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TOTAL AND PARTIAL ATOMIC-LEVEL WIDTHS*

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Total and partial atomic-level widths of the *K*-, *L*-, *M*-, and *N*-levels of the elements (covering *Z* up to 120 for *K*- and *L*-levels) are presented in graphic form. Graphs are based on theoretical predictions; total widths are natural level widths as governed by the rates of the various deexcitation processes for a single hole in that level. The drawings make possible, throughout the periodic table, a quick survey of the magnitude and trends of the total level widths, rates and yields of radiative, Auger, and Coster–Kronig processes, and widths of x-ray, Auger, and Coster–Kronig lines.

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INTRODUCTION

Until about 1970, there has been a definite lack of both experimental and theoretical data on total natural widths and their component partial widths for the atomic levels, except for the K- and L-shells. Recently however, a number of calculations[1-18] have been made covering inner levels up to the N-shell of all elements and, in several cases,[6,17] the elements $103 \leq Z \leq 120$. These calculations, most of which are based on the Herman-Skillman potential, and in some instances its relativistic version, provide us with a fair overall view of the behavior of level widths throughout the periodic table. As explained below, we have taken the theoretical predictions of Refs. 1–18 as input for our graphic representation of the total and partial level widths for the K-, L-, M-, and N-shells. The total widths are determined solely by the decay rates of a *single* hole in a given level and contain no possible contributions from other sources such as broadening by the presence of multiplets in atoms with partially filled shells.

Definitions, Relations, Conversion Factors

The natural line width Γ of a level is related to the lifetime τ of a single hole in that level by the Heisenberg uncertainty principle, namely

$$\Gamma\tau = \hbar \tag{1}$$

where $\hbar$ is the Planck constant. The transition rate $S_i = 1/\tau_i$ of a process i filling the hole is therefore

$$S_i = 1/\tau_i = \Gamma_i/\hbar \tag{2}$$

and

$$\sum_i S_i = \frac{1}{\hbar}\sum_i \Gamma_i \tag{3}$$

where Γ_i is the partial width corresponding to radiative, Auger, and Coster–Kronig processes that compete in filling a hole in a given level. Thus the total natural level width Γ is given by

$$\Gamma = \Gamma_R + \Gamma_A + \Gamma_C \tag{4}$$

where Γ_R = radiative width, Γ_A = Auger width, Γ_C = Coster–Kronig width.

Yields for the various processes are defined as follows.

Radiative or fluorescence yield	$\omega = \Gamma_R/\Gamma$	(5)
Auger yield	$a = \Gamma_A/\Gamma$	(6)
Coster–Kronig yield	$f = \Gamma_C/\Gamma$	(7)

According to (4) we have $\omega + a + f = 1$.

The width of an x-ray line is given by

$$\Gamma(X \rightarrow Y) = \Gamma(Y) + \Gamma(X) \tag{8}$$

where Y and X are the levels involved in the transition.

The width of an Auger or Coster–Kronig line is given by

$$\Gamma(X \rightarrow YZ) = \Gamma(X) + \Gamma(YZ) \tag{9}$$

or, approximately,

$$\Gamma(X \rightarrow YZ) \approx \Gamma(X) + \Gamma(Y) + \Gamma(Z) \tag{10}$$

where X is the initial single-hole and YZ is the final double-hole state, approximated in Eq. (10) by the sum of the corresponding single-hole states. For Auger transitions the levels Y and Z have a principal quantum number n different from that of the level X; for Coster–Kronig transitions at least one of the levels Y and Z has the same n as X.

