

## KLL Auger Transition Probabilities

EDWIN J. CALLAN

*Aeronautical Research Laboratory, Wright-Patterson Air Force Base, Ohio*

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*KLL* Auger transition rates have been computed for a variety of atoms  $Z=1$  to  $Z=80$  for all transitions involved. Screened nonrelativistic hydrogenic wave functions were used, with screening constants derived from the limiting screening numbers for self consistent-field functions given by Froese. Auger electron energies were derived from tabulated energy level values. Transition probabilities in the Russell-Saunders coupling forms given by Asaad and Burhop were obtained. They show smooth changes with  $Z$ , tending to saturate at high  $Z$ . The  $^1D_2$  and  $^1P_1$  probabilities show much greater increases with  $Z$  than do those of  $^1S_0$  and  $^3P_J$ . These Auger probabilities for the  $sp$  and  $p^2$  cases are opposite in strength to those found by Asaad using relativistic theory. Variations in the transition rates for several atoms were found when effective atomic charge and ejected electron energy were changed slightly. Additionally, some  $K$ -shell fluorescence yields were computed and they are compared with other values.

### INTRODUCTION

AN atom ionized in a deep ( $K$  or  $L$ ) shell may rearrange itself either through radiative or radiationless Auger transitions.<sup>1</sup> The relative probability of radiative and Auger-type transitions is called the fluorescence yield, defined by  $\omega_K = N_R / (N_R + N_A)$ , where  $N_R$  and  $N_A$  are the numbers of radiative and Auger transitions, respectively, for an initial  $K$ -shell vacancy. The present paper is concerned with the determination of the Auger transition rates and total Auger probability for the *KLL* transitions for various atoms.

Recently the theory of the  $K$ -shell Auger effect has been significantly improved by Asaad and Burhop,<sup>2</sup> who have shown the importance of intermediate coupling in arriving at satellite line energies and intensities. Transition amplitudes obtained from Russell-Saunders ( $L-S$ ) coupling of the individual transitions are used for the computations. It is noted in their work that such transition amplitudes are known for only a few values of atomic number, and are based on several different methods of computation. Therefore, in order to obtain a set of transition amplitudes for a variety of atomic numbers  $Z$ , which also were computed by the same methods, throughout, the present work was undertaken.

The basis for the calculations is the use of non-relativistic screened hydrogenic wave functions for computing the electrostatic interaction integrals involved in the Auger process. The theory is presented in the next section and the methods for obtaining screening constants follow thereafter. The ejected electron energies were computed from tables of energy levels as described later. The computations of transition rates were made for values between  $Z=12$  and  $Z=47$ , together with some additional values to  $Z=80$  for which extrapolated screening constants were used. Also,

transition rates for  $Z=1$ , the unscreened hydrogenic case, were calculated. This case has been used in earlier work.<sup>3,4</sup> In order to determine the limits of error for changes in effective charge  $Z^*$  or ejected electron energy  $k$  for a given transition, additional calculations were performed for several  $Z$  with such changes included. These are described in later sections. No relativistic corrections have been applied. Relativistic calculations for the Auger effect have been performed by Massey and Burhop<sup>5</sup> and Asaad<sup>6</sup> for Au<sup>79</sup> and Hg<sup>80</sup>. The individual transition rates, and the  $L-S$  transition amplitudes derived from them, are tabulated. However, no computation of intensities in intermediate coupling has been performed. From the total  $K$ -shell Auger transition probability, the fluorescent yield  $\omega_K$  has been computed for several  $Z$  and compared with other values. The differences are discussed.

### THEORY

The Auger transition arises from the electrostatic interaction between two electrons in an initially singly ionized atom. Following Condon and Shortley,<sup>7</sup> the interaction integrals are of the form

$$(ab|q|cd) = \int \int \bar{\psi}_1(a)\bar{\psi}_2(b) \left( \frac{e^2}{r_{12}} \right) \psi_1(c)\psi_2(d) d\tau_1 d\tau_2, \quad (1)$$

where the  $\psi$  are electron eigenfunctions. These eigenfunctions are given by Bethe and Salpeter<sup>8</sup> for the hydrogenic case. The wave function for the ejected electron of angular momentum  $l$  has been taken in the

<sup>3</sup> L. Pincherle, *Nuovo cimento* **12**, 81 (1935).

<sup>4</sup> C. Geffrion and G. Nadeau, Air Force Office of Scientific Research, Report TR 59-145, 1959 (unpublished).

<sup>5</sup> H. Massey and E. Burhop, *Proc. Roy. Soc. (London)* **A153**, 661 (1936).

<sup>6</sup> W. Asaad, *Proc. Roy. Soc. (London)* **A249**, 555 (1959).

<sup>7</sup> E. Condon and G. Shortley, *Theory of Atomic Spectra* (Cambridge University Press, New York, 1953), p. 174.

<sup>8</sup> H. Bethe and E. Salpeter, *Handbuch der Physik* edited by S. Flügge (Springer-Verlag, Berlin, 1957), Vol. XXXV, p. 379.

<sup>1</sup> E. Burhop, *The Auger Effect and Other Radiationless Transitions* (Cambridge University Press, New York, 1952).

