Natural widths of atomic *K* and *L* levels, *K*α X-ray lines and several *KLL* Auger lines

Cite as: Journal of Physical and Chemical Reference Data **8**, 329 (1979); https://doi.org/10.1063/1.555595
Published Online: 15 October 2009

M. O. Krause, and J. H. Oliver

Natural Widths of Atomic K and L Levels, $K\alpha$ X-Ray Lines and Several KLL Auger Lines

M. O. Krause and J. H. Oliver

Transuranium Research Laboratory, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830, USA

Semi-empirical values of the natural widths of K, L_1, L_2 and L_3 levels, $K\alpha_1$ and $K\alpha_2$ x-ray lines, and KL_1L_1, KL_1L_2 and KL_2L_3 Auger lines for the elements $10 \leq Z \leq 110$ are presented in tables and graphs. Level width Γ_i ($i = K, L_1, L_2, L_3$) is obtained from the relation $\Gamma_i = \Gamma_{R,i}/\omega_i$, using the theoretical radiative rate $\Gamma_{R,i}$ from Scofield's relativistic, relaxed Hartree-Fock calculation and the fluorescence yield ω_i from Krause's evaluation. X-ray and Auger line widths are calculated as the sums of pertinent level widths. This tabulation of natural level and line widths is internally consistent, and is compatible with all relevant experimental and theoretical information. Present semi-empirical widths, especially those of $K\alpha_1$ and $K\alpha_2$ x-rays, are compared with measured widths. Uncertainties of semi-empirical values are estimated.

Key words: Auger effect; Auger line width; K shell; L shell; level width; line width; natural width; x-ray line width.

1. Introduction

In the preceding paper [1][1] we presented an evaluation of fluorescence, Coster-Kronig and Auger yields for K and L shells. That evaluation utilized experimental and theoretical data up to October 1977 and led to sets of values that are internally consistent and are compatible with all relevant information. It is possible to use these fluorescence yield values, in conjunction with theoretical radiative rates, to derive reliable semi-empirical values of natural widths of K and L levels and, from these, natural widths of $K\alpha$ x-ray lines and KLL Auger lines. Such values are of importance in many areas of basic and applied science, most notably in the various branches of electron and x-ray spectrometry.

Level and line widths presented in this paper are *natural* atomic widths. In principle, natural widths are smaller than the actual widths observable in an experiment, because several effects, especially multiplet splitting and multiple ionization, may broaden a level or an emission line. However, these broadening effects are in general small, except for light elements, and will be discussed in some detail in section 5.

The most recent tabulations of x-ray line widths were made by Salem and Lee [2] and by Pessa [3]. To arrive at their recommendations of $K\alpha_1$ and $K\alpha_2$ x-ray line widths, Salem and Lee applied least-squares fits to experimental x-ray data and Pessa used x-ray and some level width data. However, line widths for $Z \leq 30$ were not reduced to natural atomic widths in either tabulation. Instead, these line widths reported in references 2 and 3 contain contributions from various broadening effects and pertain to solid systems normally encountered in practice.

Tables of K level widths, and in several cases L level widths, have been presented by Parratt [4], Blokhin [5], Meisel and Nefedov [6], Sevier [7], and Salgueiro et al. [8]. Level widths in reference 8 are based on theoretical radiative rates and semi-empirical fluorescence yields, those in references 4 to 7 are based on the relatively scarce measurements of x-ray absorption edges or absorption lines and on the more plentiful measurements of x-ray emission lines suitably adjusted for the width of the final level reached in an x-ray transition. A compilation of level width data up to about 1971 can be found in Sevier [7]; and recent theoretical results are shown in graphic form in reference 1, where also the original calculations of the partial level widths are cited.

No tabulation of KLL Auger line widths has been made to date.

It should be emphasized that, except for the theory-based $A(Z + B)^4$ relation [4,5,8], no other pertinent information has been included in past empirical efforts to systematize measured level and line widths as a function of atomic number Z and to achieve internal consistency.

2. Equations

In this work we derive the natural level width Γ_i from the radiative width (or rate) $\Gamma_{R,i}$ and the fluorescence yield ω_i of level i using the relation

$$\Gamma_i = \Gamma_{R,i}/\omega_i \tag{1}$$

where[2] $i = K, L_1, L_2, L_3$.

Natural x-ray and Auger line widths are calculated as the sums of the widths of levels involved in the transitions:

$$\Gamma(K\alpha_k) = \Gamma(K) + \Gamma(L_\ell), \tag{2}$$

[1] Figures in brackets indicate literature references at the end of this paper.

[2] The subscripts L_1, L_2, and L_3 are also written simply as 1,2,3: e.g., $\omega_{L_2} = \omega_2$.

where $k = 1, 2$; $\ell = 3, 2$; and

$$\Gamma(KL_kL_\ell) = \Gamma(K) + \Gamma(L_k) + \Gamma(L_\ell), \quad (3)$$

where $L_kL_\ell = L_1L_1, L_1L_2, L_2L_3$.

While eq (2) is exact, eq (3) is an approximation to the exact expression

$$\Gamma(KL_kL_\ell) = \Gamma(K) + \Gamma(L_kL_\ell) \quad (4)$$

and implies invariance of the decay width regardless of the number of holes present.

3. Source Material

Semi-empirical values presented in table 1 and figures 1 to 4 were obtained from eqs (1) to (3) with theoretical radiative rates $\Gamma_{R,i}$ from Scofield's relativistic, relaxed Hartree-Fock calculation [9–11] and fluorescence yields ω_i from Krause's evaluation [1]. As a consequence, the present semi-empirical level and line widths utilize the same source material as the fluorescence yields. Specifically, these widths, like the fluorescence yields, are compatible with available information on (a) fluorescence, Auger, and Coster-Kronig yields, (b) theoretical radiative and radiationless transition rates, (c) level widths, (d) x-ray and Auger line widths, (e) x-ray and Auger spectra, and (f) Coster-Kronig energies. In the evaluation of the fluorescence yields, only those level and line width data were used for which non-lifetime broadening could be presumed negligible. For further details on the evaluation procedure, the reader is referred to reference 1.

