Recommended Atomic Electron Binding Energies,

1s to $6p_{yy}$, for the Heavy Elements, Z = 84 to 103

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Recent experimental measurements of atomic electron binding energies, 1s to $6p_{3/2}$, for certain of the transuranic elements are incorporated into interpolation and extrapolation procedures yielding new recommendations for the electron binding energies from Z=84 to 103.

Key words: Atomic electron binding energies; binding energies; core electron binding energies; heavy elements: transuranic elements.

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1. Introduction

because of their physical characteristics, there are few or no direct experimental data concerning the atomic electron binding energies for several of the elements with atomic number (Z) greater than 84. Such binding energy values have been estimated [1-5] by interpolation in Z between experimental values or by extrapolation in the case of transuranic elements. In recent years new data for several transuranic elements have become available from internal conversion electron, photoelectron and x-ray studies. The present table of recommended values for Z=84–103 makes use of all experimental data available up to September 1977 for $Z\geqslant73$. Significant revisions from values recommended in [1-5] do emerge.

Experimental data are now available for both outer and inner shells for some heavy elements with several eV accura-

cy. The large differences, up to several keV, between inner shell binding energies for neighboring heavy elements makes direct interpolation to such accuracy quite difficult. The technique of subtracting most of the change with some regularly varying function of Z allows one to display the data for a single subshell over a range in Z, on a scale sufficiently expanded to exhibit the errors, to assess the errors of interpolation or extrapolation, and to obtain values for unmeasured or poorly measured cases.

One such technique which has been used before in limited regions of the periodic table is the modified Moseley plot [6] in which a parabolic (aZ^2+bZ+c) function is subtracted from the experimental values and the differences exhibited in order to visualize any small (order of 1 eV) deviation from smooth behavior of the experimental values as a function of Z. This method has been shown to work well [6] over limited ranges in Z within which a single subshell is filled, such as the 4f shell in the rare earth sequence. However, the difference as a function of Z shows large sudden excursions in its slope as subshell edges are crossed. Any such smooth polynomial function would be an unsuitable reference [7] over the range $73 \le Z \le 103$ needed here, in which several subshells are

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

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traversed. A suitable reference function must incorporate at least the major deviations from the simple quadratic Z dependence of Moseley that are associated with subshell closures at $Z=80,\,82,\,86,\,$ and 88.

The recent improvements in the quality of the numerical self-consistent-field programs for calculating relativistic eigenvalues [8] or binding energies [9] do include, in the main "electrostatic energy" term (calculated by Dirac-Fock [8] or Dirac-Slater [9] prescription) the single electron wave function configuration that minimizes the energy at each Z. Thus they each do a much better job in following the actual Z dependence of the binding energies across shell edges than polynomials we have tested. We have tested and used them both as reference functions for interpolating and smoothing the experimental data. The differences between the calculated values and the experimental values (or their averages) are plotted for each subshell as a function of Z. A smooth curve drawn through the points can be read to 1 eV accuracy, and subtracting these smooth values from the calculated values yields the recommended values for the binding energies. Thus, as we demonstrate, it is principally the experimental values that in the end determine the recommendations in this empirical analysis, the local calculated reference value "cancelling out." Both calculations [8, 9] follow the course of true binding energies sufficiently well to enable smooth interpolation of the difference function across shell edges.

As will be seen, the plotted differences (calculated — experiment) still show local waves which differ somewhat for the different reference functions. These point to residual inaccuracies in the calculations in regions where the data are known to be accurate. Such waves in the differences make it very difficult to choose a suitable order for a polynomial (nor is there any theoretical guide thereto) to be used to calculate a least squares computer fit to the differences. In comparison to a numerical fit to an arbitrary polynomial, we adopt the policy of a smooth interpolating curve without local waves. We believe the smooth curve as fit by eye with a spline yields more credible predictions for the binding energies, without additionally attenuating the accuracy (error estimates) justified by the quality of the input experimental data. We offer supporting evidence in section 2.

The eigenvalues of Desclaux [8] from which we subtract the input data are the result of a Dirac-Fock frozen orbital procedure. They are only the Koopman's theorem approximation to binding energies. The differences which we plot are, in fact, approximately the sum of the excluded relaxation and field-theoretic contributions to a complete binding energy calculation. (These terms depend smoothly on Z, being independent of particular configurations.) Thus, the differences to experimental data and their Z dependence are much larger than those referred to the true binding energies calculated by Huang et al. [9], which include the extra terms. (See ordinates of figures 2 and 3A.) Nevertheless, we find that the Desclaux eigenvalues yield binding energy predictions by our method in excellent agreement with those derived using the Huang et al. calculations as reference in the most severe test cases, the Kand L shells (see figure 4). Moreover, for the K shell the smooth interpolating curve using Desclaux's values demands lower local curvature in the region of Z=90-96 than for the Huang et al. values. Note in figure 3A (K shell; Huang et al. [9] values) the failure of the smooth curve to fit the data averages at any Z in the range 90-96 compared to the corresponding fits in figure 2 and figure 3B, which use Desclaux's [8] values and similarly locally smooth curves.

These observations and other local differences lead us to use as reference only the Desclaux values for all shells beyond the K shell. In figure 5b we also show the difference function for the L_3 shell referred to the Huang et al. values.

2. Test of the Method

In order to test the use of the calculated eigenvalues [8] and binding energies [9] as described above, we display in figure 1 the two plots for the L_2 shell differences to the data for the Z range 41 to 83 where all values are accurately measured. Note this range spans the filling of the 4d, the 5p, and the 4f (lanthanides) shells. The experimental values are taken from

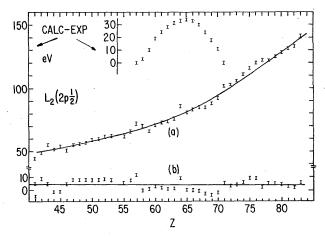


FIGURE 1. Plot of the differences between the calculated eigenvalues (a. Desclaux, ref. [8]), or binding energies (b, Huang et al. ref. [9]) and the experimental binding energies for the L_2 shell for a Z region where the values are well measured. This demonstrates the character and amplitude of the fluctuations about a smooth curve through the points which result both from experimental causes and from the calculation. The inset shows the difference between a smooth function (aZ^2+bZ+c) and the same experimental values in the lanthanide region (Z=57-71).

the table of Siegbahn et al. [2]. Bearden and Burr [1] values may differ by 1 or 2 eV and are all quoted with standard deviation $\sigma>1$ eV.

The fact that more than 5% of the points do not lie within 2σ of either smooth curve can be attributed mainly to two causes other than perhaps some optimistic assignment of a standard error by an experimenter. Most of these data rely on a photoelectron measurement on a solid sample for at least one and usually several shells for each Z, i.e., with the atom in question in a particular chemical state. No attempt is made to make any adjustment for the fact that the chemical state can affect the measured binding energy by several eV. The calculations of eigenvalues and binding energies, of course, are made for free atoms. Therefore, some of the deviations from the smooth curves can be attributed to differences in chemical shifts with Z.

The second reason for scatter around the smooth curves is due to the calculations. This assertion can be verified from a series of measurements on rare earths [6], all made with the same technique and instrumentation, in which some evidence is presented that each element was in a similar oxide state. When the results for the L_2 shell (as also for the K, L_1 and L_3 shells) from this series of measurements (all within the filling of the 4f shell) are subtracted from a parabolic function, it is clear that the values proceed smoothly, within the 1 eV errors, as a function of Z (the insert in figure 1 shows this plot; note the break at Z=57, the shell edge). Comparison to the same Z range on the other plots shows that the local deviation at Gd (Z=64) in our plots (of the differences between the calculated eigenvalues or binding energies and experimental values) is clearly due to the calculations and not to the experiment.

In the same region (lanthanides) but for the outer 6s shell, both a similar calculation [10] and the experiment show a similar local excessive increase of several eV in binding energy at Z=64 with the irregular $4f^75d6s^2$ configuration (nearby lanthanides have no 5d electrons). The local increase persists even to the innermost shells in the calculation but not experimentally. The explanation for this is not clear, but it has been suggested [11] that if the calculations were done for atoms with a configuration more appropriate to the solid state that the increase in the calculated binding energy at Z=64 would not occur.

