	208.50	204.7	209.3
3d	3/2	176.02	176.02	176.01	173.2	175.3
	5/2	169.09	169.08	169.07	166.4	168.7
4.S	1/2	57.91	57.94	57.94	55.86	59.3
4P	1/2	49.51	49.51	49.51	47.42	50.6
	3/2	41.69	41.69	41.68	39.81	43.1
4d	3/2	27.81	27.81	27.80	26.19	28.3
	5/2	26.33	26.33	26.32	24.78	26.8
4f	5/2	8.332	8.331	8.324	7.44	7.71
	7/2	8.008	8.007	7.999	7.13	7.20
5S	1/2	9.252	9.259	9.251	8.806	9.2
5P	1/2	6.429	6.429	6.421	5.997	6.8
	3/2	5.022	5.021	5.013	4.626	5.2
5d	3/2	1.175	1.174	1.167	0.858	1.0
	5/2	1.024	1.023	1.016	0.712	
6 <i>S</i>	1/2	0.7030	0.7034	0.6974	0.5665	0.7682

\* Note that the significant figures in the table are given only for the sake of comparison and they are not to be taken as representing the accuracy of the calculated eigenvalues. b Relativistic Hartree-Fock-Slater calculations with the inclusion of

<sup>b</sup> Relativistic Hartree-Fock-Slater calculations with the inclusion of finite-size effects.
 <sup>a</sup> Point-nucleus relativistic Hartree-Fock-Slater calculations.
 <sup>d</sup> Point-nucleus relativistic Hartree-Fock-Slater calculations of D. Liberman, J. T. Waber, and D. T. Cromer [Phys. Rev. 137, A27 (1965)].
 <sup>e</sup> Point-nucleus relativistic calculations (without the exchange contributions) of S. Cohen [Phys. Rev. 118, 489 (1960)].
 <sup>f</sup> S. Hagstrom, C. Nordling, and K. Siegbahn, in Alpha-, Beta-, and Gamma-Ray Spectroscopy, edited by K. Siegbahn (North-Holland Publishing Company, Amsterdam, 1965), Vol. 1, p. 854.

 $y_R$  and  $y_L$  are the respective values of F/G at this match point, when the integration was started from  $r = \infty$  and from  $r \approx 0$ . Several other precautions were taken to assure accuracy. For example, the term (W-1), which becomes extremely small for outer orbitals, was always calculated in double precision. Mesh sizes were so chosen that the calculated wave functions and the eigenvalues were insensitive to further reduction in mesh size. The identification of the various orbitals for a given n was made by a node count in F and G.

A potential  $V^{1}(\mathbf{r})$  was calculated by using the abovecalculated radial functions. In general,  $V_1(r)$  and  $V^1(r)$ are not the same. For the second iteration, a potential  $V_2(r) = \frac{1}{2} [V_1(r) + V^1(r)]$  was used and the radial functions were recalculated. This procedure was continued till the self-consistent wave functions were obtained.

In Table I we compare the eigenvalues for Hg calculated with finite-size effects included, and with the point-nucleus approximation with the calculations of Liberman et al. and Cohen. The last column contains the experimental electron binding energies.

For Z=68, 70, and 76, the calculated eigenvalues are compared in Table II with the experimental data. Note the excellent agreement.

## **B.** Continuum Wave Functions

The problems associated with the numerical integration of Eq. (1) for the appropriate potential experi-

ICC calculations and a more detailed treatment of the relativistic

Hartree-Fock-Slater Calculations. <sup>21</sup> F. Herman and S. Skillman, *Atomic Structure Calculations* (Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1963).

	Z = 0	58	Z =	70	Z =	76
Subshell	Experiment (keV)	Relativistic H-F-S (keV)	Experiment (keV)	Relativistic H-F-S (keV)	Experiment (keV)	Relativistic H-F-S (keV)
K	57.486	57.57	61.332	61.44	73.872	74.07
$L_1$	9.752	9.717	10.488	10.45	12.964	12.95
$L_2$	9.265	9.275	9.978	9.992	12.384	12.42
$L_{3}^{-}$	8.358	8.347	8.943	8.932	10.871	10.88
$M_1$	2,212	2.189	2.398	2.367	3.050	3.030
$M_2$	2.006	1.992	2.171	2.160	2,792	2.791
$M_3$	1.811	1.796	1.951	1.934	2.457	2.451
MA	1.455	1.455	1.578	1.577	2.031	2.044
$M_{5}$	1.410	1.412	1.528	1.527	1.960	1.970

TABLE II. Comparison of experimental electron binding energies<sup>a</sup> with the calculated eigenvalues<sup>b</sup> for Z = 68, 70, and 76.