<sup>2</sup> W. Asaad and E. Burhop, *Proc. Phys. Soc. (London)* **71**, 369 (1958).

form given by Gordon<sup>9</sup>:

$$\begin{aligned} \bar{\psi}_\infty = & \left(\frac{m_e}{\hbar}\right)^{\frac{1}{2}} \frac{2^{l+1}}{(2l+1)!} e^{\pi Z^*/2k} k^{l+\frac{1}{2}} |\Gamma(l+1+iZ^*/k)| \\ & \times r^l e^{-ikr} {}_1F_1(l+1+iZ^*/k; 2l+2; 2ikr) \\ & \times Y_{lm}(\theta, \phi), \quad (2) \end{aligned}$$

where  ${}_1F_1(a; b; c)$  is the confluent hypergeometric function and  $Y_{lm}$  is a spherical harmonic. It is normalized to yield one ejected electron per unit time per unit energy range. With this normalization the Auger transition rate becomes

$$W^2 = (4\pi^2/\hbar^2)(ab|q|cd)^2. \quad (3)$$

On expanding the interaction potential in a series of Legendre polynomials, the matrix element can be separated into a product of an angular factor  $Y$  and a radial factor  $R$ , so that Eq. (3) can be written

$$W^2 = Y^2 R^2. \quad (4)$$

There are twelve  $KLL$  transitions, which are listed for identification in Table I. The  $W^2$  identify the transition rates for particular transitions, values for which are given later. The angular factors  $Y^2$  are given here for convenience. There are only five distinct forms for the  $KLL$  radial integrals, but since the Auger energies are different for the particular subshells involved in a given transition, there are actually ten distinct values of these radial integrals for a given atom.

For the hydrogenic types of radial functions, we may write  $R$  in the general form

$$\begin{aligned} R = & \sum_\alpha \int_0^\infty dr_2 \left[ r_2^\alpha e^{-\alpha r_2} {}_1F_1(a, b; cr_2) \right. \\ & \times \left\{ \sum_\beta \int_0^{r_2} \left(\frac{1}{r_2^{n+1}}\right) r_1^\beta e^{-\beta r_1} dr_1 \right. \\ & \left. \left. + \sum_\gamma \int_{r_2}^\infty (r_2^n) r_1^\gamma e^{-\gamma r_1} dr_1 \right\} \right], \quad (5) \end{aligned}$$

where  $\alpha, \beta, \gamma, n$ , and the  $q$ 's are constants for a given transition. The inner integrals are of the forms

$$\int_0^{r_2} r^p e^{-qr} dr = \frac{p!}{q^{p+1}} \left(1 - e^{-qr} \sum_{i=1}^{p+1} \frac{(qr)^{p+1-i}}{(p+1-i)!}\right), \quad (6a)$$

and

$$\int_{r_2}^\infty r^p e^{-qr} dr = \frac{p!}{q^{p+1}} \left(e^{-qr} \sum_{i=1}^{p+1} \frac{(qr)^{p+1-i}}{(p+1-i)!}\right). \quad (6b)$$

The outer integrals are of the form

$$\int_0^\infty r^p e^{-qr} {}_1F_1(a; b; cr) dr = \frac{p!}{q^{p+1}} F(a; p+1; b; c/q), \quad (6c)$$

<sup>9</sup> W. Gordon, Z. Physik 48, 180 (1928).

TABLE I. Identification of transitions.<sup>a</sup>

$W$	Transition	$l_\infty$	$m_i$	$R$	$Y^2$
$W_1$	$KL_1L_1$	0	0	$R_1$	1
$W_2$	$KL_1L_2$	1	0	$R_{2a}$	1
$W_{34}$	$KL_1L_3$	1	1	$R_{3b}$	1
$W_3$	$KL_2L_{20}$	0	0	$R_{3a}$	1/9
$W_4$	$KL_2L_{22}$	2	0	$R_{4a}$	4/45
$W_5$	$KL_2L_1$	1	0	$R_{3a}$	1/9
$W_{35}$	$KL_3L_1$	1	1	$R_{3b}$	1/9
$W_6$	$KL_3L_3$	2	1	$R_{4b}$	1/15
$W_{36}$	$KL_3L_2$	2	1	$R_{4b}$	1/15
$W_7$	$KL_3L_{30}$	0	0	$R_{5b}$	1/9
$W_8$	$KL_3L_{32-}$	2	0	$R_{4c}$	1/45
$W_9$	$KL_3L_{32+}$	2	2	$R_{4c}$	2/15

<sup>a</sup>  $W^2$  = transition rate =  $Y^2R^2$ ;  $KL_iL_j = (L_i \rightarrow K; L_j \rightarrow \infty)$ ;  $l_\infty$  = angular momentum of ejected electron;  $m_i$  = projection of  $l_\infty$ ;  $R$  = radial integral of transition ( $R_{ia} = R_{ib}$  if  $k_a = k_b$ , i.e., integrals have same form, and differ only in ejected electron energy); and  $Y$  = angular factor.

where  $F(a; p+1; b; c/q)$  is the general hypergeometric function. From these forms and the tabulated constants, the radial integrals are computed. For the case of the  $KL_1L_1$  transition, as an example, the integral becomes:

$$\begin{aligned} \frac{R_1}{C} = & \left(\frac{2}{\gamma^3} - \frac{3Z_L}{\gamma^4}\right) \left[ \frac{\Gamma(2)}{\beta^2} F(\rho, 2, 2, \eta) - \frac{Z_L \Gamma(3)}{2 \beta^3} F(\rho, 3, 2, \eta) \right] \\ & - \frac{Z_L^2 \Gamma(5)}{4\gamma^2 \alpha^5} F(\rho, 5, 2, \lambda) \\ & + \left[ \frac{Z_L}{2\gamma^2} + \frac{Z_L}{2} \left(\frac{1}{\gamma^2} - \frac{2Z_L}{\gamma^3}\right) \right] \frac{\Gamma(4)}{\alpha^4} F(\rho, 4, 2, \lambda) \\ & - \left[ \left(\frac{1}{\gamma^2} - \frac{2Z_L}{\gamma^3}\right) - \frac{Z_L}{2} \left(\frac{2}{\gamma^3} - \frac{3Z_L}{\gamma^4}\right) \right] \frac{\Gamma(3)}{\alpha^3} F(\rho, 3, 2, \lambda) \\ & - \left(\frac{2}{\gamma^3} - \frac{3Z_L}{\gamma^4}\right) \frac{\Gamma(2)}{\alpha^2} F(\rho, 2, 2, \lambda), \quad (7) \end{aligned}$$

where

$$\begin{aligned} \rho = & 1 + iZ_L/k, \quad \beta = \frac{1}{2}Z_L + ik, \quad \alpha = Z_K + Z_L + ik, \\ \gamma = & Z_K + \frac{1}{2}Z_L, \quad \eta = 2ik/\beta, \quad \lambda = 2ik/\alpha, \\ C = & 2e^{\pi Z_L/2k} |\Gamma(1+iZ_L/k)| k^{\frac{1}{2}} \times Z_K^{\frac{3}{2}} Z_L^{\frac{3}{2}}. \end{aligned}$$

These integrals are of the same nature as those of Burhop.<sup>10</sup> In the present computations atomic units with  $m_e = e = \hbar = 1$  are used throughout. The transition rates  $W^2$  are then obtained using Eq. (4).