4. Estimate of Uncertainties

Uncertainties in the *level* width values are the quadratically added uncertainties in fluorescence yields ω_i and radiative rates $\Gamma_{R,i}$. We neglect correlation between the radiative rate and the fluorescence yield introduced through the evaluation process [1]. Generally, uncertainties are dominated by those assigned to ω_i [1]. Uncertainty of the theoretical K-shell rate, $\Gamma_{R,K}$, is assumed to be 3–5%, and of the L-subshell rates, Γ_{R,L_i}, to be 4–7%. These estimates rely on a comparison of theoretical rates with the following experimental data: first, the intensity ratios of x-ray transitions to levels with different principal quantum numbers [12], and second, the $K\alpha$ x-ray widths at higher Z where the radiative width predominates [2,3]. Earlier, Scofield surmised an uncertainty of about 2 % for $\Gamma_{R,K}$ on the basis of K x-ray branching ratios [11].

Uncertainties in *line* widths are the combined errors in the components.

Results are summarized in table 2. As expected, the uncertainty in the widths of the $K\alpha$ and KL_2L_3 lines are dominated by the K level width. Uncertainties are relatively large at low Z, because of large uncertainties in the fluorescence yields ω_i [1], which were obtained from the small number of experimental data and realistic calculations [13] available in this Z range. The estimates given in table 2 for light elements are conservative, at least for closed shell atoms, as can be seen from table 3 in which our semi-empirical values are compared with experimental data [14–26].

5. Effects Influencing the Widths

The natural level width, which is governed solely by the lifetime of a hole in that level, may not be observable in an experiment because of various effects influencing the width of a level. Similarly, natural line widths of transitions interconnecting levels may be difficult to delineate. General treatises of the various effects have been given in several places [4,5,7]; detailed discussions have been presented in many specific studies [27–45]. Here, only a brief outline of the most important effects and their consequences will be given in regard to the K and L shells.

Effects can be placed into two general categories: lifetime effects and non-lifetime effects. Either category can be advantageously divided into two Z ranges: (a) a range in which the levels under consideration are shallow core levels, usually in the penultimate shell, and (b) a range in which the levels are deep core levels, separated from the peripheral shell by at least one completely filled principal shell.

The lifetime of a hole in the level i is altered if additional holes are present in other levels. This lifetime effect can be substantial for shallow levels, that is in light atoms [39–41], but is negligible for deep core levels, that is in heavier atoms, provided the additional holes are in the outer shells [42]. A similar situation prevails for atoms in chemical or solid state matrices since chemical bonding entails removal or addition of peripheral charge.

If the level width is measured by photoelectron spectrometry, the widths corresponding to various hole states can generally be determined separately, for the various photolines are separated in energy [33,44]. The same holds true for x-ray lines and, especially, Auger lines of the light elements [33,44,45], unless too many hole states are present as in the case of most ion-atom collisions. A drastic change in the lifetime of the $L_{2,3}$ level of argon in the presence of an $M_{2,3}$ hole has been noted in an Auger spectrum [16,23,41], in which the single-hole, diagram line is well separated in energy from the double-hole, satellite line.

Diagram lines coincide with satellite lines in medium to heavy atoms in the case of x rays [32,36,37] and in heavy atoms in the case of Auger effect [33] assuming the additional holes are in outer levels. In these cases the line widths are affected in other ways, even though the lifetimes for the different lines may be, and usually are [42], identical.

If the peripheral electron configuration of an atom is changed, whether by multiple ionization or by chemical bonding, level energies change and Coster-Kronig decay

channels may either open or close. When this occurs, the effect on the natural level or line width is usually dramatic because of the importance of Coster-Kronig transitions. A notable example can be found in the 3*d* transition metal series, where the L_2–L_3X Coster-Kronig transition, which is forbidden in free atoms, becomes allowed in bound atoms with $26 \leq Z \leq 30$ [38] and possibly down to $Z = 22$ [1]. Hence, the L_2 level, $K\alpha_2$ x-ray and KL_2L_3 Auger lines are broader in the metal than in free atoms due to a lifetime effect. Use the ω_2 values in table 1 of the preceding paper [1] in eq (1) to obtain these natural width values pertaining to the metals of these elements.

Non-lifetime effects are caused by a myriad of effects [7,27–37], of which exchange coupling (multiplet splitting) is the most conspicuous one in the light elements [27,28]. These effects always lead to a level broadening. For example, if the energy spacings of multiplet components are less than the lifetime governed width, level broadening will result. In 3*d* elements, specifically $22 \leq Z \leq 28$, the multiplet splitting of the L_2 and L_3 levels is of such a degree that these levels as well as the pertinent x-ray and Auger lines are considerably broadened [27–29]. Although observed only in bound atoms so far, this effect is also present in free atoms. Since exchange coupling becomes weaker with increasing separation of the partially filled shells [43], *K* and *L* level widths and interconnecting transitions will experience negligible broadening from this source in the heavier elements.

Another non-lifetime effect is associated with the occurrence of multiple vacancies [32,33,36,37]. If, in addition to the hole in a deep core level, outer shell vacancies are created, as for example by photon and electron excitation, the resulting satellites will appear within the breadth of the single-hole, diagram emission line. Because the coincidence is not exact and because the satellite lines are subject to multiplet splitting, emission lines will be broadened. This has been demonstrated recently for $K\alpha$ x-ray lines in iron [37] and copper [36]. However, as *Z* increases this effect loses in significance compared with the natural width of the diagram line.

For detailed descriptions of other effects contributing to the widths of levels and lines, the reader is referred to references 7, 30, 34 and 35. The possibility that decay widths of multiplet components vary within a multiplet has been considered theoretically for light atoms [39,40].

The widths presented in table 1 and figures 1 to 4 are natural widths, in atoms with a single initial hole, on the basis of the data and procedures used (secs 2 and 3), except that small, and probably negligible, admixtures from other sources including those discussed in this section could not be completely eliminated in the evaluation process of the fluorescence yields [1].

The discussion of the most important effects influencing the widths shows that level and line widths are virtually identical with the natural widths in atoms in which *K* and *L* levels are deep core levels. On the other hand, level and line widths can deviate from the natural widths in atoms in which *K* and *L* levels are shallow levels. The dividing lines between the "deep" and "shallow" regions can be placed near $Z = 13$ for the *K* level and near $Z = 30$ for the *L* levels and for transitions between *K* and *L* levels.

