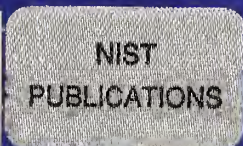


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***NIST Technical Note 1289***

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***The NIST X-Ray Photoelectron Spectroscopy (XPS)  
Database***

***Charles D. Wagner***

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# **The NIST X-Ray Photoelectron Spectroscopy (XPS) Database**

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Charles D. Wagner

Surfex Company  
29 Starview Drive  
Oakland, CA 94618

October 1991



**U.S. Department of Commerce**  
Robert A. Mosbacher, Secretary

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# The NIST X-Ray Photoelectron Spectroscopy (XPS) Database

Charles D. Wagner

*Surfex Company, 29 Starview Drive, Oakland, CA 94618*

The technique known as XPS (X-Ray Photoelectron Spectroscopy) involves x-ray irradiation of surface samples under high vacuum. Electrons escaping from the samples are sorted and arranged to form a spectrum. A compilation of data for binding energy and kinetic energy of sample electrons from all elements has been collected. Depending on the nature of the chemical bond, the chemical shift can be as much as 10 eV. Over the past 6 years the author has indexed articles related to this subject area. The data bank contains a total of 13,200 records, from a total of 800 papers.

Key words: Auger electron; Auger parameter; binding energy; chemical shift; core level; doublet separation; photoelectron; XPS; X-Ray generation.

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# THE NIST X-RAY PHOTOELECTRON SPECTROSCOPY (XPS) DATABASE

## I. Introduction

The technique of XPS was pioneered by Siegbahn and co-workers. In 1954 Siegbahn's group developed a high resolution electron spectrometer and in 1958 his group discovered that chemical shifts between copper and its oxides could readily be resolved (SNS58). Since that time there has been great interest in chemical surface analysis, encouraged by a written monograph by the Siegbahn's group (SNFN67) stating the principles of the technique. The technique is essentially nondestructive, sensitive to all elements except hydrogen and helium, and samples a shallow surface region a few nanometers thick. It is restricted to low vapor pressure compounds and can even be used to study organic materials nondestructively.

By 1973 the technique, widely known as Electron Spectroscopy for Chemical Analysis (ESCA), became widely used through the development of high-quality commercial instruments. Since that time work in the field has grown explosively. For example, by the end of 1985 over 780 papers had been written which reported measurements of photoelectron and Auger line energies.

Because of the sheer volume of this work, the number of compounds studied, and the variability of the quality of the data, it was clear that a critical compilation of available data was needed. In 1982, the author began work under the sponsorship of the then National Bureau of Standards on a data base that was to include all data on inorganic and organic compounds from refereed journals. These data were eventually to be made available for computerized retrieval.

This paper describes the structure of the resulting data bank, known as the NIST X-Ray Photoelectron Spectroscopy (XPS) Database, and the nature of the data compiled for each compound or element. At the time this paper was drafted, the author intended to include a listing of the data ordered by element through 1985 — about 13,200 records in all. However, the volume of these data was too large to make this practical. Even this compilation is not entirely complete; some references include a large number of similar compounds, and, in the interest of brevity, only representative ones were selected. Because of its size, a printed copy of the data base will be made available to interested parties upon request to Standard Reference Data, National Institute of Standards and Technology, A323 Physics Bldg., Gaithersburg, MD 20899.

## II. Structure of the NIST X-Ray Photoelectron Spectroscopy (XPS) Database

The data are organized into 13 fields.

1. *Atomic number*

This needs no elaboration.

2. *Elemental symbol*

The elements are presented in order of atomic number.

3. *Spectral line*

Included are not only photoelectron and Auger lines, but also various useful line energy differences. The following describes the different designations shown:

**Photoelectron lines** — Self-explanatory. In Figure 1 is shown a photoelectron line at 0-1070 binding energy in the reverse direction.

**Doublet separation in photoelectron lines** — This is indicated by Figure 2, simply by a  $\Delta$  followed by the line, e.g.,  $\Delta 2p$ ,  $\Delta 3p$ ,  $\Delta 3d$ ,  $\Delta 4p$ ,  $\Delta 4d$ ,  $\Delta 4f$ . Included also is the multiplet splitting of 3s, as in  $\Delta 3s$ .

**Auger lines** — The common Auger lines shown will be  $KL_{23}L_{23}(^1D)$ ,  $L_3M_{45}M_{45}(^1G)$ ,  $M_4N_{45}N_{45}$ ,  $M_5N_{67}N_{67}$ , and sometimes,  $N_6O_{45}O_{45}$ . This in the case of  $KL_{23}L_{23}$  is exemplified by Figure 1, on the kinetic energy direction. Valence type Auger lines, sometimes designated CVV, with final vacancies in valence levels, will ordinarily not be included; if they are, the notation will have V standing for

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the final vacancy, as in KVV. Other Auger lines will ordinarily be cited only as energy difference values from the above principal lines of each series (see below).

**Separation from the sharpest Auger line** — This category (Fig. 4) will be used for all Auger line energies other than KVV or  $KL_{23}L_{23}(^1D)$ , LVV or  $L_3M_{45}M_{45}(^1G)$ ,  $M_4N_{45}N_{45}$ ,  $M_5N_{67}N_{67}$ , and  $N_6O_{45}O_{45}$ . The kinetic energy of the minor line cited will be subtracted from the standard line in its series, and the energy value will have a “+” or “-.” Examples of the line designations are:

$KL_{23}L_{23}(^1S)$   
 $L_3M_{23}M_{45}(^3P)$   
 $M_{45}N_1N_{45}$   
 $M_4N_{67}N_{67}$

**Auger parameter** — In the modified form, used here in Figure 1, is the kinetic energy of the sharpest Auger line (one of those above) plus the binding energy of the most intense photoelectron line.

$\alpha 3d_5, M_4N_{45}N_{45}$

If the Auger line and the photoelectron line are supplied but not the Auger parameter, the Auger parameter was derived by the reviewer from the data. The connotation (AP derived) is indicated in the column (see Sec. 9 — *Method of compensation for steady state charge*). With charge references of photoelectron and Auger lines of doubtful value, both are omitted but the Auger parameter is retained.

**Chemical shift from the elemental form** — This is shown in Figure 3 when publications present both peaks in the same spectrum, or when the elemental peak is not in the same spectrum but in the same article. The absolute scale is not necessary because the chemical shifts are based on zero. Also the alloys constitute a special case because the chemical shifts are so minimal (a fraction of a volt in most cases). Lines cited will be strong photoelectron lines, the standard Auger lines, and Auger parameters, and there will be a “+” or “-” on the chemical shift energy.

$\gamma 2p_3$   
 $\gamma L_3M_{45}M_{45}(^1G)$   
 $\gamma \alpha 2p_3, L_3M_{45}M_{45}(^1G)$

#### 4. *Compound*

Ordinarily the simple chemical formula is used, but with complex molecules the common name can be substituted. Abbreviations commonly used in Chemical Abstracts will be used for naming the compounds.

Data are supplied for bulk condensed states believed to be pure. Gas phase data are not included. In relatively rare instances, implanted atoms or well-defined monolayers will be included, with the requirement that evidence be supplied that all of the atoms have the same environment.

If not all of the published line energy data for a compound are included in this tabulation, the compound name will be followed by a “+.”

If a compound has atoms of an element in more than one chemical state, the position of an asterisk in the structural formula will indicate the atom for which data are presented. For the special case of carbon, it is usually assumed in this data set that aliphatic or aromatic carbon bound only to carbon and hydrogen has the binding energy 284.8 eV, and so these are not usually included in the data.



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If space does not permit, an abbreviation will contain an asterisk which will refer to an asterisk with a more complete explanation such as:

With abbreviation	More complete explanation
FeCl <sub>3</sub> 2DMSO*	*DMSO = di(Me)sulfoxide

If a footnote is appropriate such as an alternative common name, it will be written out and indicated by an asterisk.

C <sub>6</sub> H <sub>6</sub> * benzene	
(COONa) <sub>2</sub> *	Na oxalate
(CH <sub>2</sub> ) <sub>6</sub> N <sub>4</sub> *	hexamethylenetetramine

Some compounds which are not obviously ionic are noted by (ionic compd) following the formula or in several cases by a plus or minus sign ending the expression. Ionic compounds such as ammonium or phosphonium are not specially indicated because they are expected to be obvious. Some abbreviations are the following:

M ox	= thin metal oxide layers formed by passive oxidation, e.g., Al ox
MY <sub>x</sub>	= non-stoichiometric binary compound (rare), such as SiN
poly(-XXXX-)	= polymer with repeat group (-XXXX-)
poly(RCH=CHX)	= vinyl polymer
p-XXXX	= para orientation on benzene ring
Am	= the element americium, or the amyl group in an organic compound
acac	= acetylacetonate
bzac or bzby	= benzoyl substitution for acetyl in acac

### 5. Empirical formula

In the case of organic compounds, the compound name is so complicated that it can be written in a multitude of ways, so that the empirical formula is the simple way out and is used.