<sup>a</sup> S. Hagstrom, C. Nordling, and K. Siegbahn, in *Alpha-*, *Beta-*, and Gamma-Ray Spectroscopy, edited by K. Siegbahn (North-Holland Publishing Company, Amsterdam, 1965), Vol. I, p. 854. <sup>b</sup> Present calculations for relativistic Hartree-Fock-Slater model with the inclusion of finite-nuclear-size effects.

enced by a conversion electron are different from the bound-state problems. Whereas the bound-state radial functions (and the eigenvalues) are not so sensitive to the choice of mesh size, the mesh size in the asymptotic region is very important for the continuum radial functions. This can be understood as follows. The ratio F/G can be calculated for  $r \approx 0$ ; one chooses one of the radial functions (say  $F_{\kappa}$ ) arbitrarily at such a point. The value of the second radial function  $(G_{\kappa})$  is then fixed by the above-mentioned ratio, which is independent of the normalization factor. In the asymptotic region, we have

$$F_{\kappa}(r) \sim -A(r) [(W-1)/\pi p]^{1/2} \sin(pr+\delta),$$
  

$$G_{\kappa}(r) \sim A(r) [(W+1)/\pi p]^{1/2} \cos(pr+\delta),$$

where A(r) approaches unity as r goes to  $\infty$ . The total electron energy W is taken to be equal to  $k+1-\epsilon_i$  (in  $mc^2$  units), where  $\epsilon_i$  is the *calculated* binding energy for a particular orbital specified by subscript i. In the calculations of Rose,  $\epsilon_i$  was taken to be the experimental binding energy, in contrast to the calculations of Sliv and Band,<sup>2</sup> where  $\epsilon_i$  is the calculated eigenvalue. The momentum of the conversion electron is denoted by p (mc units) and is equal to  $(W^2-1)^{1/2}$ . A(r) was calculated in the asymptotic region and is positive definite. It turns out that A(r) is a converging oscillating function (about unity) with a period dependent upon the momentum of the conversion electron (p).

The most crucial point in the numerical integration of the coupled differential equations is that A(r) should have at least ten points in one half cycle after reaching the asymptotic region. This corresponds to about 20 or more mesh points per cycle for the radial functions. Normalization factors tend to be in error unless the above conditions are satisfied. A large number of points (2900) were taken in the present calculation to minimize the errors arising from the mesh size. The computer program was first checked for a pure Coulomb field, where the solutions are known in closed form. It is expected that our calculated continuum wave functions for a screened field have an accuracy of better than a few tenths of 1%. We note that the uncertainties in the present calculations, as in the previous work,<sup>1,2</sup> can arise from the truncation errors, the inherent errors associated with the numerical integration of the Dirac equation, and the choice of the practical infinity for bound states. One cannot safely estimate the sum total of such uncertainties, but one may assign an upper limit on the errors of about 1% in the present calculations.

No comparison is made in this paper with the calculations of Hager and Seltzer,<sup>22</sup> who have used the nonrelativistic Hartree-Fock potential, because the relevant numerical results on their conversion coefficients are not available.

#### **III. NUMERICAL RESULTS**

All the new numerical results on internal conversion coefficients in this paper are based upon the surfacecurrent model of Sliv and Band.<sup>2</sup> Six even-even nuclei,<sup>23</sup> where the transitions are between  $2^+$  to  $0^+$  states, are considered: Gd<sup>156</sup>, Dy<sup>160</sup>, Er<sup>166</sup>, Yb<sup>170</sup>, Os<sup>186</sup>, and Os<sup>188</sup>. Internal conversion coefficients were calculated for the appropriate gamma energies, and the ratios of Lsubshell conversion coefficients are presented in Table III along with all the available experimental data. To facilitate a comparison of the new calculations with experiments weighted means for  $L_1/L_2$ ,  $L_1/L_3$ , and  $L_2/L_3$  were separately calculated in each case:

$$\bar{R} = (\sum w_i R_i) / \sum w_i$$
, where  $w_i = 1/\sigma_i^2$ .