Conversion factors are as follows:

Widths Γ:

$$1\ \mathrm{eV} = 1.6022 \times 10^{-19}\ \mathrm{J}$$
$$= 3.6748 \times 10^{-2}\ \mathrm{a.u.}$$
(atomic units of energy, hartrees)

Transition rate $S = 1/\tau$:

$$1\ \mathrm{eV}/\hbar = 1.6022 \times 10^{-19}\ \mathrm{J}/\hbar$$
$$= 1.5192 \times 10^{15}\ \mathrm{sec}^{-1}$$
$$= 3.6748 \times 10^{-2}\ (\mathrm{a.u.})^{-1}$$
(atomic units of time)

Experimental Data

Except for the K-level and the L-levels, experimental data on total level widths are virtually nonexistent. While data on K-level widths are fairly consistent, data on L-level widths may scatter considerably, often up to 100%. The experimental data collected by Sevier[20] cover the time period until about 1969. Additional data[21-24] obtained since then are referred to in Table I. Tables I and II also list recent reviews[7,20,25] that present data on widths and yields in graphic and tabular form.

Use of Graphs

The graphs are intended to provide a quick survey of the magnitude and trend of natural atomic-level widths, and partial level widths, which correspond to radiative and nonradiative decay modes. In particular, the following quantities can be readily obtained:

(a) total atomic-level widths;
(b) mean lifetimes of atomic innershell holes;
(c) total rates of radiative, Auger, and Coster–Kronig processes expressed as partial widths;
(d) yields of radiative, Auger, and Coster–Kronig transitions as fractional widths;
(e) widths of x-ray lines from the sum of the appropriate level widths; and,
(f) widths of Auger and Coster–Kronig lines from the sum of the widths of the levels involved (first approximation).

However, it should be noted that Coster–Kronig yields, which tend to be close to unity whenever Coster–Kronig transitions become energetically allowed, need be obtained with the aid of Eq. (4) or from original sources listed in the chart below, if precision is desired.

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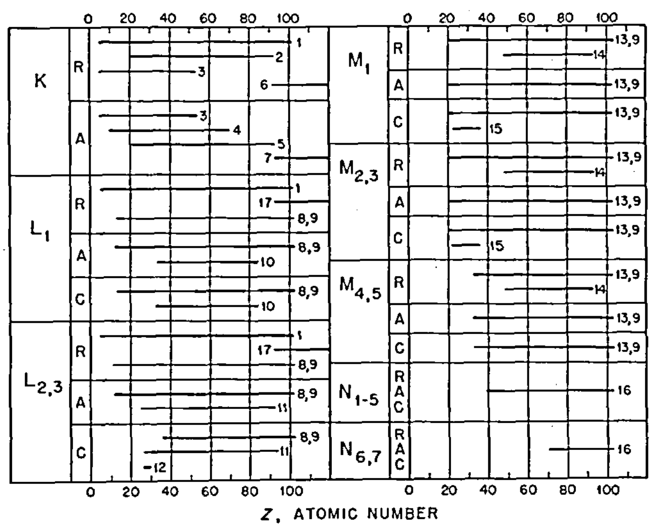


Chart showing Z-ranges of recent theoretical calculations of transition rates (partial level widths) of radiative (R), Auger (A), and Coster–Kronig (C) processes. Bold lines indicate calculations utilized for the graphs. Numbers refer to reference list. Not included in the chart are Refs. 18, 19, and 26; and work before 1970, Ref. 27. In regions where two bold lines are shown, averages were taken.

Table I. Recent reviews giving tabulations and graphs of level widths, and publications since 1969 giving experimental data on level widths

Level	Reference	Type	Remarks
K	Sevier (Ref. 20)	Exp;BF;Th	Review; graphs; tables
	Bambynek *et al.* (Ref. 7)	BF; Th	Graphs; Z > 36
	Senemaud (Ref. 21)	Exp	Z = 13
L_{1-3}	Sevier (Ref. 20)	Exp; Th	Review; graphs; tables
	Bambynek *et al.* (Ref. 7)	Th	Graph
	Wuilleumier (Ref. 22,23)	Exp	Z = 36, 54
	Krause, *et al.* (Ref. 24)	Exp	Z = 40, est. from x-rays
$L_{2,3}$	Yin *et al.* (Ref. 12)	Exp	Z = 29, 30
M_{1-5}	Sevier (Ref. 20)	Exp	Review; Z = 47,62,79,82,83,92
	Bambynek *et al.* (Ref. 7)	Th	Table from Ref. 13.
	Yin *et al.* (Ref. 15)	Exp; Th	Z = 29,30,32,40,41,47,48
	McGuire (Ref. 16)	Exp; Th	Review; Z = 40,47,58,60,63, 65, 67, 70, 71, 79
M_3	Wuilleumier (Ref. 23)	Exp	Z = 54
N_1	Krause *et al.* (Ref. 24)	Exp	Z = 40, est. from x-rays
N_{1-7}	McGuire (Ref. 16)	Exp, Th	Review; Z = 47,58,60,63,65, 67, 70, 71, 79