### 6. Physical state

When supplied in the article, some information about the physical state of the compound or element, or its method of preparation is conveyed by a code of one to three digits, as follows:

A	annealed
Ads	adsorbed
Am	amorphous
Arc	arc method
Br2	Br <sub>2</sub> -ethanol
C	cooled
CE	chemically etched
Cl	cleaved crystal
Co	co-condensed with a charge reference material
Cr	crystal
Cru	crushed
CVD	chemical vapor deposition
EO	electrolytic oxidation
ER	electrolytic reduction
Ex	exchangable
H	heated
H2	hydrogen pressure

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H&C	heated and cooled
Imp	implanted
Ind	induction heater
IR	reaction by bombarding ions
L	liquid
MBE	molecular beam epitaxy
Ml	multilayer
O2	oxygen pressure
Oxi	oxidizing atmosphere
Pc	polycrystalline
PO	passive oxide
Pwd	powder (when a special point is made in the article)
R	reacted
RF	reacted film
Red	reducing atmosphere
Sc	scraped
ScH	scraped and heated
SD	sputter deposited
Sp	sputtered
Sp*	this is an artifact made because there is no way of differentiation from Al K and Mg K. All the primary keys are identical. Therefore the Phys. St. was used as Sp*.
SpA	sputtered in argon
SpH	sputtered and heated
TF	thin film
TL	thin layer
TO	thick oxide
VC	vacuum cleaved
VD	vapor deposited
VDH	vapor deposited and heated

### 7. *Energy*

All energies are referred to the Fermi level. Ordinarily, values are shown to tenths of an eV, with some quoted to hundredths of an eV. Values are binding energies for photoelectrons and kinetic energies for Auger electrons. The data have been standardized for a voltage scale that assumes with Fermi level referencing that  $Au4f_7 = 84.0$ ,  $Ag3d_5 = 368.2$ ,  $Cu2p_3 = 932.6$ , and C1s for hydrocarbon or hydrocarbon groups equals 284.8 eV (cf below under instrument calibration and charge referencing). Data will not ordinarily be included unless correspondence with at least one point on this voltage scale can be determined, and corrections made accordingly. Energy data corrected for this are indicated by the designation "c" under the quality column.

Ordinarily there are no adequate data furnished to be assured of an energy scale of correct magnitude. When data are furnished for two widely-spaced photoelectron lines of an element corresponding to initial and final states of accurately determined x-ray transitions, the accuracy of the energy scale magnitude can be checked, and data corrected when necessary. A similar operation can be conducted if calibration lines for  $Cu2p_3$  plus either  $Au4f_7$  or  $Ag3d_5$  are furnished. Data corrected in this way for energy scale magnitude are designated by "a" in the quality column. Data from a few references performed carefully for energy scale calibration purposes have not been changed, and are designated by "A" (see Sec. 8).

All line designations beginning with  $\Delta$ , or  $\gamma$ , are difference values, and the energy values should be plus or minus except for  $\Delta$  applied to spin doublet separations or multiplet splitting (cf "Line" above). Auger parameter values (line designations beginning with  $\alpha$ ) are inherently difference values but are always positive.

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### 8. *Quality of the datum*

The uses of “c” and “a” have already been described in the paragraphs above. When the line energy is within 300 eV of a reference point on the energy scale, such as Au4f<sub>7</sub>, when a conductive material is examined, or C1s for adventitious hydrocarbon when charge referencing is done on an insulator, a “G” is included, indicating a reasonable degree of reliability. A few studies have been done very carefully and data from them are indicated by the letter “A”, representing calibration grade.

### 9. *Method of compensation for steady state charge*

Data on insulators are not included unless a technique for charge referencing is used that is believed to be valid. Some abbreviations are the following:

- a. “Cond” indicates the material is sufficiently conducting, either because of its nature, or because it is sufficiently thin not to require charge correction.
- b. “Au” indicates the gold vapor deposition method, with Au4f<sub>7</sub> assumed to be 84.0.
- c. “AC” indicates use of the C1s line of adventitious hydrocarbon, assumed to be 284.8 eV.
- d. “IC” indicates use of an internal hydrocarbon group of the compound, with the same assumed energy.
- e. “CC” indicates that a hydrocarbon was co-condensed with the vapor-deposited specimen and used as the charge reference, with value 284.8.

If use of other charge referencing values in a paper requires changes in the energy data for this set, this is indicated by the letter “c” in the Quality column.

Occasionally all energy values are referenced to a single element present in all the materials. While this does not presume to give absolute line energies, it can furnish useful data, and this method is indicated in the Charge Reference column by a phrase such as “F1s = 684.6”. A charge reference is not needed for difference values, such as those beginning with  $\Delta$ ,  $\gamma$  or  $\alpha$ .

### 10. *Instrument calibration*

The symbol FL means the instrument was calibrated to set zero binding energy at the Fermi edge of a metal with high density of states at the conduction band. The symbol ON indicates the scale was set at zero kinetic energy at the onset of electron emission. The symbol DVM indicates that voltages on the energy scale were calibrated directly with the aid of an accurate digital voltmeter.

In most studies, however, natural strong lines of conductors were used to establish the scale. For this data set it is assumed that gold, silver, and copper as calibrants have their most intense spectral lines at the following binding energies: Au4f<sub>7</sub> = 84.0, Ag3d<sub>5</sub> = 368.2, and Cu2p<sub>3</sub> = 932.6 eV. If these lines were used in the instrument calibration, the symbols Au, Ag, or Cu indicate it, and if the values used in the article were not the above, energy values for conducting species were corrected to correspond (see Energy and Quality paragraphs).

Determinations of line energies of elemental gold, silver, and copper with none of them cited as an energy scale reference are printed without change, but companion data from the same article on other materials may be corrected for deviation of these standards from the values adopted here.

If data are furnished from which the magnitude of the voltage scale can be checked (such as widely separated calibration lines, or lines for elements that represent initial and final states of x-ray transitions), these difference values are included. If the values are not those adopted for the x-ray transitions or for widely separated calibration lines, a correction of the voltage scale magnitude may be needed. When this has been done, the new and correct difference value is shown,

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energy values are corrected, and those corrected are indicated by an "a" symbol in the Quality column. It should be understood that elemental states are used for instrument calibration unless otherwise indicated.

### 11. *Compound type*

This has been used, not entirely consistently, to classify the compounds.

### 12. *Reference*

With multiple authors the first letter of each author's last name is used:

XXXX

XXX

In the case of two authors, the first two letters are used, capital and lower case:

XxXx

In the case of one author, capital and three lower case letters are used:

Xxxx

This is followed by two digits, representing the last two digits of the year of publication. This may be followed by a small letter, to distinguish between two otherwise identical reference notations.

In many cases the reference may end with a plus sign. This indicates that the reference includes a large number of similar compounds, and, in the interest of brevity, only representative ones were selected. The reader is encouraged to look for the simpler of a class of compounds, and if the reference for it contains a plus sign, to consult the reference to obtain data on similar materials. A complete list of references is given in Appendices A and B. Appendix A contains the so-called "long references" which have been separated out because of their length. Appendix B contains the majority of the references.

### 13. *Registry number*

Space is provided to enter the Chemical Abstracts Service Registry Number if it is needed in the future.

## III. Elemental Data Summary

Below (Table 2) is a summary table of the most reliable elemental photoelectron energy values through 1985. These records are about ten percent of the total bank of elemental XPS data.

## IV. Complete XPS Data

The NIST X-Ray Photoelectron Spectroscopy (XPS) Database is available from the NIST Standard Reference Data Program, National Institute of Standards and Technology, A323 Physics Bldg., Gaithersburg, MD 20899, (301) 975-2208, Joan Sauerwein. The database is complete for XPS data through 1985. It is lengthy and is not printed here, but will be sent to users on request. As an illustration, a subset for Tin (Sn) is duplicated in Table 3 and Table 4. Also a division of the records into organic and inorganic is shown. The criterion is based as a first approximation on the empirical formula for hydrogen content for organic compounds.

Also a different type of subset is shown in Table 5. In this Table are shown 800 chemical states of 84 elements, with the main photoelectron and Auger lines in detail.

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The records for the data bank include six types of spectral lines listed in Table 1 below.

TABLE 1. Distribution of Spectral lines

Type of Line	Records
Photoelectron lines	9810
Doublet separation	950
Auger lines	784
Separation from the sharpest Auger lines	168
Auger parameter	910
Chemical shifts	578

## V. Acknowledgement

This work was supported by the Department of Energy and the National Science Foundation through the Program on Critical Evaluation of Physical and Chemical Data through the Standard Reference Data Program of the National Institute of Standards and Technology.