### Screening Constants and Auger Energies

To improve on results obtained from use of unscreened hydrogenic functions, or those with essentially constant screening,<sup>11</sup> it was decided to use hydrogenic type functions, but with screening constants derived from results of the Hartree-Fock self-consistent-field (SCF) functions. This procedure permits easy variation

<sup>10</sup> E. Burhop, Proc. Roy. Soc. (London) A148, 262 (1935).

<sup>11</sup> J. Slater, Phys. Rev. 36, 57 (1930).

of  $Z$  in the calculations, yet retains some of the improvements of the SCF functions and also permits use of a single consistent method of computing the transition rates for all variations in constants. It is felt that use of more complex analytic wave functions does not offer such a clear improvement over these screened hydrogenic functions as to be worth the additional calculational complexities for computing these Auger transition rates.

The ultimate screening constants  $\sigma_0$  for an atom of number  $Z$  as the mean radius,  $\bar{r}$ ,<sup>12</sup> goes to zero have been obtained by Froese<sup>13</sup> for a series of  $Z$  up to 46, which includes the  $4d$  functions. In addition, she has obtained  $d\sigma/d\bar{r}$  for a number of configurations, also to  $Z=46$ . All these values are based on SCF functions with exchange. From these values and their variation with  $\bar{r}$ , a good screening constant can be derived for any particular subshell of a given atom, using the relation

$$\sigma = \bar{r} d\sigma/d\bar{r} + \sigma_0. \quad (8)$$

This requires a knowledge of the values of  $\bar{r}$  for each  $Z$ . Unfortunately  $\bar{r}$  is known only for a few atoms. In order to find a set of values for  $\bar{r}$ , the following relations were determined by least squares. Tabulated values of  $\bar{r}$  for neutral atoms were used, together with values for  $\bar{r}$  interpolated from those for alkali and halogen ions.

$$2s: Z = 2.4528 + 6.3405/\bar{r}, \quad (9a)$$

$$2p: Z = 3.6911 + 5.3005/\bar{r}. \quad (9b)$$

The goodness of fit of these equations is shown on Fig. 1,

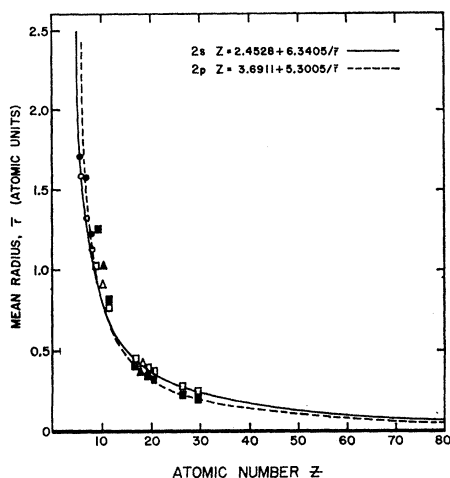


FIG. 1. Variation of mean radius ( $\bar{r}$ ) of  $2s$  and  $2p$  wave functions with atomic number ( $Z$ ). Points represent actual  $\bar{r}$  values derived from Hartree-Fock solutions, and are identified as follows:  $\circ$  and  $\bullet$  are  $2s$  and  $2p$  values of  $\bar{r}$  for neutral atoms;  $\square$  and  $\blacksquare$  are  $2s$  and  $2p$  values of  $\bar{r}$  for ions; and  $\triangle$  and  $\blacktriangle$  are  $2s$  and  $2p$  values of  $\bar{r}$  interpolated from  $\bar{r}$  values for adjacent halogen and alkali ions.

<sup>12</sup> D. Hartree, *The Calculation of Atomic Structures* (John Wiley & Sons, Inc., New York, 1957).

<sup>13</sup> C. Froese, Proc. Roy. Soc. (London) **A239**, 311 (1957); also **244**, 390 (1958) and **251**, 534 (1959).

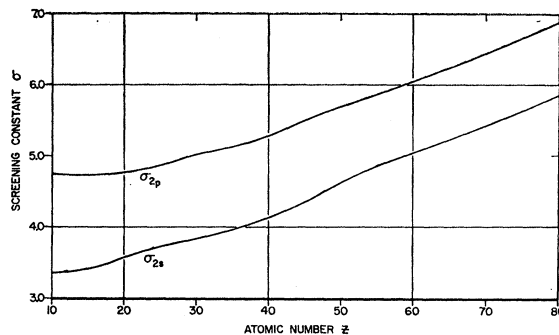


FIG. 2. Values of  $2s$  and  $2p$  screening constants ( $\sigma$ ) for various atomic numbers ( $Z$ ).

where the known  $\bar{r}$  values are from Hartree.<sup>12</sup> Beyond  $Z=46$  no values for  $\sigma_0$  and  $d\sigma/d\bar{r}$  are available, so values for  $\sigma$  have been extrapolated for higher  $Z$ . The validity of the extrapolation lies both in the regularity to  $Z=46$ , and the lessened sensitivity of the added outer electrons on the screening of the  $2s$  and  $2p$  functions for higher  $Z$ . It is considered that values of  $\sigma$  are good to within 0.1 units for  $Z < 47$ , and to within 0.2 units at high  $Z$ . Values of these screening constants are shown on Fig. 2, and may be compared to the constant value of 4.15 found by Slater's rules<sup>11</sup> for both  $2s$  and  $2p$  functions for  $Z > 10$ . These values are used to obtain effective charges  $Z^*$  for the computations. Since  $\sigma$  for the  $K$  electron shows little variation with  $Z$ ,  $Z^*$  for this shell was taken constant as  $Z-0.3$  throughout.