From the residual deviations of the accurate data from the smooth curves in the tests of the technique exhibited in figure 1, we are led to the conclusion that, using this method, an interpolated value can be assigned a "standard error" not less than about 5 eV. Errors assigned to extrapolations, of course, are increased as the distance from measured values increases (see figures 2, 3, and 4). Thus an "error band" is defined for each graph.

3. Results and Discussion

In figure 2 the differences between Desclaux's eigenvalues for the K shell and the weighted averages of the experimental data at each Z are plotted for the range 73 $Z \leq 100$. The 73000 eV span of the data is thus reduced to 700 eV, so the smoothing curve can be read to 1 eV on a 4-fold expanded plot. To show the differences on a still more expanded ordinate scale a parabolic function F(Z) following the trend of the differences was subtracted and the remainder plotted in figure 3B. Here we can also show the individual data points and their errors; solid bars denote K x-ray measurements and dashed bars denote internal conversion electron spectroscopic results. The smooth curve was drawn independently of that in figure 2. Figure 3A gives the difference between the Huang et al. K shell binding energies, as revised (personal communication [9]), and the data. Again the smooth curve is independent of the others.

Smoothed values for the K binding energies were obtained from all three curves. The differences among these, each referred to the value from the figure 2 curve, are shown in figure 4 as grouped triads of error bars at each Z, as a function of Z. Clearly the differences among the three sets of values are nowhere as large as the individual assigned errors. Thus we

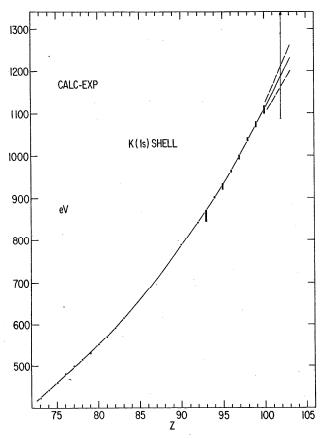


FIGURE 2. Plots of the differences between the calculated eigenvalues (Desclaux, ref. [8]), and the weighted averages of the experimental values for the K shells at each Z vs. Z from Z=73-100. These plots (figs. 2, 3, 5-9) are used for interpolation and extrapolation to obtain the recommended values of the binding energies for the unknown or poorly known cases.

give the average of the three values at each Z as our recommendation for the K binding energy, with an error assignment given by the envelope of figure 4.

We call attention to a thus far inexplicable trend in the K shell data. In both figures 3a and 3b one observes an increasing deviation above Z=95 between the smooth (solid) curve through the averages of all the data, determined mainly by the many accurate K x-ray measurements at Z=95–100 but including the data from the internal conversion electron spectroscopy at Z=98 and 100, and the dashed curve which follows the trend of the latter measurements only. (The dashed curve leads to higher K binding energies.) The latter measurements are our own [12, 13] and are themselves averages of many measurements, e.g., ten at Z=100; in view of the deviation we have carefully reanalyzed them and find no reason to change them.

Thus the trend of the deviation, while not outside reasonable statistical expectations, is perhaps suggestive of the onset at very high Z, where K vacancy lifetimes $\approx 10^{-17}$ s, of a significant reduction of K x-ray energies below the difference of the adiabatic binding energies of the initial and final vacancy states. In earlier work [14] we have shown that, at Z=95, such possible non-adiabaticity equals 0 ± 12 eV. At Z=100 the deviation is about +30 eV, twice the assigned (external) error of our recommended binding energy, which is

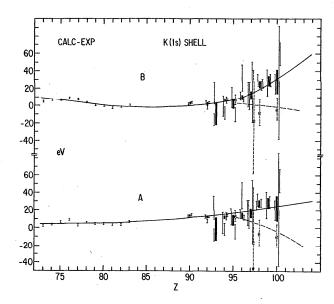


FIGURE 3. B) Plots of K shell differences (as in fig. 2) from which a function $F(Z) = aZ^2 + bZ + c$ (which follows the trend of the curve in fig. 2) has been subtracted. All individual data shown; solid error bars from K x-ray measurements, dashed error bars from internal conversion electron spectroscopy. Error bars spaced out slightly at each Z for visibility. Solid smooth curve follows data averages (heavy error bars); dashed curve follows dashed error bars. See text. A) Plot of the differences of calculated K shell binding energies (Huang et al. [9]) and experimental values. Remaining description same as above.

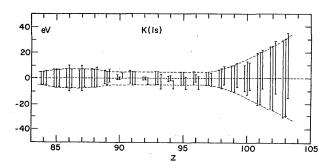


FIGURE 4. Plots of differences of smooth-curve values of K binding energies from figures 2, 3A and 3B, referred to those from curve of figure 2. Error bars grouped in triads at each Z; right hand member from curve 3A (Huang et al.) and left hand member from curve 3B (Desclaux-F(Z)). Center member from figure 2 plotted at 0 eV ordinate. Errors assigned to recommended K-shell binding energies given by envelope of error bars at each Z.

based on the average of all the data. In addition, one can see from the comparisons of our recommended K binding energies at Z=100 in table 2 to four theoretical calculations, columns 6, 7, 8 and 9, that the calculations are much closer to the binding energy derived from the internal conversion electron spectroscopic results than to our average value. This question

is challenging for future experiments, and may conceal fundamental physics.

In figures 5–9 are shown the plots for the other individual shells. These plots all refer to Desclaux's [8] eigenvalues except figure 5b for which the references are the L_3 binding energies of Huang et al. [9]. The L_3 binding energies obtained from this smooth curve agree with those from curve 5a within the range -1 to +3 eV from $84 \le Z \le 103$, with an average difference of 0.7 eV compared to our average assigned error of 4.5 eV in this range. (See table 1.) On the basis of this excellent agreement we refer all the other plots only to Desclaux's eigenvalues.

In a few cases where experiments report averages for unresolved spin-orbit splitting in the outer shells we have

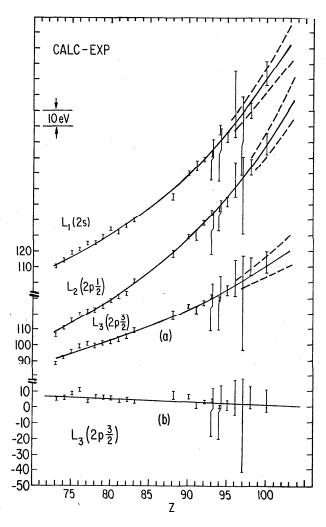


Figure 5. Plots of differences of calculated eigenvalues (Desclaux [8]) and experimental values for the L subshells. Figure 5b, L₃ differences from Huang et al. [9] binding energies.

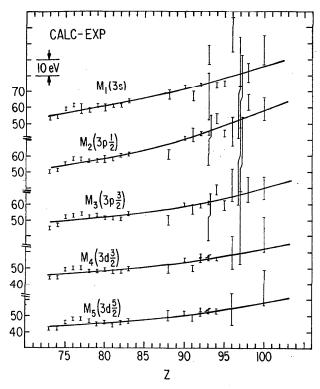


Figure 6. Plots of differences of calculated eigenvalues (Desclaux [8]) and experimental values for the M subshells.

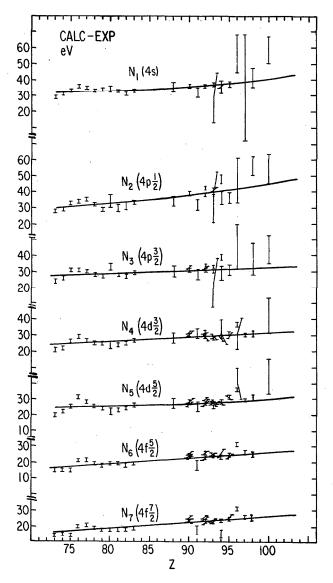


FIGURE 7. Plots of differences of calculated eigenvalues (Desclaux [8]) and experimental values for the N subshells.

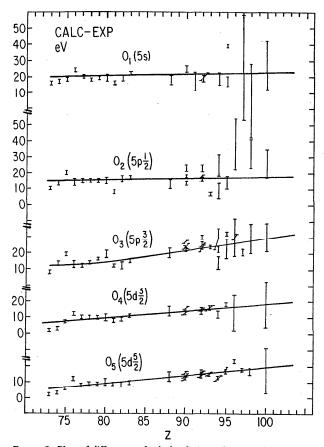


Figure 8. Plots of differences of calculated eigenvalues (Desclaux [8]) and experimental values for the ${\it O}$ subshells.