Exp = Experimental, BF = Best Fit and Th = Theory

Table II. Recent reviews on fluorescence yields ω and Coster-Kronig yields f [a]

Level ω	Level f	Reference	Type	Remarks
K	-	Burhop and Asaad (Ref. 25)	BF	Review
		Bambynek *et al.* (Ref. 7)	BF;Exp;Th	Review
L_{1-3}	$L_{1,2}$	Sevier (Ref. 20)	BF;Th	Review
L_{1-3}	$L_{1,2}$	Bambynek *et al.* (Ref. 7)	Exp;Th	Review[b]
L_2	L_1	Burhop and Asaad (Ref. 25)	Exp;Th	Review
$\overline{M}$	-	Bambynek *et al.* (Ref. 7)		Review. Note special definitions

a. Notations same as Table I

b. Also given is the average L shell fluorescence yield

GRAPHS OF TOTAL AND PARTIAL LEVEL WIDTHS

Explanation

Widths are given in eV, full width at half maximum (FWHM). Widths smaller than 10^{-4} eV are not displayed. Graphs are based on the theoretical calculations indicated in the preceding chart.

Γ or $\Gamma(X)$	Total natural width of level indicated
Γ_R	Radiative width
Γ_A	Auger width
Γ_C	Coster–Kronig width

Basis of Graphs

In the chart we show the quantities and ranges that are covered by the calculations on which the graphs are based. The bold lines in the chart indicate the sections we actually utilized. More than one bold line shown in a given region indicates averaged results of the theoretical predictions. However, the following specifics should be noted:

K-Shell

The *K*-shell radiative widths Γ_R are based principally on the relativistic Herman–Skillman calculations made by Scofield,[1] and by Rosner and Bhalla.[2] These calculations agree well and, for light elements, agree with McGuire's[3] nonrelativistic calculations. The Auger widths Γ_A are averaged from the values given by McGuire,[3] Kostroun *et al.*,[4] and Bhalla *et al.*,[5] whose results deviate by less than 30% in ranges where the calculations overlap. For $Z > 93$, Auger widths are deduced from the radiative widths reported by Lu *et al.*[6] and the extrapolated best fit fluorescence yield curve of Bambynek *et al.*[7]

L-Shell

The Auger widths $\Gamma_A(L_1)$ are those of McGuire[8,9] and Crasemann *et al.*,[10] averaged where applicable; and the Auger widths $\Gamma_A(L_{2,3})$, taken as $[\Gamma_A(L_2) + \Gamma_A(L_3)]/2$, since $\Gamma_A(L_2) \approx \Gamma_A(L_3)$, are those of McGuire[8,9] averaged with the predictions of Chen *et al.*[11] for $32 \leq Z \leq 93$. In the critical region around $Z = 28$ we rely on the values of Yin *et al.*[12]

The Coster–Kronig widths $\Gamma_C(L_1)$ are obtained from the data of Crasemann *et al.*[10] and the yields reported by McGuire.[8,9] However, in the regions near $Z = 40$ and $Z = 80$, we give perference to Crasemann *et al.*'s predictions, since their lower values are closer to the experimental observation.