For the *KLL* Auger transitions, the energies of the ejected electrons are given by

$$k = [(K - L_{Zi} - L_{(Z+1)j})/13.605]^{1/2}, \quad (10)$$

where  $k$  is the Auger energy in atomic units,  $K$  is the  $K$ -shell energy level (in eV) for atomic number  $Z$ ,  $L_{Zi}$  is the  $L_i$ -subshell energy level (in eV) for atomic number  $Z$ , and  $L_{(Z+1)j}$  is the  $L_j$ -subshell energy level (in eV) for atomic number  $Z+1$ . It is to be noted that the energy level for the second electron is taken as that for an atom of next higher  $Z$ . This is because the atom can then be considered as singly ionized, and thus approximately equivalent to an un-ionized atom of  $Z+1$ . Other workers<sup>4,14</sup> consider that the Auger electron energy is better given by

$$k = [(K - L_{Zi} - L_{(Z+n)j})/13.605]^{1/2},$$

where  $0 < n < 1$ , and with  $n$  varying among  $Z$  and subshells for any  $Z$ . According to reference 14 for  $\text{Hg}^{80}$ ,  $n=0.55$  for the  $L_1$  and  $L_2$  subshells, and  $n=0.76$  for the  $L_3$  subshell. The difference in taking  $n=1$ , as done here, or less than 1 results in insignificant differences in the Auger transition amplitudes, as will be shown later from study of the variations in transition rates with changes in  $k$ , the Auger energy.

<sup>14</sup> I. Bergstrom and R. Hill, Arkiv Fysik **8**, 2 (1954).

TABLE II. Auger transition rates for various values of  $Z$ .<sup>a</sup>

$Z$	$W_1^2$	$W_2^2$	$W_3^2$	$W_4^2$	$W_5^2$	$W_6^2$	$W_7^2$	$W_8^2$	$W_9^2$	$W_{34}^2$	$W_{35}^2$	$W_{36}^2$
1	248 752	194 337	62 808	301 265	67 204	225 949	62 808	75 316	451 898	194 337	67 204	225 949
12	244 165	081 376	04 144	022 314	20 972	016 679	04 130	05 560	033 359	081 140	20 960	016 679
13	249 051	091 870	05 561	029 611	24 425	022 142	05 544	07 381	044 283	091 635	24 414	022 142
14	252 514	100 232	06 971	036 801	27 529	027 601	06 952	09 175	055 051	100 232	27 529	026 701
15	255 981	108 041	08 332	043 693	30 204	032 770	08 310	10 896	065 377	107 819	30 197	032 770
16	258 262	114 200	09 642	050 297	32 590	037 296	09 506	12 404	074 421	112 929	32 552	037 296
17	259 962	120 375	10 982	057 014	34 763	042 671	10 838	14 075	084 449	120 170	34 759	042 671
18	260 940	125 672	12 327	063 723	36 796	047 701	12 302	15 900	095 403	125 475	36 793	047 701
19	261 363	129 543	13 520	069 663	38 554	052 152	13 468	17 352	104 114	129 543	38 554	052 152
20	261 851	133 450	14 634	075 185	40 086	056 293	14 581	18 732	112 394	133 270	40 084	056 293
21	261 940	136 117	15 635	080 155	41 548	060 019	15 581	19 974	119 846	135 946	41 547	060 019
22	262 800	139 056	16 535	084 612	42 750	063 363	16 481	21 089	126 532	138 727	42 750	063 363
23	263 073	141 379	17 385	088 815	43 850	066 419	17 304	22 108	132 647	141 064	43 852	066 419
24	262 864	143 663	18 236	093 018	44 927	069 572	18 128	23 127	138 763	143 210	44 931	069 572
25	262 803	145 440	19 042	096 992	45 925	072 554	18 934	24 122	144 729	145 006	45 929	072 554
26	262 873	147 151	19 758	100 521	46 784	075 109	19 624	24 974	149 843	146 734	46 789	075 109
27	262 398	148 574	20 408	103 734	47 582	077 522	20 276	25 779	154 674	148 174	47 589	077 522
28	261 772	149 617	21 050	106 894	48 330	079 895	20 893	26 540	159 242	149 233	48 337	079 895
29	261 250	150 883	21 729	110 228	49 060	082 308	21 547	27 345	164 072	150 390	49 071	082 308
30	260 591	152 395	22 479	113 877	49 731	085 047	22 271	28 229	169 377	151 801	49 747	085 047
31	259 855	152 252	22 921	116 082	50 355	086 707	22 691	28 755	172 531	151 682	50 369	086 707
32	260 105	154 125	23 533	119 074	50 950	088 868	23 280	29 477	176 864	153 571	50 967	088 868
33	259 688	155 013	24 093	121 813	51 534	090 841	23 817	30 137	180 822	154 371	51 554	090 841
34	259 687	156 115	24 610	124 339	52 033	092 743	24 314	30 744	184 466	155 388	52 058	092 743
35	259 400	157 180	25 170	127 061	52 542	094 622	24 803	31 345	188 070	156 374	52 572	094 622
36	259 048	157 980	25 657	129 444	53 042	096 501	25 294	31 946	191 677	157 295	53 068	096 501
37	258 817	158 796	26 108	131 640	53 463	097 993	25 726	32 474	194 843	158 035	53 494	097 992
38	258 593	159 442	26 478	133 446	53 818	099 359	26 078	32 905	197 433	158 609	53 853	099 359
39	258 375	160 049	26 855	135 279	54 155	100 586	26 391	33 292	199 751	159 149	54 194	100 586
40	259 050	160 621	27 194	136 931	54 475	101 838	26 736	33 713	202 276	159 658	54 519	101 838
41	258 722	161 846	27 518	138 512	54 745	102 961	27 022	34 065	204 391	160 734	54 800	102 961
44	257 286	162 376	28 414	142 881	55 620	106 059	27 789	35 013	210 075	161 192	55 680	106 059
45	257 020	162 740	28 689	144 223	55 875	106 938	28 031	35 311	211 865	161 430	55 942	106 938
46	256 763	163 086	28 954	145 514	56 120	107 853	28 242	35 574	213 445	161 731	56 190	107 853
47	256 597	163 488	29 209	146 757	56 350	108 734	28 466	35 850	215 101	162 090	56 424	108 734
50	256 407	165 059	29 939	150 308	57 060	111 119	29 050	36 574	219 443	163 540	57 143	111 119
55	255 660	166 729	30 997	155 455	57 991	114 587	29 870	37 597	225 584	164 657	58 113	114 587
57	255 143	167 026	31 400	157 424	58 367	115 871	30 159	37 961	227 769	164 854	58 498	115 871
70	251 926	167 619	32 812	164 485	60 086	119 624	30 691	38 739	232 432	164 065	60 302	119 624
72	251 325	167 654	32 936	165 136	60 298	119 808	30 653	38 717	232 303	163 745	60 534	119 808
80	249 322	167 146	33 331	167 233	61 085	120 088	30 339	38 437	230 620	162 269	61 362	120 088