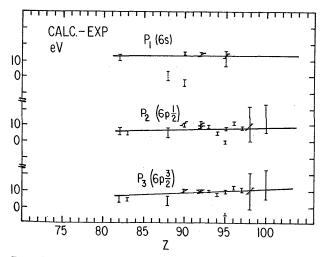


Figure 9. Plots of differences of calculated eigenvalues (Desclaux [8]) and experimental values for the P subshells.

made use of plots of experimental spin-orbit splitting as a function of Z to assign experimental values to the individual components. There is evidence that $5d_{3/2}$ peaks in photoelectron experiments [15] are smeared in energy ($\sim 10 \text{ eV}$) for those cases in which the 5f shell is partially filled. No values for this subshell are given in [15].

In the region from Z = 73-94 no attempt has been made to adjust any experimental value for the chemical nature of the source. For $Z \ge 94$ we have plotted the experimental values

adjusted, if necessary, to the "metal" or "condensed elemental" state. If, for example, the original experimental work indicates source deposition in an isotope-separator with low ion energy or thin vacuum-evaporated films, both exposed to air in the source handling process, the quoted experimental values have been reduced by 3 eV for inner shells and 2 eV for the P shells to account for the shift from the oxide environment to a "metal" environment.

One other adjustment we have made occurs at Z=96 at the irregular $5f^76d7s^2$ configuration analogous to the half-filled 4f shell at Z=64. Fortunately we have some photoelectron data [15] for the outer shells which confirms a smooth experimental behavior compared to a jump in both the calculated eigenvalue [8] and calculated binding energy [9] at Z=96. Consequently, we have recommended values at Z=96 which are smooth interpolations between neighboring recommended values. The adjustment is 5 to 6 eV for the inner shells and becomes smaller for the outer shells.

The binding energies given in table 1 are the energies required to move an electron from the particular orbit to the Fermi level in a solid source. The electronic work function of the material, typically 3-5 eV, is not included; see discussions in [1-3]. In comparing these energies to those from calculations for free atoms, the neglect of the electron work function, as well as the neglect of the energy needed to extract the resulting inner-vacancy ion from the solid, this latter energy being very difficult to measure or to estimate, must be taken into account. These corrections may total + (5-10) eV. However, since these corrections should depend very little on the particular inner shell ionized, they would not affect comparison to calculated x-ray energies.

In table 2 is exhibited a comparison of some of the present recommended values with others which have appeared as well as some calculations where they exist. For Z=87, which falls roughly in the middle of the interpolation region between Z=83 to 90, we see that the present recommended values are generally 2 to 14 eV lower than the Bearden and Burr interpolation (up to N_5) and the ESCA interpolation (from N_5 to the outer shells) except at N_2 and N_3 where our values are ~20 eV larger, significant compared to our estimated errors of ~ 5 eV. At Z=100 we see an example of the very poor K shell values which were the result of early calculations [16] quoted in Bearden and Burr (98 < Z < 103) and in subsequent tabulations [2,5] but corrected by the semi-empirical calculations of Carlson et al. [4]. Note also the high P shell extrapolation of Lotz [3] at Z=100 and 103 made without benefit of recent experimental values for $Z \ge 92$.

In table 3 we compare the energies of $K_{\alpha 1}$ x-ray transitions $(2p_3/2-1s)$ from the recommended binding energies of table 1 with those from the least-squares fit of an even Z^8 polynomial to the data from Z=90-100 by Krause and Nestor [17], and with the recent calculations by Carlson and Nestor [17], and from the (revised) binding energies of Huang et al. [9]. One sees the tendency of the polynomial fit, column 3, to deviate sharply above its fitting range. In early attempts we have made similar observations. The aggreement with the semi-empirically fitted calculations of Carlson and Nestor [17] is much more uniform and the values from Huang et al. [9] tend to diverge significantly at higher Z.

Prefatory Comments on Table 1

Recommended values for each subshell are underlined. Recommended values marked * are actual experimental values (or averages) instead of value from graphical smoothing procedure. This choice is made only if error bar of experimental average lies entirely inside estimated error band of graph.

Standard errors given as less than 1 eV in input data are given here as 1 eV. Errors assigned to averages of input data are larger of internal and external errors. For the K shell the error assignments are given by the envelope of the error bars in figure 4. The error band width for the L and higher shells is ± 5 eV from Z=83-96; at higher Z it flares out as shown in figure 5 and in this table.

Under each recommended value are listed all input data

with references. Each reference is coded with the measuring technique:

p=photoelectron spectroscopy;

e=internal conversion electron spectroscopy;

a=x-ray absorption edge;

x=x-ray transition R_iS_j plus S_j -shell binding energy (S_j -shell binding energy from this table for Z above 83, or from refs. [1 and 2] for $73 \le Z \le 83$).

For the range $73 \le Z \le 83$ used in the interpolating graphs the references to input data are: p—19, 20, 21, 22; x—18.

All those experimental input values for Z > 94 derived from internal conversion or photoelectron spectroscopy on oxide-coated sources have been reduced by 3 eV for shells K to O_5 and by 2 eV for the P shell, in the smoothing graphs and in this table, to account for the shift from the oxide environment to a "metal" environment.

TABLE1. Recommended values for atomic electron binding energies to the Fermi level in solids for the heavy elements (Z=84-103). Values in eV with estimate of standard errors.

Shell	84 Po	ref. 85 At	ref. 86 Rn	ref. 87 Fr	ref. 88 Ra	ref.
K(1s)	93100 ±5	95724 ±7	98397 ±7	101130 ±7	103915 ±7	
L ₁ (2s)	16928 ±5	17482 ±5	18048 ±5	18634 ±5	19232 ±5 19237 ±2 19236	x18 a18
L ₂ (2p _{1/2})	16237 ±5	16776 ±5	17328 ±5	17899 ±5	18484 ±2* 18484 ±2 18486	x18 a18
L ₃ (2p _{3/2})	13810 ±5	14207 ±5	14610 ±5	15025 ±5	15444 ±2* 15444 ±2 15444	x18 a18
M _] (3s)	4152 ±5	4310 ±5	4473 ±5	4644 ±5	4822 ±2* 4822 ±2	x18
M ₂ (3p _{1/2})	3844 ±5	3994 ±5	4150 ±5	4315 ±5	4483 ±5 4489 ±3	x18
M ₃ (3p _{3/2})	3293 ±5	3409 ±5	3529 ±5	<u>3656 ±5</u>	$\frac{3785 \pm 5}{3792 \pm 3}$	x18
M ₄ (3d _{3/2})	2794 ±5	2901 ±5	3012 ±5	3129 ±5	3248 ±2* 3248 ±2	x18
M ₅ (3d _{5/2})	2680 ±5	2781 ±5	2884 ±5	2994 ±5	3105 ±2* 3105 ±2	x18
N ₁ (4s)	987 ±5	1038 ±5	1090 ±5	1148 ±5	1208 ±2* 1208 ±2	x18
N ₂ (4p _{1/2})	851 ±5	897 ±5	944 ±5	999 ±5	1055 ±5 1058 ±3	x18
N ₃ (4p _{3/2})	715 ±5	751 ±5	<u>790 ±5</u>	834 ±5	879 ±3* 879 ±3	x18
N ₄ (4d _{3/2})	495 ±5	<u>527 ±5</u>	<u>558 ±5</u>	<u>597 ±5</u>	$\frac{636 \pm 2*}{636 \pm 2}$	x18
N ₅ (4d _{5/2})	469 ±5	499 ±5	530 ±5	<u>567 15</u>	603 ±3*	x18
N ₆ (4f _{5/2})	184 ±5	206 ±5	229 ±5	<u>258 ±5</u>	<u>287 ±5</u>	
N ₇ (4f _{7/2})	<u>178 +5</u>	199 +5	222 +5	249 +5	<u>279 +5</u>	
0 ₁ (5s)	176 ±5	<u>192 ±5</u>	<u>208 ±5</u>	229 ±5	251 ±5 254 ±3	x18
0 ₂ (5p _{1/2})	132 ±5	144 ±5	158 ±5	178 ±5	197 ±5 200 ±3	x18
0 ₃ (5p _{3/2})	102 ±5	113 ±5	123 ±5	138 ±5	153 ±3* 153 ±3	x18
0 ₄ (5d _{3/2})	34 ±5	41 ±5	48 ±5	<u>60 ±5</u>	72 ±5 ^a	
0 ₅ (5d _{5/2})	30 ±5	37 ±5	43 ±5	<u>55 ±5</u>	66 ±5 a	
P ₁ (6s)	<u>9 ±5</u>	<u>13 ±5</u>	<u>16 ±5</u>	<u>24 ±5</u>	31 ±5 44 ±3	x18
P ₂ (6p _{1/2})	4 ±5	6 ±5	<u>8 ±5</u>	<u>14 ±5</u>	20 ±5 a	
P ₃ (6p _{3/2})	1 ±5	<u>1 ±5</u>	<u>2 ±5</u>	<u>7 ±5</u>	12 ±5 a	

