Reevaluation of X-Ray Atomic Energy Levels

J. A. BEARDEN, A. F. BURR*
The Johns Hopkins University, Baltimore, Maryland

All of the x-ray emission wavelengths have recently been reevaluated and placed on a consistent Å* scale. For most elements these data give a highly overdetermined set of equations for energy level differences, which have been solved by least-squares adjustment for each case. This procedure makes "best" use of all x-ray wavelength data, and also permits calculation of the probable error for each energy difference. Photoelectron measurements of absolute energy levels are more precise than x-ray absorption edge data. These have been used to establish the absolute scale for eighty-one elements and, in many cases, to provide additional energy level difference data. The x-ray absorption wavelengths were used for eight elements and ionization measurements for two; the remaining five were interpolated by a Moseley diagram involving the output values of energy levels from adjacent elements. Probable errors are listed on an absolute energy basis. In the original source of the present data, a table of energy levels in Rydberg units is given. Difference tables in volts, Rydbergs, and milli-Å* wavelength units, with the respective probable errors, are also included there.

CONTENTS

INTRODUCTION

Manne Siegbahn[1,2] developed the first extensive evaluation of atomic energy levels from x-ray absorption edges and emission lines. The energy of the well-defined L_{III} absorption edge was chosen as the fundamental reference level for most of the periodic system; K edges were used for the lower atomic numbers. Other levels of each element were determined from the wavelengths of the emission lines as suggested by Idei.[3]

As improved x-ray data have become available, several reviews have appeared.[4–9] Different energy units have been used to facilitate use by special groups. Cauchois[6,7] improved the consistency of the rare-earth evaluations by a series of controlled absorption measurements. Theoretical calculations of many parameters often require ionization energies. Slater[9] has calculated these for all atomic numbers less than 42. For the outer electrons he used optical data, for the inner electrons, x-ray data.

Magnetic spectrometer[10] measurements of the kinetic energy of photoelectrons released by irradiation with x rays of known wavelength furnish a method for direct measurement of energy levels. Recently Kai Siegbahn[11] and co-workers have used a high-precision iron-free spectrometer to determine energy levels directly from x-ray photoelectron measurements. For elements where photoelectron values are not available and x-ray absorption edge values existed, the latter are used to help complete the table; in other instances, interpolated or extrapolated values are listed. All values are given to the nearest eV.

X-ray emission wavelengths provide accurate data for evaluating the atomic energy levels on a relative scale,[3] but only recently[12] has full advantage been taken of all the information available. The number of available lines is usually considerably greater than the number of energy levels involved. For such problems, which yield an overdetermined set of linear equations, the method of least squares furnishes a convenient and consistent means of obtaining "best" values and also probable errors for each of the values. Recently re-evaluated wavelengths[13] of the x-ray emission lines provide most of the input data. In place of the x-ray absorption edge values, previously used to establish the absolute scale, photoelectron measurements are substituted, wherever available.

* Present address: Physics Department, New Mexico State University, University Park, N.M. 88070.

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[2] D. L. Webster, W. W. Nicholas, and M. Siegbahn, *International Critical Tables*, E. W. Washburn, Ed. (McGraw-Hill Book Co., Inc., New York, 1929), Vol. 6, p.35.
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[9] J. C. Slater, Phys. Rev. **98**, 1039 (1955).
[10] H. R. Robinson, J. P. Andrews, and E. J. Irons, Proc. Roy. Soc. (London) **A143**, 48 (1933); H. R. Robinson: Proc. Phys. Soc. (London) **46**, 693 (1934); Phil. Mag. **18**, 1086 (1934); also see Kretschmar, Phys. Rev. **43**, 417 (1933).
[11] S. Hagström, C. Nordling, and K. Siegbahn, *Alpha-, Beta-, and Gamma-Ray Spectroscopy*, K. Siegbahn, Ed. (North-Holland Publ. Co., Amsterdam, 1965), Vol. 1, p. 845.
[12] J. A. Bearden and A. F. Burr, *Atomic Energy Levels*, NYO 2543-1 (Federal Sci. and Tech. Inf., U.S. Dept. of Commerce, Springfield, Va. 122151).
[13] J. A. Bearden, Rev. Mod. Phys. **39**, 78 (1967), preceding article. J. A. Bearden, *X-Ray Wavelengths*, NYO 10586 (Federal Sci. and Tech. Inf., U.S. Dept. of Commerce, Springfield, Va. 122151).

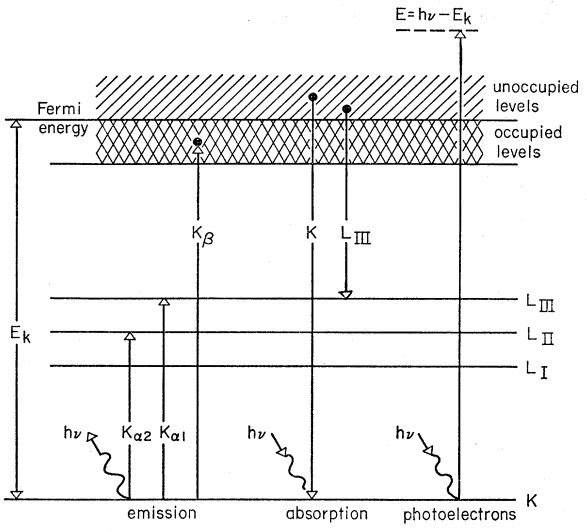

FIG. 1. Schematic of the principles involved in evaluating atomic energy levels.

METHODS OF EVALUATING ENERGY LEVELS

The principles involved in evaluating atomic energy levels are shown schematically in Fig. 1. The energy of a $K\alpha_1$ emission photon is just the difference between the K and L_{III} levels; similarly the $K\alpha_2$ corresponds to that difference between K and L_{II}. Usually the energy difference between a pair of levels can be obtained in two or more ways. For example, the difference between L_{II} and L_{III} can be evaluated from $K\alpha_1 - K\alpha_2$ (expressed in energy units). Alternatively it can be found from $L\beta_1 - L\alpha_2$, which represent the $L_{II}M_{IV}$ and $L_{III}M_{IV}$ transitions, respectively (omitted from Fig. 1 in the interest of simplicity). In the case of thorium, ninety-nine equations (including sixteen photoelectron measurements as discussed below) can be set up with only twenty-five unknown levels. A least-squares solution of this set yields the desired energy levels.

In order to determine these values on an absolute scale, the energy required to raise an electron from at least one energy state to the Fermi level energy (zero) must be included among the input data. In the center of Fig. 1 a K and an L_{III} absorption edge are indicated; experimental measurements of these edges give (approximately) the energy difference between the Fermi level and the K and L_{III} states, respectively. The theoretical corrections that must be made to these values for fine structure effects in the edges (due to differing transition probabilities and other causes) constitutes the principal uncertainty[8,14] in the use of present x-ray absorption edge measurements.

The photoelectron method measures the energy of various states relative to the Fermi level. In this case the incident photon (usually originating from an x-ray spectral line) has an energy $h\nu$, normally much larger than that of the energy level under study. If, for example, the photoelectron comes from the K level, it emerges with an energy $(h\nu - E_K)$. To determine the exact kinetic energy, a work function correction is required. This is more amenable to analysis[15] than the corrections to x-ray absorption measurements. This fact constitutes a major advantage of this method. This procedure is discussed in a later section.

[14] L. G. Parratt, Rev. Mod. Phys. **31**, 616 (1959).

EXPERIMENTAL MEASUREMENTS

X-Ray Measurements of Wavelengths and Absorption Edges

The principles of precise measurement of x-ray wavelengths have been summarized in the foregoing paper.[13] Absorption edge wavelength measurements require the same techniques, but are subject to additional complications. The thickness[14,16] of the absorber can displace the observed edge and, of course, the chemical state of the absorber is important. However, in spite of the uncertainty in the correction for fine-structure effects and difficulties of precise x-ray measurements, a number of the results are in excellent agreement with the photoelectron values. Thus it appears that with sufficient care the x-ray absorption measurements could be made competitive with the photoelectron method.

X-Ray Photoelectron Measurements

The precision β-ray spectrograph developed by Kai Siegbahn[17] and his collaborators at Uppsala provides an instrument of high accuracy for the measurement of photoelectron energies. The precision of these measurements is approximately one hundred times that of the older magnetic spectrometer values[10]; for some elements they are an order of magnitude better than existing x-ray ones.

