158, 34 (1967); R. F. Gentner and E. A. Burke, Phys. Rev. **176,** 63 (1968).
[10]J. S. Sims and S. Hagstrom, Phys. Rev. A **4,** 908 (1971).
[11]T. Kinoshita, Phys. Rev. **105,** 1490 (1957); C. L. Pekeris, Phys. Rev. **112,** 1649 (1958); C. Schwarz, Phys. Rev. **128,** 1146 (1962); A. M. Ermolaev and G. B. Sochilin, Dokl. Akad. Nauk Uzb. SSR **155,** 1050 (1964) [Sov. Phys.-Dokl. **9,** 292 (1964)]; K. Frankowski and C. L. Pekeris, Phys. Rev. **146,** 46 (1966).
[12]J. C. Slater, Phys. Rev. **31,** 333 (1928).
[13]T. Kato, Commun. Pure Appl. Math. **10,** 151 (1957).
[14]S. Larsson and V. H. Smith, Jr., Int. J. Quantum Chem. **6,** 1019 (1972).
[15]R. A. Sack, J. Math. Phys. **5,** 245 (1964).
[16]A. Weiss, Astrophys. J. **138,** 1262 (1963).
[17]C. L. Pekeris, Phys. Rev. **126,** 143 (1962).
[18]I. Johansson, Ark. Fys. **15,** 169 (1959).
[19]C. W. Scherr, J. N. Silverman, and F. A. Matsen, Phys. Rev. **127,** 830 (1962).
[20]S. Larsson and V. H. Smith, Jr., Phys. Rev. **178,** 137 (1969).
[21]P. O. Löwdin, Phys. Rev. **97,** 1474 (1955).
[22]S. Larsson, Phys. Rev. A **2,** 1248 (1970).
[23]J. D. Lyons and T. P. Das, Phys. Rev. A **2,** 2250 (1970).
[24]J. D. Lyons, R. T. Pu and T. P. Das, Phys. Rev. **178,** 103 (1959).
[25]R. K. Nesbet, Phys. Rev. A **2,** 661 (1970); J. D. Lyons and R. K. Nesbet, Phys. Rev. Lett. **24,** 433 (1970).
[26]S. Hameed and H. M. Foley, Phys. Rev. A **6,** 1399 (1972).
[27]R. J. S. Crossley, in *Advances in Atomic and Molecular Physics,* edited by D. R. Bates (Academic, New York, 1969), Vol. 5, p. 237.
[28]O. S. Heavens, J. Opt. Soc. Am. **51,** 1058 (1961); D. R. Bates and A. Damgaard, Philos. Trans. R. Soc. Lond. **242,** 101 (1949). A slightly incorrect normalization is used in these works, see Ref. 27, p. 269.
[29]K. C. Brog, T. G. Eck, and H. Wieder, Phys. Rev. **153,** 91 (1967).

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K-LL Auger Transition Probabilities for Elements with Low and Intermediate Atomic Numbers*†

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Radiationless K-LL transition probabilities have been calculated nonrelativistically in j-j coupling and in intermediate coupling, without and with configuration interaction, for elements with atomic numbers $13 \leq Z \leq 47$. The system is treated as a coupled two-hole configuration. The single-particle radial wave functions required in the calculation of radial matrix elements, and in the calculation of mixing coefficients in the intermediate-coupling scheme, were obtained from Green's atomic independent-particle model. Comparison with previous theoretical work and with experimental data is made. The effects of intermediate coupling, configuration interaction, and relativity are noted. Agreement of the calculated Z dependence of K-LL relative intensities with experiment has been somewhat improved.

I. INTRODUCTION

The K-LL Auger spectrum is the simplest Auger spectrum and has been thoroughly studied both experimentally and theoretically. The theoretical work is surveyed in the review article of Bambynek *et al.*[1]; the experimental relative intensities of K-LL Auger transitions have been compiled by Ramsdale.[2] In a recent thorough review of K-shell Auger spectra, Geiger[3] conclusively demonstrated the importance of relativistic effects for intermediate and high Z. The relative intensities of K-LL Auger lines calculated in LS or j-j coupling agree poorly with experiment.[4-7] Application of the intermediate-coupling scheme in the calculation of the K-LL Auger spectrum by Asaad and Burhop[4] and Asaad[5] modified the usual six-line K-LL spectrum expected in j-j coupling into a nine-line spectrum. The predicted nine K-LL lines were observed from several elements of intermediate atomic number.[8-14] Although the inclusion of the effects of intermediate coupling and configuration interaction in the calculation of K-LL Auger transition probabilities improved agreement with experimental data on relative intensities,[4-7] discrepancies remained even at relatively low Z which could be due to the inaccuracy of the transition amplitudes used in the early calculations.[4-7] To test this hypothesis, we have recalculated the K-LL Auger transition probabilities in j-j coupling, and in intermediate coupling without and with configuration interaction, for elements with atomic numbers $13 \leq Z \leq 47$, using wave functions determined from Green's atomic independent-particle model (IPM).[15] The central IPM potential provides a complete and orthogonal basis set for all the electrons in an atom. Although it contains only two adjustable parameters (one established for the entire periodic table, the other, adjusted for each element), it has proved