 $R_i$  is one of the above experimental ratios.

An estimate of the error in the weighted mean of the experimental data was made by two methods:

(a) 
$$\sigma(\bar{R}) = (\sum w_i)^{-1/2}$$

and

(b) 
$$\sigma(\bar{R}) = [(n-1)^{-1} \sum w_i (\bar{R} - R_i)^2 / \sum w_i]^{1/2}.$$

 $<sup>^{22}</sup>$  R. Hager and E. Seltzer, Phys. Letters 18, 163 (1965).  $^{23}$  We do not consider here the 130-keV transition in Tm<sup>169</sup>, because this transition is not a pure E2 transitions. Furthermore, the inclusion of this case would have added little to the essential conclusions of this paper.

Nucleus (γ Energy in keV)	Reference	$10^{3} \times L_{1}/L_{2}$	$10^{3} \times L_{1}/L_{3}$	$10^{3} \times L_{2}/L_{3}$
Gd <sup>156</sup> (88.97)	Present calculations <sup>a</sup> Chalk River (Ref. 3) Percent difference between expt	$168.9 \\ 180\pm 5$	$160.6 \\ 170 \pm 3$	950.8 943±10
	and present calculations	$6.2 \pm 2.8$	$5.5 \pm 1.8$	$-(0.98 \pm 1.0)$
Dy <sup>160</sup> (86.79)	Present calculations BNL (Ref. 4)—Nobel Chalk River (Ref. 3) Uppsala (Ref. 5) Weighted mean <sup>b</sup> of all experiments (w) Percent difference of w from present calculations	$127.1 \\ 134 \pm 4 \\ 136 \pm 5 \\ 137 \pm 8 \\ 135.1 \pm 5.8 \\ 5.9 \pm 4.3$	$122.8 \\ 130\pm 2 \\ 129\pm 3 \\ 135\pm 8 \\ 12.9\pm 3.2 \\ 5.5\pm 2.5$	$\begin{array}{c} 966.7\\ 967{\pm}14\\ 949{\pm}10\\ 967{\pm}14\\ 958{\pm}14\\ 0.9{\pm}1.5 \end{array}$
Er <sup>166</sup> (80.57)	Present calculations Chalk River (Ref. 3) BNL (Ref. 4)—Nobel Belgrade (Ref. 6) Berkeley (Ref. 7) Weighted mean of all experiments (w) Percent difference of w from present calculations	$83.790.6\pm 391.0\pm 3104\pm 1193\pm 891.4\pm 4.08.4\pm 4.4$	$\begin{array}{c} 81.24\\ 87.2\pm2.0\\ 85.9\pm1.5\\ 102\pm11\\ 91\pm8\\ 86.7\pm2.0\\ 6.3\pm2.3\end{array}$	$971962 \pm 10944 \pm 14978 \pm 15970 \pm 10964 \pm 120.7 \pm 1.2$
Yb <sup>170</sup> (84.26)	Present calculations BNL (Ref. 4)—Nobel Chalk River (Ref. 3) Vanderbilt (Ref. 8) Belgrade (Ref. 6) Uppsala (Ref. 5) Weighted mean of all experiments (w) Percent difference of w from present calculations	$75.8 \\ 81.3 \pm 2.3 \\ 80.0 \pm 2.6 \\ 89 \pm 8 \\ 93 \pm 10 \\ 86 \pm 6 \\ 81.8 \pm 3.2 \\ 7.3 \pm 3.9$	$76.5 \\ 81.0 \pm 1.2 \\ 79.6 \pm 1.8 \\ 88 \pm 7 \\ 95 \pm 10 \\ 85 \pm 6 \\ 80.97 \pm 1.94 \\ 5.5 \pm 2.4$	$1009996\pm14994\pm101000\pm301020\pm20983\pm11994\pm121.5\pm1.2$
Os <sup>186</sup> (137.15)	Present calculations BNL (Ref. 4)—Nobel Berkeley (Ref. 7) Belgrade (Ref. 6) Weighted mean of all experiments (w) Percent difference of w from present calculations	$145.1 \\ 156\pm6 \\ 156\pm12 \\ 163\pm15 \\ 156.8\pm10 \\ 7.5\pm6.4$	$187.1 \\ 200 \pm 5 \\ 199 \pm 14 \\ 215 \pm 20 \\ 200.3 \pm 9.2 \\ 6.6 \pm 4.6$	$1290 \\ 1280 \pm 20 \\ 1280 \pm 17 \\ 1330 \pm 30 \\ 1288 \pm 24 \\ 0.2 \pm 1.9$
Os <sup>188</sup> (155.03)	Present calculations BNL (Ref. 4)—Nobel Belgrade (Ref. 6) Chalk River (Ref. 9) Weighted mean of all experiments (w) Present difference of w from present calculations	$189.6 \\ 193 \pm 7 \\ 210 \pm 20 \\ 195 \pm 11 \\ 195 \pm 11 \\ 2.8 \pm 5.6$	$256.4 266\pm 6 296\pm 30 269\pm 15 268\pm 11 4.3\pm 4.1$	$1353 \\ 1380 \pm 20 \\ 1370 \pm 30 \\ 1380 \pm 50 \\ 1377 \pm 31 \\ 1.7 \pm 2.25$