6. Comparison With Experimental Data

In this section, we compare our semi-empirical values with various experimental data on level and line widths. Such comparisons provide an overview of the present state of the art and may pinpoint areas where improvements are needed.

In table 3, free-atom data [14–26], mostly of recent origin, are compared with semi-empirical values. Generally, satisfactory accord is noted except for the KL_1L_1 and KL_1L_2 widths of argon. These discrepancies in the argon Auger line widths may be due, at least in part, to the use of the approximate expression eq (3).

Semi-empirical natural line widths of $K\alpha_1$ and $K\alpha_2$ x-rays are compared in figures 2, 3, 5 and 6 with both fitted and selected original experimental data. As seen in figures 2 and 3, semi-empirical widths show the expected smooth increase with atomic number, while fitted data [2,3] exhibit some undulations. Part of the increased width observed in experiments with atoms in solids [2,3] between $Z = 21$ and 28 is due to exchange interactions of a 2*p* hole with the incomplete 3*d* shell [7,27,28]. Starting with $Z = 29$ [30], x-ray widths are essentially lifetime governed.

The deviation of the fitted values by Salem and Lee [2] from the present semi-empirical values (fig 5) occurs in several, but nonidentical, regions for $K\alpha_1$ and $K\alpha_2$ lines and might be attributed to their use of inaccurate input data. Values tabulated by Pessa [3] agree satisfactorily with our semi-empirical values except in the vicinity of $Z = 90$. Measurements by Nelson and Saunders [46], though exhibiting relatively larger scatter, agree satisfactorily with present values if the *average* percent-deviation ($\leq 2\%$) is considered.

In figure 6, level width differences $\Delta\Gamma(L_{2,3}) = \Gamma(L_2) - \Gamma(L_3)$ taken from various sources are plotted for $Z > 30$. We note small fluctuations in the present values, probably due to uncorrelated errors in $\Gamma(L_2)$ and $\Gamma(L_3)$, and find good agreement with $\Delta\Gamma(L_{2,3}) = \Gamma(L_2M_4\beta_1) - \Gamma(L_3M_5\gamma_1)$ of Salem and Lee's [2] fitted values. To be rigorous, the $L_3M_4\alpha_2$ line width should be used for calculating the difference $\Delta\Gamma(L_{2,3})$; but we preferred to base comparison on the $L_3M_5\alpha_1$ line width since the $L\alpha_1$ line is the much stronger line and the width of the M_4 level is nearly the same[3] as the width of the M_5 level except for $Z \geq 90$. While the width differences $\Delta\Gamma(L_{2,3})$ derived from *L* x-ray emission lines agree well with the differences obtained in this work, those derived from the $K\alpha$ doublet, $\Delta\Gamma(L_{2,3}) = \Gamma(KL_2\alpha_2) - \Gamma(KL_3\alpha_1)$ are in very poor agreement. In fact, the large scatter in the values based on $K\alpha$ width determinations indicates a need for improved measurements of $K\alpha$ line widths.

[3] Like *L* Coster-Kronig rates (see ref (1)), the Coster-Kronig rate M_4–M_5X is probably greatly overestimated by theory [47].

Table 1. Natural widths of K and L levels, Kα x-ray lines, and several KLL Auger lines in eV. (FWHM)[a]

Element	Level				X-ray line		Auger line		
	K	L_1	L_2	L_3	$K\alpha_1$	$K\alpha_2$	KL_1L_1	KL_1L_2	KL_2L_3
10 Ne	0.24	(<0.1)	(0.000)	(0.000)	0.24	0.24	(<0.4)	(<0.3)	0.24
11 Na	0.30	(0.2)	(0.000)	(0.000)	0.30	0.30	(0.7)	(0.5)	0.30
12 Mg	0.36	0.41	0.001	0.001	0.36	0.36	1.19	0.77	0.36
13 Al	0.42	0.73	0.004	0.004	0.43	0.43	1.89	1.16	0.43
14 Si	0.48	1.03	0.015	0.014	0.49	0.49	2.54	1.52	0.51
15 P	0.53	1.26	0.032	0.033	0.57	0.56	3.04	1.82	0.60
16 S	0.59	1.49	0.054	0.054	0.65	0.64	3.56	2.13	0.70
17 Cl	0.64	1.58	0.083	0.087	0.72	0.72	3.80	2.30	0.81
18 Ar	0.68	1.63	0.126	0.128	0.81	0.80	3.93	2.43	0.93
19 K	0.74	1.92	0.152	0.156	0.89	0.89	4.57	2.81	1.05
20 Ca	0.81	2.07	0.17	0.17	0.98	0.98	4.94	3.04	1.15
21 Sc	0.86	2.21	0.19	0.19	1.05	1.06	5.27	3.26	1.25
22 Ti	0.94	2.34	0.24	0.22	1.16	1.18	5.62	3.52	1.40
23 V	1.01	2.41	0.26	0.24	1.26	1.28	5.84	3.69	1.52
24 Cr	1.08	2.54	0.29	0.27	1.35	1.37	6.15	3.90	1.64
25 Mn	1.16	2.62	0.34	0.32	1.48	1.50	6.40	4.12	1.82
26 Fe	1.25	2.76	0.37	0.36	1.61	1.62	6.77	4.38	1.99
27 Co	1.33	2.79	0.43	0.43	1.76	1.76	6.91	4.56	2.19
28 Ni	1.44	2.89	0.52	0.48	1.94	1.96	7.22	4.85	2.44
29 Cu	1.55	3.06	0.62	0.56	2.11	2.17	7.67	5.23	2.73
30 Zn	1.67	3.28	0.72	0.65	2.32	2.39	8.22	5.66	3.04
31 Ga	1.82	3.38	0.83	0.76	2.59	2.66	8.59	6.04	3.42
32 Ge	1.96	3.53	0.95	0.82	2.78	2.92	9.02	6.45	3.73
33 As	2.14	3.79	1.03	0.94	3.08	3.17	9.71	6.96	4.11
34 Se	2.33	3.94	1.13	1.00	3.33	3.46	10.2	7.40	4.46
35 Br	2.52	4.11	1.21	1.08	3.60	3.73	10.8	7.84	4.81
36 Kr	2.75	4.28	1.31	1.17	3.92	4.06	11.3	8.34	5.23
37 Rb	2.99	4.44	1.43	1.27	4.26	4.92	11.9	8.85	5.69
38 Sr	3.25	4.67	1.54	1.39	4.63	4.79	12.6	9.45	6.17
39 Y	3.52	4.71	1.65	1.50	5.02	5.18	13.0	9.89	6.68
40 Zr	3.84	4.78	1.78	1.57	5.40	5.62	13.4	10.4	7.18
41 Nb	4.14	3.94	1.87	1.66	5.80	6.01	12.0	9.9	7.67
42 Mo	4.52	4.25	1.97	1.78	6.31	6.49	13.0	10.7	8.28
43 Tc	4.91	4.36	2.08	1.91	6.82	6.99	13.6	11.4	8.90
44 Ru	5.33	4.58	2.23	2.00	7.33	7.56	14.5	12.1	9.55
45 Rh	5.77	4.73	2.35	2.13	7.90	8.12	15.2	12.9	10.2
46 Pd	6.24	4.93	2.43	2.25	8.49	8.67	16.1	13.6	10.9
47 Ag	6.75	4.88	2.57	2.40	9.16	9.32	16.5	14.2	11.7
48 Cd	7.28	4.87	2.62	2.50	9.79	9.91	17.0	14.8	12.4
49 In	7.91	5.00	2.72	2.65	10.56	10.63	17.9	15.6	13.3
50 Sn	8.49	2.97	2.84	2.75	11.2	11.3	14.4	14.3	14.1
51 Sb	9.16	3.13	3.00	2.87	12.0	12.2	15.4	15.3	15.0
52 Te	9.89	3.32	3.12	2.95	12.8	13.0	16.5	16.3	16.0
53 I	10.6	3.46	3.25	3.08	13.7	13.8	17.5	17.3	16.9
54 Xe	11.4	3.64	3.40	3.13	14.6	14.8	18.7	18.5	18.0
55 Cs	12.3	3.78	3.51	3.25	15.6	15.8	19.9	19.6	19.1
56 Ba	13.2	3.92	3.57	3.32	16.5	16.8	21.1	20.7	20.1
57 La	14.1	4.06	3.68	3.41	17.6	17.8	22.3	21.9	21.2
58 Ce	15.1	4.21	3.80	3.48	18.6	18.9	23.6	23.2	22.5
59 Pr	16.2	4.34	3.89	3.60	19.8	20.1	24.9	24.4	23.7