TABLE I. Radial matrix elements for K-LL Auger transitions, in atomic units.[a]

Element	$\{(2s)^2, 0, 0\}$	$\{(2s)(2p), 0, 1\}$	$\{(2p)(2s), 1, 1\}$	$\{(2p)^2, 1, 0\}$	$\{(2p)^2, 1, 2\}$
$_{13}$Al	0.033 33	0.027 736	0.044 256	−0.042 160	0.107 61
$_{15}$P	0.035 169	0.029 619	0.047 902	−0.045 841	0.116 40
$_{18}$Ar	0.036 874	0.031 472	0.051 096	−0.049 731	0.125 15
$_{20}$Ca	0.037 885	0.032 464	0.053 193	−0.051 674	0.129 75
$_{23}$V	0.038 898	0.033 547	0.055 675	−0.053 788	0.135 13
$_{25}$Mn	0.039 480	0.034 172	0.057 025	−0.055 049	0.138 20
$_{28}$Ni	0.040 257	0.034 989	0.058 799	−0.056 750	0.142 01
$_{30}$Zn	0.040 746	0.035 505	0.059 745	−0.057 889	0.144 59
$_{33}$As	0.041 369	0.036 086	0.061 134	−0.058 959	0.147 12
$_{35}$Br	0.041 738	0.036 436	0.061 929	−0.059 596	0.148 63
$_{40}$Zr	0.042 465	0.037 094	0.063 604	−0.060 704	0.151 27
$_{47}$Ag	0.043 457	0.038 031	0.065 825	−0.062 216	0.155 47

[a] Matrix elements are denoted in the conventional manner by $\{(nl)(n'l'), \nu, l_A\}$, where the quantum numbers n, l characterize the electron that fills the initial vacancy, and n', l', the electron that is ejected (in the direct transition) into a continuum state of angular momentum $l_A\hbar$. In the exchange transition, these quantum numbers are interchanged. The integer ν characterizes the pertinent term in the expansion of the Coulomb interaction potential in scalar products of irreducible tensor operators (see, e.g., Ref. 1).

to be accurate, versatile, and very convenient for the calculation of radiationless transition probabilities.[16,17] We compare the results with other theoretical predictions and with experimental information.

II. THEORY

The radiationless transition probabilities were calculated nonrelativistically in the customary manner, with the Coulomb interaction between two electrons treated as a perturbation. The hole representation of the system consisted in assuming that the initial inner-shell hole is coupled to a hole in the continuum representing the missing Auger electron, and the two final inner-shell vacancies are coupled. The holes were described by single-particle wave functions.

Spherical symmetry of the potential was assumed, so that the Auger matrix elements could be separated into angular and radial factors. The single-particle radial wave functions required in the calculation of radial factors were obtained by solving the Schrödinger equation numerically in the analytic potential of Green's atomic independent-particle model.[15] Details of the calculation have been described elsewhere.[16]

The theory of intermediate coupling and configuration interaction as applied to K-LL Auger transitions has been worked out by Asaad and Mehlhorn[5-7]; the reader is referred to their papers for details.

Numerical values of the mixing coefficients in the intermediate coupling scheme without configuration interaction were calculated in the present work; configuration-interaction mixing coefficients were taken from Mehlhorn and Asaad.[7]

III. RESULTS AND DISCUSSION

A. Radial Matrix Elements

The numerical values of the radial matrix elements for radiationless K-LL transitions are listed in Table I for 12 elements with atomic numbers $13 \leq Z \leq 47$.

For comparison with the results of Walters and Bhalla,[18] the matrix elements of the present work must be divided by $(2\pi)^{1/2}$, due to a difference in the normalization of the continuum-state wave functions. Walters and Bhalla[18] used wave functions determined from a Hartree-Fock-Slater (HFS) approach with Kohn-Sham and Gaspar exchange. The present results agree with those of Walters and Bhalla to better than 3% for all matrix elements.