## VI. Reference

An additional discussion of the NIST X-Ray Photoelectron Spectroscopy (XPS) Database is given below.

C. J. Powell, "Formal Databases for Surface Analysis: The current Situation and Future Trends" in *Quantitative Surface Analysis* (London, Nov. 13-16, 1990).

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TABLE 2. The best values of elemental photoelectric energies as of 1985

1s									
3	Li	54.8	G <sup>x</sup>	KLMP	73				
4	Be	111.8	G	WRDM	79				
5	B	(186.5) <sup>y</sup>	G	SMS	80				
6	C	284.45	G	WVB	80				
						2p			
11	Na	1071.8	G	BaSt	75	30.8	G	BaSt	75
						30.52	G	Citr	73
12	Mg	1303.2	G	Fugg	77	49.6	G	Fugg	77
						49.6	G	VaTr	79a
13	Al					72.85	G	Tayl	82
						72.92	G	WPHK	82
14	Si					(99.44)	G	WPHK	82
15	P					(130.00)	G	NSDU	75
16	S					164.1	G	Brio	80
						164.15	G	WRDM	79
						164.25	G	RiVe	83
						2p <sub>3</sub>			
18	Ar	(241.8)	G	KiWi	75				
19	K	294.7	G	PeKa	77				
20	Ca	345.9	G	VaVe	80				
21	Sc	(398.3)	G	MFA	85				
22	Ti	453.89	A <sup>z</sup>	LANM	81	32.5	A <sup>z</sup>	LANM	81
		453.73	A	ALMP	82				
23	V	512.14	A	LANM	81	37.2	A	LANM	81
24	Cr	574.26	A	LANM	81	42.3	A	LANM	81
25	Mn	638.78	A	LANM	81	47.2	A	LANM	81
						3p			
26	Fe	706.74	A	LANM	81	52.5	A	LANM	81
		706.82	A	Asam	86				
27	Co	778.32	A	LANM	81	58.9	A	LANM	81
28	Ni	852.68	A	LANM	81	66.1	A	LANM	81
		852.8	A	PEJ	82	66.5	A	PEJ	82
		852.73	A	ALMP	82				
29	Cu	932.57	A	LANM	81	75.13	A	LANM	81
		932.7	A	PEJ	82	75.20	A	PEJ	82
		932.67	A	AnSe	84				
		932.55	A	ALMP	82				
		932.62	A	BiSw	80				
		932.70	A	BiSw	80				
30	Zn	1021.82	A	LANM	81	10.00	A	LANM	81
		1021.70	A	Evan	85	9.78	A	Evan	85
		1021.96	A	LKMP	73	10.18	A	LKMP	73
31	Ga	1116.67	A	Evan	85	18.69	A	Evan	85
32	Ge	1217.28	A	Evan	85	29.45	A	Evan	85
		1217.38	A	Evan	85	29.65	A	Evan	85
		1217.2	A	McWe	76	29.3	A	McWe	76
						29.0	A	SFS	77
33	As					41.5	G	BWWI	76
						3d <sub>5</sub>			
34	Se	55.1	A	BWI	80				
37	Rb	112.0	G	EbSi	79				
38	Sr	134.4	G	VaVe	80				
39	Y	155.8	A	NyMa	80				
40	Zr	178.79	A	NyMa	80				
41	Nb	202.26	A	NyMa	80				
42	Mo	227.94	A	NyMa	80				
44	Ru	280.02	A	NyMa	80				
45	Rh	307.18	A	NyMa	80				
46	Pd	335.08	A	NyMa	80				
		335.18	A	VaTr	79				
		335.20	A	Asam	86				
		335.2	A	JHBK	73				
						4p <sub>3</sub>			
						27.1	A	NyMa	80
						30.8	A	NyMa	80
						35.5	A	NyMa	80
						43.4	A	NyMa	80
						47.3	A	NyMa	80

# THE NIST X-RAY PHOTOELECTRON SPECTROSCOPY (XPS) DATABASE

TABLE 2. The best values of elemental photoelectric energies as of 1985 — Continued

		3d <sub>5</sub>							
47	Ag	335.20	A	BiSw	80				
		335.47	A	BiSw	80				
		368.2	A	JHBK	73				
		368.22	A	NyMa	80				
		368.23	A	Asam	86				
		368.28	A	AnSe	84				
		368.10	A	BiSw	80				
48	Cd	368.16	A	BiSw	80				
		368.21	A	BiSw	80				
		405.15	A	NyMa	81				
49	In	443.86	A	NyMa	81				
50	Sn	484.8	A	VaTr	79				
		484.92	A	NyMa	80				
51	Sb	528.2	A	VaTr	79				
						10.2	A	PLJL	73
						10.47	A	PKLS	72
						16.74	A	PKLS	72
						24.04	A	VaTr	79
						23.95	A	NyMa	80
						23.68	A	PKLS	72
24.1	A	SFS	77						
32.3	A	VaTr	79						
32.07	A	NyMa	80						
32.1	A	SFS	77						
32.14	A	PKLS	72						
40.44	A	NyMa	80						
40.5	A	SFS	77						
40.31	A	PKLS	72						
52	Te	572.98	A	NyMa	80				
		573.0	A	SFS	77				
53	I	(619.9)		DMKK	84				
		(619.9)		Sher	76				
55	Cs	726.0	G	KDR	77	77.3	A	SLCO	83
56	Ba	780.6	G	KoGr	85	90.2	G	KoGr	85
						90.4	G	VaVe	80
57	La	(835.9)		SOS	82	103.7	G	KEML	74
		(835.9)		SeSc	82				
58	Ce	(883.2)		PKHL	80	(111.2)		NIS	72
		(883.9)		SOS	82				
		(883.9)		ScOs	82				
59	Pr	(932.0)		FuOs	84				
62	Sm	(1081.2)		DKMB	76				
						128.4	G	NNBF	68
						141.7	G	TeLe	79
		4d <sub>5</sub>							
70	Yb	(181.4)	G	HHL	70				
		(181.4)	G	KEML	74				
		(182.7)	G	LPWF	75				
		(183.0)	G	PLNW	77				
71	Lu	(196.1)	G	KEML	74				
		(196.3)	G	LPWF	75				
		(196.6)	G	PLNW	77				
72	Hf	211.5	A	NBM	80				
73	Ta	226.4	A	NBM	80				
74	W	243.5	A	NBM	80	14.23	A	NBM	80
75	Re	260.5	A	BNMN	79	21.61	A	NBM	80
76	Os	278.5	A	BNMN	79	21.64	A	VHE	82
77	Ir	296.3	A	NMB	80	31.32	A	NBM	80
78	Pt	314.6	A	NMB	80	40.46	A	BNMN	79
		314.6	A	KNNH	68	50.7	A	BNMN	79
						60.75	A	NMB	80
						71.07	A	NMB	80
						71.0	A	JHBK	73
						71.07	A	VaTr	79
		4f <sub>7</sub>							

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TABLE 2. The best values of elemental photoelectric energies as of 1985 — Continued

		4d <sub>s</sub>				4f <sub>7</sub>			
79	Au	334.7	A	VaTr	79	83.97	A	VaTr	79
		335.2	A	NBM	80	84.00	A	NBM	80
		335.1	A	PEJ	82	84.0	A	MKLP	73
					84.00	A	AnSe	84	
					84.07	A	Asam	86	
					84.1	A	PEJ	82	
					84.15	A	ALMP	82	
					83.86	A	BiSw	80	
					83.98	A	BiSw	80	
80	Hg	359.3	G	SMBM	76	99.9	G	SMBM	76
81	Tl	385.0	G	MBN	80	117.73	G	MBN	80
82	Pb	412.0	A	NBM	80	136.78	A	NBM	80
		412.0	A	SFS	77	136.8	A	SFS	77
83	Bi	440.1	A	NBM	80	156.85	A	NBM	80
		440.3	A	VaTr	79	156.88	A	VaTr	79
		440.4	A	SFS	77	156.9	A	SFS	77
					157.0	A	LKMP	73	
90	Th	(675.2)		FBWF	74	333.1	G	ScLa	81
		(675.2)		ScLa	81	333.25	G	WRDM	79
92	U	(736.0)		FBWF	74	376.9	G	VRPC	74
		(736.4)		ScLa	81	377.1	G	ACCT	74
		(736.8)		ACCT	74	377.1	G	Chad	73
					377.4	G	ScLa	81	
					377.4	G	WRDM	79	

<sup>a</sup>When the data are within 300 eV of a point of reference, they are indicated by a "G".

<sup>b</sup>When the data are enclosed by a parenthesis, it is indicated that the data are not within bounds of 300 eV, or if they are within "G", they are still so scattered that several competing data must be supplied.

<sup>c</sup>A few data have been done very carefully, and all of these data are indicated by the letter "A", representing calibration grade.