Table 1. Natural widths of K and L levels, Kα x-ray lines, and several KLL Auger lines in eV. (FWHM)[a] – continued.

Element	Level				X-ray line		Auger line		
	K	L_1	L_2	L_3	$K\alpha_1$	$K\alpha_2$	KL_1L_1	KL_1L_2	KL_2L_3
60 Nd	17.3	4.52	3.97	3.65	20.9	21.3	26.3	25.8	24.9
61 Pm	18.5	4.67	4.06	3.75	22.2	22.5	27.8	27.2	26.3
62 Sm	19.7	4.80	4.15	3.86	23.6	23.8	29.3	28.6	27.7
63 Eu	21.0	4.91	4.23	3.91	24.9	25.2	30.8	30.1	29.1
64 Gd	22.3	5.05	4.32	4.01	26.4	26.7	32.4	31.7	30.7
65 Tb	23.8	5.19	4.43	4.12	27.9	28.2	34.1	33.4	32.3
66 Dy	25.2	5.25	4.55	4.17	29.4	29.8	35.7	35.0	34.0
67 Ho	26.8	5.33	4.66	4.26	31.1	31.5	37.5	36.8	35.7
68 Er	28.4	5.43	4.73	4.35	32.7	33.1	39.2	38.5	37.5
69 Tm	30.1	5.47	4.79	4.48	34.6	34.9	41.0	40.3	39.3
70 Yb	31.9	5.53	4.82	4.60	36.5	36.7	42.9	42.2	41.3
71 Lu	33.7	5.54	4.92	4.68	38.4	38.7	44.8	44.2	43.4
72 Hf	35.7	5.63	5.02	4.80	40.5	40.7	47.0	46.3	45.5
73 Ta	37.7	5.58	5.15	4.88	42.6	42.9	48.9	48.5	47.8
74 W	39.9	5.61	5.33	4.98	44.9	45.2	51.1	50.8	50.2
75 Re	42.1	6.18	5.48	5.04	47.2	47.6	54.5	53.8	52.6
76 Os	44.4	7.25	5.59	5.16	49.6	50.0	58.9	57.2	55.1
77 Ir	46.8	8.30	5.69	5.25	52.1	52.5	63.4	60.8	57.7
78 Pt	49.3	9.39	5.86	5.31	54.6	55.2	68.1	64.6	60.5
79 Au	52.0	10.5	6.00	5.41	57.4	58.0	72.9	68.4	63.4
80 Hg	54.6	11.3	6.17	5.50	60.1	60.8	77.3	72.1	66.3
81 Tl	57.4	12.0	6.32	5.65	63.1	63.8	81.4	75.7	69.4
82 Pb	60.4	12.2	6.48	5.81	66.2	66.8	84.8	79.1	72.7
83 Bi	63.4	12.4	6.67	5.98	69.4	70.1	88.2	82.5	76.1
84 Po	66.6	12.6	6.83	6.13	72.7	73.4	91.9	86.1	79.6
85 At	69.8	12.8	7.01	6.29	76.1	76.8	95.5	89.7	83.1
86 Rn	73.3	13.1	7.20	6.41	79.7	80.5	99.4	93.5	86.9
87 Fr	76.8	13.3	7.47	6.65	83.4	84.2	103	97.5	90.9
88 Ra	80.4	13.4	7.68	6.82	87.2	88.1	107	101	94.9
89 Ac	84.1	13.6	7.95	6.98	91.1	92.0	111	106	99.0
90 Th	88.0	13.7	8.18	7.13	95.2	96.2	115	110	103
91 Pa	91.9	14.3	8.75	7.33	99.3	100.7	121	115	108
92 U	96.1	14.0	9.32	7.43	103.5	105.4	124	119	113
93 Np	100	14.0	9.91	7.59	108	110	128	124	118
94 Pu	105	13.5	10.5	7.82	113	115	132	129	123
95 Am	109	13.3	10.9	8.04	117	120	136	133	128
96 Cm	114	13.6	11.4	8.26	122	125	141	139	133
97 Bk	119	13.8	11.8	8.55	127	130	146	144	138
98 Cf	124	14.0	12.2	8.75	132	136	151	150	144
99 Es	129	14.3	12.7	9.04	138	141	157	155	150
100 Fm	135	14.4	13.1	9.33	144	148	164	162	157
101 Md	140	14.8	13.6	9.61	150	153	170	168	163
102 No	145	15.1	14.0	9.90	155	159	176	175	169
103 Lr	150	15.9	14.4	10.1	161	165	182	181	175
104	156	16.2	14.9	10.5	167	171	189	188	182
105	162	16.5	15.5	10.8	173	177	195	194	188
106	168	16.8	15.9	11.2	179	184	201	200	195
107	174	17.0	16.4	11.6	185	190	208	207	202
108	181	17.2	17.0	12.0	193	198	215	215	210
109	187	17.6	17.5	12.3	200	205	222	222	217
110	193	18.1	18.1	12.7	206	211	229	229	224