B. K-LL Auger Transition Probabilities

Numerical values of the various K-LL Auger transition probabilities in j-j coupling and in intermediate coupling without and with configuration interaction are listed in Tables II, III, and IV. The total K-LL transition probabilities are plotted in Fig. 1 as a function of atomic number. For

TABLE II. K-LL Auger transition probabilities (in multiples of 10^{-3} a.u.),[a] calculated in j-j coupling.

Element	K-L_1L_1	K-L_1L_2	K-L_1L_3	K-L_2L_2	K-L_2L_3	K-L_3L_3	TOTAL
$_{13}$Al	1.111	1.156	2.311	0.198	5.146	2.965	12.887
$_{15}$P	1.237	1.319	2.637	0.234	6.024	3.477	14.927
$_{18}$Ar	1.360	1.490	2.977	0.275	6.960	4.025	17.087
$_{20}$Ca	1.435	1.586	3.168	0.297	7.480	4.328	18.295
$_{23}$V	1.513	1.696	3.387	0.322	8.114	4.690	19.722
$_{25}$Mn	1.559	1.760	3.515	0.338	8.487	4.904	20.564
$_{28}$Ni	1.621	1.847	3.687	0.360	8.975	5.187	21.676
$_{30}$Zn	1.660	1.903	3.798	0.375	9.306	5.378	22.420
$_{33}$As	1.711	1.968	3.925	0.390	9.638	5.566	23.199
$_{35}$Br	1.742	2.007	4.002	0.399	9.839	5.680	23.668
$_{40}$Zr	1.803	2.084	4.150	0.415	10.201	5.878	24.531
$_{47}$Ag	1.889	2.195	4.365	0.438	10.790	6.191	25.868

[a] One atomic unit (a.u.) $=4.134\times10^{16}$ sec^{-1} $=27.212$ eV/$\hbar$.

comparison, the results of McGuire,[19] Walters and Bhalla,[18,20] and Ramsdale[2] are also indicated. McGuire's work[19] is based on a Hartree-Slater calculation with straight-line approximation to the Herman-Skillman[21] potential, so that the radial wave equation can be solved exactly in terms of Whittaker functions. Ramsdale's calculation[2] is based on the relativistic HFS model. The results from the present work are quite consistent with those of Walters and Bhalla[18,20] and of Ramsdale,[2] but McGuire's results[19] exceed those of the present calculation by 10–30% for $22 \leq Z \leq 47$.

Individual probabilities of the six K-LL Auger transitions in j-j coupling are compared with the results of other calculations in Figs. 2 and 3. From these comparisons, one can draw the following conclusions:

(1) The results of the present work agree well with Rubenstein's self-consistent field calculation,[22] except for K-L_2L_3 and K-L_3L_3 transitions, but differ drastically from Callan's results[23] derived from screened hydrogenic single-particle wave functions.

(2) The K-L_1L_1 and K-L_1L_2 transition probabilities are strongly modified by relativistic effects. Relativity becomes important for elements heavier

TABLE III. K-LL Auger transition probabilities (in multiples of 10^{-3} a.u.), calculated in intermediate coupling.

Element	K-L_1L_1	K-L_1L_2		K-L_1L_3		K-L_2L_2	K-L_2L_3	K-L_3L_3	
	$(^1S_0)$	$(^1P_1)$	$(^3P_0)$	$(^3P_1)$	$(^3P_2)$	$(^1S_0)$	$(^1D_2)$	$(^3P_0)$	$(^3P_2)$
$_{13}$Al	a	2.707	0.084	0.251	0.422	0.591	7.701	0.001	0.019
$_{15}$P		3.115	0.093	0.281	0.466	0.697	8.977	0.003	0.056
$_{18}$Ar		3.522	0.104	0.319	0.521	0.810	10.251	0.014	0.191
$_{20}$Ca		3.765	0.109	0.340	0.543	0.859	10.863	0.031	0.360
$_{23}$V		4.031	0.112	0.378	0.562	0.880	11.414	0.084	0.759
$_{25}$Mn		4.166	0.115	0.421	0.575	0.868	11.623	0.142	1.110
$_{28}$Ni		4.297	0.118	0.529	0.592	0.815	11.739	0.259	1.706
$_{30}$Zn		4.326	0.122	0.646	0.608	0.772	11.814	0.345	2.124
$_{33}$As		4.265	0.123	0.887	0.617	0.701	11.747	0.458	2.683
$_{35}$Br		4.163	0.125	1.098	0.625	0.661	11.706	0.523	3.021
$_{40}$Zr		3.766	0.126	1.711	0.630	0.587	11.558	0.641	3.697
$_{47}$Ag		3.257	0.129	2.526	0.645	0.539	11.674	0.751	4.440

[a] See Table I; the K-L_1L_1 transition probability is independent of the coupling scheme.