TABLE 1. Recommended values for atomic electron binding energies to the Fermi level in solids for the heavy elements (Z = 84-103). Values in eV with estimate of standard errors..continued

She11	89 Ac	ref. 90	Th	ref.	91 Pa	ref.	92 U	ref.	93 Np	ref.
K (1s)	106756 ±5	<u>10965</u> 10965 10964		x18 x24	112596 ±5		115602 ±1* 115606 ±2 115601 ±1 115601 ±2	x18 x24 x30	118669 ±5 118690 ±7 118659 ±13 118663 ±31	x33 x30 e51
1 ^(2s)	19846 ±5	2047 2047	2 ±1* 2 ±1	x18	21105 ±3* 21105 ±3 21128	x18 a18	21758 ±1* 21758 ±1	x18	22427 ±2* 22427 ±2 22431 ±13 22445 ±14	x18 e51 e52
2 ^{(2p} 1/2)	19081 ±5	1969 1969	3 ±1* 3 ±1	x18	20314 ±3* 20314 ±3 20319	x18 a18	20948 ±1* 20948 ±1	x18	21600 ±1* 21600 ±1 21612 ±14 21618 ±14	x18 e51 e52
3 ^{(2p} 3/2)	15870 ±5	1630 1630 1630	0 ±1* 0 ±1 0 ±1	x18 p23	16733 ±2* 16733 ±2 16733	x18 a18	17168 ±1* 17166 ±1 17168 ±1	x18 p26	17610 ±1* 17610 ±1 17617 ±15 17627 ±14	x18 e51 e52
₁ (3s)	4999 ±5	518: 518: 518:	2 ±1* 2 ±1 2 ±1	x18 p23	5361 ±5 5367 ±3	x18	5548 ±1* 5548 ±1	x18	5739 ±5 5723 ±5 5748 ±15 5750 ±15	x18 e51 e52
2 ^{(3p} 1/2)	<u>4655 ±5</u>	483 483 483	1 ±1* 0 ±1 1 ±1	x18 p23	5001 ±4* 5001 ±4	x18	5181 ±1* 5182 ±1 5181 ±1	x18 p26	5366 ±1* 5366 ±1 5366 ±1 5370 ±16 5377 ±19	x18 p32 e51 e52
3 ^{(3p} 3/2)	3915 ±5	4040 4040 4040	6 ±1* 6 ±1 6 ±1	x18 p23	4174 ±3* 4174 ±3	x18	4304 ±1* 4303 ±1 4304 ±1	x18 p26	4435 ±1* 4435 ±1 4435 ±1 4444 ±15 4446 ±19	x18 p32 e51 e52
; ^{(3d} 3/2)	3370 ±5	349 ¹ 349 ¹ 349 ¹	1 ±1* 1 ±1 1 ±1	x18 p23	3606 ±5 3608 3611 ±2	a18 x18	3726 ±1* 3728 ±1 3728 ±1 3725 ±1	x18 p26 x31	3849 ±1* 3850 ±1 3850 ±1 3848 ±1 3858 ±19	x18 p32 x34 e52
(^{3d} 5/2)	3219 ±5	3332 3332 3332	2 ±1* 2 ±1 2 ±1	x18 p23	3442 ±2* 3436 3442 ±2	a18 x18	3550 ±1* 3552 ±1 3552 ±1 3549 ±1	x18 p26 x31	3664 ±1* 3666 ±1 3664 ±1 3663 ±1 3674 ±24 3670 ±19	x18 p32 x34 e51 e52
(4s)	1269 ±5	1330 1330 1330) ±]*) ±]) ±]	x18 p23	1383 ±5 1387 ±3	x18	1441 ±1* 1441 ±1 1441 ±1	x18 p26	1501 ±1* 1501 ±1 1501 ±1 1509 ±16 1506 ±23	x18 p32 e51 e52
(4p _{1/2})	1112 ±5	1168 1168	3 ±1 3 ±1 3 ±1	x18 p23	1217 ±5 1224 ±2	x18	1271 ±2* 1273 ±1 1273 ±1 1269 ±1	x18 p26 x31	1328 ±2* 1328 ±1 1328 ±1 1327 ±1 1331 ±16 1334 ±23	x18 p32 x34 e51 e52
(4p _{3/2})	924 ±5	968	/ ±]* / ±] 3 ±] 5 ±]	x18 p23 p28	1004 ±5 1007 ±3	x18	1043 ±1* 1045 ±1 1045 ±1 1042 ±1 1043 ±1	x18 p26 x31 p28	1085 ±2* 1087 ±1 1087 ±1 1084 ±1 1094 ±16 1093 ±25	x18 p32 x34 e51 e52

TABLE 1. Recommended values for atomic electron binding energies to the Fermi level in solids for the heavy elements (Z = 84-103). Values in eV with estimate of standard errors.--continued.

Shell	89 Ac	ref.	90 Th	ref.	91 Pa	ref.	92 U	ref.	93 Np	ref.
N ₄ (4d _{3/2})	<u>676 ±5</u>		713 ±1* 714 ±1 714 ±1 713 ±2 712 ±1	x18 p23 p15 p28	743 ±3* 743 ±3	`-x18	779 ±1* 780 ±1 780 ±1 780 ±2 777 ±1 778 ±1	x18 p26 p15 p29 p28	816 ±1* 816 ±1 817 ±1 816 ±2 816 ±1 831 ±30	x18 p32 p15 p34 e52
N ₅ (4d _{5/2})	640 ±5		677 ±1* 676 ±1 676 ±1 676 ±2 678 ±1	x18 p23 p15 p25	708 ±3* 708 ±3	x18	737 ±1* 738 ±1 738 ±1 735 ±1 738 ±2 736 ±1	x18 p26 p29 p15 p28	771 ±1* 770 ±1 773 ±1 771 ±1 771 ±1 786 ±30	x18 p32 p15 p34 e52
N ₆ (4f _{5/2})	316 ±5		344 ±1* 344 ±1 344 ±1 344 ±1 345 ±1 342 ±1	x18 p23 p15 p25 p28	366 ±5 371 ±2	x18	389 ±1* 391 ±1 391 ±2 388 ±1 398 ±1	x18 p15 p28 p29	414 ±1* 415 ±1 414 ±1 414 ±1	p32 p15 p34
N ₇ (4f _{7/2})	<u>307 ±5</u>		335 ±1* 335 ±1 335 ±1 335 ±2 333 ±1 335 ±1	x18 p23 p15 p28 p25	355 ±5 360 ±3	x18	379 ±1* 381 ±2 378 ±1 380 ±1 377 ±1	x18 p29 p15 p28	403 ±1* 403 ±1 403 ±1 404 ±1	p34 p15 p32
0 ₁ (5s)	272 ±5		290 ±1* 290 ±1	x18	305 ±5 310 ±7	x18	324 ±2* 324 ±2 323 ±2	x18 p29	338 ±5	
o ₂ (5 _{P1/2})	217 ±5		236 ±1* 229 ±2 238 ±1 234 ±1	x18 p25 p28	245 ±5		257 ±1* 259 ±1 253 ±2 258 ±1	x18 p29 p28	274 ±5 283 ±1	p32
0 ₃ (5 _{P3/2})	168 ±5		180 ±1* 182 ±1 182 ±1 179 ±2 180 ±1 177 ±1	x18 p23 p15 p25 p28	188 ±5		194 ±2* 195 ±2 190 ±1 197 ±2 195 ±1	x18 p29 p15 p28	206 ±1* 206 ±1 206 ±2	p32 p15
⁰ 4 ^{(5d} 3/2)	<u>84 ±5</u>		94 ±1* 94 ±1 94 ±1 95 ±1 92 ±1	x18 p23 p25 p28	<u>97 ±5</u>		104 ±1* 105 ±1 103 ±1 103 ±1	x18 p28 p29	109 ±1* 109 ±1 109 ±1	x18 p32
0 ₅ (5d _{5/2})	76 ±5		87 ±1* 88 ±1 88 ±1 07 ±2 88 ±1 85 ±1	x18 p23 p15 p25 p28	90 ±5		95 ±2* 96 ±2 96 ±1 93 ±1 94 ±1	x18 p15 p29 p28	101 ±1* 101 ±1 101 ±1 101 ±2	x18 p32 p15
P ₁ (6s)	<u>37 ±5</u>		41 ±1* 60 ±2 41 ±1	x18 p28	43 ±5		44 ±1* 71 ±2 44 ±1 74 ±3 44 ±1	x18 p28 p29 p27	47 ±5	
P ₂ (6p _{1/2})	<u>24 ±5</u>		24 ±1* 49 ±4 25 ±2 24 ±1	x18 p15 p28	<u>27 ±5</u>		27 ±1* 42 ±13 27 ±1 26 ±1 28 ±2 58 ±3	x18 p28 p27 p15 p29	29 ±1* 29 ±1	p15
P ₃ (6p _{3/2})	15 ±5		17 ±1* 43 ±4 17 ±1 17 ±1	x18 p28 p15	<u>17 ±5</u>		17 ±1* 32 ±13 17 ±1 17 ±1 32 ±4 17 ±1	x18 p15 p28 p29 p27	18 ±1* 18 ±1	p15