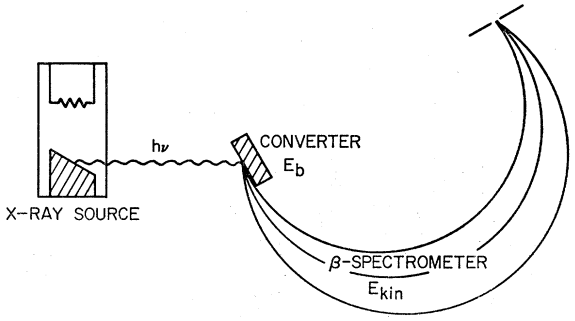

FIG. 2. Schematic of the use of a β-ray spectrometer for determining energy levels.

[15] E. Sokolowski, Arkiv Fysik **15**, 1 (1959).
[16] O. Beckman, B. Axelsson, and P. Bergvall, Arkiv Fysik **15**, 567 (1959).
[17] K. Siegbahn, *Alpha-, Beta-, and Gamma-Ray Spectroscopy*, K. Siegbahn, Ed. (North-Holland Publ. Co., Amsterdam, 1965), Chap. III.

The use of a β-ray spectrometer for determining energy levels is shown schematically in Fig. 2. X rays strike the material under study (the converter) and release photoelectrons, whose kinetic energy is measured by the spectrometer. In its simplest form Einstein's photoelectric law states that $E_{pe}=h\nu-E_B$, where E_{pe} is the kinetic energy of the photoelectron, $h\nu$ that of the incident photon, and E_B the binding energy of the electron.

However, the measured photoelectron energy is decreased by the work function of the converter, ϕ. Since the converter and the slit are electrically connected, their Fermi levels are identical. Thus, if ϕ_s is the work function of the spectrometer slit system, there is an increase in kinetic energy, $\phi-\phi_s$, due to contact potential. With these corrections, the photoelectric equation becomes

$$E_{pe}=h\nu-E_B-\phi+(\phi-\phi_s)=h\nu-E_B-\phi_s.$$

Hence the net correction involves only the work function of the slits (oxidized Cu) and is independent of the work function of the converter.

In general, intense K lines were used to produce photoelectrons. Each x-ray line ejects photoelectrons from all levels whose energies are less than $h\nu-\phi$ in absolute value (e.g., photons energetic enough to remove K electrons also eject these from L_{I}, L_{II}, L_{III}, and other levels). The observed β-ray spectrum is composed of a number of lines due to the multiplicity in both the primary x-ray wavelengths and the energy levels of the converter. The resolution of the spectrometer was sufficient to exclude the influence of the α_2 lines on α_1 measurements.[11] Likewise the electrons undergoing discrete energy losses did not displace the observed spectra to lower energies.

Calculation of the electron energy in terms of the observed current in the magnetic coils of the spectrometer requires an involved procedure which has been discussed in several papers and recently reviewed, in detail, by Kai Siegbahn.[17] This treatise should be consulted for theory, procedures, and resulting reference standards, which are used for all subsequent measurements.

Hagström and Karlsson[18] showed that the method is not limited to conductors or even semiconductors. They found that, if the sample under study was insulated with thin mylar from the aluminum backing plate, (which was electrically connected to the spectrometer slit), the intense ionization due to the direct x-ray beam kept the potential of the insulating sample constant. Hence, even in this case, the observed binding energies were still measured with respect to the zero or Fermi energy. Thus insulating compounds could be attached in thin layers directly to the aluminum backing plate and their level energies measured in this manner.

[18] S. Hagström and S.-E. Karlsson, Arkiv Fysik **26**, 451 (1964); and S. Hagström, Z. Physik **178**, 82 (1964).

INPUT DATA USED IN EVALUATING ENERGY LEVEL VALUES

A separate least-squares evaluation was carried out on each element for which an overdetermined set of data was available. Wavelengths and probable errors of emission lines (all expressed in eV units) are taken from the previous paper.[13] If photoelectron measurements are available for two or more levels, they are included in the least-squares adjustment for that element. If only a single level is determined by the photoelectron method, this establishes one energy level; the others are found from energy differences obtained by a least-squares adjustment of the emission line data.

Wavelength measurements[13] of critical absorption edges are used to establish the absolute scale for eight elements for which no photoelectron measurements are available. In a few cases, where neither photoelectron nor x-ray measurements exist, a Moseley diagram of the final output values of adjacent elements is used to establish one level of the element. The remaining levels are then calculated with emission lines as above. If two or more absorption wavelengths are available for an element, these are also treated by the least-squares method.

The values of the x-ray photoelectron measurements used are listed in brackets in Table I, together with references to the original publications. The published values have been adjusted slightly to make them consistent with the new x-ray emission wavelengths[13] and more recent values of the atomic constants.[19] In the original data most of the errors are 2σ values; these have been changed to probable errors as shown in Table I. For comparison, all the more accurately measured x-ray absorption wavelengths (converted to eV by the factor 12398.1 Å*—eV) are listed in parentheses in Table I. The x-ray absorption data are used for establishing the absolute energy level scale in only eight elements; the other listed values are for comparison only.

EVALUATION OF THE ATOMIC ENERGY LEVELS

Since nearly all elements involve many emission line measurements interconnecting a lesser number of energy levels, an overdetermined set of equations results. As indicated above, a least-squares adjustment provides an appropriate way of solving this set of equations in order to obtain maximum information from the available data. Justification for this procedure and derivations of the equations involved have been presented in many sources.[20–22] A clear explanation of

[19] E. R. Cohen and J. W. M. DuMond, Rev. Mod. Phys. **37**, 537 (1965).

[20] E. Whittaker and G. Robinson, *The Calculus of Observations* (New York, 1944), 4th ed., Chap. 9.

[21] I. F. Sokolnikoff and R. M. Radheffer, *Mathematics of Physics and Modern Engineering* (McGraw-Hill Book Co., Inc., New York, 1958), Chap. IX, Sec. 11.

[22] E. R. Cohen, Rev. Mod. Phys. **25**, 709 (1953).

TABLE I. Recommended values of the atomic energy levels, and probable errors in eV. Where available, photoelectron direct measurements are listed in brackets [ ] immediately under the recommended values. The measured values of the x-ray absorption energies (from Ref. 13) are shown in parentheses ( ). Interpolated values are enclosed in angle brackets ⟨ ⟩.

Level	1 H	2 He	3 Li	4 Be	5 B	6 C	7 N	8 O
K	13.59811[a]	24.58678[b]	54.75±0.02	111.0±1.0	188.0±0.4	283.8±0.4	401.6±0.4	532.0±0.4
					[188.0][c]	[283.8][c]	[401.6][c]	[532.0][c]
			(54.75)	(111.0)		(283.8)		
L_{I}								23.7±0.4
								[23.7][d]
$L_{\mathrm{II,III}}$					4.7±0.9	6.4±1.9	9.2±0.6	7.1±0.8
	9 F	10 Ne	11 Na	12 Mg	13 Al	14 Si	15 P	16 S
K	685.4±0.4	866.9±0.3	1072.1±0.4	1305.0±0.4	1559.6±0.4	1838.9±0.4	2145.5±0.4	2472.0±0.4
	[685.4][c]		[1072.1][c]	[1305.0][c]	[1559.6][c]	[1838.9][c]	[2145.5][d]	[2472.0][c]
		(866.9)	(1072.)	(1303.)	(1559.8)			(2470.)
L_{I}	⟨31.⟩	⟨45.⟩	63.3±0.4	89.4±0.4	117.7±0.4	148.7±0.4	189.3±0.4	229.2±0.4
			[63.3][d]	[89.4][d]	[117.7][d]	[148.7][d]	[189.3][d]	[229.2][d]
				(63.)	(87.)			
$L_{\mathrm{II,III}}$	8.6±0.8	18.3±0.4	31.1±0.4	51.4±0.5	73.1±0.5	99.2±0.5	132.2±0.5	164.8±0.7
			(31.)	(50.)	(72.8)	(100.6)	(132.)	
	17 Cl	18 Ar	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr
K	2822.4±0.3	3202.9±0.3	3607.4±0.4	4038.1±0.4	4492.8±0.4	4966.4±0.4	5465.1±0.3	5989.2±0.3
	[2822.4][c]		[3607.4][c]	[4038.1][c]	[4492.8][c]	[4966.4][d]	[5465.1][c]	[5989.2][c]
	(2020.)	(3202.9)	(3607.8)	(4038.1)		(4964.5)	(5464.)	(5989.)
L_{I}	270.2±0.4	320.	377.1±0.4	437.8±0.4	500.4±0.4	563.7±0.4	628.2±0.4	694.6±0.4
	[270.2][d]	⟨320.⟩[d]	[377.1][d]	[437.8][d]	[500.4][d]	[563.7][d]	[628.2][d]	[694.6][d]
L_{II}	201.6±0.3	247.3±0.3	296.3±0.4	350.0±0.4	406.7±0.4	461.5±0.4	520.5±0.3	583.7±0.3
L_{III}	200.0±0.3	245.2±0.3	293.6±0.4	346.4±0.4	402.2±0.4	455.5±0.4	512.9±0.3	574.5±0.3
M_{I}	17.5±0.4	25.3±0.4	33.9±0.4	43.7±0.4	53.8±0.4	60.3±0.4	66.5±0.4	74.1±0.4
$M_{\mathrm{II,III}}$	6.8±0.4	12.4±0.3	17.8±0.4	25.4±0.4	32.3±0.5	34.6±0.4	37.8±0.3	42.5±0.3
$M_{\mathrm{IV,V}}$					6.6±0.5	3.7	2.2±0.3	2.3±0.4