TABLE IV. K-LL Auger transition probabilities (in multiples of 10^{-3} a.u.), calculated in intermediate coupling with configuration interaction.

Element	K-L_1L_1	K-L_1L_2		K-L_1L_3		K-L_2L_2	K-L_2L_3	K-L_3L_3	
	$(^1S_0)$	$(^1P_1)$	$(^3P_0)$	$(^3P_1)$	$(^3P_2)$	$(^1S_0)$	$(^1D_2)$	$(^3P_0)$	$(^3P_2)$
$_{13}$Al	0.826	a		a		0.877	a	0.001	a
$_{15}$P	0.864					1.068		0.005	
$_{18}$Ar	0.955					1.212		0.017	
$_{20}$Ca	0.992					1.287		0.046	
$_{23}$V	1.073					1.269		0.136	
$_{25}$Mn	1.120					1.227		0.222	
$_{28}$Ni	1.250					1.117		0.327	
$_{30}$Zn	1.286					1.064		0.428	
$_{33}$As	1.340					0.955		0.575	
$_{35}$Br	1.382					0.893		0.652	

[a] See Table III; these transition probabilities are not affected by configuration interaction.

than bromine ($Z=35$) in K-L_1L_1 transitions and zirconium ($Z=40$) in K-L_1L_2 transitions. This conclusion agrees with Ramsdale's observation.[2]

(3) For K-L_1L_3, K-L_2L_2, and K-L_2L_3 transitions, relativistic effects are small for atomic numbers below $Z=50$. Results of the present calculation and Ramsdale's relativistic HFS results[2] are quite consistent for these transition probabilities.

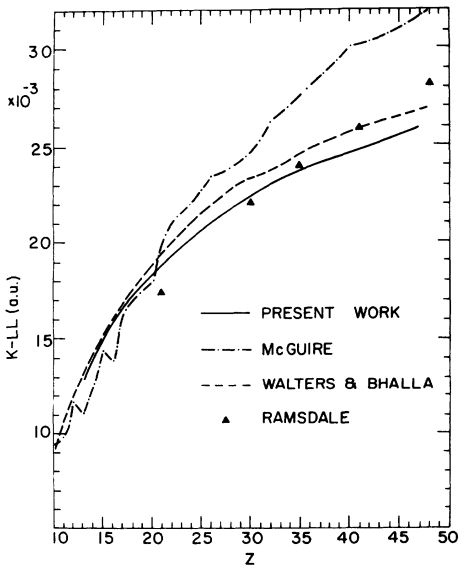

FIG. 1. Theoretical total K-LL Auger transition probability as a function of atomic number. The results from the present calculation are compared with those of McGuire (Ref. 19), Walters and Bhalla (Ref. 20), and Ramsdale (Ref. 2).

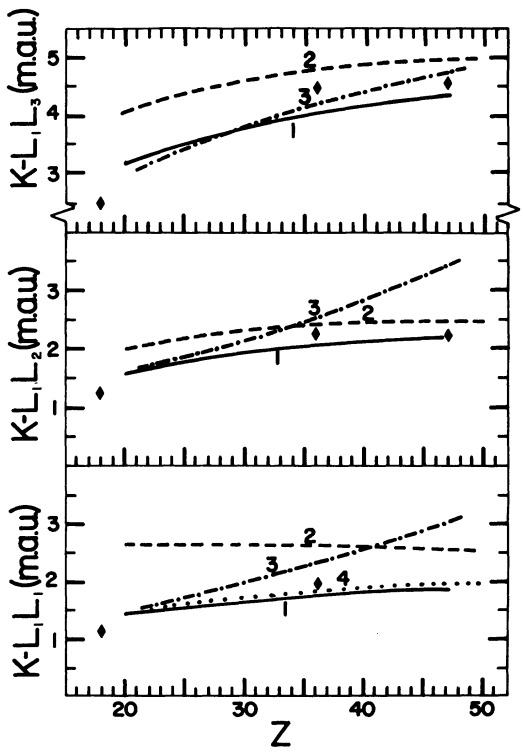

FIG. 2. Theoretical K-L_iL_j Auger transition probabilities (in milli-atomic-units), in j-j coupling, as functions of atomic number. Curves indicate 1: present results; 2: Callan's results from screened hydrogenic wave functions (Ref. 23); 3: Ramsdale's relativistic HFS calculation (Ref. 2); 4: nonrelativistic HFS calculation of Walters and Bhalla (Ref. 20). Diamonds represent Rubenstein's predictions from nonrelativistic Hartree wave functions (Ref. 22).