## THE NIST X-RAY PHOTOELECTRON SPECTROSCOPY (XPS) DATABASE

TABLE 3. Inorganic compounds for which Sn was being observed by photoelectron or Auger spectroscopy.

Spectral Line	Compound	Physical State	Energy (eV)	Quality	Charge Reference	Calibration Method	Reference
<b>Binding Energy</b>							
3s	Sn	Sc	885.3	A	Au	Au	NyMa 80
3p3	K2SnF6		717.2	c	AC		MoVa 73
3p3	Sn	Sc	714.6	A	Cond	Au4f7 = 83.97 Pd3d5 = 335.18	VaTr 79
3p3	Sn	Sc	714.7	A	Au	Au	NyMa 80
3p3	Sn	Sc	714.7	A	Cond	Au, Na1s-2p = 1041.1	SFS 77
3p3	SnF2		716.3	c	AC		MoVa 73
3p3	SnO		716.2	c	AC		MoVa 73
3p3	SnO2		716	c	AC		MoVa 73
3d5	(NH4)2SnCl6		486.7	c	Au		GZF 73+
3d5	Ag95Sn5		485.6	G	Cond	Au,Ag,Cu	HSBS 81
3d5	Ba(SnCl3)2		486.8	Gc	AC	FL	WVW 79+
3d5	BaSnCl4		486.8	Gc	AC	FL	WVW 79+
3d5	Cd2SnO4		486	Gc	AC	Au	GHMH 83
3d5	Cd996Sn4		485.3	G	Cond	Au,Ag,Cu	HSBS 81
3d5	CdSnO3		486.1	Gc	AC	Au	GHMH 83
3d5	Co20Sn80	Sp	484.7		Cond	Au	ThSh 78
3d5	K2SnF6		487.6	Gc	AC		MoVa 73
3d5	KSnF3		486.7	c	Au		GZF 73+
3d5	Na2SnO3		486.2	Gc	AC		MoVa 73
3d5	Na2SnO3		486.7	Gc	AC	Au,Cu	Wagn 75
3d5	Na2SnO3		486.8	Gc	AC		Shut 80
3d5	Na2SnO3		487.2	Gc	AC		ADPS 77
3d5	NaSnF3		487.4	Gc	AC	Au,Cu	Wagn 75
3d5	Pb98Sn2		486.4	G	Cond	Au,Ag,Cu	HSBS 81
3d5	Sb95Sn5		485.2	G	Cond	Au,Ag,Cu	HSBS 81
3d5	Sn		484.4		Cond	FL	WVW 79+
3d5	Sn		484.7	Gc	AC		FaGo 77
3d5	Sn		484.8		Cond	ON	PWA 79
3d5	Sn		484.8	Gc	AC		Shut 80
3d5	Sn		484.87	G	Cond	Vacuum Ne1s = 870.27 (Ne2s = 48.47)	VeCa 85
3d5	Sn		484.9		Cond	Au	TLR 78
3d5	Sn		484.9	G	AC		LAK 77
3d5	Sn		485.2	Gc	AC		OCH 79
3d5	Sn	Sc	484.8	A	Cond	Au4f7 = 83.97 Pd3d5 = 335.18	VaTr 79
3d5	Sn	Sc	484.92	A	Au	Au	NyMa 80
3d5	Sn	Sc	485	Gc	Cond	Au,Cu	Wagn 75
3d5	Sn	Sc	485.1	A	Cond	Au, Na1s-2p = 1041.1	SFS 77
3d5	Sn	Sp	484.3	c	Cond	Au	ADPS 77
3d5	Sn	Sp	484.7		Cond	Au	ThSh 78
3d5	Sn	Sp	484.85	Gc	Cond	Au,Cu	WRDM 79
3d5	Sn	SpA	485		Cond		SHR 82
3d5	Sn	VD	484.8		Cond		BVWW 80
3d5	Sn	VD	484.87	G	Cond	Ag	PVVA 79
3d5	Sn,alpha		486.72		Au		WaHu 74
3d5	Sn,alpha	SpA	485	G	Cond	AuCu	Hegd 82
3d5	Sn,beta		484.6	G	Cond	Au,Ag,Cu	HSBS 81
3d5	Sn,beta		486.1		Au		WaHu 74
3d5	Sn,beta	SpA	484.6	G	Cond	AuCu	Hegd 82

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TABLE 3. Inorganic compounds for which Sn was being observed by photoelectron or Auger spectroscopy — Continued

Spectral Line	Compound	Physical State	Energy (eV)	Quality	Charge Reference	Calibration Method	Reference
Binding Energy							
3d5	SnBr2		486.9	c	Au		GZF 73+
3d5	SnCl2		486.5	c	Au		GZF 73+
3d5	SnCl2		486.7	Gc	AC	FL	WV 79+
3d5	SnF2		487	Gc	AC		MoVa 73
3d5	SnF2		487.1	c	Au		GZF 73+
3d5	SnF2		487.4	Gc	AC		Shut 80
3d5	SnF4		487.9	c	Au		GZF 73+
3d5	SnF4		488.2	Gc	AC		Shut 80
3d5	SnMo6S8		486.2	Gc	AC		MAS 85
3d5	SnO		485.6	Gc	AC		Shut 80
3d5	SnO		486	Gc	AC		ADPS 77
3d5	SnO		486.6	c	Au		GZF 73+
3d5	SnO		486.9	Gc	AC	FL	WV 79+
3d5	SnO		487	Gc	AC		MoVa 73
3d5	SnO	Sc	487	Gc	AC		FaGo 77
3d5	SnO2		486.1	Gc	AC		Shut 80
3d5	SnO2		486.2	Gc	AC	Au	GHH 83
3d5	SnO2		486.5	Gc	AC		ADPS 77
3d5	SnO2		486.6	Gc	AC		MoVa 73
3d5	SnO2		486.6	Gc	AC	Au,Cu	WRDM 79
3d5	SnO2		486.7	Gc	AC		NGDS 75
3d5	SnO2		486.7	Gc	AC	FL	WV 79+
3d5	SnO2		486.7	c	Au		GZF 73+
3d5	SnO2		486.8	Gc	AC	Au	TLR 78
3d5	SnO2	PO	486.6	G	AC		LAK 77
3d5	SnO2	Sc	486.5	Gc	AC		FaGo 77
3d5	SnS		485.6	Gc	AC	Au,Cu	Wagn 75
3d5	SnS		486.4	Gc	AC		MoVa 73
3d5	SnS	Cl	485.7	G	Cond	Au, Na1s-2p = 1041.1	SFS 77
3d5	SnS2		486.8	Gc	AC		MoVa 73
3d5	SnSe	Cl	485.7	G	Cond	Au, Na1s-2p = 1041.1	SFS 77
3d5	SnTe	Sc	485.6	G	Cond	Au, Na1s-2p = 1041.1	SFS 77
4s	Sn	Sc	136.8	A	Cond	Au4f7 = 83.97 Pd3d5 = 335.18	VaTr 79
4s	Sn	Sc	137.2	A	Au	Au	NyMa 80
4p	Sn	Sc	85.2	A	Cond	Au4f7 = 83.97 Pd3d5 = 335.18	VaTr 79
4d	Sn		24.5		Cond	ON	PWA 79
4d	Sn	SpA	24.2		Cond		SHR 82
4d5	Sn		23.68	G	Cond	Vacuum Ne1s = 870.27 (Nc2s = 48.47)	VeCa 85
4d5	Sn	Cr	23.68	A	Cond	Au FL	PKLS 72
4d5	Sn	Sc	23.95	A	Au	Au	NyMa 80
4d5	Sn	Sc	24.04	A	Cond	Au4f7 = 83.97 Pd3d5 = 335.18	VaTr 79
4d5	Sn	Sc	24.1	A	Cond	Au, Na1s-2p = 1041.1	SFS 77
4d5	Sn	VD	23.68		Cond	Ag	PVVA 79
4d5	SnS	Cl	24.8	G	Cond	Au, Na1s-2p = 1041.1	SFS 77
4d5	SnSe	Cl	24.7	G	Cond	Au, Na1s-2p = 1041.1	SFS 77
4d5	SnTe	Sc	24.5	G	Cond	Au, Na1s-2p = 1041.1	SFS 77

## THE NIST X-RAY PHOTOELECTRON SPECTROSCOPY (XPS) DATABASE

TABLE 3. Inorganic compounds for which Sn was being observed by photoelectron or Auger spectroscopy – Continued