TABLE I (*Continued*)

	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge
K	6539.0±0.4 [6539.0][e] (6538.)	7112.0±0.9 [7111.3][e,f] (7111.2)	7708.9±0.3 [7708.9][e] (7709.5)	8332.8±0.4 [8332.8][e] (8331.6)	8978.9±0.4 [8978.9][e,g] (8980.3)	9658.6±0.6 [9658.6][g] (9660.7)	10367.1±0.5 [10367.1][g] (10368.2)	11103.1±0.7 [11103.8][g] (11103.6)
L_{I}	769.0±0.4 [769.0][d]	846.1±0.4 [846.1][d]	925.6±0.4 [925.6][d]	1008.1±0.4 [1008.1][d]	1096.6±0.4 [1096.0][d]	1193.6±0.9	1297.7±1.1	1414.3±0.7 [1413.6][g]
L_{II}	651.4±0.4	721.1±0.9 (720.8)	793.6±0.3 (793.8)	871.9±0.4 (870.6)	951.0±0.4 [950.0][h] (953.)	1042.8±0.6 (1045.)	1142.3±0.5	1247.8±0.7 (1249.)
L_{III}	640.3±0.4	708.1±0.9 (707.4)	778.6±0.3 (779.0)	854.7±0.4 (853.6)	931.1±0.4 [931.4][h] (933.)	1019.7±0.6 (1022.)	1115.4±0.5 (1117.)	1216.7±0.7 (1217.0)
M_{I}	83.9±0.5	92.9±0.9	100.7±0.4	111.8±0.6	119.8±0.6	135.9±1.1	158.1±0.5	180.0±0.8
M_{II} M_{III}	48.6±0.4	54.0±0.9 (54.)	59.5±0.3 (61.)	68.1±0.4 (66.)	73.6±0.4 (75.)	86.6±0.6 (86.)	106.8±0.7 102.9±0.5	127.9±0.9 120.8±0.7
$M_{\mathrm{IV,V}}$	3.3±0.5	3.6±0.9	2.9±0.3	3.6±0.4	1.6±0.4	8.1±0.6	17.4±0.5	28.7±0.7
	33 As	34 Se	35 Br	36 Kr	37 Rb	38 Sr	39 Y	40 Zr
K	11866.7±0.7 [11866.7][i] (11865.)	12657.8±0.7 [12657.8][g] (12654.5)	13473.7±0.4 (13470.)	14325.6±0.8 (14324.4)	15199.7±0.3 (15202.)	16104.6±0.3 (16107.)	17038.4±0.3 (17038.)	17997.6±0.4 (17999.)
L_{I}	1526.5±0.8 (1529.)	1653.9±3.5 (1652.5)	1782.0±0.4 [1782.0][j]	1921.0±0.6 [1921.2][k]	2065.1±0.3 [2065.4][j]	2216.3±0.3 [2216.2][l]	2372.5±0.3 [2372.7][l]	2531.6±0.3 [2531.6][l]
L_{II}	1358.6±0.7 (1358.7)	1476.2±0.7 (1474.7)	1596.0±0.4 [1596.2][j]	1727.2±0.5 [1727.2][k] (1730.)	1863.9±0.3 [1863.4][j]	2006.8±0.3 [2006.6][l] (2008.5)	2155.5±0.3 [2155.0][l] (2154.0)	2306.7±0.3 [2306.5][l] (2305.3)
L_{III}	1323.1±0.7 (1323.5)	1435.8±0.7 (1434.0)	1549.9±0.4 [1549.7][j]	1674.9±0.5 [1674.8][k] (1677.)	1804.4±0.3 [1804.6][j]	1939.6±0.3 [1939.9][l] (1941.)	2080.0±0.3 [2080.2][l] (2079.4)	2222.3±0.3 [2222.5][l] (2222.5)
M_{I}	203.5±0.7	231.5±0.7	256.5±0.4		322.1±0.3	357.5±0.3	393.6±0.3	430.3±0.3
M_{II}	146.4±1.2	168.2±1.3	189.3±0.4	222.7±1.1	247.4±0.3	279.8±0.3	312.4±0.4	344.2±0.4

TABLE I (*Continued*)

	33 As	34 Se	35 Br	36 Kr	37 Rb	38 Sr	39 Y	40 Zr
M_{III}	140.5±0.8	161.9±1.0	181.5±0.4	213.8±1.1	238.5±0.3	269.1±0.3	300.3±0.4	330.5±0.4
M_{IV}	41.2±0.7	56.7±0.8	70.1±0.4	88.9±0.8	111.8±0.3	135.0±0.3	159.6±0.3	182.4±0.3
M_V			69.0±0.4		110.3±0.3	133.1±0.3	157.4±0.3	180.0±0.3
N_I			27.3±0.5	24.0±0.8	29.3±0.3	37.7±0.3	45.4±0.3	51.3±0.3
N_{II}	2.5±1.0	5.6±1.3	5.2±0.4	10.6±1.9	14.8±0.4	19.9±0.3	25.6±0.4	28.7±0.4
N_{III}			4.6±0.4		14.0±0.3			
	41 Nb	**42 Mo**	**43 Tc**	**44 Ru**	**45 Rh**	**46 Pd**	**47 Ag**	**48 Cd**
K	18985.6±0.4 (18987.)	19999.5±0.3 (20004.)	21044.0±0.7	22117.2±0.3 (22119.)	23219.9±0.3 (23219.8)	24350.3±0.3 (24348.)	25514.0±0.3 (25516.)	26711.2±0.3 (26716.)
L_I	2697.7±0.3 [2697.7][l]	2865.5±0.3 [2866.0][l]	3042.5±0.4 [3042.5][l]	3224.0±0.3 [3224.3][l]	3411.9±0.3 [3412.0][l] (3417.)	3604.3±0.3 [3604.6][l] (3607.)	3805.8±0.3 [3806.2][m] (3807.)	4018.0±0.3 [4018.1][m] (4019.)
L_{II}	2464.7±0.3 [2464.7][l]	2625.1±0.3 [2624.5][l] (2627.)	2793.2±0.4 [2973.2][l]	2966.9±0.3 [2966.8][l] (2966.3)	3146.1±0.3 [3146.3][l] (3145.)	3330.3±0.3 [3330.3][l] (3330.3)	3523.7±0.3 [3523.6][g,m] (3526.)	3727.0±0.3 [3727.1][m] (3728.)
L_{III}	2370.5±0.3 [2370.6][l]	2520.2±0.3 [2520.2][l] (2523.2)	2676.9±0.4 [2676.9][l]	2837.9±0.3 [2837.7][l] (2837.7)	3003.8±0.3 [3003.5][g,l] (3002.)	3173.3±0.3 [3173.0][g,l] (3173.0)	3351.1±0.3 [3350.8][g] (3351.0)	3537.5±0.3 [3537.3][g] (3537.6)
M_I	468.4±0.3	504.6±0.3		585.0±0.3	627.1±0.3	669.9±0.3	717.5±0.3	770.2±0.3
M_{II}	378.4±0.4	409.7±0.4	444.9±1.5	482.8±0.3	521.0±0.3	559.1±0.3	602.4±0.3	650.7±0.3
M_{III}	363.0±0.4	392.3±0.3	425.0±1.5	460.6±0.3	496.2±0.3	531.5±0.3	571.4±0.3	616.5±0.3
M_{IV}	207.4±0.3	230.3±0.3	256.4±0.5	283.6±0.3	311.7±0.3	340.0±0.3	372.8±0.3	410.5±0.3
M_V	204.6±0.3	227.0±0.3	252.9±0.4	279.4±0.3	307.0±0.3	334.7±0.3	366.7±0.3	403.7±0.3
N_I	58.1±0.3	61.8±0.3		74.9±0.3	81.0±0.3	86.4±0.3	95.2±0.3	107.6±0.3
N_{II}	33.9±0.4	34.8±0.4	38.9±1.9	43.1±0.4	47.9±0.4	51.1±0.4	62.6±0.3	66.9±0.4
N_{III}							55.9±0.3	
$N_{IV,V}$	3.2±0.3	1.8±0.3		2.0±0.3	2.5±0.4	1.5±0.3	3.3±0.3	9.3±0.3