TABLE III.	Comparison of new	theoretical ICC	calculations wit	h experimental.	L-subshell ratios
	for some	e E2 transitions	in the rare-earth	1 region.	

<sup>a</sup> Present calculations are based upon a relativistic self-consistent Hartree-Fock potential in the Slater exchange approximation.

<sup>b</sup> Weighted mean and the estimate of errors were calculated as follows:  $\overline{R} = \sum_i w_i R_i / \sum w_i$ , where  $w_i = 1/\sigma_i^2$ . An estimate of  $\sigma(\overline{R})$  was made by two methods: (1)  $\sigma(\overline{R}) = (\sum w_i)^{-1/2}$  and (2)  $\sigma(\overline{R}) = [(n-1)^{-1} \sum w_i (\overline{R} - R_i)^2 / \sum w_i]^{1/2}$ . The larger of these two  $\sigma(\overline{R})$  was taken, and multiplied by 2, corresponding to a confidence level of about 90%.

The total number of independent experiments is denoted by n. To obtain an approximate 90% confidence level, the uncertainty, quoted in Table III, is taken as twice the larger  $\sigma(\vec{R})$  calculated by (a) and (b). The percent deviation of the weighted mean from the new calculations is given in Table III for the six transitions.<sup>23a</sup>

The interpolated *L*-subshell ratios from the tables of Rose<sup>1</sup> and of Sliv and Band<sup>2</sup> are not given in Table III.

The reason is that the interpolations<sup>24</sup> introduce additional uncertainties in the subshell ratios. However, Table IV contains a comparison of the new calculations with those of Refs. 1 and 2 for the tabulated values of gamma energies. The choice of these two gamma energies, 0.15 and 0.20 in  $mc^2$  units, was dictated by the fact that the appropriate gamma energies in all six cases do lie between these values. The percentage differences between the new ICC and those of Sliv and Band<sup>1</sup> (and

<sup>&</sup>lt;sup>23a</sup> Note added in proof. S. Karlsson, I. Andersson, Ö. Nilsson, G. Malmsten, C. Nordling, and Kai Siegbahn have also accurately measured *L*-subshell ratios (private communication). The results are in agreement with the Chalk River and the BNL-Nobel groups.