[a] Semi-empirical values (eqs. (1) to (3)); values in parentheses are estimated. Uncertainties are listed in Table 2.

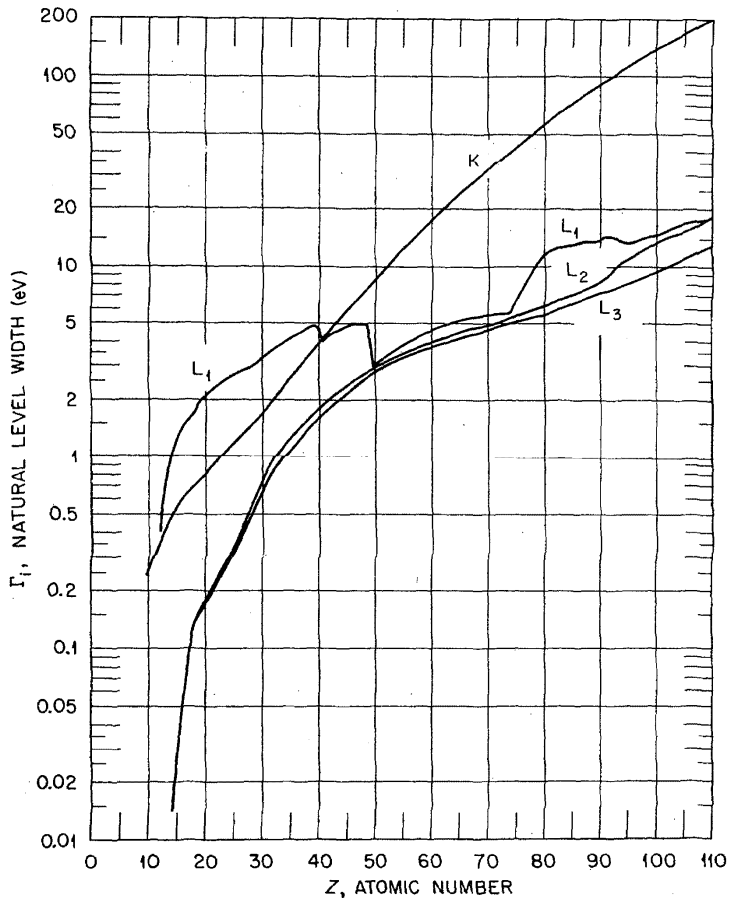

FIGURE 1. Natural widths of K and L levels. Graphic display of table 1.

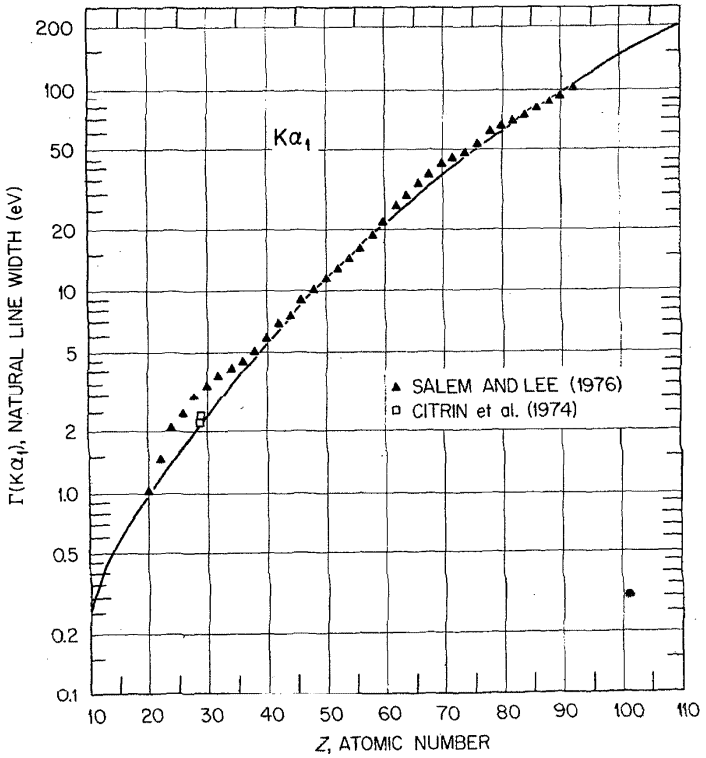

FIGURE 2. Natural widths of $K\alpha_1$ x-ray lines. Graphic display of table 1. Values of reference 2 are also shown.