TABLE I (*Continued*)

	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe	55 Cs	56 Ba
K	27939.9±0.3	29200.1±0.4 (29195.)	30491.2±0.3 (30486.)	31813.8±0.3 (31811.)	33169.4±0.4 (33167.)	34561.4±1.1 (34590.)	35984.6±0.4 (35987.)	37440.6±0.4 (37452.)
L_{I}	4237.5±0.3 [4237.7][m] (4237.3)	4464.7±0.3 [4464.5][g] (4464.8)	4698.3±0.3 [4698.3][m] (4698.4)	4939.2±0.3 [4939.3][m] (4939.7)	5188.1±0.3 [5188.1][j]	5452.8±0.4 (5452.8)	5714.3±0.4 [5712.7][j] (5721.)	5988.8±0.4 [5986.8][j] (5996.)
L_{II}	3938.0±0.3 [3937.8][m] (3939.3)	4156.1±0.3 [4156.2][g] (4157.)	4380.4±0.3 [4380.6][m] (4382.)	4612.0±0.3 [4612.0][m] (4612.6)	4852.1±0.3 [4852.0][j]	5103.7±0.4 (5103.7)	5359.4±0.3 [5359.5][j] (5358.)	5623.6±0.3 [5623.6][j] (5623.3)
L_{III}	3730.1±0.3 [3730.0][g] (3730.2)	3928.8±0.3 [3928.8][g] (3928.8)	4132.2±0.3 [4132.2][g] (4132.3)	4341.4±0.3 [4341.2][g] (4341.8)	4557.1±0.3 [4557.1][j]	4782.2±0.4 (4782.2)	5011.9±0.3 [5012.0][j] (5011.3)	5247.0±0.3 [5247.3][j] (5247.0)
M_{I}	825.6±0.3	883.8±0.3	943.7±0.3	1006.0±0.3	1072.1±0.3		1217.1±0.4	1292.8±0.4
M_{II}	702.2±0.3	756.4±0.4	811.9±0.3	869.7±0.3	930.5±0.3	999.0±2.1	1065.0±0.5	1136.7±0.5
M_{III}	664.3±0.3	714.4±0.3	765.6±0.3	818.7±0.3	874.6±0.3	937.0±2.1	997.6±0.5	1062.2±0.5
M_{IV}	450.8±0.3	493.3±0.3	536.9±0.3	582.5±0.3	631.3±0.3		739.5±0.4	796.1±0.3
M_{V}	443.1±0.3	484.8±0.3	527.5±0.3	572.1±0.3	619.4±0.3	672.3±0.5	725.5±0.5	780.7±0.3
N_{I}	121.9±0.3	136.5±0.4	152.0±0.3	168.3±0.3	186.4±0.3		230.8±0.4	253.0±0.5
N_{II}	77.4±0.4	88.6±0.4	98.4±0.5	110.2±0.5	122.7±0.5	146.7±3.1	172.3±0.6	191.8±0.7
N_{III}							161.6±0.6	179.7±0.6
N_{IV}	16.2±0.3	23.9±0.3	31.4±0.3	39.8±0.3	49.6±0.3		78.8±0.5	92.5±0.5
N_{V}							76.5±0.5	89.9±0.5
O_{I}	0.1±4.5	0.9±0.5	6.7±0.5	11.6±0.6	13.6±0.6		22.7±0.5	39.1±0.6
O_{II}	0.8±0.4	1.1±0.5	2.1±0.4	2.3±0.5	3.3±0.5		13.1±0.5	16.6±0.5
O_{III}							11.4±0.5	14.6±0.5

	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd
K	38924.6±0.4 (38934.)	40443.0±0.4 (40453.)	41990.6±0.5 (42002.)	43568.9±0.4 (43574.)	45184.0±0.7 (45198.)	46834.2±0.5 (46849.)	48519.0±0.4 (48519.)	50239.1±0.5 (50233.)

TABLE I (*Continued*)

	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd
L_{I}	6266.3±0.5 [6266.3][n]	6548.8±0.5 [6548.5][n]	6834.8±0.5 [6834.9][n]	7126.0±0.4 [7125.8][n] (7129.)	7427.9±0.8 [7427.9][o]	7736.8±0.5 [7736.2][n] (7748.)	8052.0±0.4 [8051.7][n] (8061.)	8375.6±0.5 [8375.4][n] (8386.)
L_{II}	5890.6±0.4 [5890.7][n]	6164.2±0.4 [6164.3][n]	6440.4±0.5 [6440.2][n]	6721.5±0.4 [6721.8][n] (6723.)	7012.8±0.6 [7012.8][o]	7311.8±0.4 [7312.0][n] (7313.)	7617.1±0.4 [7617.6][n] (7620.)	7930.3±0.4 [7930.5][n] (7931.)
L_{III}	5482.7±0.4 [5482.6][n]	5723.4±0.4 [5723.6][n]	5964.3±0.4 [5964.3][n]	6207.9±0.4 [6208.0][n] (6209.)	6459.3±0.6 [6459.4][o]	6716.2±0.5 [6716.8][n] (6717.)	6976.9±0.4 [6976.7][n] (6981.)	7242.8±0.4 [7242.8][n] (7243.)
M_{I}	1361.3±0.3	1434.6±0.6	1511.0±0.8	1575.3±0.7		1722.8±0.8	1800.0±0.5	1880.8±0.5
M_{II}	1204.4±0.6	1272.8±0.6	1337.4±0.7	1402.8±0.6	1471.4±6.2	1540.7±1.2	1613.9±0.7	1688.3±0.7
M_{III}	1123.4±0.5	1185.4±0.5	1242.2±0.6	1297.4±0.5	1356.9±1.4	1419.8±1.1	1480.6±0.6	1544.0±0.8
M_{IV}	848.5±0.4	901.3±0.6	951.1±0.6	999.9±0.6	1051.5±0.9	1106.0±0.8	1160.6±0.6	1217.2±0.6
M_{V}	831.7±0.4	883.3±0.5	931.0±0.6	977.7±0.6	1026.9±1.0	1080.2±0.6	1130.9±0.6	1185.2±0.6
N_{I}	270.4±0.8	289.6±0.7	304.5±0.9	315.2±0.8		345.7±0.9	360.2±0.7	375.8±0.7
N_{II}	205.8±1.2	223.3±1.1	236.3±1.5	243.3±1.6	242.±16.	265.6±1.9	283.9±1.0	288.5±1.2
N_{III}	191.4±0.9	207.2±0.9	217.6±1.1	224.6±1.3		247.4±1.5	256.6±0.8	270.9±0.9
$N_{IV,V}$	98.9±0.8	110.0±0.6	113.2±0.7	117.5±0.7	120.4±2.0	129.0±1.2	133.2±0.6	140.5±0.8
$N_{VI,VII}$		0.1±1.2	2.0±0.6	1.5±0.9		5.5±1.1	0.0±3.2	0.1±3.5
O_{I}	32.3±7.2	37.8±1.3	37.4±1.0	37.5±0.9		37.4±1.5	31.8±0.7	36.1±0.8
$O_{II,III}$	14.4±1.2	19.8±1.2	22.3±0.7	21.1±0.8		21.3±1.5	22.0±0.6	20.3±1.2

	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	72 Hf
K	51995.7±0.5 (52002.)	53788.5±0.5 (53793.)	55617.7±0.5 (55619.)	57485.5±0.5 (57487.)	59389.6±0.5	61332.3±0.5 (61300.)	63313.8±0.5 (63310.)	65350.8±0.6 (65310.)
L_{I}	8708.0±0.5 [8707.6][n] (8717.)	9045.8±0.5 [9046.5][n]	9394.2±0.4 [9394.3][n] (9399.)	9751.3±0.4 [9751.5][n] (9757.)	10115.7±0.4 [10115.6][n] (10121.)	10486.4±0.4 [10487.3][n] (10490.)	10870.4±0.4 [10870.1][n] (10874.)	11270.7±0.4 [11271.6][o] (11274.)