<sup>&</sup>lt;sup>24</sup> C. P. Bhalla, M. S. Freedman, F. T. Porter, and F. Wagner, Phys. Letters 23, 116 (1966). Also see T. Novakov, J. M. Hollander, and R. L. Graham, University of California Radiation Laboratory Report No. UCRL-1140, 1963 (unpublished).

		k	=0.15			k = 0.20	
Nucleus	Reference	$L_1$	$L_2$	$L_3$	$L_1$	$L_2$	$L_3$
$\mathrm{Gd}^{156}$	Present calculation Sliv and Band Rose	$\begin{array}{c} 1.924(-1) \\ 1.91(-1) \\ 1.90(-1) \end{array}$	1.658 1.67 1.59	1.810 1.80 1.75	9.932(-2) 1.00(-1) 9.72(-2)	$\begin{array}{c} 4.304(-1) \\ 4.33(-1) \\ 4.17(-1) \end{array}$	$\begin{array}{c} 4.355(-1) \\ 4.33(-1) \\ 4.25(-1) \end{array}$
Dy <sup>160</sup>	Present calculation Sliv and Band Rose	1.826(-1) 1.79(-1) 1.81(-1)	$\begin{array}{c} 1.995 \\ 1.95 \\ 1.92 \end{array}$	2.131 2.12 2.07	9.74(-2) 9.81(-2) 9.58(-2)	5.190(-1) 5.20(-1) 5.04(-1)	5.122(-1) 5.09(-1) 5.01(-1)
Er <sup>166</sup>	Present calculation Sliv and Band Rose	1.734(-1) 1.71(-1) 1.74(-1)	2.393 2.33 2.31	2.494 2.50 2.44	9.526(-2) 9.62(-2) 9.42(-2)	6.241(-1) 6.20(-1) 6.06(-1)	6.002(-1) 5.97(-1) 5.91(-1)
Yb <sup>170</sup>	Present calculation Sliv and Band Rose	1.663(-1) 1.63(-1) 1.67(-1)	$2.865 \\ 2.80 \\ 2.77$	2.914 2.93 2.87	9.328(-2) 9.42(-2) 9.26(-2)	7.488(-1) 7.41(-1) 7.28(-1)	7.013(-1) 6.98(-1) 6.96(-1)
Os <sup>186</sup>	Present calculation Sliv and Band Rose	1.656(-1) 1.68(-1) 1.69(-1)	4.855 4.80 4.72	4.578 4.65 4.61	9.193(-2) 9.32(-2) 9.28(-2)	1.281 1.30 1.24	1.103 1.12 1.12

TABLE IV. Comparison of present calculations<sup>a</sup> of E2 internal conversion coefficients with those of Rose and of Silv and Band for two  $\gamma$  energies.<sup>b</sup> The number in parentheses after an entry is the power of 10 to be multiplied by it.

<sup>a</sup> Based on completely relativistic Hartree-Fock-Slater treatment.
 <sup>b</sup> This choice of the two γ energies is made because the appropriate k-values of the E2 transitions in Table I lie between 0.15 and 0.20.

those of Rose<sup>2</sup>) are less than 1% for 17 (7) cases, are 1-2% for 10 (7) cases, and are 2-3% for 3 (9) cases. There are seven ICC where Rose's results differ from the present calculations by more than 3%. Considering these 30 cases, one can conclude that most of the

TABLE V. Results of new ICC calculations for K shell and L subshells. The number in parentheses following an entry is the power of 10 to be multiplied by it.

	Gamma energy (keV)	$\alpha_2(K)$	$\alpha_2(L_1)$	$\alpha_2(L_2)$	α2(L3)
Gd156	88.97	1.540(0)	1.388(-1)	8.215(-1)	8.640(-1)
$\mathrm{Dy^{160}}$	86.79	1.531(0)	1.412(-1)	1.1107(0)	1.149(0)
$\mathrm{Er}^{166}$	80.57	1.616(0)	1.581(-1)	1.890(0)	1.946(0)
$\mathrm{Yb^{170}}$	84.26	1.358(0)	1.392(-1)	1.838(0)	1.821(0)
Os186	137.15	4.278(-1)	4.866(-2)	3.355(-1)	2.601(-1)
Os <sup>188</sup>	155.03	3.202(-1)	3.673(-2)	1.938(-1)	1.432 (-1)

relevant calculations of Sliv and Band are within the assigned uncertainty of  $\pm 2\%$ . For  $L_1/L_2$  conversion ratios, Sliv and Band agree within 1% for seven cases and differ by 1–2% for three cases; the corresponding results for Rose's calculations are one ratio within 1%, three differing by 1–2%, and five differing by 2–3%. In the above comparisons, we have not included a

possible uncertainty resulting from the Z interpolation made in Refs. 1 and 2.