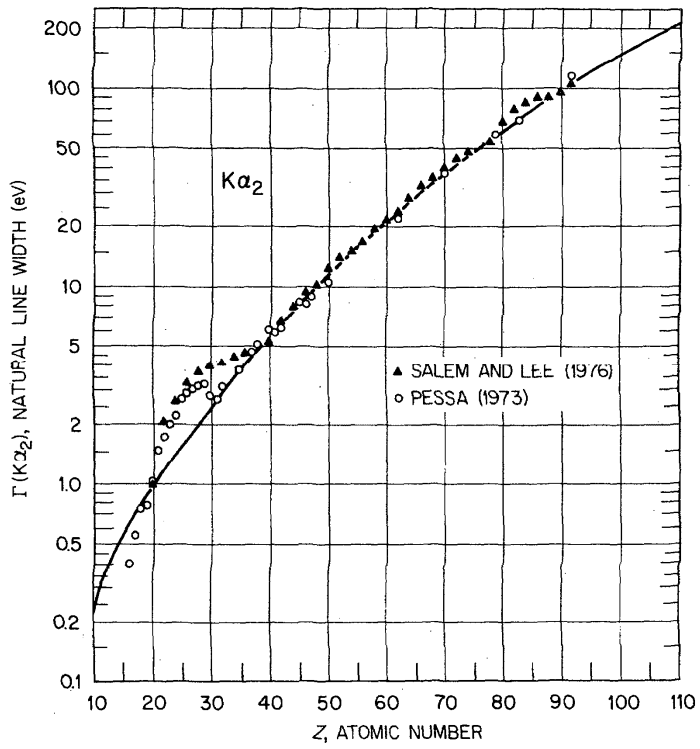

FIGURE 3. Natural widths of $K\alpha_2$ x-ray lines. Graphic display of table 1. Values of references 2 and 3 are also shown.

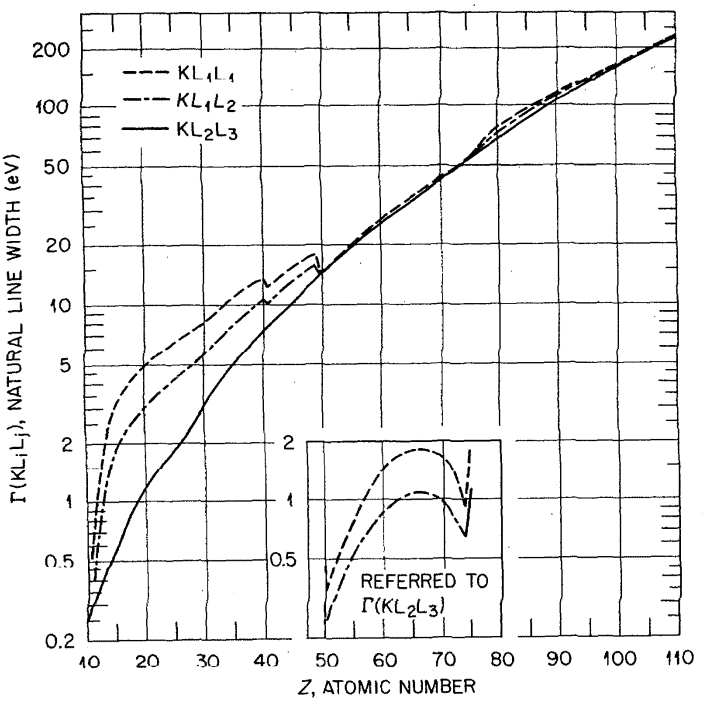

FIGURE 4. Natural widths of three *KLL* Auger lines. Graphic display of table 1. Note magnification of width differences shown in inset for $50 \leq Z \leq 75$.

Table 2. Estimated uncertainties (in percent) of semi-empirical values of natural level and line widths.

Level or Line	Range of atomic numbers									
	10–20	20–30	30–40	40–50	50–60	60–70	70–80	80–90	90–100	100–110
K	10[a]	5	5	4	4	3	3	3	4	5
L_1	30[a]	30[a]	30[b]	25[b]	20	15	15	15	20	20
L_2	25[a]	25[a]	25[b]	20	10	10	10	10	10[b]	15
L_3	25[a]	25[a]	20	15	10	10	8	8	8	10
$K\alpha_{1,2}$	10[a]	7[a]	6	5	4	4	3	3	4	5
KL_1L_1[c]	25[a]	25[a]	20[b]	10[b]	8	5	5	5	5	6
KL_1L_2[c]	25[a]	20[a]	15[b]	10[b]	5	5	5	4	4	6
KL_2L_3[c]	10[a]	10[a]	10	8	5	5	4	3	4	6

[a]Uncertainties from neglect of multi-body effects not included.

[b]Near Coster-Kronig discontinuities, uncertainties may exceed those listed; cutoffs or onsets may be shifted for KL_1L_1 Auger transitions.

[c]Errors due to the use of approximate formula eq. 3 are not included.

Table 3. Experimental free-atom data compared with semi-empirical natural level and line widths (in eV)

Element	Level or Line[a]	Natural width		Notes and references
		Semi-empirical[b]	Expt.	
10 Ne	K	0.24	0.27(1)	Photoelectron; Svensson et al., Ref. 14
	$K\alpha_{1,2}$	0.24[c]	0.27(5)	Electron exc.; Ågren et al., Ref. 15
	KL_2L_3	0.24	0.21(2)	Proton exc.; Stolterfoht, Ref. 16
11 Na	$L_1L_{2,3}M_1$	0.2	0.24(2)	Electron exc.; Breuckmann et al., Ref. 17
18 Ar	K	0.68	0.68(3)	X-ray absorption; Watanabe, Ref. 18
	KL_1L_1	3.93	7.5(9)	Electron exc.; Krause, Ref. 19
	KL_1L_2	2.43	3.6(3)	Electron exc.; Krause, Ref. 19
	KL_2L_3	0.93	1.0(1)	Electron exc.; Krause, Ref. 19
	KL_2L_3	0.93	0.92	Electron exc.; Asplund et al., Ref. 20
	$L_1M_{2,3}$	1.63	1.3	Electron exc.; Nordgren et al., Ref. 21
	L_1	1.63	1.8(2)	Electron exc.; Mehlhorn, Ref. 22
	$L_{2,3}M_1$	0.127	0.12	Electron exc.; Nordgren et al., Ref. 21
	$L_{2,3}M_{2,3}M_{2,3}$	0.127	0.10(2)	Proton exc.; Ridder et al., Ref. 23
			0.10(2)	Electron exc.; Kondow et al., Ref. 24
			0.16(2)	Electron exc.; Mehlhorn, Ref. 22
30 Zn	$L_{2,3}M_{4,5}M_{4,5}$	0.70	0.50(15)	Electron exc.; Aksela et al., Ref. 25
36 Kr	L_2	1.31	1.3	X-ray absorption; Wuilleumier, Ref. 26
	L_3	1.17	1.2	X-ray absorption; Wuilleumier, Ref. 26

[a]Widths of M levels are negligibly small.