TABLE I (*Continued*)

	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	72 Hf
L_{II}	8251.6±0.4 [8251.8][n] (8253.)	8580.6±0.4 [8580.4][n] (8583.)	8917.8±0.4 [8918.2][n] (8916.)	9264.3±0.4 [9264.3][n] (9262.)	9616.9±0.4 [9617.1][n] (9617.1)	9978.2±0.4 [9977.9][n] (9976.)	10348.6±0.4 [10349.0][n] (10345.)	10739.4±0.4 [10738.9][o] (10736.)
L_{III}	7514.0±0.4 [7514.2][n] (7515.)	7790.1±0.4 [7789.6][n] (7789.7)	8071.1±0.4 [8070.6][n] (8068.)	8357.9±0.4 [8357.6][n] (8357.5)	8648.0±0.4 [8647.8][n] (8649.6)	8943.6±0.4 [8942.6][n] (8944.1)	9244.1±0.4 [9243.8][n]	9560.7±0.4 [9560.4][o] (9558.)
M_I	1967.5±0.6	2046.8±0.4	2128.3±0.6	2206.5±0.6	2306.8±0.7	2398.1±0.4	2491.2±0.5	2600.9±0.4
M_{II}	1767.7±0.9	1841.8±0.5	1922.8±1.0	2005.8±0.6	2089.8±1.1	2173.0±0.4	2263.5±0.4	2365.4±0.4
M_{III}	1611.3±0.8	1675.6±0.9	1741.2±0.9	1811.8±0.6	1884.5±1.1	1949.8±0.5	2023.6±0.5	2107.6±0.4
M_{IV}	1275.0±0.6	1332.5±0.4	1391.5±0.7	1453.3±0.5	1514.6±0.7	1576.3±0.4	1639.4±0.4	1716.4±0.4
M_V	1241.2±0.7	1294.9±0.4	1351.4±0.8	1409.3±0.5	1467.7±0.9	1527.8±0.4	1588.5±0.4	1661.7±0.4
N_I	397.9±0.8	416.3±0.5	435.7±0.8	449.1±1.0	471.7±0.9	487.2±0.6	506.2±0.6	538.1±0.4
N_{II}	310.2±1.2	331.8±0.6	343.5±1.4	366.2±1.5	385.9±1.6	396.7±0.7	410.1±1.8	437.0±0.5
N_{III}	385.0±1.0	292.9±0.6	306.6±0.9	320.0±0.7	336.6±1.6	343.5±0.5	359.3±0.5	380.4±0.5
N_{IV}, N_V	147.0±0.8	154.2±0.5	161.0±1.0	176.7±1.2 167.6±1.5	179.6±1.2	198.1±0.5 184.9±1.3	204.8±0.5 195.0±0.4	223.8±0.4 213.7±0.5
$N_{VI,VII}$	2.6±1.5	4.2±1.6	3.7±3.0	4.3±1.4	5.3±1.9	6.3±1.0	6.9±0.5	17.1±0.5
O_I	39.0±0.8	62.9±0.5	51.2±1.3	59.8±1.7	53.2±3.0	54.1±0.5	56.8±0.5	64.9±0.4
O_{II}, O_{III}	25.4±0.8	26.3±0.6	20.3±1.5	29.4±1.6	32.3±1.6	23.4±0.6	28.0±0.6	38.1±0.6 30.6±0.6

	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg
K	67416.4±0.6 (67403.)	69525.0±0.3 (69508.)	71676.4±0.4 (71658.)	73870.8±0.5	76111.0±0.5	78394.8±0.7 (78381.)	80724.9±0.5 (80720.)	83102.3±0.8
L_I	11681.5±0.3 [11680.2][p] (11682.)	12099.8±0.3 [12098.2][p] (12099.6)	12526.7±0.4 (12530.)	12968.0±0.4 (12972.)	13418.5±0.3 (13423.)	13879.9±0.4 (13883.)	14352.8±0.4 (14353.7)	14839.3±1.0 (14842.)

TABLE I (*Continued*)

	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg
L_{II}	11136.1±0.3 [11136.1]^{p} (11132.)	11544.0±0.3 [11541.4]^{p} (11538.)	11958.7±0.3 [11956.9]^{p} (11954.)	12385.0±0.4 (12381.)	12824.1±0.3 [12824.0]^{e,p} (12820.)	13272.6±0.3 [13272.6]^{e,p} (13272.3)	13733.6±0.3 [13733.5]^{e,p} (13736.)	14208.7±0.7 (14215.)
L_{III}	9881.1±0.3 [9880.3]^{p} (9877.7)	10206.8±0.3 [10204.2]^{p} (10200.)	10535.3±0.3 [10534.2]^{p} (10531.)	10870.9±0.3 [10870.7]^{p} (10868.)	11215.2±0.3 [11215.1]^{e,p} (11212.)	11563.7±0.3 [11563.7]^{e,p} (11562.)	11918.7±0.3 [11918.2]^{e,p} (11921.)	12283.9±0.4 [12284.0]^{e,p} (12286.)
M_{I}	2708.0±0.4	2819.6±0.4	2931.7±0.4	3048.5±0.4	3173.7±1.7	3296.0±0.9	3424.9±0.3 [3424.8]^{p}	3561.6±1.1
M_{II}	2468.7±0.3 [2468.6]^{p}	2574.9±0.3 [2575.0]^{p}	2681.6±0.4	2792.2±0.3 [2791.9]^{p}	2908.7±0.3 [2909.1]^{p}	3026.5±0.4 [3026.5]^{p} (3029.)	3147.8±0.4 [3149.5]^{p}	3278.5±1.3
M_{III}	2194.0±0.3 [2194.1]^{p}	2281.0±0.3 [2281.0]^{p}	2367.3±0.3 [2367.3]^{p}	2457.2±0.4 [2457.4]^{p}	2550.7±0.3 [2550.5]^{p} (2550.5)	2645.4±0.4 [2645.5]^{p} (2645.9)	2743.0±0.3 [2743.1]^{p} (2744.0)	2847.1±0.4 [2847.1]^{p}
M_{IV}	1793.2±0.3 [1793.1]^{p}	1871.6±0.3 [1871.4]^{p}	1948.9±0.3 [1948.9]^{p}	2030.8±0.3 [2031.0]^{p}	2116.1±0.3 [2116.1]^{p}	2201.9±0.3 [2201.9]^{p}	2291.1±0.3 [2291.2]^{p} (2307.)	2384.9±0.3 [2384.9]^{p}
M_{V}	1735.1±0.3 [1735.2]^{p}	1809.2±0.3 [1809.3]^{p}	1882.9±0.3 [1882.9]^{p}	1960.1±0.3 [1960.2]^{p}	2040.4±0.3 [2040.5]^{p}	2121.6±0.3 [2121.6]^{p}	2205.7±0.3 [2206.1]^{p} (2220.)	2294.9±0.3 [2294.9]^{p}
N_{I}	565.5±0.5	595.0±0.4	625.0±0.4	654.3±0.5	690.1±0.4	722.0±0.6	758.8±0.4	800.3±1.0
N_{II}	464.8±0.5	491.6±0.4	517.9±0.5	546.5±0.5	577.1±0.4	609.2±0.6	643.7±0.5	676.9±2.4
N_{III}	404.5±0.4	425.3±0.5	444.4±0.5	468.2±0.6	494.3±0.6	519.0±0.6	545.4±0.5	571.0±1.4
N_{IV}	241.3±0.4	258.8±0.4	273.7±0.5	289.4±0.5	311.4±0.4	330.8±0.5	352.0±0.4	378.3±1.0
N_{V}	229.3±0.3	245.4±0.4	260.2±0.4	272.8±0.6	294.9±0.4	313.3±0.4	333.9±0.4	359.8±1.2
N_{VI}	25.0±0.4	36.5±0.4	40.6±0.4	46.3±0.6	63.4±0.4	74.3±0.4	86.4±0.4	102.2±0.5
N_{VII}		33.6±0.4			60.5±0.4	71.1±0.5	82.8±0.5	98.5±0.5
O_{I}	71.1±0.5	77.1±0.4	82.8±0.5	83.7±0.6	95.2±0.4	101.7±0.4	107.8±0.7	120.3±1.3
O_{II}	44.9±0.4	46.8±0.5	45.6±0.7	58.0±1.1	63.0±0.6	65.3±0.7	71.7±0.7	80.5±1.3
O_{III}	36.4±0.4	35.6±0.5	34.6±0.6	45.4±1.0	50.5±0.6	51.7±0.7	53.7±0.7	57.6±1.3
$O_{IV,V}$	5.7±0.4	6.1±0.4	3.5±0.5		3.8±0.4	2.2±1.3	2.5±0.5	6.4±1.4