TABLE 1. Recommended values for atomic electron binding energies to the Fermi level in solids for the heavy elements (Z = 84-103). Values in eV with estimate of standard errors.--continued.

Shell	94 Pu	ref.	95 Am	ref.	96 Cm	ref.	97 Bk	ref.	98 Cf	ref.
(1s)	121791 ±2*		124982 ±5		128241 ±3*		131556 ±5*		134939 ±7	
	121805 ±7	x33	124982 ±6	e39	128239 ±5	x41	131587 ±60	e42	134968 ±15	e13
	121790 ±1	x24	124997 ±8	x33	128218 ±15	x37	131553 ±35	x44	134930 ±7	x37
	121788 ±4	x30	124978 ±12	x39	128243 ±3	x30	131557 ±16	x41	134936 ±5	x43
	121794 ±12	x37					131548 ±7	×43	134934 ±5	x41
	121798 ±23	e36					131563 ±7	x30		
	121790 123	630						****		
1201	23104 ±5		23808 ±3*		24526 ±5		25256 +5		26010 ±7	
1 ^(2s)	23097 ±2	x18	23808 ±3	e39	24515 ±21	e40	25256 ±5 25272 ±25	e42	26016 ±5	e13
			23000 13	633	24313 121	•	20272 220		200.0 20	•.•
	23113 ±17	e36								
			00000 .0+		00051 .5		24271 . E		25100 +5+	
2 ^{(2p} 1/2)	22266 ±1*		22952 ±3*		23651 ±5 23651 ±11		24371 ±5 24832 ±25	e42	25108 ±5* 25108 ±5	e13
,-	22266 ±1	x18	22952 ±3	e39	23651 ±11	e40	24832 ±25	642	20100 ID	613
	22270 ±10	e36							•	
3 ^{(2p} 3/2)	18057 ±1*		18510 ±3*		18970 ±5		19435 ±5		19907 ±5	
3 3/2	18057 ±1	x18	18510 ±3	e39	18970 ±11	e40	19449 ±30	e42	19901 ±6	e13
	18060 ±17	e36								
1 ₁ (3s)	5933 +2*		6133 ±2*		6337 ±5		6545 ±7		6761 ±6*	
7,237	5933 ±2* 5933 ±2	x18	6133 ±2	e39	6314 ±11	e40	6553 ±31	e42	6761 ±6	e13
	3933 IL	XIO	0133 22	637	0017 211	2.10	0000 201		V/V/ 20	•.•
1 (30)	5547 ±5		5739 ±5		5937 ±5		6138 ±5		6345 ±6	
2 ^{(3p} 1/2)	5547 ±3	x18	5744 ±2	e39	5947 ±9	e40	6144 ±46	e42	6337 ±5	e13
• •	3341 I3	XIO	3/44 IZ	633	3347 13	640	0144 140	CTL	0557 25	
			4600 . 5		4000 5		4076 .5		E116 .E	
3 ^{(3p} 3/2)	4563 ±5 4557 ±2		4698 ±5 4703 ±3		4838 ±5 4835 ±10		4976 ±5 4974 ±46		5116 ±5	.10
J 5/L	4557 ±2	x18	4703 ±3	e39	4835 ±10	e40	49/4 ±46	e42	5115 ±8	e13
4 ^{(3d} 3/2)	3970 ±1*		4096 ±5		4224 ±5		4353 ±5	,	4484 ±6	
4. 3/2.	3970 ±1* 3970 ±1	p35			4227 ±10	e40				
		F								
5 ^{(3d} 5/2)	3775 +1*		3890 ±5		4009 ±5		4127 ±5		4247 ±6	
51-5/2	3775 ±1* 3775 ±1	p35			4014 ±10	e40				
	0	,,,,			, , , , , , , , , , , , , , , , , , , ,					
(4s)	1559 +1*		1620 ±2*		1684 ±5		1748 ±6		1813 ±6*	
11.75	1559 ±1* 1559 ±1	x18	1620 ±2	e39	1671 ±12	e40	1752 ±33	e42	1813 ±6	e13
	1560 ±4	e36	1020 12		1071 212	240	1702 200		7010 20	
	1300 14	630								
14- 1	1200 45		1420 ±E		1498 ±5		1558 ±8		1620 ±10	
2 ^{(4p} 1/2)	1380 ±5 1372 ±3	10	1438 ±5 1443 ±3	e39	1490 ±3 1497 ±14	e40	1330 IO		1607 ±6	e13
	13/2 I3	x18	1443 IS	633	. 149/ II4	240			1007 10	613
	1384 ±4	e36								
	,,,,,		11.00 4:		1007 5		3040 5		1000 6	
3 ^{(4p} 3/2)	1123 ±5		1165 ±3*		1207 ±5		1249 ±5		1292 ±6	• •
/-	1115 ±2	x18	1165 ±3	e39	1197 ±14	e40			1286 ±10	e13
	1125 ±4	e 36								
4 ^{(4d} 3/2)	846 ±1*		880 ±1*		916 ±2*		955 ±2*		991 ±2* 991 ±2	
4. 3/2.	846 ±1	p35	880 ±2	p15	916 ±2	p15	955 ±2	p15	991 ±2	p15
	847 ±2	p15	880 ±1	p38	922 ±10	e40				
	843 ±8	e36		•		7				
-(44)	798 ±1*		829 ±1*		862 ±2*		898 ±2*		930 +2*	
5 ^{(4d} 5/2 ⁾	708 +1	n35	829 ±1	p15	962 +2	p15	898 ±2	p15	930 ±2* 930 ±2	p15
	798 ±1 799 ±1	p35 p15	829 ±1	p38	862 ±2 858 ±10	e40	070 IZ	p15	930 ±2	pro
	133 11	hia	073 71	μυσ	030 110	240				
114 1	42C . 0±		AC1 .1+		404 .04		E11 .0±		E20 .0±	
6 ^{(4f} 5/2)	436 ±2*		461 ±1*	. 1 -	484 ±2*		511 ±2*		538 ±2* 538 ±2	
	436 ±2	p15	460 ±2	p15	484 ±2	p15	511 ±2	p15	538 ±2	p15
3,2		x18	461 ±1	p38						
0 0,1	443 ±3	×10								
		×10	_				_			
	424 ±2*		446 ±1*		470 ±2*		495 ±2*		520 ±2*	
7 ^{(4f} 7/2 ⁾		p15	446 ±1* 445 ±2	p15	470 ±2* 470 ±2	p15	495 ±2* 495 ±2	p15	520 ±2* 520 ±2	p15
	424 ±2*		446 ±1* 445 ±2 446 ±1	p15 p38	470 ±2* 470 ±2	p15	495 ±2* 495 ±2	p15	520 ±2* 520 ±2	p15

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TABLE 1. Recommended values for atomic electron binding energies to the Fermi level in solids for the heavy elements (Z = 84-103). Values in eV with estimate of standard errors.--continued.