[b]This work.

[c]Multiply by ≈ 1.15 to include splitting of doublet.

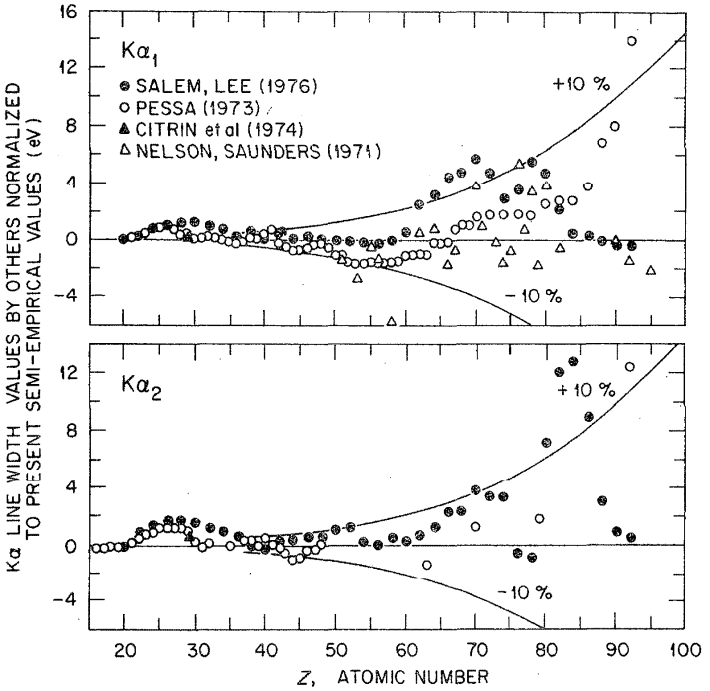

FIGURE 5. $K\alpha$ line widths recommended by Salem and Lee [2] and by Pessa [3], and reported by Citrin et al., [30], and by Nelson and Saunders [46] are normalized to present semi-empirical values. For clarity, only the $K\alpha_1$ values of reference 46 are shown. Note the arbitrarily chosen ± 10% uncertainty limits.

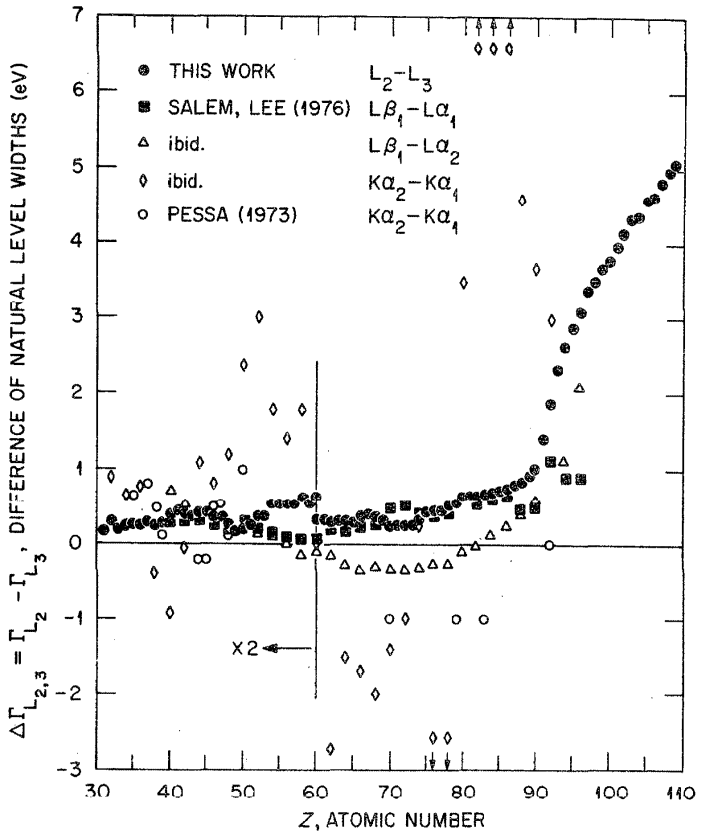

FIGURE 6. Differences of natural level widths, $\Delta\Gamma(L_{2,3}) = \Gamma(L_2) - \Gamma(L_3)$, from table 1 and other sources [2,3].

Acknowledgements

This work was sponsored by the U. S. Department of Energy, Division of Nuclear Sciences, Office of Basic Energy Sciences, under contract W-7405-eng-26 with the Union Carbide Corporation, operator of the Oak Ridge National Laboratory.