Spectral Line	Compound	Physical State	Energy (eV)	Quality	Charge Reference	Calibration Method	Reference
<b>Auger</b>							
M455	Na <sub>2</sub> SnO <sub>3</sub>		431.7	Gc	AC	Au,Cu	Wagn 75
M455	NaSnF <sub>3</sub>		430.8	Gc	AC	Au,Cu	Wagn 75
M455	Sn		437.27	G	Cond	Vacuum Ne1s = 870.27 (Ne2s = 48.47)	VeCa 85
M455	Sn		437.5		AC		LAK 77
M455	Sn	Sc	437.4	Gc	Cond	Au,Cu	Wagn 75
M455	Sn	Sc	437.5	A	Cond	Au4f7 = 83.97 Pd3d5 = 335.18	VaTr 79
M455	Sn	Sp	437.6	Gc	Cond	Au,Cu	WRDM 79
M455	Sn	VD	437.27		Cond	Ag	PVVA 79
M455	SnO <sub>2</sub>	PO	432.6		AC		LAK 77
M455	SnS		435.7	Gc	AC	Au,Cu	Wagn 75
M555	Sn		428.85	G	Cond	Vacuum Ne1s = 870.27 (Ne2s = 48.47)	VeCa 85
M555	Sn		428.9		Cond	ON	PWA 79
M555	Sn	Sc	429	A	Cond	Au4f7 = 83.97 Pd3d5 = 335.18	VaTr 79
<b>Auger Parameter</b>							
3d5-M4	Na <sub>2</sub> SnO <sub>3</sub>		918.4	G		Au,Cu	Wagn 75
3d5-M4	NaSnF <sub>3</sub>		918.2	G		Au,Cu	Wagn 75
3d5-M4	Sn		922.14			Vacuum Ne1s = 870.27 (Ne2s = 48.47)	VeCa 85
3d5-M4	Sn		922.4				LAK 77
3d5-M4	Sn	Sc	922.4	G		Au,Cu	Wagn 75
3d5-M4	Sn	Sp	922.45	G		Au,Cu	WRDM 79
3d5-M4	Sn	VD	922.14			Ag	PVVA 79
3d5-M4	SnO <sub>2</sub>	PO	919.2				LAK 77
3d5-M4	SnS		921.3	G		Au,Cu	Wagn 75
3d5-M5	Sn		913.7			ON	PWA 79
3d5-M5	Sn		913.72			Vacuum Ne1s = 870.27 (Ne2s = 48.47)	VeCa 85
4d5-M4	Sn		460.95			Vacuum Ne1s = 870.27 (Ne2s = 48.47)	VeCa 85
4d5-M5	Sn		452.53			Vacuum Ne1s = 870.27 (Ne2s = 48.47)	VeCa 85
<b>Chemical Shift</b>							
3p3	AuSn	Sc	+0.2	A	Cond	Au4f7 = 83.97 Pd3d5 = 335.18	VaTr 79
3d5	Ag <sub>95</sub> Sn <sub>5</sub>		+1		Cond	Au,Ag,Cu	HSBS 81
3d5	Ag <sub>95</sub> Sn <sub>5</sub>	SpA	+1	G	Cond	AuCu	Hegd 82
3d5	AuSn		+0.4			Au	FHPW 73
3d5	AuSn	Sc	+0.3	A	Cond	Au4f7 = 83.97 Pd3d5 = 335.18	VaTr 79
3d5	AuSn <sub>4</sub>		+0.1			Au	FHPW 73
3d5	Cd <sub>99.5</sub> Sn <sub>5</sub>	SpA	+0.7	G	Cond	AuCu	Hegd 82
3d5	Cd <sub>99.6</sub> Sn <sub>4</sub>		+0.7		Cond	Au,Ag,Cu	HSBS 81
3d5	CsSn	RF	+0.0				BVWW 80
3d5	Cu <sub>95</sub> Sn <sub>5</sub>	SpA	+1	G	Cond	AuCu	Hegd 82
3d5	In <sub>95</sub> Sn <sub>5</sub>	SpA	+0.6	G	Cond	AuCu	Hegd 82
3d5	Pb <sub>95</sub> Sn <sub>5</sub>	SpA	+1.8	G	Cond	AuCu	Hegd 82
3d5	Pb <sub>98</sub> Sn <sub>2</sub>		+1.6		Cond	Au,Ag,Cu	HSBS 81
3d5	Sb <sub>95</sub> Sn <sub>5</sub>		+0.6			Au,Ag,Cu	HSBS 81
3d5	Sb <sub>95</sub> Sn <sub>5</sub>	SpA	+0.6	G	Cond	AuCu	Hegd 82
3d5	Sn ox	RF	+1.5				WaBi 73
3d5	Sn <sub>5</sub> Cu <sub>95</sub>		+1			Au	HeSi 83
4d	Sn ox	RF	+1.2				WaBi 73

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TABLE 3. Inorganic compounds for which Sn was being observed by photoelectron or Auger spectroscopy – Continued

Spectral Line	Compound	Physical State	Energy (eV)	Quality	Charge Reference	Calibration Method	Reference
<b>Auger Parameter</b>							
d5	AuSn	Sc	+0.3	A	Cond	Au4f7 = 83.97 Pd3d5 = 335.18	VaTr 79
M455	AuSn	Sc	-0.3	A	Cond	Au4f7 = 83.97 Pd3d5 = 335.18	VaTr 79
M455	Sn ox	PO	-3.4				SHR 82
M455	Sn ox	RF	-3.9				WaBi 73
M455	Sn ox	RF	-4.1	G			BBG 79
M555	AuSn	Sc	+0.3	A	Cond	Au4f7 = 83.97 Pd3d5 = 335.18	VaTr 79
3d5-M4	AuSn	Sc	+0.0	A	Cond (AP derived)	Au4f7 = 83.97 Pd3d5 = 335.18	VaTr 79
3d5-M4	Sn ox	RF	-2.4				WaBi 73
<b>Doublet Separation</b>							
3p	Sn	Sc	41.9			Au, Na1s-2p = 1041.1	SFS 77
3p	Sn	Sc	41.9	A		Au	NyMa 80
3p	Sn	Sc	41.9	A	Cond	Au4f7 = 83.97 Pd3d5 = 335.18	VaTr 79
3d	Sn		8.4				FaGo 77
3d	Sn		8.45			Vacuum Ne1s = 870.27 (Ne2s = 48.47)	VeCa 85
3d	Sn	Sc	8.3			Au, Na1s-2p = 1041.1	SFS 77
3d	Sn	Sc	8.4	A	Cond	Au4f7 = 83.97 Pd3d5 = 335.18	VaTr 79
3d	Sn	Sc	8.41	A		Au	NyMa 80
3d	Sn	Sp	8.5			Au,Cu	WRDM 79
3d	Sn	VD	8.45			Ag	PVVA 79
3d	SnMo6S8		8.5				MAS 85
3d	SnO		8.5				FaGo 77
3d	SnO2		8.5				FaGo 77
4d	Sn		1.08			Vacuum Ne1s = 870.27 (Ne2s = 48.47)	VeCa 85
4d	Sn	Cr	1.08			Au FL	PKLS 72
4d	Sn	Sc	0.98	A	Cond	Au4f7 = 83.97 Pd3d5 = 335.18	VaTr 79
4d	Sn	Sc	1.05	A		Au	NyMa 80
4d	Sn	VD	1.08			Ag	PVVA 79
<b>Separation from Strongest Auger Line</b>							
M555	Sn	VD	-8.5	G			BBG 79

# THE NIST X-RAY PHOTOELECTRON SPECTROSCOPY (XPS) DATABASE

TABLE 4. Organic compounds for which Sn was being observed by photoelectron or Auger spectroscopy.