TABLE I (*Continued*)

	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn	87 Fr	88 Ra
K	85530.4±0.6	88004.5±0.7 (88005.)	90525.9±0.7 (90534.)	93105.0±3.8	95729.9±7.7	98404.±12.	101137.±13.	103921.9±7.2
L_{I}	15346.7±0.4 (15343.)	15860.8±0.5 (15855.)	16387.5±0.4 (16376.)	16939.3±9.8	17493.±29.	18049.±38.	18639.±40.	19236.7±1.5 (19236.0)
L_{II}	14697.9±0.3 [14697.3]^{p} (14699.)	15200.0±0.4 (15205.)	15711.1±0.3 [15708.4]^{p} (15719.)	16244.3±2.4	16784.7±2.5	17337.1±3.4	17906.5±3.5	18484.3±1.5 (18486.0)
L_{III}	12657.5±0.3 [12656.3]^{e,p} (12660.)	13035.2±0.3 [13034.9]^{e,p} (13041.)	13418.6±0.3 [13418.3]^{e,p} (13426.)	13813.8±1.0 ⟨13813.8⟩	14213.5±2.0 ⟨14213.5⟩	14619.4±3.0 ⟨14619.4⟩	15031.2±3.0 ⟨15031.2⟩	15444.4±1.5 (15444.0)
M_{I}	3704.1±0.4	3850.7±0.5	3999.1±0.3 [3999.1]^{p}	4149.4±3.9	⟨4317.⟩	⟨4482.⟩	⟨4652.⟩	4822.0±1.5
M_{II}	3415.7±0.3 [3415.7]^{p}	3554.2±0.3 [3554.2]^{p}	3696.3±0.3 [3696.4]^{p}	3854.1±9.8	4008.±28.	4159.±38.	4327.±40.	4489.5±1.8
M_{III}	2956.6±0.3 [2956.5]^{p}	3066.4±0.4 [3066.3]^{p}	3176.9±0.3 [3176.8]^{p}	3301.9±9.9	3426.±29.	3538.±38.	3663.±40.	3791.8±1.7
M_{IV}	2485.1±0.3 [2485.2]^{p}	2585.6±0.3 [2585.5]^{p} (2606.)	2687.6±0.3 [2687.4]^{p}	2798.0±1.2	2908.7±2.1	3021.5±3.1	3136.2±3.1	3248.4±1.6
M_{V}	2389.3±0.3 [2389.4]^{p}	2484.0±0.3 [2484.2]^{p} (2502.)	2579.6±0.3 [2579.5]^{p}	2683.0±1.1	2786.7±2.1	2892.4±3.1	2999.9±3.1	3104.9±1.6
N_{I}	845.5±0.5	893.6±0.7	938.2±0.3 [938.7]^{p}	995.3±2.9	⟨1042.⟩	⟨1097.⟩	⟨1153.⟩	1208.4±1.6
N_{II}	721.3±0.8	763.9±0.8	805.3±0.3 [805.3]^{p}	851.±12.	886.±30.	929.±40.	980±42.	1057.6±1.8
N_{III}	609.0±0.5	644.5±0.6	678.9±0.3 [678.9]^{p}	705.±14.	740.±30.	768.±40.	810±43.	879.1±1.8
N_{IV}	406.6±0.4	435.2±0.5	463.6±0.3 [463.6]^{p}	500.2±2.4	533.2±3.2	566.6±4.0	603.3±4.1	635.9±1.6
N_{V}	386.2±0.5	412.9±0.6	440.0±0.3 [440.1]^{p}	473.4±1.3			577.±34.	602.7±1.7

TABLE I (*Continued*)

	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn	87 Fr	88 Ra
N_{VI}	122.8±0.4	142.9±0.4	161.9±0.5					
N_{VII}	118.5±0.4	138.1±0.4	157.4±0.6					298.9±2.4
O_I	136.3±0.7	147.3±0.8	159.3±0.7					254.4±2.1
O_{II}	99.6±0.6	104.8±1.0	116.8±0.7					200.4±2.0
O_{III}	75.4±0.6	86.0±1.0	92.8±0.6					152.8±2.0
O_{IV}	15.3±0.4	21.8±0.4	26.5±0.5	31.4±3.2				
O_V	13.1±0.4	19.2±0.4	24.4±0.6					67.2±1.7
P_I		3.1±1.0						43.5±2.2
$P_{II,III}$		0.7±1.0	2.7±0.7					18.8±1.8

	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm
K	106755.3±5.3	109650.9±0.9	112601.4±2.4	115606.1±1.6	118678.±33.	121818.±44.	125027.±55.	128220
L_I	19840.±18.	20472.1±0.5	21104.6±1.8	21757.4±0.3	22426.8±0.9	23097.2±1.6	23772.9±2.0	24460
		(20464.)	(21128.)	(21771.)		(23109.)	⟨23772.9⟩	
L_{II}	19083.2±2.8	19693.2±0.4	20313.7±1.5	20947.6±0.3	21600.5±0.4	22266.2±0.7	22944.0±1.0	23779
		(19683.)	(20319.)	(20945.)		(22253.)		
L_{III}	15871.0±2.0	16300.3±0.3	16733.1±1.4	17166.3±0.3	17610.0±0.4	18056.8±0.6	18504.1±0.9	18930
	⟨15871.0⟩	[16299.6][q]		[17168.5][r]				
		(16299.)	(16733.)	(17165.)	(17606.2)	(18053.1)	(18504.1)	
M_I	⟨5002.⟩	5182.3±0.3	5366.9±1.6	5548.0±0.4	5723.2±3.6	5932.9±1.4	6120.5±7.5	6288
		[5182.3][q]						
M_{II}	4656.±18.	4830.4±0.4	5000.9±2.3	5182.2±0.4	5366.2±0.7	5541.2±1.7	5710.2±2.1	5895
		[4830.6][q]		[5180.9][r]	[5366.4][s]			
M_{III}	3909.±18.	4046.1±0.4	4173.8±1.8	4303.4±0.3	4434.7±0.5	4556.6±1.5	4667.0±2.1	4797
		[4046.1][q]		[4303.6][r]	[4434.6][s]			
		(4041.)		(4299.)				
M_{IV}	3370.2±2.1	3490.8±0.3	3611.2±1.4	3727.6±0.3	3850.3±0.4	3972.6±0.6	4092.1±1.0	4227
		[3490.7][q]		[3728.1][r]	[3849.8][s]	[3972.7][t]		
		(3485.)	(3608.)	(3720.)				