<sup>a</sup> All values are in units of  $10^{-8}$  atomic unit.

Energy level values of Sandstrom<sup>15</sup> were used, with a few level values from Siegbahn<sup>16</sup> for low  $Z$  values. These energy level values agree usually to within 10 eV (or about one part in  $10^4$ ) with the values of Wapstra *et al.*<sup>17</sup> Experimental values for Auger energies were not used in the computations, primarily because it was desired to maintain consistency in the values for different  $Z$ . This could best be done through use of the energy tables of Sandstrom and Siegbahn. The differences between computed and experimental energies would in most cases not exceed 0.1 units, so that the choice of which energies to use is not critical for  $K$ -shell computations. In the case of  $L$ -shell Auger transitions, on the other hand, it would be very desirable to use experimental values since in many cases these can be

determined with greater precision than the energy level values. Particularly for  $Z$  values near the limits for the Coster-Kronig processes,<sup>18</sup> use of the experimental energy values could be important for valid comparisons with the sharp cutoff of satellite intensities at these limits.

#### CALCULATIONS AND RESULTS

Based on the integrals using the  $Z^*$  and  $k$  values derived as described in the preceding section, the transition rates were calculated for a variety of atomic numbers, ranging from  $Z=12$  to 80, together with values for the unscreened hydrogenic case  $Z=1$  for which  $k=\sqrt{2}/2$ . The program used included generation of the hypergeometric functions, followed by computation of the radial integral values. Then the  $W^2$  values were obtained by multiplying the radial values by the angular constants. The hypergeometric functions were generated using a matrix routine based on standard

<sup>15</sup> A. Sandstrom, *Handbuch der Physik* edited by S. Flügge (Springer-Verlag, Berlin, 1959), Vol. XXX, p. 224.

<sup>16</sup> K. Siegbahn, *Beta- and Gamma-Ray Spectroscopy* (North-Holland Publishing Company, Amsterdam, 1955).

<sup>17</sup> A. Wapstra, G. Nijgh, and R. Van Lieshout, *Nuclear Spectroscopy Tables* (North-Holland Publishing Company, Amsterdam, 1959).

<sup>18</sup> D. Coster and R. Kronig, *Physica* 2, 13 (1935).

recursion relations.<sup>19</sup> This method obviates summing of series and is good to seven or more places, as found through comparison of test values with those found using an independent double precision routine programmed for another problem. The computations were conducted using the WADD Univac 1103 A, and the results are good to at least six significant figures, for the  $Z^*$  and  $k$  values chosen. The results for the individual transitions are given in Table II. These provide for further calculations of the transition amplitudes in any coupling scheme.

Several of the coupling schemes have been utilized in the theory of complex spectra, and have been applied to the Auger transitions. The most successful to date has been the intermediate coupling scheme as used by Asaad and Burhop.<sup>2</sup> This starts from the Russell-Saunders ( $L-S$ ) transition probabilities. These are given in terms of functions  $K\{ \}$  of reference 2, which are related to the  $W^2$  transition rates as follows:

$$s^2\ ^1S_0: K\{(2s)^2\ ^1S_0\} = R_1^2 = W_1^2,$$

$$sp\ ^1P_1: K\{(2s)(2p)\ ^1P_1\} = \frac{3}{2}(R_2 + R_3/3)^2 \\ = \frac{3}{2}(W_2^2 + W_5^2 + 2W_2W_5),$$

$$^3P_J: K\{(2s)(2p)\ ^3P_J\} = \frac{2J+1}{2}(R_2 - R_3/3)^2 \\ = \frac{2J+1}{2}(W_2^2 + W_5^2 - 2W_2W_5),$$

$$p^2\ ^1S_0: K\{(2p)^2\ ^1S_0\} = R_5^2/3 = 3W_3^2,$$

$$^3P_J: 0$$

$$^1D_2: K\{(2p)^2\ ^1D_2\} = 2R_4^2/3 = 10W_6^2.$$

These transition probabilities are shown on Fig. 3. These curves demonstrate the saturation effects at high  $Z$ , which are also noticeable in the transition rates  $W^2$ , and which are discussed later. From the  $L-S$  amplitudes and separately computed spin-orbit interactions, the intermediate coupling can be performed. Because of the form of these  $L-S$  amplitudes, which are based on the use of a single  $Z_L$  value for each atom, it is necessary to make the following approximations in the  $W^2$ :

$$W_2 = W_{34}, \quad W_3 = W_7, \quad W_4 = 2W_8, \\ W_4 = (2/3)^{1/2}W_9, \quad W_5 = W_{35}, \quad W_6 = (3/4)^{1/2}W_4.$$