Spectral Line	Compound	Physical State	Energy (eV)	Quality	Charge Reference	Calibration Method	Reference
Binding Energy							
3p3	Ph4Sn		716	c	IC		MoVa 73
3d5	(Et4N)2SnBr6		487	Gc	IC	FL	WVV 79+
3d5	(Et4N)3Pt(SnCl3)5		486.9	Gc	IC		Rigg 72+
3d5	(Me4N)2 < Pt(SnCl3)2Cl2 >		486.7	Gc	IC		AKSK 82+
3d5	(Me4N)2 < Pt(SnCl3)5 >		486.8	Gc	IC		AKSK 82+
3d5	(Me4N)2SnCl6		486.7	Gc	IC		AKSK 82+
3d5	(Me4N)SnCl3		485.3	Gc	IC		AKSK 82+
3d5	(PhCH2)2SnCl2		487.6	Gc	IC		MoVa 73
3d5	(PhCH2)3SnCl		486.9	Gc	IC		MoVa 73
3d5	AgSnCl3(Ph3P)3		487	Gc	IC		GZF 73+
3d5	Br4Sn(pyrazine)		487.4	Gc	IC		FMPB 81
3d5	Bu2SnO		485.6	Gc	IC	FL	WVV 79+
3d5	Cl2Ph2Sn(pyrazine)		487.5	Gc	IC		FMPB 81
3d5	Cl3BuSn(pyrazine)		487.6	Gc	IC		FMPB 81
3d5	Cl3MeSn(pyrazine)		487.5	Gc	IC		FMPB 81
3d5	Cl3OctSn(pyrazine)		487.6	Gc	IC		FMPB 81
3d5	Cl3PhSn(pyrazine)		487.9	Gc	IC		FMPB 81
3d5	Cl3SnCo(CO)3AsPh3		487.2	Gc	IC		WVV 79+
3d5	Cl3SnMo(CO)3(C5H5)		487.1	Gc	IC		WVV 79+
3d5	Cl3SnMo(CO)3(C5H5)		487.3	Gc	IC		WWVV 77
3d5	Cl3SnW(CO)3(C5H5)		487	Gc	IC		WVV 79+
3d5	Cl3SnW(CO)3(C5H5)		487	Gc	IC		WWVV 77
3d5	Cl4Sn(pyrazine)		487.8	Gc	IC		FMPB 81
3d5	Cl4Sn(pyrazine)2		488.1	Gc	IC		FMPB 81
3d5	Et2Sn(5-Ac-8-quinolinol)2		487.4	Gc	IC		UBS 83+
3d5	EtSnCl3(pyridine)2		487.2	Gc	IC	FL	WVV 79+
3d5	I4Sn(pyrazine)		487.6	Gc	IC		FMPB 81
3d5	Mc2ClSnMo(CO)3(C5H5)		486.3	Gc	IC		WWVV 77
3d5	Me2ClSnW(CO)3(C5H5)		486	Gc	IC		WWVV 77
3d5	Me2Sn(MeCOCHCOMe)2	VD	486.81		Cond	Pt4f7 = 71.2	BALS 76+
3d5	Me2Sn(8-quinolinol)2		486.96	Gc	IC		UBS 83+
3d5	Mc2Sn(PhCOCHCOPh)2	VD	486.87		Cond	Pt4f7 = 71.2	BALS 76+
3d5	Mc2SnCl2(DMSO)2		487	Gc	IC		WVV 79+
3d5	Me2SnF2		487.1	Gc	IC	FL	WVV 79+
3d5	Me2SnI2(bipyridyl)		486.3	Gc	IC		WVV 79+
3d5	Me2SnSO4		487	Gc	IC	FL	WVV 79+
3d5	Me3SnF		486.7	Gc	IC	FL	WVV 79+
3d5	Me3SnMo(CO)3(C5H5)		485.3	c	Au		GrMa 75+
3d5	Me3SnW(CO)3(C5H5)		485.8	Gc	IC		WWVV 77
3d5	Me4NSnCl3		486.1	Gc	IC		GZF 73+
3d5	McCl2SnW(CO)3(C5H5)		486.3	Gc	IC		WWVV 77
3d5	Ph2Sn(PhCOCHCOPh)2	VD	486.64		Cond	Pt4f7 = 71.2	BALS 76+
3d5	Ph3Sn(8-quinolinol)		487	Gc	IC		UBS 83+
3d5	Ph3Sn(PhCOCHCOPh)	VD	486.55		Cond	Pt4f7 = 71.2	BALS 76+
3d5	Ph3SnBr		487.5	Gc	IC		HWVV 74
3d5	Ph3SnCl		486.3	Gc	IC	FL	WVV 79+
3d5	Ph3SnCl		487	Gc	IC		MoVa 73
3d5	Ph3SnCl		487.6	Gc	IC		HWVV 74
3d5	Ph3SnF		486.2	Gc	IC	FL	WVV 79+
3d5	Ph3SnF		487.3	Gc	IC		HWVV 74
3d5	Ph3SnFc(CO)2(C5H5)		485.4	Gc	IC		WVV 79+

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TABLE 4. Organic compounds for which Sn was being observed by photoelectron or Auger spectroscopy — Continued

Spectral Line	Compound	Physical State	Energy (eV)	Quality	Charge Reference	Calibration Method	Reference
Binding Energy							
3d5	Ph3SnGePh3		485.1	Gc	IC	FL	WVV 79+
3d5	Ph3SnI		486.3	Gc	IC	FL	WVV 79+
3d5	Ph3SnI		487.5	Gc	IC		HWVV 74
3d5	Ph3SnMo(CO)3(C5H5)		486	Gc	IC		WWVV 77
3d5	Ph3SnOH		485.6	Gc	IC	FL	WVV 79+
3d5	Ph3SnOSnPh3		485.6	Gc	IC	FL	WVV 79+
3d5	Ph3SnSSnPh3		485.3	Gc	IC	FL	WVV 79+
3d5	Ph3SnW(CO)3(C5H5)		485.8	Gc	IC		WVV 79+
3d5	Ph3SnW(CO)3(C5H5)		486.1	Gc	IC		WWVV 77
3d5	Ph4Sn		485.1	Gc	IC	FL	WVV 79+
3d5	Ph4Sn		486.3	Gc	IC		MoVa 73
3d5	Ph4Sn		487.1	Gc	IC		HWVV 74
3d5	Ph4Sn	VD	485.85		Cond	Pt4f7 = 71.2	BALS 76+
3d5	PhClSn(PhCOCHCOPh)2	VD	487.18		Cond	Pt4f7 = 71.2	BALS 76+
3d5	PhSnCl3(pyridine)2		487.2	Gc	IC	FL	WVV 79+
3d5	Sn(5,7-Cl2-8-quinolinol)2		487.18	Gc	IC		UBS 83+
3d5	Sn(8-quinolinol)2		488.1	Gc	IC		UBS 83+
3d5	SnCl4(Me2SO)2		487.1	Gc	IC		GZF 73+
3d5	SnCl4(dimethylsulfone)2		486.9	Gc	IC		WVV 79+
3d5	SnCl4(pyridine)2		487.3	Gc	IC		WVV 79+
4d	Ph3SnBr		26.6	Gc	IC		HWVV 74
4d	Ph3SnCl		26.9	Gc	IC		HWVV 74
4d	Ph3SnF		26.4	Gc	IC		HWVV 74
4d	Ph3SnI		26.6	Gc	IC		HWVV 74
4d	Ph4Sn		26.5	Gc	IC		HWVV 74
Doublet Separation							
3d	Ph4Sn	VD	8.39			Pt4f7 = 71.2	BALS 76+

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TABLE 5. A subset of values of photoelectron binding energies and Auger kinetic energies for all the elements.

	Values in Chemical State		Ref. (median)
		Values in Error ( 0.5 eV)	
		1s	
<b>LITHIUM</b>			
Li	3	54.8	KLMP 73
LiO		55.6	CSFG 79
LiOH		54.9	CSFG 79
LiCl	3	56.1	MVS 73
LiF	3 1	55.7	MVS 73
Li <sub>2</sub> CO <sub>3</sub>	2	55.2	CSFG 79
<b>BERYLLIUM</b>			
Be	3	111.8	WRDM 79
BeO	4	113.7	NFS 82
BeF <sub>2</sub>	2 1	115.3	NKBP 73
NaBeF <sub>3</sub>		115.3	NKBP 73
<b>BORON</b>			
B	2 1	186.5	SMS 80
TiB <sub>2</sub>		187.5	MECC 73
BN	4	190.5	WRDM 79
B <sub>2</sub> O <sub>3</sub>	4	193.1	SMS 80
H <sub>3</sub> BO <sub>3</sub>	2	193.0	SMS 80
Na <sub>2</sub> B <sub>4</sub> O <sub>7</sub>		191.8	SMS 80
NaBF <sub>4</sub>	2	194.9	RNS 73
<b>CARBON</b>			
C <sub>graphite</sub>	5	284.5	SmBl 84
TiC	3	281.5	IKIM 73
C <sub>6</sub> H <sub>6</sub>	3	284.9	CKAM 72
Na <sub>2</sub> CO <sub>3</sub>	2	289.4	HHDD 81
CO <sub>2</sub>		291.9	GHHL 70
CCl <sub>4</sub>		292.4	GHHL 70
CF <sub>2</sub> CF <sub>2</sub>	2 1	292.6	Tayl 78
<b>NITROGEN</b>			
CrN		396.8	STAB 76
Si <sub>3</sub> N <sub>4</sub>	3 1	397.7	TLR 78
BN	4 1	398.1	WRDM 79
NH <sub>3</sub>	3 1	398.8	LaLu 79
NH <sub>4</sub> Cl	4 1	401.7	BTE 77
NH <sub>4</sub> NO <sub>3</sub>	4 2	401.9	BCM 78
NaNO <sub>2</sub>	5 2	403.8	DML 84
NaNO <sub>3</sub>	5 2	407.3	DML 84
<b>OXYGEN</b>			
CdO	4	529.2	NFS 82
NiO	10	529.5	LoSt 84
Ni(OH) <sub>2</sub>	9	531.2	LoSt 84
CuO	9 1	529.6	MSSS 81
Cu <sub>2</sub> O	7 1	530.4	MSSS 81
CoO	7	530.2	NGDS 75
Co <sub>3</sub> O <sub>4</sub>	6	530.2	NGDS 75
MoO <sub>3</sub>	11 2	530.62	BFCB 83
Al <sub>2</sub> O <sub>3</sub>	17 4	531.0	StHe 84
KClO <sub>3</sub>	3	531.87	TCCW 85
KClO <sub>4</sub>	3	532.92	TCCW 85
poly(CH <sub>2</sub> CHOH)	3	532.6	PRCV 77
H <sub>2</sub> O	3	533.1	WZR 80
Co(CO) <sub>6</sub>	5 1	533.9	KTWY 76