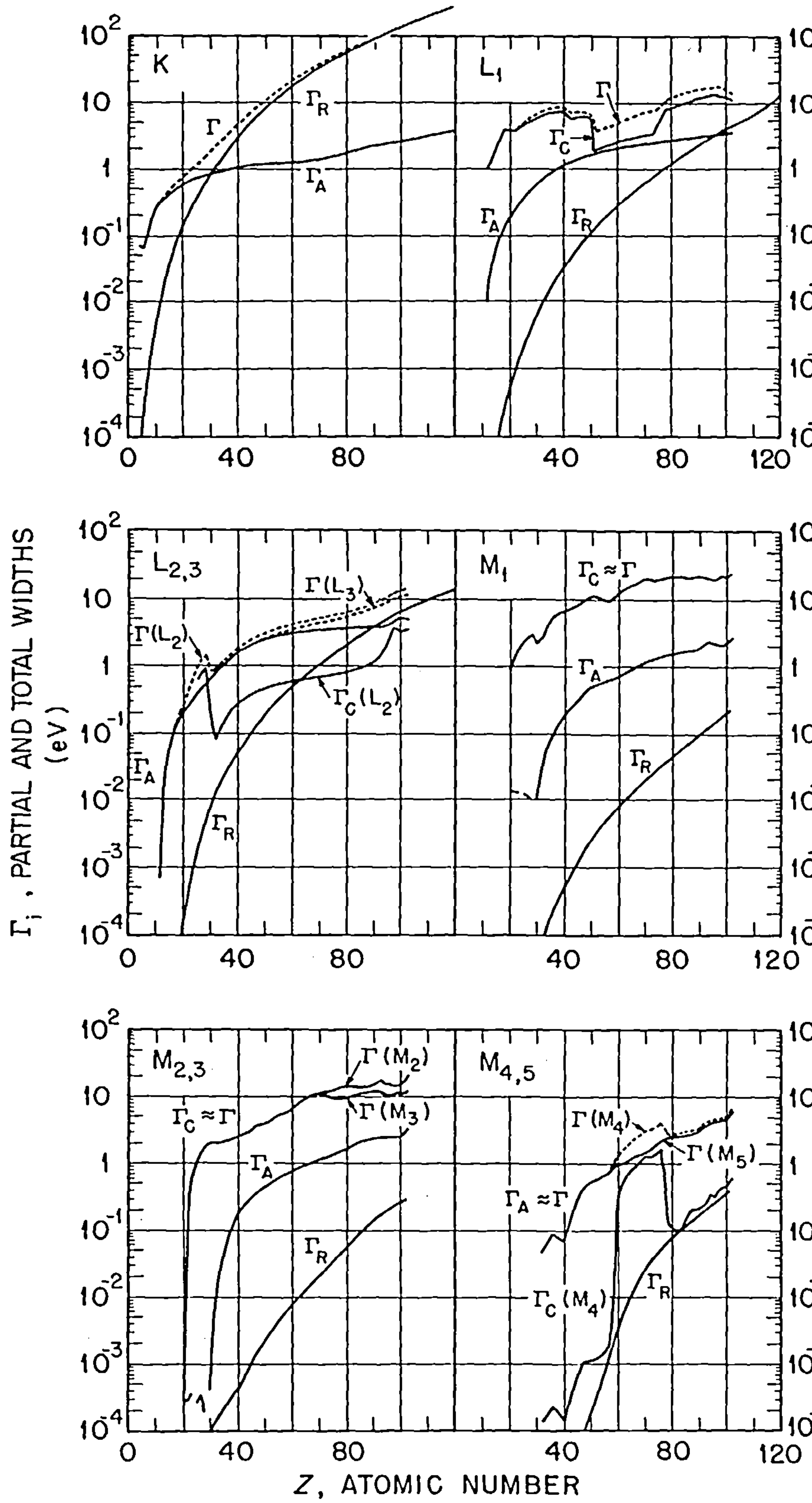
The partial widths $\Gamma_C(L_2)$ for $36 \leq Z \leq 93$ represent the average between data from Refs. 8 and 11, but for $Z > 93$, Ref. 9 is the only source. In the region around $Z = 30$, theoretical results differ considerably depending upon whether or not L_2–$L_3M_{4,5}$ transitions are considered energetically possible. Here we adopt the values of Yin *et al.*[12] who use experimental information to select the most probable value.