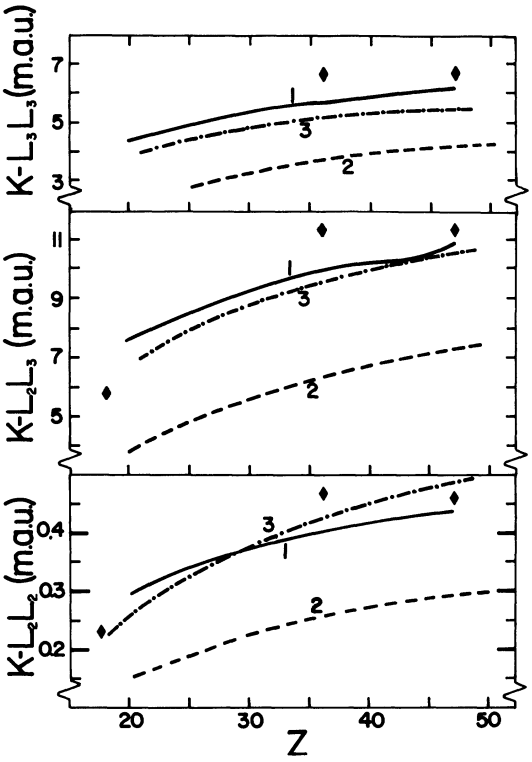

FIG. 3. Theoretical K-L_2L_1 and K-L_3L_3 Auger transition probabilities (in milli-atomic-units), in j-j coupling, as functions of atomic number. The key is as in Fig. 2.

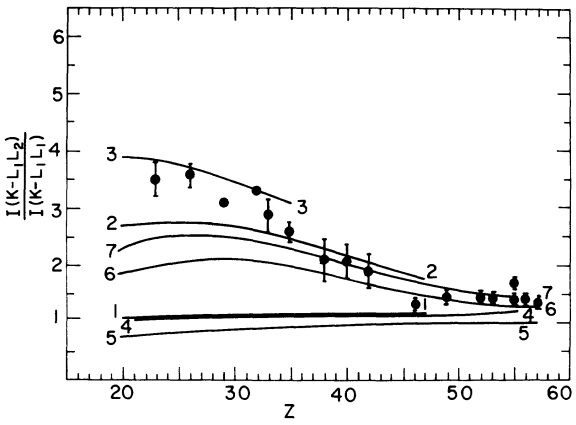

FIG. 4. Intensity of the K-L_1L_2 transition relative to the K-L_1L_1 transition, as a function of atomic number. Dots represent experimental data (reproduced from Ref. 2). The curves indicate theoretical ratios from 1: present work, in j-j coupling; 2: present work, in intermediate coupling; 3: present work, in intermediate coupling with configuration interaction; 4: relativistic HFS calculation in j-j coupling by Ramsdale (Ref. 2); 5: nonrelativistic calculation in j-j coupling by Callan, with screened hydrogenic wave functions (Ref. 23); 6: nonrelativistic calculation in intermediate coupling by Asaad using Callan's amplitudes (Ref. 5); 7: nonrelativistic calculations in intermediate coupling with configuration interaction by Asaad (Ref. 6) and by Mehlhorn and Asaad (Ref. 7), based on Callan's amplitudes.

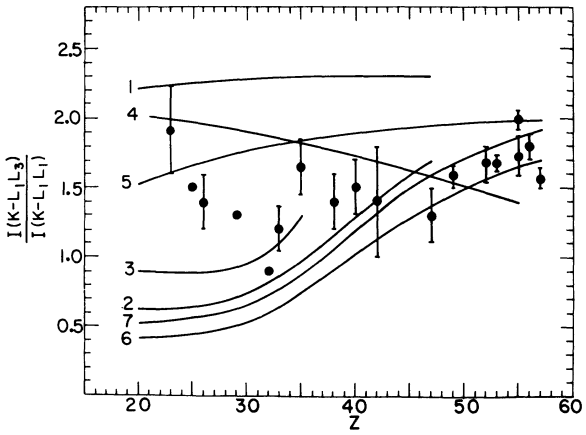

FIG. 5. K-L_1L_3 transition probability relative to the K-L_1L_1 transition probability, as a function of atomic number. The dots represent experimental data (reproduced from Ref. 2). Curves indicate theoretical ratios, keyed as in Fig. 4.