This says that  $R_{ia} = R_{ic} = R_{ie}$  ( $i=1 \dots 5$ ). For a single  $Z_L$  and  $k$  value, this equivalence of radial integrals holds, while for distinct  $Z_L$  and  $Z_L'$  and different  $k$  values, the integrals are not identical. The differences are slight as seen from Table II, and the approximations are quite reasonable. A corrected coupling scheme

<sup>19</sup> C. Snow, Nat. Bur. Standards (U.S.), Applied Math. Series 19 (U. S. Government Printing Office, Washington, D. C., 1952).

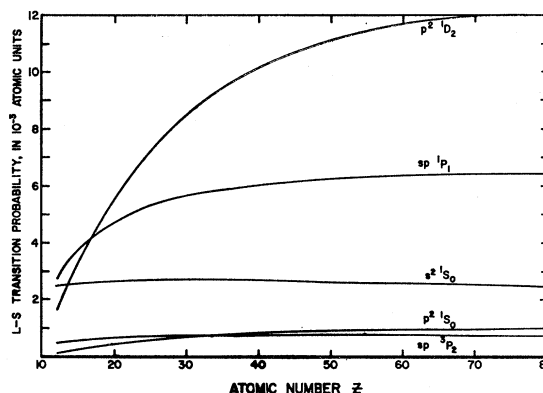


FIG. 3. Variation of  $KLL$  Auger transition probabilities in Russell-Saunders ( $L-S$ ) coupling, with atomic number ( $Z$ ).

could be obtained, but the smallness of the differences indicate that these transition probabilities would be relatively unaffected.

The progression with increasing  $Z$  of the transition probabilities is seen to be quite smooth, as shown on Fig. 3. The increase with  $Z$  of the  $^1D_2$  and  $^1P_1$  amplitudes is much greater than for the others. The  $^1S_0$  amplitudes stay fairly constant with  $Z$ . There is also seen a levelling-off of all amplitudes for high  $Z$ , rather than a continuous increase toward the values for the unscreened hydrogenic case. The values for the pure hydrogenic case  $Z=1$  represent an ultimate limit as  $Z \rightarrow \infty$ , since  $\bar{r}=0$  for this case, and higher  $Z$  atoms tend toward  $\bar{r} \rightarrow 0$  in the limit. However, in the present computations the loss of this tendency toward  $Z=1$  values is seen around  $Z=50$ . The reason appears to be due to the fact that the Auger energies are derived from the energy levels. These energy levels are lowered due to relativistic effects. Thus, there is an indication of the effect on the Auger transition rate due to relativistic effects, although the computations are not relativistic. For  $Z=80$ , the lowering from  $Z=1$  values is of the order of 40% for the  $p^2$  terms, about 15% for the  $sp$  terms, and does not appear for the  $s^2$  term. In absolute value, however, only in the case of  $Z=80$  is there any actual decline in any of the transition rates other than  $KL_1L_1$ . This decline is quite small, being of the order of  $2 \times 10^{-5}$  atomic units, or about 1% of the transition rate for this case.

The case of  $KL_1L_1$  is somewhat different; the transition rate going through a broad and shallow maximum at about  $Z=23$ . This maximum is only about 10% higher than either the low- or high- $Z$  limit values for the transition. It is a true maximum however, since the variations are considerably greater than would be due to computation errors, or expected errors in  $Z^*$  or  $k$  values. A variation of 0.1 unit in  $Z^*$  or  $k$  would only result in a difference of 1%, rather than the 10% found. The reason for this maximum occurring at  $Z=23$  is not understood. This point deserves further study.

In addition to the transition amplitudes, the total

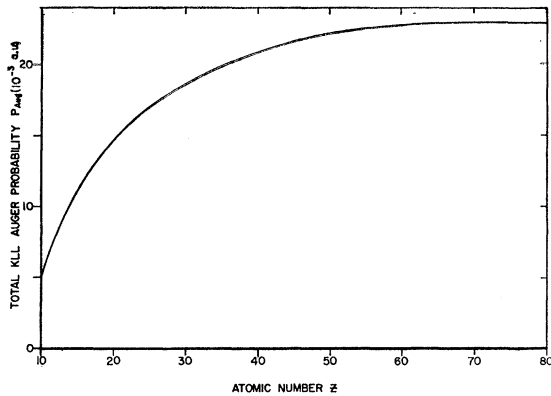


FIG. 4. Total *KLL* Auger Transition probability as a function of atomic number (*Z*).

*KLL* Auger probability was computed using the relation

$$P_{\text{Aug}} = W_1^2 + 6(W_2^2 + W_6^2 - W_2W_6) + 3W_3^2 + 10W_6^2.$$

It is shown in Fig. 4 where the saturation effect with increasing *Z* is seen clearly. The total probabilities are independent of the coupling model and are used later in the computation of fluorescence yields.