Shell	94 Pu	ref.	95 Am	ref.	96 Cm	ref.	97 Bk	ref.	98 C f	ref.
) _[(5s)	350 ±5 352 ±4	x18	365 ±5 370 ±3 348 ±1	e39 p38	383 ±5		399 ±5 395 ±33	e42	$\frac{416 \pm 5}{433 \pm 23}$	el3
)2 ^{(5p} 1/2)	283 ±5 274 ±7 290 ±5	x18 e36	298 ±5 300 ±4	e39	313 ±5 296 ±16	e40	326 ±7		341 ±9 326 ±9	el3
) ₃ (5p _{3/2})	213 ±2* 206 ±7 218 ±4 213 ±2	x18 e36 p15	219 ±5 222 ±6 213 ±1	e39 p38	229 ±2* 229 ±12 229 ±2	e40 p15	237 ±5 243 ±2	p15	245 ±6 244 ±9	el3
) ₄ (5d _{3/2})	113 ±5 116 ±2	x18	116 ±1* 116 ±1	р38	124 ±5 132 ±11	e40	130 ±5		137 ±6	
) ₅ (5d _{5/2})	102 ±2* 105 ±2 102 ±2	x18 p15	106 ±1* 105 ±2 106 ±1	p15 p38	110 ±2* 110 ±2	p15	117 ±2* 117 ±2	p15	122 ±2* 122 ±2	p15
(6s)	46 ±5		48 ±1* 50 ±5 48 ±1	e39 p38	50 ±5		52 ±5		54 ±8	
2 ^{(6p} 1/2)	29 ±2* 29 ±2	p15	29 ±2* 29 ±2 38 ±1	p15 p38	30 ±2* 30 ±2	p15	32 ±2* 32 ±2	p15	33 ±2*b	
(6p _{3/2})	16 ±2* 16 ±2	p15	16 ±2* 16 ±2 30 ±1	p15 p38	16 ±2* 16 ±2 31 ±27	p15 e40	16 ±2* 16 ±2	p15	17 ±2*b	p15

TABLE 1. Recommended values for atomic electron binding energies to the Fermi level in solids for the heavy elements (Z = 84-103). Values in eV with estimate of standard errors.--continued.

Shell	99 Es	ref.	100 Fm	ref.	101 Md	ref. 102 No	ref.	103 Lw	ref.
((1s)	138396 ±10 138394 ±15 138391 ±7	x41 x37	141926 ±15 141960 ±13 141931 ±11 141930 ±65 141897 ±13	e12 x46 x45 x47	145526 ±20	149208 ±25 149103 ±200	x48	152970 ±30	
-1 ^(2s)	26/82 ±/	,	2/5/4 ±8 27570 ±8	e12	28387 ±8	29221 ±10		30083 ±12	
·2 ^{(2p} 1/2)	25865 ±6		26641 ±7* 26641 ±7	e12	27438 ±10	28255 ±11		29103 ±12	
·3 ^{(2p} 3/2)	20384 ±6		20868 ±7 20865 ±7	e12	21356 ±7	<u>21851 ±8</u>		22359 ±10	
1 ₁ (3s)	6981 ±7		7208 ±9 7197 ±9	e12	7440 ±10	7678 ±11		7930 ±12	
1 ₂ (3p _{1/2})	6558 ±7		6776 ±7* 6776 ±7	e12	7001 ±8	7231 ±9		7474 ±10	
1 ₃ (3p _{3/2})	5259 ±6		5405 ±7* 5405 ±7	e12	5552 ±8	5702 ±9		5860 ±10	
1 ₄ (3d _{3/2})	4617 ±6		4752 ±7 4743 ±11	e12	4889 ±9	5028 ±11		5176 ±13	
15 ^{(3d} 5/2)	4368 ±8		4491 ±10 4481 ±11	e12	4615 ±11	4741 ±13		4876 ±15	
1 ^(4s)	1883 ±11		1952 ±14 1937 ±11	e12	2024 ±18	2097 ±21		2180 ±25	
2 ^{(4p} 1/2 ⁾	1683 ±11		1749 ±13 1740 ±9	e12	1816 ±15	<u>1885</u> ±17		1963 ±20	
3 ^{(4p} 3/2)	1336 ±8		1379 ±10 1368 ±9	e12	1424 ±11	1469 ±13		1523 ±17	
4 ^{(4d} 3/2)	1029 ±9		1067 ±11 1056 ±11	e12	1105 ±13	1145 ±16		1192 ±18	
5 ^{(4d} 5/2)	965 ±9		1000 ±15 986 ±11	e12	1034 ±18	1070 ±20		1112 ±24	
6 ^{(4f} 5/2)	564 ±6		591 ±8		618 ±10	645 ±13		680 ±15	
7 ^{(4f} 7/2)	546 ±6		572 ±8		597 ±10	624 ±13		658 ±15	
1 ^{(5s})	434 ±7		452 ±9 447 ±15	e12	471 ±11	490 ±13		516 ±15	
2 ^{(5p} 1/2)	357 ±11		$\frac{373 \pm 9}{364 \pm 9}$	el2	389 ±16	406 ±18		429 ±20	
3 ^{(5p} 3/2)	255 ±7		262 ±9* 262 ±9	e12	272 ±9	280 ±10		296 ±12	
4 ^{(5d} 3/2)	142 ±7		149 ±9 ^C		154 ±10	<u>161 ±11</u>		174 ±12	
5 ^{(5d} 5/2)	127 ±7		133 ±9 ^C		137 ±10	142 ±11		154 ±12	
(6s)	57 ±9		59 ±10		61 ±11	63 ±12		71 ±13	
, 2 ^{(6p} 1/2)	35 ±6		36 ±7 ^C		37 ±8	38 ±10		44 ±11	
3 ^{(6p} 3/2)	17 ±6		17 ±7°		17 ±8	18 ±10		21 ±11	

 $^{^{}a}$ Experimental points (x 18) on figures 8 and 9 from unresolved 0 4,5 and p 2,3 peaks, using extrapolated spin-orbit splitting.

bExperimental points with larger error bars [el3] on figure 9 from unresolved P2,3 peak using extrapolated spin-orbit splitting.

 $^{^{}c}$ Experimental points [el2] on figure 8 from unresolved 0 4,5 and p 2,3 peaks using extrapolated spin-orbit splitting.

TABLE 2. Comparison of atomic electron binding energies at three values of the atomic number (2).

Column two in eV. Other columns give excess over values in column two in eV. Standard errors given in eV.

		-	usted compilat	ions	••••	Calculat	ions	
Shell	Recommended values (TABLE 1) ^a	ESCA	Bearden and Burr ^C	Lotz ^d	Huang et al ^e	Carlson et al ^f		Frick et al
			<u>Z = 87</u>					
K(ls)	101130 ±7	+7	+7 ±20	+4	+9			
L ₁ (2s)	18634 ±5	+5	+5 ±60	+3	+14			
L ₂ (2p _{1/2})	17899 ±5	+7	+7 ±5	+4	+5			
L ₃ (2p _{3/2})	15025 ±5	+6	+6 ±5	+3	+6			
M ₇ (3s)	4644 ±5	+8	+8	+8	+27			
M ₂ (3p _{1/2})	4315 ±5	+12	+12 ±60	+9	+15			
M ₃ (3p _{3/2})	3656 ±5	+7	+7 ±60	+10	+14			
M ₄ (3d _{3/2})	3129 ±5	+7	+7 ±5	+5	+9			
M ₅ (3d _{5/2})	2994 ±5	+6	+6 ±5	+4	+9			
N ₁ (4s)	1148 ±5	+5	+5	+5	+18	•		
N ₂ (4p _{1/2})	999 ±5	-19	-19 ±60	+4	+17			
N ₃ (4p _{3/2})	834 ±5	-24	-24 ±60	+5	+14			
N ₄ (4d _{3/2})	597 ±5	+6	+6 ±6	+6	+10			
N ₅ (4d _{5/2})	567 ±5	+10	+10 ±50	+5	+11			
16 ^{(4f} 5/2)	258 ±5 (. 7.4		+10	+7			
N7 ^{(4f} 7/2)	249 ±5 \$	+14		+11	+9			
) ₁ (5s)	229 ±5	+5		+2	+15			
O ₂ (5p _{1/2})	178 ±5	+4		+5	+9			
) ₃ (5p _{3/2})	138 ±5	+2		+9	+14			
) ₄ (5d _{3/2})	60 ±5)	•		+5	+8			
0 ₅ (5d _{5/2})	55 ±5∫	0		+6	+8			
7(6s)	24 ±5	+10		+19	+11			
² (6p _{1/2})	14 ±5)	. 4		+3	+5			
3 ^{(6p} 3/2)	7 ±5∮	+4		+6	+7			

TABLE 2. Comparison of atomic electron binding energies at three values of the atomic number (2).