C. Relative Intensities of Individual K-LL Lines Compared with the K-L_1L_1 Line

The relative intensities in j-j coupling, intermediate coupling, and in intermediate coupling with configuration interaction are shown in Figs. 4 to 8. Intensity ratios from other theoretical calculations and from experimental data are also included. The following conclusions can be drawn from these figures:

(1) The effects of intermediate coupling and configuration interaction are very important in the determination of relative intensities for atomic numbers $20 \leq Z \leq 50$. This fact had been established previously.[5-7]

(2) The results from the present calculation

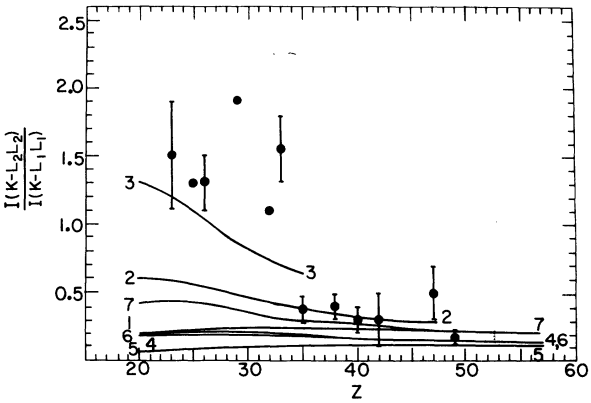

FIG. 6. K-L_2L_2 transition probability relative to the K-L_1L_1 transition probability, as a function of atomic number. Dots represent experimental data (taken from Ref. 2). Curves indicate theoretical ratios, keyed as in Fig. 4.

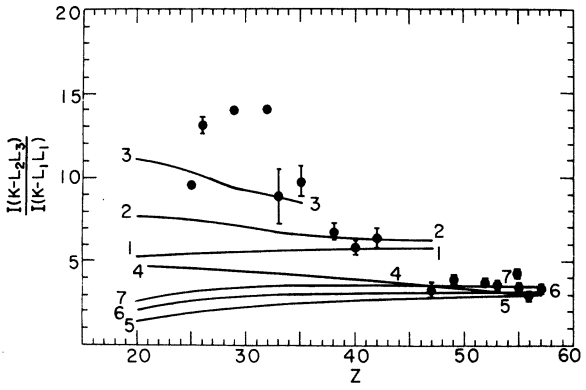

FIG. 7. K-L_2L_3 transition probability relative to the K-L_1L_1 transition probability, as a function of atomic number. Dots represent experimental data (reproduced from Ref. 2). Curves indicate theoretical ratios, keyed as in Fig. 4.

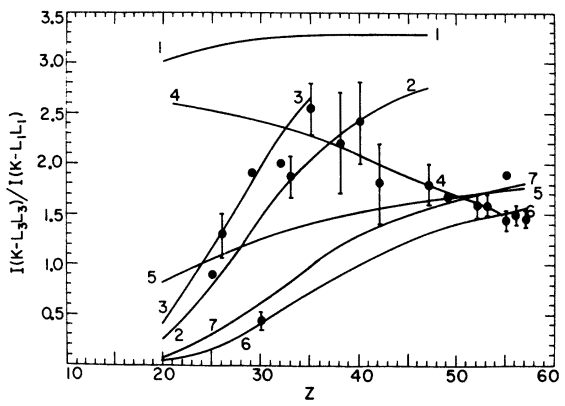

FIG. 8. K-L_3L_3 transition probability relative to the K-L_1L_1 transition probability, as a function of atomic number. Dots represent experimental ratios (reproduced from Ref. 2). Curves indicate theoretical ratios, keyed as in Fig. 4.

using intermediate coupling with configuration interaction agree better with experimental intensity ratios for $20 \leq Z \leq 35$ than other theoretical results. However, owing to the neglect of relativistic effects, the intensity ratios $I(KL_3L_3)/I(KL_1L_1)$ and $I(KL_2L_3)/I(KL_1L_1)$ of the present calculation with intermediate coupling for elements with $35 \leq Z \leq 47$ display the wrong trend with Z, compared with experimental results.