Numerical results are also presented in Tables V and VI for K shell, L subshells, and M subshells for all the E2 transitions discussed in this paper.

The differences between the ICC calculated from the relativistic and the nonrelativistic Hartree-Fock-Slater models were found to be at most 1%, and normally about 0.7%. The *L*-subshell ICC ratios for the cases under discussion were the same within  $\approx 0.4\%$  for the two models. We note here that some of the numerical results based upon the nonrelativistic model, which were privately circulated, were slightly in error, mainly because the contributions inside the nucleus were not calculated correctly in the computer program for *E*2 transitions.

## IV. DISCUSSION AND CONCLUSIONS

Figure 1 contains a summary of comparisons between the present calculations and the weighted mean of experimental data relevant to  $L_1/L_2$  and  $L_1/L_3$  as a function of mass number A. The weighted means of the percentage deviations from the calculations for the six cases are  $(6.5\pm2.0)\%$  and  $(5.7\pm1.2)\%$ , respectively,

TABLE VI. *M*-subshell ICC for some  $2^+ \rightarrow 0^+$  transitions. The number in parentheses following an entry is the power of 10 to be multiplied by it.

Transition (Energy in keV)	$lpha_2({M}_1)$	$lpha_2(M_2)$	$lpha_2(M_3)$	$lpha_2(M_4)$	$lpha_2(M_5)$
$\begin{array}{c} {\rm Gd^{156}} \\ {\rm Gd^{156}} \left( {88.97} \right) \\ {\rm Dy^{160}} \left( {86.79} \right) \\ {\rm Er^{166}} \left( {80.57} \right) \\ {\rm Yb^{170}} \left( {84.26} \right) \\ {\rm Os^{186}} \left( {137.15} \right) \\ {\rm Os^{188}} \left( {155.03} \right) \end{array}$	$\begin{array}{c} 2.958(-2)\\ 3.079(-2)\\ 3.566(-2)\\ 3.221(-2)\\ 1.136(-2)\\ 8.479(-3)\end{array}$	1.918(-1)2.630(-1)4.518(-1)4.447(-1)8.422(-2)4.872(-2)	$\begin{array}{c} 2.066(-1)\\ 2.787(-1)\\ 4.778(-1)\\ 4.533(-1)\\ 6.765(-2)\\ 3.730(-2)\end{array}$	$\begin{array}{c} 1.930 (-3) \\ 2.754 (-3) \\ 5.032 (-3) \\ 4.928 (-3) \\ 7.569 (-4) \\ 4.089 (-4) \end{array}$	1.868(-3)2.588(-3)4.629(-3)4.416(-3)5.753(-4)3.045(-4)

for  $L_1/L_2$  and  $L_1/L_3$  at about 90% confidence level. The experimental values of  $L_2/L_3$  agree extremely well with the calculations.

A brief discussion regarding these observed deviations in  $L_1/L_2$  and  $L_1/L_3$  is presented next.

(a) It has been pointed out by Church and Weneser<sup>11</sup> that dynamic effects, when significant at all, influence only the K and  $L_1$  conversion coefficients appreciably, and those of higher subshells negligibly. The dynamic effects, if present in these transitions, can either remove completely or reduce appreciably the aforementioned deviations. This argument, however, is not strong, because the observed gamma transition rates have enhancement factors as large as 100 when compared with the single-particle transition rates. This enhancement tends to suppress the contribution of dynamic effects. Additional experiments are needed before this conjecture can be discarded completely. The relevant experiments are to measure the  $K/L_3$ ,  $L_3/\sum_i M_i$ , and M subshell ratios; in the presence of dynamic effects, the ratio involving the K conversion coefficient should be most influenced, in contrast to the other ratios, which should agree with the present calculation.

Several measurements<sup>25-44</sup> of K conversion coefficients have unfortunately large (5-12%) errors, thus arriving at meaningful conclusions unlikely at the present time. However, a summary of the comparison between the present calculations and the experimental data is given in Table VII. Further experimental work needs to be done.

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TABLE VII. Comparison of theory and experiments<sup>a</sup> on  $\alpha_K$  for Z = 66, 68, and 70.