Column two in eV. Other columns give excess over values in column two in eV. Standard errors given in eV. --continued..

		Adju	sted Compilat	ions		.Calculat	ions	
Shell .	Recommended	ESCA ^b	Bearden and Burr ^C	Lotz ^d	Huang et al.e	Carlson et al ^f		Fricke et al ^h
			7 100					
			Z = 100					
K(1s)	141926 ±15	+1164	+1164	+913	+25	+17 ±34	+30 ~±25	+27 ±26
L ₁ (2s)	27574 ±8	+126	+126	- 15	+19	+10 ±25		+7 ±20
L ₂ (2p _{1/2})	26641 ±7	+169	+169	-27	0	+2 ±16		+5 ±10
L ₃ (2p _{3/2})	20868 ±7	+32	+32	-8	+1	+4 ±14		+1 ±10
M ₁ (3s)	7208 ±9	-3	-3	0	+30	-2 ±12		+5 ±15
M ₂ (3p _{1/2})	6776 ±7	+17	+17	+3	+17	+7 ±11		+7 ±4
M ₃ (3p _{3/2})	5405 ±7	-8	-8	+21	+14	+9 ±11	•	
M ₄ (3d _{3/2})	4752 ±7	+14	+14	+14	+5	+5 ±11		
M ₅ (3d _{5/2})	4491 ±10	+7	+7	+17	+6	+6 ±11		
N ₁ (4s)	1952 ±14	-15	-15	-13	+15	+2 ±20		
N ₂ (4p _{1/2})	1749 ±13	-2	-2	-10	+15	+4 ±20		
N ₃ (4p _{3/2})	1379 ±10	-13	-13	-6	+9	+4 ±20		
N ₄ (4d _{3/2})	1067 ±11			+2	+8	+4 ±10		
N ₅ (4d _{5/2})	1000 ±15			+2	+8	+5 ±10		
N ₆ (4f _{5/2})	591 ±8			+24	+4			
N ₇ (4f _{7/2})	572 ±8			+27	+4			
0 ₁ (5s)	452 ±9	+2	+2	+13	+10			
0 ₂ (5p _{1/2})	373 ±9			+4	+5	+2 ±15		
0 ₃ (5 _{P3/Z})	262 ±9			+8	+19			
0 ₄ (5d _{3/2})	149 ±9			+17	+10	+4 ±15		
0 ₅ (5d _{5/2})	133 ±9			+10	+9	+5° ±15		
P ₁ (6s)	59 ±10			+55	+9			
P ₂ (6p _{1/2})	36 ±7			+57	+5			
P ₃ (6p _{3/2})	17 ±7			+58	+8			

TABLE 2. Comparison of atomic electron binding energies at three values of the atomic number (Z).

Column two in eV. Other columns give excess over values in column two in eV. Standard errors given in eV. --continued.

5			usted Compila					
Shell	Recommended	ESCA ^b	Bearden C	Lotz ^d	Huang	Carlson	Mann	Fricke
	values (TABLE 1) ^a		and Burr ^C		et al ^e	et al f	et al ^g	et al ⁿ
			<u>'</u> = 103					
K(1s)	152970 ±30	+1410	+1410	+766	+36	+11 ±62		
L _] (2s)	30083 ±12	+157	+157	-60	+20	+7 ±44		
L ₂ (2p _{1/2})	29103 ±12	+177	+177	-76	0	-4 ±25		
L ₃ (2p _{3/2})	22359 ±10	1+1	+1	-27	+2	+1 ±22.		
M ₁ (3s)	7930 ±12	-30	-30	-5	+32	-9 ±20		
M ₂ (3p _{1/2})	7474 ±10	-14	-14	-5	+17	0 ±17		
M ₃ (3p _{3/2})	5860 ±10	-50	-150	+31.	+14	+3 +17		
M ₄ (3d _{3/2})	5176 ±13	-26	-26	+20	+5	-3 ±17		
M ₅ (3d _{5/2})	4876 ±15	-16	-16	+25	+6	+2 ±17		
N ₁ (4s)	2180 ±25	-40	- 40	-33	+15	-6 ±20		
N ₂ (4p _{1/2})	1963 ±20	-33	-33	-17	+15	-4 ±20		
N ₃ (4p _{3/2})	1523 ±17	-43	-43	-17	+7	-4 ±20		
N ₄ (4d _{3/2})	1192 ±18			-4	+7	-3 ±15		
N ₅ (4d _{5/2})	1112 ±24			-3	+9	0 ±15		
N ₆ (4f _{5/2})	680 ±15			+36	+4			
N ₇ (4f _{7/2})	658 ±15			+39	+4			
0 ₁ (5s)	516 ±15	-26	-26	+3	+9			
0 ₂ (5p _{1/2})	429 ±20			+1	+4	-5 ±15		
0 ₃ (5p _{3/2})	296 ±12			+4	+21			
0 ₄ (5d _{3/2})	174 ±12			+24	+9	-3 ±15		
0 ₅ (5d _{5/2})	154 ±12			+9	+12	-ļ ±15		
P ₁ (6s)	71 ±13			+63	+8			
2 ^{(6p} 1/2 ⁾	44 ±11			+69	+6			
P ₃ (6p _{3/2})	21 ±11			+72	+9			

^aBinding energies to Fermi level in condensed source.

^bRef. 2; binding energies to Fermi level in condensed source. Ref. 5; same values for Z=87, 100, 103.

^CRef. 1; binding energies to Fermi level in condensed source.

 $^{^{}m d}$ Ref. 3; binding energies for free atoms, i.e., includes work function of 5 eV. Standard error estimates are stated for Z=87 as < 3 eV; for Z=100 and 103 error estimates are stated to be > 15 but < 90 eV.

 $^{^{\}rm e}$ Ref. 9; calculations for free atoms. Expected to be $^{\sim}$ 5 eV higher than experimental values for binding energies to Fermi level of a condensed source.

fT. A. Carlson and C. W. Nestor, Jr., ref. 17. Errors from this ref. only; no contribution from error in column 2. Calculations for free atoms.

gRef. 29. Error from this ref. only; no contribution from error in column 2. Calculations for free atoms.

hRef. 50. Error from this ref. only; no contribution from error in column 2. Calculations for free atoms.

TABLE 3. Comparison of $K\alpha_1$ (1s-2 $p_{3/2}$) x-ray transition energies.

Z	This paper	Empirical Fit ^a	Calculationb	Calculation ^C
89	90886 ±7	-6 ±11		+5
90	93350 ±2	-2 ±3		+6
91	95863 ±5	+2 ±3		+12
92	98434 ±3	-1 ±3	+9	+9
93	101059 ±5	-3 ±3		+9
94	103734 ±2	+1 ±3	•	+13
95	106472 ±3	0 ±3	+11 ±29	+13
96	109271 ±6	-3 ±3	+8 ±49	+8
97	112121 ±7	+5 ±5	+10 ±49	+15
98	115032 ±9	+13 ±6	+15 ±49	+22
99	118012 ±12	+14 ±8	+13 ⊥49	+23
100	121058 ±17	+12 ±13	+13 ±37	+24
101	124170 ±21	+6 ±29	+15 ±65	+29
102	127357 ±27	-12 ±59	+11 ±65	+31
103	130611 ±31	-38 ±111	+10 ±65	+34

^aM. O. Krause and C. W. Nestor, Jr., ref. 17. Error from this ref. only.