TABLE I (*Continued*)

	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm
M_V	3219.0±2.1	3332.0±0.3 [3332.1][q] (3325.)	3441.8±1.4 (3436.)	3551.7±0.3 [3551.7][r] (3545.)	3665.8±0.4 [3664.2][s]	3778.1±0.6 [3778.0][t]	3886.9±1.0	3971
N_I	⟨1269.⟩	1329.5±0.4 [1329.8][q]	1387.1±1.9	1440.8±0.4 [1441.3][r]	1500.7±0.8 [1500.7][s]	1558.6±0.8	1617.1±1.1	1643
N_{II}	1080.±19.	1168.2±0.4 [1168.3][q]	1224.3±1.6	1272.6±0.3 [1272.5][r]	1327.7±0.8 [1327.7][s]	1372.1±1.8	1411.8±8.3	1440
N_{III}	890.±19.	967.3±0.4 [967.6][q]	1006.7±1.7	1044.9±0.3 [1044.9][r]	1086.8±0.7 [1086.8][s]	1114.8±1.6	⟨1135.7⟩	1154
N_{IV}	674.9±3.7	714.1±0.4 [714.4][q]	743.4±2.1	780.4±0.3 [779.7][r]	815.9±0.5 [817.1][s]	848.9±0.6 [848.9][t]	878.7±1.0	
N_V		676.4±0.4 [676.4][q]	708.2±1.8	737.7±0.3 [737.6][r]	770.3±0.4 [773.2][s]	801.4±0.6 [801.4][t]	827.6±1.0	
N_{VI}		344.4±0.3 [344.2][q]	371.2±1.6	391.3±0.6	415.0±0.8 [415.0][s]	445.8±1.7		
N_{VII}		335.2±0.4 [335.0][q]	359.5±1.6	380.9±0.9	404.4±0.5 [404.4][s]	432.4±2.1		
O_I		290.2±0.8	309.6±4.3	323.7±1.1		351.9±2.4		385
O_{II}		229.4±1.1	222.9±3.9	259.3±0.5	283.4±0.8 [283.4][s]	274.1±4.7		
O_{III}		181.8±0.4 [181.8][q]		195.1±1.3	206.1±0.7 [206.1][s]	206.5±4.7		
O_{IV}		94.3±0.4 [94.4][q]	94.1±2.8	105.0±0.5	109.3±0.7 [108.8][s]	116.0±1.2	115.8±1.3	
O_V		87.9±0.3 [88.1][q]		96.3±1.4	101.3±0.5 [101.4][s]	105.4±1.0	103.3±1.1	
P_I		59.5±1.1		70.7±1.2				
P_{II}		49.0±2.5		42.3±9.0				
P_{III}		43.0±2.5		32.3±9.0				

TABLE I (*Continued*)

	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lw
K	[131590±40][u]	135960	139490	143090	146780	150540	154380
L_{I}	[25275±17][u]	26110	26900	27700	28530	29380	30240
L_{II}	[24385±17][u]	25250	26020	26810	27610	28440	29280
L_{III}	[19452±20][u]	19930	20410	20900	21390	21880	22360
M_{I}	[6556±21][u]	6754	6977	7205	7441	7675	7900
M_{II}	[6147±31][u]	6359	6574	6793	7019	7245	7460
M_{III}	[4977±31][u]	5109	5252	5397	5546	5688	5710
M_{IV}	4366	4497	4630	4766	4903	5037	5150
M_{V}	4132	4253	4374	4498	4622	4741	4860
N_{I}	[1755±22][u]	1799	1868	1937	2010	2078	2140
N_{II}	1554	1616	1680	1747	1814	1876	1930
N_{III}	1235	1279	1321	1366	1410	1448	1480
O_{I}	[398±22][u]	419	435	454	472	484	490

[a] J. E. Mack, 1949, as given in C. E. Moore, *Atomic Energy Levels* (U. S. National Bureau of Standards, Washington, D. C., 1949), Vol. 1, p. 1.
[b] G. Herzberg, 1957, as given in C. E. Moore, *Atomic Energy Levels* (U. S. National Bureau of Standards, Washington, D. C., 1958), Vol. 3, p. 238.
[c] See Ref. 18.
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[r] C. Nordling and S. Hagström, Arkiv Fysik **15,** 431 (1959).
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[t] A. Fahlman, K. Hamrin, R. Nordberg, C. Nordling, K. Siegbahn, and L. W. Holm, Phys. Letters **19,** 643 (1966).
[u] J. M. Hollander, M. D. Holtz, T. Novakov, and R. L. Graham ,Arkiv Fysik **28,** 375 (1965).

the procedure followed here is given by Bearden and Thomsen.[23]

Two methods are used to check the consistency of the input data with the output data. The first is the use of the χ^2 test, where

$$\chi^2=\sum(d_i/\sigma_i)^2, \tag{1}$$

with d_i representing the difference between the ith experimental input value and that computed from the adjusted energy levels, and σ_i representing the corresponding standard deviation. It is well known[23] that, in any least-squares adjustment of data with Gaussian error distribution, χ^2 can be expected to equal the number of degrees of freedom; that is, the difference between the number of equations and the number of unknowns which the system possesses. When all the data for all elements are considered as a group, the resultant system possesses about 1300 degrees of freedom and a χ^2 of approximately 3300.

The procedure discussed above is strictly applicable only when the errors are known to be Gaussian.[24] A second check is made by calculating the ratio, r, of the residuals, d_i, to the value to be expected from consideration of the input errors. This ratio can be estimated by following and extending the arguments presented by Cohen and DuMond.[25] Let y stand for a particular energy level difference and p stand for the corresponding probable error. Let a subscript 1 indicate the experimental input value, either an emission line or a photoelectric measurement, subscript 2 indicate the least-squares output value, and subscript 3 indicate the output value of a least-squares adjustment made *without* including the experimental datum y_1. The probable error of the difference y_1-y_2 is desired; however, this error cannot be found directly, since the fact that y_1 was included in the set of data which produced y_2 means that their errors are correlated. However, y_2 can also be obtained by an appropriate average of y_1 and y_3. Since y_3 is obtained from a set of data which excludes y_1, they are independent, and y_2 and p_2 can be computed by simply taking a weighted average of y_1 and y_3, with weights inversely proportional to the squares of the probable errors. Hence the sum of the weights is

$$1/p_2^2=1/p_1^2+1/p_3^2 \tag{2}$$

and

$$y_2=p_2^2[(y_1/p_1^2)+(y_3/p_3^2)]. \tag{3}$$

From (2) one obtains

$$p_2^2=p_1^2p_3^2/(p_1^2+p_3^2) \tag{4}$$

and

$$p_3^2=p_1^2p_2^2/(p_1^2-p_2^2). \tag{5}$$

Since y_1 and y_3 are independent, the probable error squared of the difference y_1-y_3 can be written down immediately as $p_1^2+p_3^2$, but the probable error squared of the difference y_1-y_2 must be computed by first expressing y_1-y_2 in terms of y_1 and y_3. By using (3) and (4) to express y_2 we obtain

$$y_1-y_2=[p_1^2/(p_1^2+p_3^2)](y_1-y_3). \tag{6}$$

hence p_{12}^2, the probable error squared of y_1-y_2, is

$$p_{12}^2=[p_1^2/(p_1^2+p_3^2)]^2(p_1^2+p_3^2). \tag{7}$$

Substituting (5) into (7) to eliminate p_3^2 gives the desired probable error in the form

$$p_{12}=(p_1^2-p_2^2)^{\frac{1}{2}}. \tag{8}$$

Thus the desired ratio r between the actual difference and its statistically expected value is given by

$$r=(y_1-y_2)/(p_1^2-p_2^2)^{\frac{1}{2}}. \tag{9}$$

A study of r as calculated for each input datum reveals the extent to which each datum fitted in with the data as a whole. If the input errors are chosen properly, then according to the definition of probable error, fifty percent of the ratios should be less than one. For all the elements as a group, the actual percentage of error ratios less than one is just 50; the extremely close agreement is doubtless partly fortuitous.

The conclusion from this percentage is that the errors assigned to the input data, including the data from the previous article, are substantially correct. On the other hand, from the fact that χ^2 exceeded the degrees of freedom, it would appear that there are a greater number of large deviations than would be expected from a Gaussian error distribution. The likelihood of this had been emphasized by the authors.

Not only are half the error ratios less than one for the whole mass of the data, but the figure for each element individually is usually close to 50%; hence output errors as calculated directly by the computer (on the basis of internal consistency) are used. In a few cases (32 Ge, 33 As, 34 Se, and 80 Hg) the percentages are unusually low; in order to avoid understating any errors, all errors for these elements are reported on the basis of external consistency.

The comparison of the residuals (differences between the input values and the corresponding values as calculated on the basis of the adjusted energy levels) with the statistically expected differences proved very useful in other ways. When this error ratio is very large, a renewed investigation of that input often revealed a misprint, misidentification, or other mistake. However, in some cases this ratio is uncomfortably large, and no specific reason can be found for rejecting that input item. Those items which have an error ratio greater than 5.0 are rejected.[12]

There appears to be no significant pattern in these rejected input data. Almost as many have negative

[23] J. A. Bearden and J. S. Thomsen, Nuovo Cimento **5**, 267 (1957).
[24] J. S. Thomsen, Bull. Am. Phys. Soc. **10**, 547 (1965).
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error ratios as positive ones; no level or pair of levels predominates in the list. The rejected data are distributed among the K, L, and M, and photoelectron categories roughly in proportion to the amount of input data in each category. As one progresses up the periodic table, it seems that the initial measurement of various lines is often accompanied by high errors. This is not surprising, since these lines are weak and sometimes diffuse, making their identification and detection unusually difficult and subject to errors which are easy to underestimate.