(3) For elements heavier than tin ($Z = 50$), intensity ratios from the relativistic HFS calculation of Ramsdale[2] appear to agree best with experimental ratios.

D. Transition Probabilities to Final-State Configurations $(2s)(2p)^5$ and $(2s)^2(2p)^4$, Compared with Those to Configuration $(2s)^0(2p)^6$

These ratios are independent of the coupling scheme in the nonrelativistic calculation without configuration interaction. The results from the present work are compared with other theoretical predictions and with experimental results in Fig. 9. There is excellent agreement among the theoretical results without configuration interaction from the present work, from McGuire[19] and from Walters and Bhalla.[20] However, the Z dependence of these theoretical ratios shows a different trend from that displayed by the experimental results.

Inclusion of configuration interaction in the present calculations improves agreement with experimental data in the range of atomic numbers $20 \leq Z \leq 35$. Nonrelativistic calculations for elements heavier than bromine ($Z = 35$) are not accurate because of the neglect of important relativistic effects.

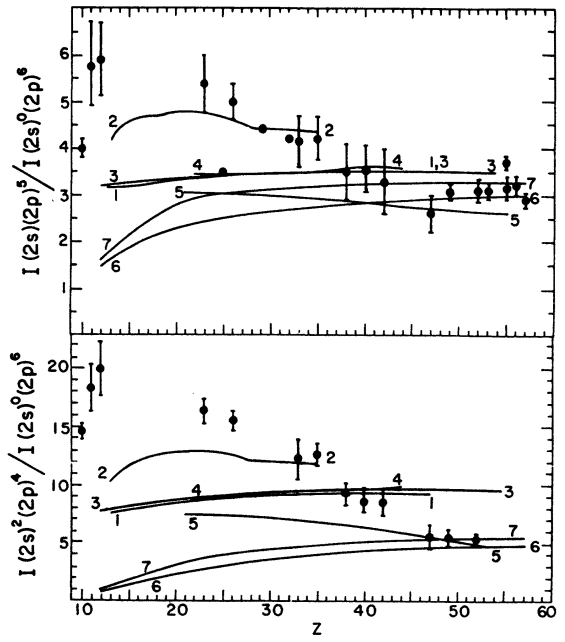

FIG. 9. The total K-LL transition probabilities to the final-state configurations $(2s)(2p)^5$ and $(2s)^2(2p)^4$, divided by those to the configuration $(2s)^0(2p)^6$. Dots indicate experimental ratios (reproduced from Ref. 2). Curves indicate theoretical ratios, 1: present work without configuration interaction; 2: present work with configuration interaction; 3: nonrelativistic HFS calculation in LS coupling by Walters and Bhalla (Ref. 20); 4: nonrelativistic Hartree-Slater calculation in LS coupling by McGuire (Ref. 19); 5: relativistic HFS calculation in j-j coupling by Ramsdale (Ref. 2); 6: nonrelativistic calculation in j-j coupling using screened hydrogenic wave functions, by Callan (Ref. 23); 7: nonrelativistic calculation with configuration interaction, using Callan's amplitudes, by Asaad (Ref. 6) and by Mehlhorn and Asaad (Ref. 7).

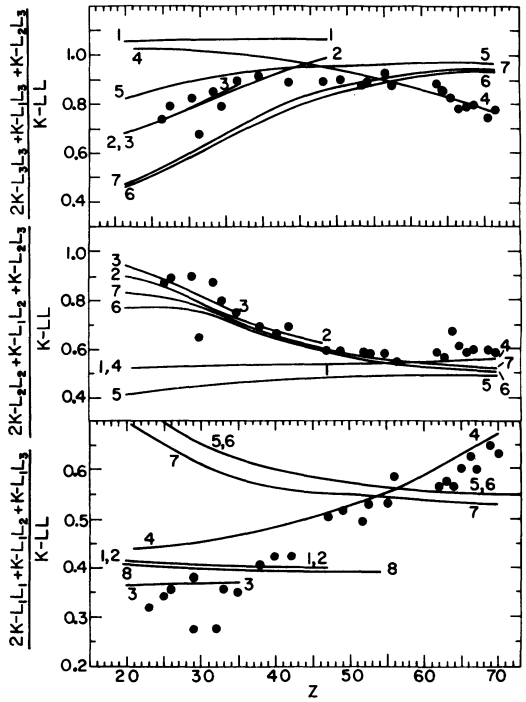

FIG. 10. The probability of producing an L_i-subshell vacancy, per K-LL transition, vs atomic number. The points are experimental ratios (reproduced from Ref. 24). Theoretical ratios are indicated by curves keyed as in Fig. 4. Curve 8 represents the results from a nonrelativistic HFS calculation by Walters and Bhalla (Ref. 20).