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TABLE 5. A subset of values of photoelectron binding energies and Auger kinetic energies for all the elements – Continued

		Values in Chemical State					
		Values in Error ( 0.5 eV)					
		1s			Ref.		
					(median)		
<b>FLUORINE</b>							
CaF2	4	684.8			WRDM	79	
LiF	5 1	685.0			NBK	74	
NaF	5 1	684.5			NBK	74	
KF	4	683.9			NBK	74	
MgF2	4	685.52			MuTh	80	
UF4	4 1	684.8			Chad	73	
K2NbF7	2	685.2			NBK	74	
Ni(OOCCF3)2		688.4			WRDM	79	
poly(CF2CF2)	3 1	690.0			CFKM	73	
C6F6		690.9			CKAM	72	
NF4BF4		694.2			RNS	73	
		1s	KL <sub>23</sub> L <sub>23</sub>	α			
<b>NEON</b>							
Ne(implanted in Fe)		863.4	818.0	1681.4	Wagn	75	
Ne(implanted in diamond)		863.1	818.7	1681.8	Evan	80	
Ne(implanted in Ag)		862.4			CiHa	74	
<b>SODIUM</b>							
Na	4	1071.8	994.3	2066.1	BaSt	75	
Na3Sb				2064.8	BaGa	80	
Na2O		1072.5	989.8	2062.3	BaSt	75	
NaNO2		1071.6	989.8	2061.4	Wagn	75	
NaNO3		1071.4	989.4	2060.8	WGR	79	
Na3PO4	3	1071.1	990.2	2061.3	Swif	82	
NaPO3	3	1071.6	989.4	2061.0	Swif	82	
Na2SO3	3 1	1071.4	990.2	2061.6	WGR	75	
Na2SO4	3 1	1071.2	989.8	2061.0	Wagn	75	
Na2CrO4	2	1071.2	990.9	2062.1	WGR	79	
Na2MoO4	2 1	1070.9	991.0	2061.9	WGR	79	
NaBiO3		1071.3	990.9	2062.2	WGR	79	
NaI	2	1071.6	991.2	2062.8	Wagn	75	
NaBr	3 1	1071.7	990.6	2062.3	Wagn	75	
NaCl	8 5	1071.6	990.3	2061.9	Wagn	75	
NaOOCH		1071.1	989.8	2060.9	WGR	79	
NaOAc	2 1	1071.1	989.9	2061.0	Wagn	75	
natrolite(Na2Al2Si3O10)		1072.4	988.5	2060.9	WPHK	82	
Na zeolite A (NaAlSiO4)	2	1071.7	988.9	2060.6	WPHK	82	
Na2ZrF6		1071.5	988.7	2060.2	Wagn	75	
NaF	4 1	1071.2	988.6	2059.8	Wagn	75	
NaBF4		1072.7	987.1	2059.8	Wagn	75	
Na2SiF6	2	1071.7	987.7	2059.4	Wagn	75	
		2p	KL <sub>23</sub> L <sub>23</sub>	α	1s		
<b>MAGNESIUM</b>							
Mg	9	49.6	1185.6	1235.2	1303.2	Fugg	77
Mg2Cu		49.5	1186.0	1235.5	1302.6	FWPF	75
Mg3Bi		50.3	1184.9	1235.2	1303.6	FWPF	75
MgO		50.4	1180.4	1230.8	1304.0	WRDM	79
Mg(OH)2		49.5	1302.7			HKNU	78
MgAl2O4		50.4	1304.0			HNUW	78
MgF2	2	50.95	1178.15	1229.1	1305.0	Wagn	80
Mg acetylacetonate		50.1	1180.5	1230.6	1304.0	WGR	79
Mg erucate		50.7	1180.2	1230.9	1304.4	WGR	79



# THE NIST X-RAY PHOTOELECTRON SPECTROSCOPY (XPS) DATABASE

TABLE 5. A Subset of values of photoelectron binding energies and Auger kinetic energies for all the elements – Continued

		Values in Chemical State				
		Values in Error ( 0.5 eV)				
		2p	KL <sub>23</sub> L <sub>23</sub>	α	Ref.	
					(median)	
<b>ALUMINIUM</b>						
Al	9 1	72.85	1393.29	1466.14	Tayl	82
AlAs		73.6	1391.2	1464.8	Tayl	82
AlN	2	74.0	1388.9	1462.9	TaRa	81
Al <sub>2</sub> O <sub>3</sub> ,alpha	3 1	73.85	1388.24	1462.09	WSJT	81
Al <sub>2</sub> O <sub>3</sub> ,gamma	6	73.72	1377.83	1461.55	WSJT	81
Al <sub>2</sub> O <sub>3</sub> ,sapphire	2	74.10	1387.87	1461.97	WPHK	82
Al(OH) <sub>3</sub>	2	74.3	1387.7	1462.0	Tayl	82
CuAl <sub>2</sub> O <sub>4</sub>	2	74.2			SLFH	85
natrolite		74.25	1386.53	1460.78	WPHK	82
sillimanite		74.58	1386.86	1461.44	WPHK	82
molecular sieve type A	2	73.66	1386.90	1460.56	WPHK	82
<b>SILICON</b>						
Si	11 1	99.44	1616.68	1716.12	WSJT	81
MoSi <sub>2</sub>		99.56	1617.2	1716.76	WSJT	81
PtSi		100.5			GMM	82
SiC		100.4			SmBl	84
Si <sub>3</sub> N <sub>4</sub>	5	101.9	1612.2	1714.1	Tayl	81
Ph <sub>4</sub> Si		101.2			GCH	76
SiO <sub>2</sub>	12	103.4	1608.8	1712.2	KBHN	74
SiO <sub>2</sub> α-quartz		103.65	1608.6	1712.25	WPHK	82
SiO <sub>2</sub> Vycor		103.5	1608.5	1712.0	Wagn	78
SiO <sub>2</sub> gel		103.59	1607.87	1711.46	WPHK	82
methylsilicone resin		102.92	1608.80	1711.72	WPHK	82
poly-dimethylsilicone		102.40	1609.38	1711.78	WPHK	82
pyrophyllite		102.88	1609.20	1712.08	WPHK	82
spodumene		102.46	1609.59	1712.05	WPHK	82
albite		102.63	1609.26	1711.89	WPHK	82
natrolite		102.22	1609.62	1711.84	WPHK	82
hydroxysodalite		101.65	1610.7	1712.35	WPHK	82
molecular sieve type A	2	101.65	1610.09	1711.52	Tayl	81
Na <sub>2</sub> SiF <sub>6</sub>		104.3			NSLS	77
<b>PHOSPHORUS</b>						
P (red)	7 1	(130.2)	1857.0	1987.2	ScBr	81
BP		130.3			PHHJ	70
CrP		129.6			PHHJ	70
GaP		128.7	1858.9	1987.6	WaTa	80
InP	5 1	129.7			Bert	81
P <sub>2</sub> O <sub>5</sub>	6	135.2			CFRS	80
Ph <sub>3</sub> P	18 3	130.9			BMPN	85
Ph <sub>3</sub> PO	9 1	132.5			Wagn	75
Ph <sub>3</sub> PS	5	132.5			Wagn	75
NaPO <sub>3</sub>	5 2	134.7	1848.3	1983.0	Wagn	78
Na <sub>2</sub> HPO <sub>4</sub>	4	133.1	1850.8	1983.9	WaTa	80
Na <sub>3</sub> PO <sub>4</sub>	5	132.3			Swif	82
<b>SULFUR</b>						
S	7 1	164.25			RiVe	83
ZnS	4 1	161.7	2114.4	2276.1	Wagn	78
NiS	4	162.8	2116.1	2278.9	WaTa	80
WS <sub>2</sub>	5 2	162.8	2115.6	2278.4	Wagn	78
Na <sub>2</sub> SO <sub>3</sub>	5 1	166.6	2108.5	2275.1	WaTa	82
Na <sub>2</sub> S <sub>2</sub> O <sub>3</sub> (ccntral S)	3 1	168.6	2107.8	2276.4	Wagn	78
Na <sub>2</sub> S <sub>2</sub> O <sub>3</sub> (periphcral S)		162.5	2112.5	2275.0	Wagn	78
CuSO <sub>4</sub>	3 1	169.1	2108.0	2277.1	WaTa	80
Na <sub>2</sub> SO <sub>4</sub>	5 1	169.1	2105.9	2275.0	Wagn	78
SF <sub>6</sub>		174.4	2100.45	2274.85	WaTa	82
CS <sub>2</sub>		163.6	2111.65	2275.25	WaTa	82
SO	2	167.4	2106.2	2273.6	WaTa	82