It is interesting to note that no $K\alpha_1$, $K\alpha_2$, nor any of the best measured L lines appear in the rejected group, despite the fact that they had been assigned the lowest errors. Furthermore, in no case did the error ratio for these lines become suspiciously large. A few difficulties, particularly with the value of the L_I level in the light elements, did appear, and are discussed further in the detailed energy level report.[12]

ENERGY LEVEL TABLE

The adjusted values for the various energy levels, together with the respective probable errors, are listed in Table I. These errors are primarily due to three causes: (1) those due to the photoelectron measurements, which may be subdivided into two parts: (a) random variations introduced by counting statistics which affects *even* the spacing between levels of a single element, and (b) systematic errors in the main calibration line (usually common to a group of elements) and the spectrometer slit work function, which affect the absolute accuracy relative to the Fermi level energy and amount to approximately 0.3 eV for all elements; (2) the probable errors in the x-ray emission wavelengths relative to the W $K\alpha_1$ standard and that of the primary standard to the absolute angstrom scale (5 parts per million); (3) the probable error in the wavelength to energy ($V\lambda = 12398.10 \pm 0.13$ eV—Å*) conversion factor.

Recently[26] photoelectron measurements of the L_I energy in the elements sodium ($Z=11$) to copper ($Z=29$) have been reported. The values from sodium ($Z=11$) to vanadium ($Z=23$) have been used to replace the interpolated values shown in our previous report.[12] The remaining new values have been used with the older K-level values to redetermine new level energies for the elements vanadium ($Z=23$) to copper ($Z=29$). The K-level energies of the elements from sodium to chromium were also redetermined. Agreement with previous values[18] to within 0.5 eV was obtained for all elements except titanium. The new value for titanium is 1.2 eV higher than that of the earlier work, and while no explanation of the discrepancy is available, this new value has been substituted for the older value. This indicates a need for further redeterminations of all the older values as a check on the estimated accuracies and on unsuspected experimental variations.

For some elements the K level alone has been used to determine the absolute values. In these cases when new photoelectron measurements are available, all the remaining levels can be adjusted by the difference in the new and old values for each element. However, three or more level energies have been measured for the heavier elements (sixteen for thorium) and when new measurements are available for these, a new least-squares readjustment will be necessary to obtain corrected energy level values for an element.

Some energy levels were obtained by interpolation or calculation. The interpolation was performed by passing a fourth order polynomial through the nearest fifteen energy values. The level for atomic numbers 96 and 98 through 103 were obtained from a relativistic self-consistent Slater–Dirac energy level calculation.[27] The results of an extrapolation vary greatly with the order of the polynomial used, and therefore should be considered rough values only.

The best of the x-ray absorption edge measurements, listed in parentheses ( ), are generally in good agreement with the photoelectron values. From these it would appear that the x-ray measurements have been made relative to the Fermi energy level with higher accuracy than previously estimated. New x-ray measurements with modern techniques should certainly be competitive with the photoelectron measurements.

ERROR CORRELATION AND ENERGY DIFFERENCES

The errors shown in Table I are not statistically independent and hence can not be combined without some knowledge of the correlation coefficients. For example, consider the L_{II}–L_{III} energy difference of chromium. As in the case of other lighter elements, the K level energy was determined by the photoelectron method. The error involved in this measurement, item (1) in the first paragraph of the preceding section, is considerably greater than that in the emission line wavelengths, item (2); consequently all stated errors are strongly correlated through this common source. Thus, since in Table I the value of the L_{II} level is (583.7 ± 0.3) eV, and that for the L_{III} level is (574.5 ± 0.3) eV, one might erroneously conclude that the difference is (9.2 ± 0.4) eV, which would be true only if the major errors were uncorrelated. However, the wavelengths of chromium $K\alpha_1$ and $K\alpha_2$ emission lines which connect the L_{III} and L_{II} levels to the K level are known with probable errors of ten and one parts per million respectively; hence most of the errors in both the L_{II} and L_{III} levels come from the errors in the absolute value of the K level.

[26] R. Nordberg, K. Hamrin, A. Fahlman, C. Nordling, and K. Siegbahn, Z. Physik **192**, 462 (1966).

[27] J. T. Waber (private communication, 1964); D. Liberman, J. T. Waber, and D. T. Cromer, Phys. Rev. **137**, A27 (1965).

TABLE II. Examples of energy level differences and corresponding probable errors for the case of 24 chromium. Entries above the principal diagonal represent differences while those below give corresponding probable errors.

24 Cr	Energy level differences in electron volts						
	K	*L*1	*L*2	*L*3	*M*1	*M*23	*M*45
K		5292.77	5405.51	5414.72	5915.09	5946.71	5986.93
*L*1	0.70		112.74	121.95	622.31	653.93	694.16
*L*2	0.05	0.69		9.21	509.58	541.20	581.42
*L*3	0.07	0.70	0.05		500.36	531.98	572.21
*M*1	0.21	0.72	0.20	0.19		31.62	71.85
*M*23	0.08	0.69	0.06	0.07	0.21		40.23
*M*45	0.18	0.71	0.17	0.17	0.26	0.18	
24 Cr	Energy level difference errors in electron volts						

24 Cr	Energy level differences in Rydberg units						
	K	*L*1	*L*2	*L*3	*M*1	*M*23	*M*45
K		389.022	397.308	397.985	434.762	437.086	440.043
*L*1	131		8.286	8.963	45.740	48.064	51.021
*L*2	5.1	6152		0.677	37.454	39.778	42.735
*L*3	10	5700	5179		36.777	39.101	42.058
*M*1	33	1158	387	385		2.324	5.281
*M*23	10	1057	106	139	6497		2.957
*M*45	28	1028	289	304	3603	4403	
24 Cr	Energy level difference errors in ppm Rydberg units						

24 Cr	Energy level differences in wavelength (mÅ*)						
	K	*L*1	*L*2	*L*3	*M*1	*M*23	*M*45
K		2342.459	2293.606	2289.703	2096.01	2084.86	2070.86
*L*1	131		109975	101666	19922	18959	17860
*L*2	1.3	6152		1345646	24330	22908	21323
*L*3	8.7	5700	5179		24778	23305	21667
*M*1	33	1158	387	385		392094	172564
*M*23	9.6	1057	106	139	6497		308210
*M*45	28	1028	289	304	3603	4403	
24 Cr	Energy level difference errors in ppm Å*						

Indeed the correlation coefficient between these two levels is almost unity. When this is taken into account, the value of the above difference becomes (9.21±0.05) eV.

Thus energy level differences and corresponding errors can not in general be accurately obtained from the data in Table I alone. For this reason the original report included three tables of energy level differences, in units of electron-volts, Rydbergs, and equivalent wavelength in milli Å* (abbreviated mÅ*). Table II shows examples of each, presented in matrix form, for the specific case of chromium ($Z=24$).

For example, the $L_{II}L_{III}$ difference which was discussed above is found in the first matrix at the intersection of the *L*2 row and the *L*3 column, above the principal diagonal, and is 9.21 eV. The correspond ing element in the lower half of the matrix gives the probable error (calculated with proper consideration of error correlation), viz. 0.05 eV. The last two matrices are similar in form, but errors are given in parts per million rather than absolute units.

It will be noted that the equivalent wavelength values in the mÅ* units carry the smallest probable errors. Since all the x-ray emission line input data used

in this report were given in Å*, values on this scale involve little or no error due to conversion factor uncertainties. These energy level differences represent possible x-ray emission lines; therefore this table should be of value to investigators looking for new lines or seeking possible identification of observed lines. One should note, however, that all possible differences are listed, no matter how the transition may be forbidden by selection rules. The values in this table will differ slightly from the corresponding entries in the preceding article,[12] because the latter values are a weighted mean of the *actual* observations on a given *line*, while the former represent values based on all the available information for the given *element*. Usually any difference is within the experimental error; in the few cases where a definite disagreement arose, the value based on direct observation was discarded in this work.

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