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References

- [1] Bearden, J. A., and Burr, A. F., Rev. Mod. Phys. 39, 125 (1967).
- [2] Siegbahn, K., Nordling, C., Fahlman, A., Nordberg, R., Hamrin, K., Hedman, J., Johansson, C., Bergmark, T., Karlsson, S.-E., Lindgren, I., and Lindberg, B., ESCA—Atomic, Molecular and Solid State Structure Studied by Means of Electron Spectroscopy, (Almqvist and Wiksells Boktryckeri AB, Uppsala, Sweden, 1967) Appendix I.
- [3] Lotz, W., J. Opt. Soc. Am. 60, 206 (1970).
- [4] Carlson, T. A., Nestor, C. W., Jr., Malik, F. B., and Tucker, T. C., Nucl. Phys. A135, 57 (1969).
- [5] Sevier, K. D., Low Energy Electron Spectrometry (Wiley—Interscience, New York, 1972) Appendix F.
- [6] Bergvall, P., and Hagström, S., Arkiv. Fysik. 17, 61 (1960).
- [7] We have also tried including a Z⁴ term as suggested by S. Hagström [Z. Physik 178, 82 (1964)] to reduce the total span of the data. While such a function does indeed reduce the total range of the differences and is good for interpolation, we find it poor for extrapolation.
- [8] Desclaux, J. P., Atomic Data Nucl. Data Tables, 12, 312 (1973). We have compared the calculations of Desclaux with those of J. B. Mann and J. T. Waber (ref. 10 and private communication) and find them to be the same (within ~ 1 eV) for the cases we have checked.
- [9] Huang, K-N, Aoyagi, M., Chen, M. H., Crasemann, B. and Mark, H., Atomic Data and Nuclear Data Tables, 18, 243 (1976). This calculation of binding energies includes relaxation and field-theoretic contri-

butions. Approximations to the form of the Breit interaction and to the form of the nuclear charge distribution used in the program for the published table lead to rapidly increasing deviations from K shell experimental values above Z=90. The Huang et al. values we use for the K shell were revisions based on corrections of these factors (Dr. Chen private communication) above Z=80, extrapolated by us down to Z=73.

- [10] Mann, J. B., and Waber, J. T., Atomic Data 5, 201 (1973).
- [11] Mann, J. B., private communication.
- [12] Porter, F. T., and Freedman, M. S., Phys. Rev. Letters 27, 293 (1971).
- [13] Porter, F. T., and Freedman, M. S., unpublished work, based on: Freedman, M. S., Ahmad, I., Porter, F. T., Sjoblom, R. K., Barnes, R. P., Lerner, J., and Fields, P. R., Phys. Rev. C 15, 760 (1977).
- [14] Freedman, M. S., and Porter, F. T., Phys. Rev. A 6, 659 (1972).
- [15] Veal, B. W., Lam, D. J., Diamond, H., and Hoekstra, H. R., Phys. Rev. B 15, 2929 (1977); Veal, B., Lam, D. J., Carnall, W. T., and Hoekstra, H. R., Phys. Rev. B 12, 5651 (1975).
- [16] Liberman, D., Waber, J. T., and Cromer, D. T., Phys. Rev. 137, A 27 (1965).
- [17] Krause, M. O., and Nestor, C. W., Jr., Proc. Symposium on Electron Spectroscopy, Uppsala, 1977. Physica Scripta.—Suppl. issue; Carlson, T. A. and Nestor, C. W. Jr., At. Data Nucl. Data Tables, 19, 153 (1977).
- [18] Bearden, J. A., Rev. Mod. Phys. 39, 78 (1967) and ref. 1.
- [19] Fahlman, A. and Hagström, S., Arkiv Fysik 27, 69 (1964).
- [20] Nordling, R., Hedman, J., Nordling, C., and Siegbahn, K., unpublished, quoted in ref. 2.
- [21] Sokolowski, E., Arkiv Fysik 15, 1 (1959).
- [22] Karlsson, S.-E., Norbert, C.-H., Nilsson, Ö., Högberg, S., el-Farrash, A. H., Nordling, C., and Siegbahn, K., unpublished, quoted in ref. 2.

 b_{T} . C. Carlson and C. W. Nestor, Jr., ref. 17. Error from this ref. only.

CHuang et al., ref. 9.

- [23] Nordling, C., and Hagström, S., Z. Phys. 178, 418 (1964).
- [24] Borchert, G. L., and Fricke, B., Abstr., 5th Int. Conf. Atomic Physics, Marrus, R., Prior, M. H., Shugart, H. A., eds., Berkeley 1976, p. 321; Borchert, G. L., Z. Naturf. 31a, 102 (1976).
- [25] Bancroft, G. Michael and Sham, Tsun, K., Chem. Phys. Lett. 46, 551 (1977).
- [26] Nordling, C., and Hagotröm, S., Arkiv Fysik 15, 431 (1959).
- [27] Verbist, J., Riga, J., Pireaux, J. J. and Caudano, R., J. Elec. Spec. Rel. Phenom. 5, 193 (1974).
- [28] Fuggle, J. C., Burr, A. F., Watson, L. M., Fabian, D. J., and Lang, W., J. Phys. F. 4, 335 (1974).
- [29] Park, R. L., and Houston, J. E., Phys. Rev. A. 7, 1447 (1973).
- [30] Börner, H., (personal communication).
- [31] Keski-Rahkonen, O. and Krause, M. O., Phys. Rev. A 15, 959 (1977).
- [32] Hagström, S., Bull. Am. Phys. Soc., 11, 389 (1966).
- [33] Nelson, G. C., Saunders, B. G., and Salem, S. I., Z. Physik 235, 308 (1970).
- [34] Krause, M. O., Nestor, C. W., Jr., and Oliver, J. H., Phys. Rev. A 15, 2335 (1977).
- [35] Fahlman, A., Hamrin, K., Nordling, R., Nordling, C., Siegbahn, K., and Holm, L. W., Phys. Letters 19, 643 (1966).
- [36] Porter, F. T., Ahmad, I., Freedman, M. S., Barnes, R. F., Sjoblom, R. K., Wagner, F., Jr., and Fields, P. R., Phys. Rev. C 5, 1738 (1972).
- [37] Ahmad, I., unpublished work (personal communication).
- [38] Krause, M. O., and Wuilleumier, F., Electron Spectroscopy (Ed. Shirley, D. A., North Holland Publishing Co., Netherlands, 1972) p. 759.

- [39] Porter, F. T., Ahmad, I., Freedman, M. S., Milsted, J., and Friedman, A. M., Phys. Rev. C 10, 803 (1974) gives experimental data only. Binding energy calculation unpublished.
- [40] Chu, Y. Y., Perlman, M. L., Dittner, P. F., and Bemis, C. E., Jr., Phys. Rev. A 5, 67 (1972).
- [41] Dittner, P. F., and Bemis, C. E., Jr., Phys. Rev. A 5, 481 (1972).
- [42] Hollander, J. M., Holtz, M. D., Novakov, T., and Graham, R. L., Arkiv Fysik, 28, 375 (1965).
- [43] Helmer, R. G., unpublished work (personal communication).
- [44] Fields, P. R., Ahmad, I., Barnes, R. F., Sjoblom, R. K., and McHarris, W. C., Nuc. Phys. A208, 269 (1973).
- [45] Dittner, P. F., Bemis, C. E., Hensley, D.C., Silva, R. J., and Goodman, C. D., Phys. Rev. Letters 17, 1037 (1971).
- [46] Ahmad, I., Diamond, H., Milsted, J., Lerner, J., and Sjoblom, R. K., Nucl. Phys. A208, 287 (1973); Ahmad, I., private communication.
- [47] Clark, R. G., and Glendenin, L. E., unpublished work (personal communication).
- [48] Bemis, C. E., Jr., Silva, R. J., Hensley, D. C., Keller, O. L., Jr., Tarrant, J. R., Hunt, L. D., Dittner, P. F., Hahn, R. L., and Goodman, C. D., Phys. Rev. Lett. 31, 647 (1973).
- [49] Freedman, M. S., Porter, F. T., and Mann, J. B., Phys. Rev. Lett. 28, 711 (1972).
- [50] Fricke, B., Desclaux, J. P., and Waber, J. T., Phys. Rev. Lett. 28, 714 (1972).
- [51] Yamazaki, T., and Hollander, J. M., Nucl. Phys. 84, 505 (1966).
- [52] Wolfson, J. L., and Park, J. J. H., Can. J. Phys. 42, 1387 (1964).