References

[1] Krause, M. O., J. Phys. Chem. Ref. Data, **8**, 307 (1979); preceding paper.
[2] Salem, S. I., and Lee, D. L., At. Data Nucl. Data Tables, **18**, 233 (1976).
[3] Pessa, V. M., X-Ray Spectrometry, **2**, 169 (1973).
[4] Parratt, L. G., Rev. Mod. Phys. **31**, 616 (1959).
[5] Blokhin, M. A., Physik der Röntgenstrahlen, 470 pp., VEB Verlag Technik, Berlin (1965). Blokhin, M. A. and Sachenko, V. P., Bull. Acad. Sci., USSR, Phys. Ser. **21**, 1343 (1957).
[6] Meisel, A., and Nefedov, W., Ann. Physik (Leipzig) **9**, 48 (1961).
[7] Sevier, K. D., *Low Energy Electron Spectrometry*, 397 pp. Wiley, New York, N. Y. (1972).
[8] Salgueiro, L., Ramos, M. R., and Ferreira, J. G., Portugaliae Physica **6**, 183 (1971).
[9] Scofield, J. H., Phys. Rev. **A9**, 1041 (1974).
[10] Scofield, J. H., Phys. Rev. **A10**, 1507 (1974).
[11] Scofield, J. H., "Radiative Transitions" in *Atomic Innershell Processes*, B. Crasemann, editor, Vol. I, pp. 265–288, Academic Press, Inc., New York (1975).
[12] Salem, S. I., Panossian, S. L., and Krause, R. A., At. Data Nucl. Data Tables, **14**, 91 (1974).
[13] Kelly, H. P., "Many-Body Perturbation Approaches to the Calculation of Transition Probabilities," in *Atomic Inner Shell Processes*, B. Crasemann, editor, Vol. I, pp. 331–351, Academic Press, Inc., New York (1975).
[14] Svensson, S., Mårtensson, N., Basilier, E., Malmquist, P. Å., Gelius, U., and Siegbahn, K., Physica Scripta, **14**, 141 (1976).
[15] Ågren, H., Nordgren, J., Selander, L., Nordling, C., and Siegbahn, K., UUIP-944 report, Uppsala University, Institute of Physics, Dec. 1976.
[16] Stolterfoht, N., *4th Conf. Appl. Small Accelerators*, Publ. No. 76CH117-9 NTS: Denton, Texas, 1976.
[17] Breuckmann, E., Breuckmann, B., Mehlhorn, W., and Schmitz, W., J. Phys., B**10**, 3135 (1977).
[18] Watanabe, T., Phys. Rev. **139**, 1747 (1965).
[19] Krause, M. O., Phys. Rev. Lett. **34**, 633 (1975).
[20] Asplund, L., Kelfre, P., Blomster, B., Siegbahn, H., and Siegbahn, K., Physica Scripta, **16**, 268 (1977).
[21] Nordgren, J., Ågren, H., Nordling, C., and Siegbahn, K., Physica Scripta, **16**, 280 (1977).
[22] Mehlhorn, W., Z. Physik, **208**, 1 (1968).
[23] Ridder, D., Dieringer, J., and Stolterfoht, N., J. Phys. B**9**, L307 (1976).
[24] Kondow, T., Kawai, T., Kunimori, K., Onishi, T., and Tamura, K., J. Phys. B**6**, L156 (1973).
[25] Aksela, S., Väyrynen, J., and Aksela, H., Phys. Rev. Lett., **33**, 999 (1974).
[26] Wuilleumier, F., J. Phys. (Paris), **32**, C4–88 (1971).
[27] Meisel, A., and Nefedov, W., Ann. Physik (Leipzig), **9**, 53 (1961); Nefedov, W. I., Bull. Acad. Sci. USSR, Phys. Ser. **28**, 724 (1964).
[28] Kowalczyk, S. P., Ley, L., McFeely, F. R., and Shirley, D. A., Phys. Rev. B**11**, 1721 (1975).
[29] Gupta, R. P., and Sen, S. K., Phys. Rev. B**10**, 71 (1974).
[30] Citrin, P. H., Eisenberger, P. M., Marra, W. C., Åberg, T., Utriainen, J. and Källne, E., Phys. Rev. B**10**, 1762 (1974).
[31] Krause, M. O., "Electron Spectrometry" in *Atomic Innershell Processes*, B. Crasemann, editor, Vol. II, pp. 33–81, Academic Press, Inc., New York (1975).
[32] Krause, M. O., Wuilleumier, F., and Nestor, C. W., Jr., Phys. Rev. **A6**, 871 (1973).
[33] Krause, M. O., "Creation of Multiple Vacancies" in *Proceedings International Conference on Innershell Ionization Phenomena*, R. W. Fink, et al., editors, pp. 1586–1616, USAEC CONF-720404 (1973).
[34] Boehm, F., "Isotope Shifts, Chemical Shifts, and Hyperfine Interaction of Atomic K X rays" in *Atomic Innershell Processes*, B. Crasemann, editor, Vol. 1, pp. 412–442, Academic Press, Inc., New York (1975).
[35] Hüfner, S., and Wertheim, G. K., Physics Letters, **51A**, 301 (1975).
[36] Sauder, W. C., Huddle, J. R., Wilson, J. D., and LaVilla, R. E., Physics Letters, **63A**, 313 (1977).
[37] Chevallier, P., Tavernier, M., and Briand, J. P., J. Phys. B **11**, L171 (1978).
[38] Yin, L. I., Adler, I., Chen, M. H., and Crasemann, B., Phys. Rev. **A7**, 897 (1973).
[39] Chen, M. H., and Crasemann, B., Phys. Rev. **A12**, 959 (1975).
[40] Bhalla, C. P., J. Phys. B**8**, 2792 (1975).
[41] Chen, M. H., and Crasemann, B., Phys. Rev. **A10**, 2232 (1974).
[42] Manson, S. T., Dehmer, J. L., and Inokuti, M., Bull Am. Phys. Soc., **22**, 1332 (1977).
[43] Van Vleck, J. H., Phys. Rev. **45**, 405 (1934); Bagus, P. S., Freeman, A. J., and Sasaki, F., Phys. Rev. Lett. **30**, 850 (1973).
[44] Siegbahn, K., J. Electr. Spectrosc., **5**, 3 (1974).
[45] Faegri, K., Jr., and Keski-Rahkonen, O., J. Electr. Spectrosc. **11**, 275 (1977).
[46] Nelson, G. C., and Saunders, B. G., J. Phys. (Paris), **32**, C4–97 (1971).
[47] McGuire, E. J., Phys. Rev. **A5**, 1043 (1972); Phys. Rev. **A6**, 851 (1972).

Note Added in Proof

Since submitting this manuscript, the following data on level and line widths have come to my attention: Ar$L_{2,3}$ = 0.127(10) eV [G. C. King et al., J. Phys. B**12**, 2479 (1978)]; Eu$K\alpha_1$ = 24.8(4) eV, Tm$K\alpha_1$ = 34.4(7) eV, Ta$K\alpha_1$ = 42.9(1.1) eV [K. C. Wang et al., Phys. Rev. A**17**, 1735 (1978)]; Ne$K\alpha_{1,2}$ = 0.24 eV [T. P. Tooman and R. J. Liefeld, *Int. Conf. Phys. X-Ray Spectra*, Extended abstracts, R. D. Deslattes, editor, pp. 352–354, NBS (1976)]; and N($K \rightarrow \pi 2p$) = 0.128(6) eV in N_2 [G. C. King et al., Chem. Phys. Lett. **52**, 50 (1977)]. On the basis of the line width of 0.04 eV measured for Ar($L_{2,3}M_{2,3} \rightarrow M_1M_{2,3}$) [21], the widths of Ne$K$ reported in reference 16 and Ar$L_{2,3}$ reported in reference 23 should be changed to 0.23(3) eV and 0.12(2) eV, respectively, [D. Ridder, private communication (1978)].