Isotope	Reference	$\alpha_K$
Dy <sup>160</sup>	Dingus et al. <sup>b</sup> Erman and Hultherg <sup>e</sup> Jansen et al. <sup>d</sup> Thosar et al. <sup>e</sup> Fossan and Herskind <sup>f</sup> Bernstein <sup>g</sup> Clark <sup>h</sup> Joshi et al. <sup>i</sup> McGowan <sup>i</sup> Present calculation (theory)	$\begin{array}{c} 1.54 \pm 0.06 \\ 1.55 \pm 0.15 \\ 1.73 \pm 0.08 \\ 1.52 \pm 0.06 \\ 1.94 \pm 0.15 \\ 2.05 \pm 0.22 \\ 1.5 \pm 0.3 \\ 2.0 \pm 0.2 \\ 1.65 \pm 0.2 \\ 1.531 \end{array}$
$\mathrm{Er}^{166}$	Erman and Hultberg <sup>e</sup> Thosar <sup>d</sup> Present calculation (theory)	$1.68 \pm 0.12$ 1.67 1.616
Yb <sup>170</sup>	Nelson and Hatch <sup>k</sup> Dingus <i>et al.</i> <sup>b</sup> Erman and Hultburg <sup>e</sup> Jansen and Wapstra <sup>1</sup> Hatch <i>et al.</i> <sup>m</sup> Croft <i>et al.</i> <sup>n</sup> Hootan <sup>o</sup> Thosar <i>et al.</i> <sup>e</sup> Jansen and Wapstra <sup>p</sup>	$\begin{array}{c} 1.43 {\pm} 0.04 \\ 1.47 {\pm} 0.05 \\ 1.37 {\pm} 0.07 \\ 1.32 {\pm} 0.05 \\ 1.47 {\pm} 0.09 \\ 1.52 {\pm} 0.07 \\ 1.46 {\_} 0.3^{\pm 0.05} \\ 1.31 {\pm} 0.08 \\ 1.36 {\pm} 0.10 \end{array}$
	Fossan and Herskind <sup>e</sup> Berstein <sup>f</sup> McGowan and Stelson <sup>q</sup> Houtermans <sup>r</sup> Bisi <i>et al.</i> <sup>s</sup> Liden and Starfelt <sup>t</sup> Graham <i>et al.</i> <sup>u</sup> Present calculations (theory)	$\begin{array}{c} 1.52{\pm}0.11\\ 1.41{\pm}0.11\\ 1.65{\pm}0.12\\ 1.34{\pm}0.07\\ 1.69{\pm}0.02\\ 1.56{\pm}0.15\\ 1.60{\pm}0.15\\ 1.358\end{array}$

<sup>a</sup> See J. F. W. Jansen and A. H. Wapstra, Ref. 35, for a discussion of the corrections which need be applied to the measurements with the scintillation methods

<sup>b</sup> Reference 25.	<sup>1</sup> Reference 35.
<ul> <li>Reference 26.</li> </ul>	<sup>m</sup> Reference 36.
<sup>d</sup> Reference 27.	<sup>n</sup> Reference 37.
<ul> <li>Reference 28.</li> </ul>	<ul> <li>Reference 38.</li> </ul>
f Reference 29.	P Reference 39.
g Reference 30.	q Reference 40.
<sup>h</sup> Reference 31.	r Reference 41.
<sup>i</sup> Reference 32.	<sup>s</sup> Reference 42.
<sup>i</sup> Reference 33.	<sup>t</sup> Reference 43.
<sup>k</sup> Reference 34.	<sup>u</sup> Reference 44.