M-Shell

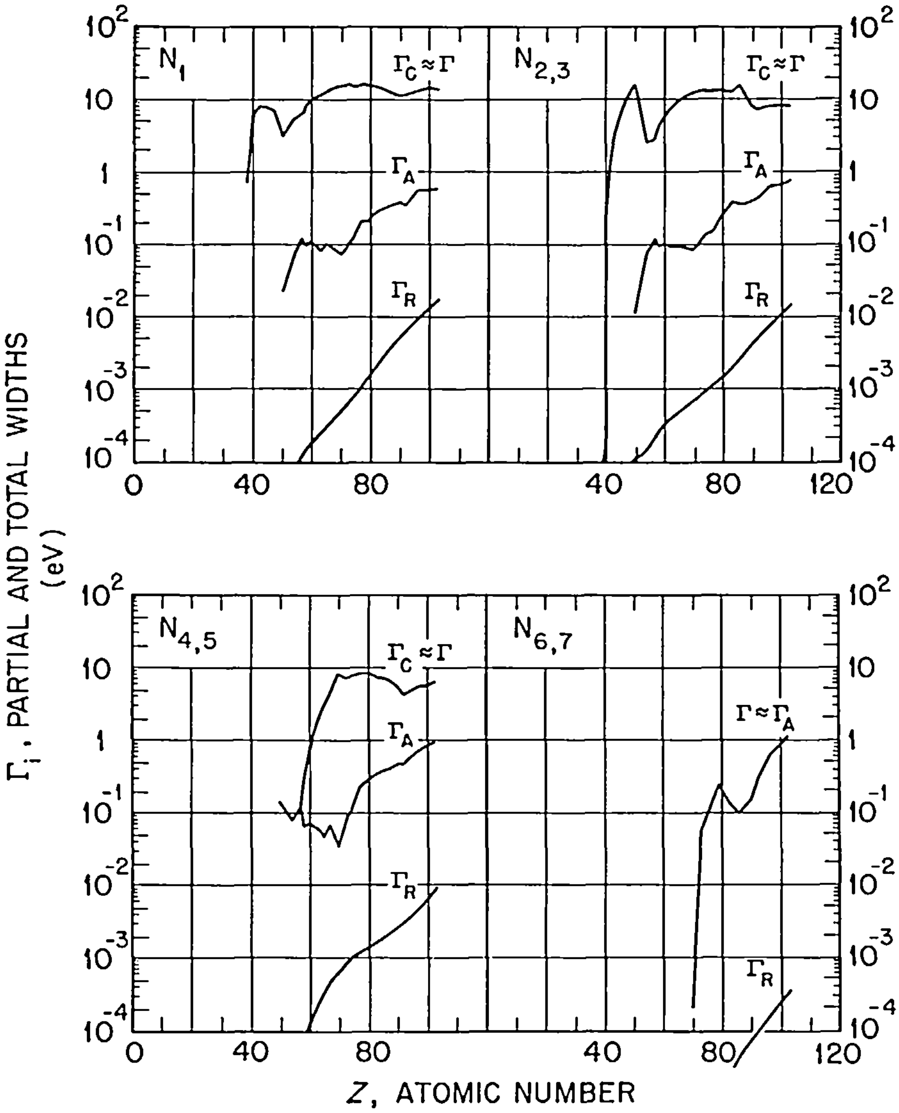
A comprehensive calculation of total widths and yields for all *M*-subshells was made by McGuire.[9,13] Our plotting is based on his results with the following exceptions. (a) The relativistic results of Bhalla[14] and the nonrelativistic Herman–Skillman results of Manson[18] are also taken into account to arrive at the radiative widths Γ_R. (b) Total M_1, M_2, and M_3 widths, which are approximately equal to Coster–Kronig widths for $22 \leq Z \leq 36$, are taken from Yin *et al.*[15] because their calculation is more refined and, in addition, in satisfactory accord with experiment.

N-Shell

McGuire[16] and Manson[18] supply the data for Γ_R; but in the absence of any other work, we transcribe the table values of McGuire[16] into the graphic form for Γ_A and Γ_C.



See page 143 for Explanation



See page 143 for Explanation

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