Although the *K*-shell transition rates are not grossly sensitive to variations in *Z*, there is sufficient change to warrant a study of the effects due to differences in *Z*\* and *k* from their true values. The anticipated errors in *Z*\* or *k* are only of the order of 0.1, or at most 0.2 unit. Since the variations in transition rates are not great, it was decided to examine them for changes in *Z*\* and *k* of 0.5 unit so as to magnify the variations and to set outside limits on the computed transition rates for a given *Z*. *Z*\* and *k* were varied independently by 0.5 unit and also the value of *Z<sub>K</sub>* was increased independently by 0.1 unit. The transition rates were then computed for the cases *Z*=20, 40, 47, and 80, for each of these changes. The radial integrals *R<sub>ia</sub>* (*i*=1...5) for these cases are given in Table III. The variations for *R<sub>ib</sub>* and *R<sub>ic</sub>* are essentially the same as for *R<sub>ia</sub>*. The results show the variations to be far greater than the normal changes which occur in successive *Z* values, although still of small absolute magnitude. It is also seen that some transitions like *KL<sub>1</sub>L<sub>2</sub>* (*R<sub>2</sub>*) are more sensitive to changes in *k* than *Z*\*, while others such as *KL<sub>3</sub>L<sub>3</sub>* (*R<sub>4</sub>*) are more sensitive to changes in *Z*\* than changes in *k*.

#### COMPARISON WITH OTHER RESULTS

It has been shown that the *K*-shell Auger transition probabilities increase with increasing *Z* for all transitions except *KL<sub>1</sub>L<sub>1</sub>*. This differs from the results for the unscreened hydrogenic case, where the Auger probabilities would be independent of *Z*. As a check on the computations, the rates for *Z*=1 were computed and found to agree closely with those of Geffrion and Nadeau.<sup>4</sup> The total *KLL* Auger probability for this case was identical with theirs to the sixth significant

figure. For other values of *Z* there are few reported values of the transition probabilities. Therefore, the earlier values of Burhop<sup>10</sup> were checked for the case of silver (*Z*=47), both for the values chosen for *Z*\* and *k*, and for the present values for these constants. Additionally, the results for the same *Z* from the self-consistent-field values of Rubinstein and Snyder as quoted by Asaad<sup>6</sup> are compared. They are in terms of the radial integrals, as follows:

	B <sub>0</sub>	B <sub>1</sub>	R-S	C
<i>R<sub>1</sub></i>	0.0504	0.05043	0.0438	0.05066
<i>R<sub>2</sub></i>	0.0433	0.04254	0.0389	0.04043
<i>R<sub>3</sub></i>	0.0832	0.07548	0.0669	0.07121
<i>R<sub>4</sub></i>	0.1551	0.14892	0.1602	0.12771
<i>R<sub>5</sub></i>	-0.0564	-0.05984	-0.0645	-0.05127

Here B<sub>0</sub> and B<sub>1</sub> are the Burhop original and recomputed values, R-S is the Rubinstein-Snyder value, and C is the value obtained in the present work; all in atomic units. The comparison is interesting in showing the divergence between these values for cases of different total angular momentum. For *L*=1 (*KL<sub>2</sub>L<sub>2</sub>* and *KL<sub>1</sub>L<sub>3</sub>*), the present values are higher than the R-S values and closer to the Burhop results, while for *L*=2 (*KL<sub>2</sub>L<sub>2</sub>*, *KL<sub>2</sub>L<sub>3</sub>*, and *KL<sub>3</sub>L<sub>3</sub>*) the present values are lower than the R-S ones. For the case of Hg<sup>80</sup>, the pattern holds for the Asaad<sup>6</sup> (A) and present values, but is more marked. The transition rates differ by about 50% for the *L*=2 case, and about 10% for the *L*=1 case, for this atom.

TABLE III. Variations in radial integral values with changes in *Z*\* and *k* for *KLL* Auger transitions.<sup>a</sup>

Case <sup>b</sup>	<i>R<sub>1</sub></i> <sup>2</sup>	<i>R<sub>2</sub></i> <sup>2</sup>	<i>R<sub>3</sub></i> <sup>2</sup>	<i>R<sub>4</sub></i> <sup>2</sup>	<i>R<sub>5</sub></i> <sup>2</sup>
<i>Z</i> =20					
Basic	261 851	133 450	360 774	844 395	131 706
A	249 701	124 705	359 325	774 720	120 186
B	274 453	142 733	360 459	918 960	144 189
C	261 132	138 401	391 257	991 980	155 601
D	261 039	127 613	330 624	712 155	110 394
E	263 760	134 096	356 247	834 195	130 113
<i>Z</i> =40					
Basic	259 050	160 621	490 275	1 527 570	244 746
A	254 142	156 277	491 823	1 469 940	234 558
B	264 010	165 050	488 124	1 586 865	255 303
C	256 871	161 788	505 701	1 630 995	261 774
D	260 900	159 194	474 786	1 428 255	228 402
E	260 173	161 102	487 314	1 519 080	243 459
<i>Z</i> =47					
Basic	256 597	163 488	507 150	1 631 010	262 881
A	252 572	159 827	508 779	1 579 215	253 638
B	260 653	167 206	505 071	1 684 050	272 412
C	254 623	164 331	520 236	1 722 150	277 947
D	258 338	162 456	494 001	1 542 840	248 310
E	257 559	163 915	504 549	1 623 390	261 720
<i>Z</i> =80					
Basic	249 322	167 146	549 765	1 801 320	299 979
A	247 162	165 068	550 935	1 768 170	293 859
B	251 490	169 239	548 442	1 834 935	306 207
C	248 065	167 500	557 541	1 856 955	309 384
D	250 506	166 728	541 962	1 746 690	290 736
E	249 888	167 409	548 145	1 796 595	299 250

<sup>a</sup> All values are in units of 10<sup>-8</sup> atomic unit. Basic values are for *ZL* and *k* as chosen for atomic number *Z*.

<sup>b</sup> A—values for *k*+½; B—values for *k*-½; C—values for *ZL*+½; D—values for *ZL*-½; E—values for *Z<sub>K</sub>*+0.1.