(b) Parity violation in electromagnetic transitions has been advanced as one possibility<sup>45</sup> for explaining the anomalies observed in the highly retarded E1 L-subshell ratios of Hf<sup>180m</sup>. Hager and Seltzer<sup>46</sup> have invoked the contribution of dynamic effects as a possible explanation; their obtained values of  $\lambda(\mathbf{j} \cdot \mathbf{r})$  and  $\lambda(\mathbf{j} \cdot \nabla)$ are not unreasonable. Lawson and Segel<sup>47</sup> conclude that the hypothesis of parity mixing, if valid, leads to results which are inconsistent with the properties of the 501-keV crossover to the 6<sup>+</sup> state. We note here that the differences between the E2 cases and theory in the present work are of the correct sign to be explained by a small admixture of M2 to the E2 contribu-

<sup>&</sup>lt;sup>25</sup> R. S. Dingus, W. L. Talbert, Jr., and M. G. Stewart, Nucl. Phys. 83, 545 (1966). <sup>26</sup> P. Erman and S. Hultberg, in *Internal Conversion Processes*,

<sup>&</sup>lt;sup>45</sup> G. Scharff-Goldhaber and M. McKeown, Proceedings of the Argonne International Conference on Weak Interactions, 1965, Argonne National Laboratory Report No. ANL 7130 (unpublished). This experiment involved the measurement of Lsubshell internal conversion coefficients in the  $8^- \rightarrow 8^+$  transition of Hf180m

<sup>&</sup>lt;sup>46</sup> R. Hager and E. Seltzer, Phys. Letters 20, 180 (1966)

<sup>&</sup>lt;sup>47</sup> R. D. Lawson and R. E. Segel, Phys. Rev. Letters 16, 1008 (1966).



FIG. 1. Ratios of the weighted mean of experimental  $L_1/L_2$  and  $L_1/L_3$  to the appropriate calculated values, versus the mass number. The uncertainties assigned to the ratios correspond to an error estimate at about 90% confidence level  $(2\sigma)$ . The weighted mean of all cases is also shown.

tion. However, the single-particle E2 transition rates have enhancement factors  $\approx 50$  in the deformed nuclear region, whereas M2's are generally hindered by a factor  $\approx 200$ . If one accepts this retardation factor for M2 in the cases under discussion, it appears difficult to explain the observed gamma transition rates.<sup>48</sup>

(c) Finally, it should be noted that all the numerical results for ICC involve considering a nucleus as a sphere of uniform charge distribution with a nuclear radius of  $1.2A^{1/3}$  F. A variation of nuclear radius would have an

insignificant effect<sup>2,11</sup> on ICC. However, the assumption of a spherically symmetric nucleus is not valid in the rare-earth region. Consequently, the effects of nuclear deformation on the L-subshell ratios cannot be dismissed. Church and Weneser<sup>49</sup> discuss the modifications of radial functions for the unscreened Coulomb field. A possible contribution to ICC will result only from the mixing of bound-state wave functions in  $2^+ \rightarrow 0^+$ transitions. The inclusion of nuclear-deformation effects works in the right direction. Quantitative estimates of this effect on the numerical results presented in this paper cannot be made at the present time. It is not unlikely that the calculated values of  $L_1/L_2$  and  $L_1/L_3$ , given in this paper, may increase by 1-2% with the inclusion of this effect. Additional experiments of Lsubshell ratios, with an accuracy attained at Brookhaven National Laboratory,<sup>4</sup> and Chalk River Laboratory,3 are desirable in the region of spherical nuclei. M-subshell measurements, if feasible in the rare-earth region, could also lead to significant information, inasmuch as  $M_1/M_2$ ,  $M_1/M_3$ , etc. are expected to be in agreement with the present calculation.

The conjecture involving possible contributions to ICC arising from nuclear deformation is the most attractive at the present time. The possibility of an adequate explanation appears small in the framework of present theory (ignoring higher-order terms) if (1) the *M*-subshell measurements in the rare-earth region should also disagree with the present calculation, and (2) if the experimental  $L_1/L_2$  and  $L_1/L_3$  in the spherical nuclear region should establish about the same order of deviations as observed now in the rare-earth region.

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<sup>&</sup>lt;sup>48</sup> It should be noted that in the analyses involving the parity mixing, E2 and M2 contribute coherently to the amplitude in transition probabilities; therefore the cross terms will be present. The relevant expressions for ICC and the gamma emission do not, as yet, appear in the literature. Such calculations are in progress at the present time.

<sup>&</sup>lt;sup>49</sup> E. Church and J. Weneser, Bull. Am. Phys. Soc. **3**, 184 (1958); also see the review article by Church and Weneser, Ref. 11, p. 208.