E. Probabilities of Producing an L_i-Subshell Vacancy Per K-LL Auger Transition

These probabilities have been discussed by Rao *et al.*[24] Good agreement is found between the results of the present calculation with intermediate coupling and configuration interaction and experimental values for $20 \leq Z \leq 35$, as illustrated in Fig. 10. Theoretical results from Ramsdale,[2] Walters and Bhalla,[20] Callan,[23] Asaad,[5,6] and Mehlhorn and Asaad[7] are included for comparison. For elements with atomic numbers above $Z = 50$, the predictions from the relativistic HFS calculation of Ramsdale[2] agree fairly well with experimental results.

IV. CONCLUDING REMARKS

Although agreement between theory and experiment has been improved by the present calculations of K-LL relative intensities, some discrepancies remain. It appears that the K-LL Auger spectra for atomic numbers $13 \leq Z \leq 60$ should be computed in intermediate coupling with configuration interaction, taking account of correlation effects. Above $Z = 35$, relativistic effects need to be taken into consideration, particularly in the L_1 shell.

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[1]W. Bambynek, B. Crasemann, R. W. Fink, H. U. Freund, Hans Mark, R. E. Price, P. Venugopala Rao, and C. D. Swift, Rev. Mod. Phys. **44**, 716 (1972).
[2]D. J. Ramsdale, Ph.D. thesis (Kansas State University, 1969) (unpubished).
[3]J. S. Geiger, in Inner-Shell Ionization Phenomena and Future Applications, Proceedings of the Atlanta Conference, edited by R. W. Fink, S. T. Manson, J. M. Palms, and P. Venugopala Rao, U.S. Atomic Energy Commission Report No. CONF-720404, 1973 (unpublished).
[4]W. N. Asaad and E. H. S. Burhop, Proc. Phys. Soc. Lond. **71**, 369 (1958).
[5]W. N. Asaad, Nucl. Phys. **44**, 399 (1963).
[6]W. N. Asaad, Nucl. Phys. **66**, 494 (1965).
[7]W. Mehlhorn and W. N. Asaad, Z. Phys. **191**, 231 (1966).
[8]G. T. Ewan, J. S. Geiger, R. L. Graham, and D. R. MacKenzie, Can. J. Phys. **37**, 174 (1959).
[9]G. T. Ewan, R. L. Graham, and L. Grodzins, Can. J. Phys. **38**, 163 (1960).
[10]G. T. Ewan and J. S. Merritt, Can. J. Phys. 38, 324 (1960).
[11]R. L. Graham and J. S. Merritt, Can. J. Phys. **39**, 1058 (1961).
[12]R. L. Graham, F. Brown, G. T. Ewan, and J. Uhler, Can. J. Phys. **39**, 1086 (1961).
[13]E. Sokolowski and C. Nordling, Ark. Fys. **14**, 557 (1959).
[14]R. L. Graham, I. Bergström, and F. Brown, Nucl. Phys. **39**, 107 (1962).
[15]A. E. S. Green, D. L. Sellin, and A. S. Zachor, Phys. Rev. **184**, 1 (1969).
[16]M. H. Chen and B. Crasemann, in Ref. 3, p. 43.
[17]L. I Yin, I. Adler, M. H. Chen, and B. Crasemann, Phys. Rev. A **7**, 897 (1973).
[18]D. L. Walters and C. P. Bhalla, At. Data 3, 301 (1971).
[19]E. J. McGuire, Phys. Rev. A **2**, 273 (1970).
[20]D. L. Walters and C. P. Bhalla, Phys. Rev. A **3**, 1919 (1971).
[21]F. Herman and S. Skillman, *Atomic Structure Calculations* (Prentice-Hall, Englewood Cliffs, N.J., 1963).
[22]R. A. Rubenstein, Ph.D. thesis (University of Illinois, 1955) (unpublished).
[23]E. J. Callan, Phys. Rev. **124**, 793 (1961).
[24]P. Venugopala Rao, M. H. Chen, and B. Crasemann, Phys. Rev. A **5**, 997 (1972).