Further comparison with the results of Ramberg and Richtmyer<sup>20</sup> (R-R) for Au<sup>79</sup> shows the following, in  $10^8$  atomic units:

	A	R-R	C
$KL_1L_1$	2.034	2.021	2.493
$KL_1L_{2,3}$	4.992	7.093	7.965
$KL_{2,3}L_{2,3}(l_\infty=0)$	1.492	1.433	1.000
$KL_{2,3}L_{2,3}(l_\infty=2)$	16.328	17.824	12.009

The R-R results are for a Thomas-Fermi field; the A for a self-consistent field, and the present for screened hydrogenic functions. It is not clear why the large discrepancy in the  $l_\infty=2$  case arises; it would be necessary to increase  $Z_L$  by about two units to raise the  $R_4$  value close to that for the R-R and R-S cases, but this seems an unlikely correction. The lower values now found for the  $KL_{2,3}L_{2,3}$  transitions are closer to the observed relative intensities, although still high by a factor of about 2. The intensity values are also in general agreement as to order, but not as to numerical values, with the experimental results of Sokolowski and Nordling<sup>21</sup> for Cu and Ge, both for the present results and those of reference 2. Use of the present transition probabilities in intermediate coupling has not been accomplished, but could result in closer agreement with these experimental values.

Comparison of these probabilities in  $L-S$  coupling with those done relativistically is of interest. In the nonrelativistic case, the transitions of total angular momentum  $L=0$ , or the  $s^2\ ^1S_0$  cases are close to their  $Z=1$  value throughout, while the  $sp\ ^1P_1$  and  $^3P$  cases reach about 85% of their  $Z=1$  values at  $Z=50$ , and the  $L=2$  transitions  $p^2\ ^1D_2$  and  $^1S_0$  have reached only about 50% of the  $Z=1$  value at  $Z=50$ . The  $L=2$  transitions level off considerably more than do the  $L=1$  transitions, but they are higher in actual value than the  $L=1$  transitions for all  $Z$  above about 18. In the relativistic case, the reverse is true,<sup>6</sup> the  $L=1$  lines being stronger than the  $L=2$  lines for Hg<sup>80</sup>. Asaad discusses this reversal which appears to be due to lowering of the Coulomb integrals when treated in relativistic fashion. The relativistic increase in the  $KL_1L_1$  transition rate markedly lowers the ratios of intensities of other lines, in agreement with experiment.

The unscreened hydrogenic  $Z=1$  case represents a limiting case for high  $Z$  when there are no relativistic corrections. For the lighter atoms particularly, the differences between the transition rates found here and those for  $Z=1$  are rather large. The rates are much lower for lighter atoms and tend to zero for all but  $KL_1L_1$ , as would be expected. As a measure of comparison, the  $K$ -shell fluorescent yields were computed for some atoms using the present Auger transition rates. The scheme of computation was to take the present rate, assume a value for the  $KLX/KLL$  ratio, and thus obtain the total  $K$  Auger probability. This ratio varies considerably with  $Z$ , being about 0.4 for  $Z$  near 40 and

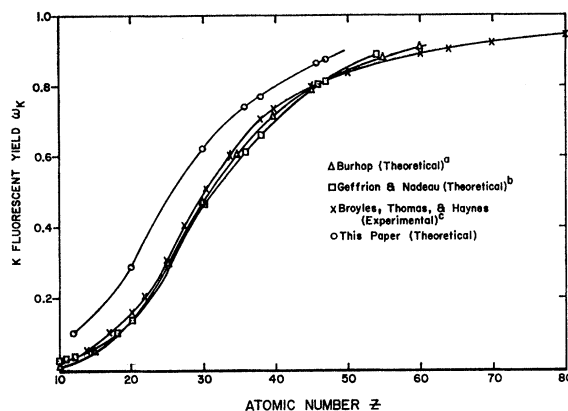


FIG. 5. Comparison of  $K$ -shell fluorescent yields ( $\omega_K$ ) with atomic number ( $Z$ ).  $\Delta$  represent values from Burhop (reference 23);  $\square$  represent values from Geffrion and Nadeau (reference 4);  $\times$  represent values from experimental curves given by Broyles *et al.* (reference 22); and  $\circ$  represent present values.

about 0.8 for  $Z$  near 60.<sup>22</sup> The  $KXY$  values were not computed, and would add to the total  $K$  rate. Geffrion and Nadeau also computed the  $K$ -shell fluorescent yields,<sup>4</sup> based on the hydrogenic transition rates. Their total transition rates would correspond to a  $(KLY+KXY)/KLL$  ratio value about 1.0. For comparison it was decided to use their ratio, and also their values for the radiative transition probabilities. The results are plotted on Fig. 5, together with those of Geffrion and Nadeau, and the values given by Burhop.<sup>23</sup> The experimental value curve given by Broyles *et al.*<sup>22</sup> is also shown. It is seen that the present results are higher than the other curves. Since the  $Z=1$  case represents an upper limit for the nonrelativistic transition probabilities, the  $K$ -shell fluorescent yields computed from it represent lower limits to the actual values. As the Auger rates obtained here are lower than for  $Z=1$  at the same time that the  $\omega_K$  values are too high, the indication is that the radiative transition probabilities computed on the hydrogenic basis are also too high. Although values for the  $1s-2p$  oscillator strengths are rather scarce in the literature for medium- and high- $Z$  atoms, generally they are found to be considerably lower than those for hydrogen. In Bethe and Salpeter<sup>8</sup> the actual oscillator strengths for alkali doublets are quoted as between 10 and 100 times lower than the comparable hydrogenic ones. Such a lowering of the radiative probabilities would lead to lowering of the  $\omega_K$  values.

#### ACKNOWLEDGMENTS

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<sup>21</sup> E. Sokolowski and C. Nordling, Arkiv Fysik **14**, 557 (1959).

<sup>22</sup> C. Broyles, D. Thomas, and S. Haynes, Phys. Rev. **89**, 715 (1953).

<sup>23</sup> E. Burhop, J. phys. radium **16**, 625 (1955).