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TABLE 5. A subset of values for photoelectron binding energies and Auger kinetic energies for all the elements – Continued

		Values in Chemical State					
		Values in Error ( 0.5 eV)					
		2p	KL <sub>23</sub> L <sub>23</sub>	α	Ref.		
						(median)	
<b>CHLORINE</b>							
NaCl	5	198.6			NSLS	77	
KCl	4	198.4			NSLS	77	
KClO <sub>3</sub>	2	206.16			TCCW	85	
KClO <sub>4</sub>	2	208.33			TCCW	85	
K <sub>2</sub> PtCl <sub>4</sub>	4 1	198.7			NSBM	80	
K <sub>2</sub> PtCl <sub>6</sub>	5 1	198.9			NSBM	80	
NiCl <sub>2</sub>	2	199.4			KIHe	83	
RhCl <sub>3</sub>	3 1	198.6			NSBM	80	
poly-(vinyl chloride)		200.1			WRDM	79	
<b>ARGON</b>							
		2p <sub>3</sub>					
Ar(implanted in Fe)		241.7			Wagn	75	
Ar(implanted in graphite)		241.5			Wagn	78	
<b>POTASSIUM</b>							
		2p <sub>3</sub>	L <sub>3</sub> M <sub>2</sub> M <sub>3</sub>	L <sub>2</sub> M <sub>2</sub> M <sub>3</sub>	α		
K		294.7				PeKa 77	
KI		292.8			543.6*	Wagn 75	
KBr	3	293.1	248.3	250.7	542.6	WRDM 79	
KCl	4	292.8				NSLS 77	
KF		292.8				Wagn 75	
K <sub>2</sub> O <sub>s</sub> Cl <sub>6</sub>	3	293.0				LZML 83	
KSbF <sub>6</sub>		293.7				Wagn 75	
*Peaks composed mainly of L <sub>3</sub> M <sub>23</sub> M <sub>23</sub> and L <sub>2</sub> M <sub>23</sub> M <sub>23</sub> respectively.							
<b>CALCIUM</b>							
		2p <sub>3</sub>	L <sub>3</sub> M <sub>2</sub> M <sub>3</sub> ,L <sub>2</sub> M <sub>2</sub> M <sub>3</sub>	α			
Ca		345.9	298.2	644.1		VaVe 80	
CaS		346.45				KMUK 77	
CaO	4	347.3	292.5	639.8		VaVe 80	
CaCl <sub>2</sub>	3	348.3	291.9	640.2		Wagn 77	
CaF <sub>2</sub>	3 1	347.9	288.9	636.8		Wagn 77	
CaCO <sub>3</sub>	4	347.0	291.8	638.5		WRDM 79	
CaSO <sub>4</sub>		348.0				CLSW 83	
CaHPO <sub>4</sub>		347.6				LaMa 84	
<b>SCANDIUM</b>							
Sc		398.3				MFA 85	
ScP		399.4				MFA 85	
ScN		400.7				STAB 76	
ScS		402.9				FUMT 76	
Sc <sub>2</sub> O <sub>3</sub>	4	401.9	334.9	736.8		WRDM 79	
ScF <sub>3</sub>		405.0	329.8	734.8		AWH 81	
<b>TITANIUM</b>							
		2p <sub>3</sub>	L <sub>3</sub> M <sub>23</sub> V	α			
Ti	6	453.89				LANM 81	
TiP		454.8				MFA 85	
TiN		455.8				STAB 76	
TiC		454.6	418.2	872.8		WGR 79	
TiO <sub>2</sub>	10 2	458.7				WRDM 79	
TiCl <sub>4</sub>		458.5				MRV 83	
BaTiO <sub>3</sub>	2	458.55				MWI 75	
Na <sub>2</sub> TiF <sub>6</sub>		462.6	409.8	872.4		WGR 79	
K <sub>2</sub> TiF <sub>6</sub>		462.1	409.4	871.5		WGR 79	

# THE NIST X-RAY PHOTOELECTRON SPECTROSCOPY (XPS) DATABASE

TABLE 5. A subset of values for photoelectron binding energies and Auger kinetic energies for all the elements — Continued

		Values in Chemical State				
		Values in Error ( 0.5 eV)				
		2p <sub>3</sub>	L <sub>3</sub> M <sub>23</sub> V	α		Ref. (median)
<b>VANADIUM</b>						
V	10 2	512.15	472.0	984.15	WRDM	79
VN	2	514.3			STAB	76
VS		513.9			FUMT	76
V <sub>2</sub> O <sub>3</sub>	4 2	515.8			HSGH	81
V <sub>2</sub> O <sub>5</sub>	16 6	517.65			WRDM	79
Na <sub>3</sub> VO <sub>4</sub>		517.3			NFS	82
V(C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub>	2	512.9			GSMJ	74
V(acac) <sub>3</sub>		514.2			LFS	73
<b>CHROMIUM</b>						
Cr	10 1	574.3	527.2	1101.5	WRDM	79
ZrCr <sub>2</sub>		573.9			RKOS	84
Cr <sub>2</sub> O <sub>3</sub>	16 3	576.6			BDFP	81
CrO <sub>3</sub>	4 2	580.1			Shut	80
Na <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub>	4	579.8			NSSP	80
Cr(C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub>	3	574.8			GSMJ	74
CrCl <sub>3</sub>	2	577.8			AITu	76
CrF <sub>3</sub>	3 1	579.4			MMP	82
<b>MANGANESE</b>						
Mn		638.78			LANM	81
MnP		639.0			MFA	85
MnN		641.3			CSC	72
Mn <sub>2</sub> O <sub>3</sub>	9 1	641.6			StHe	84
Mn <sub>3</sub> O <sub>4</sub>	6	641.4			INZI	82
MnO <sub>2</sub>	7 2	642.6			INZI	82
MnBr <sub>2</sub>	2	642.1			Aoki	76
MnCl <sub>2</sub>	2	642.0			Aoki	76
KMnO <sub>4</sub>		647.0			UmRe	78
		2p <sub>3</sub>	L <sub>3</sub> VV	α		
<b>IRON</b>						
Fe	19 3	706.95	702.4	1409.35	WRDM	79
FeP	2	707.1			MFA	85
FeB	2	707.4			JJH	80
Fe <sub>3</sub> Si		707.5			ShTr	75
Fe <sub>3</sub> C		708.1			ShTr	75
FeS <sub>2</sub>	5 1	706.7			VHVH	80
FeO	6 2	709.6			NDKS	83
Fe <sub>2</sub> O <sub>3</sub>	14 3	710.9			WRDM	79
FeF <sub>2</sub>	2	711.4			KaUr	79
Fe(C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub>	4	707.8			Nefe	78
<b>COBALT</b>						
Co	6	778.2	773.0	1551.2	HaWi	77
CoS <sub>2</sub>	2	778.1			VHVH	80
CoO	13 1	780.4			NFS	82
CoOOH	2	780.3			SDM	83
Co(OH) <sub>2</sub>	2	781.3			SDM	83
CoAl <sub>2</sub> O <sub>4</sub>	3	780.8			OkHi	76
CoMoO <sub>4</sub>	2	781.3			KGBP	83
K <sub>3</sub> Co(CN) <sub>6</sub>	3 1	781.9	766.8	1548.7	WGR	79
Co(NH <sub>3</sub> ) <sub>6</sub> Cl <sub>3</sub>	4 1	781.7	768.6	1550.3	WGR	79

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TABLE 5. A subset of values for photoelectron binding energies and Auger kinetic energies for all the elements — Continued

		Values in Chemical State				
		Values in Error ( 0.5 eV)				
		2p <sub>3</sub>	L <sub>3</sub> VV	α	Ref. (median)	
<b>NICKEL</b>						
Ni	18 1	852.7	846.2	1698.9	PEJ	82
Al3Ni		853.75			HFBZ	82
AuNi		852.15			HFBZ	82
NiB		853.2			SMS	80
Ni2Si	3	853.0			GGM	82
NiS	2	852.8			ShRe	79
NiO	18 7	854.4			GGM	82
Ni2O3	2	856.0			SMSB	81
Ni(OH)2	9 2	855.9			SMSB	81
Ni(CO)4	2	854.4			KMI	81
NiCl2	4	856.7			KIHe	83
NiAl2O4	6 2	856.2			SMSB	81
NiSO4	4	856.8			ShRe	79
Ni(dimethylglyoxime)2	4	854.8	842.4	1697.2	WGR	79
NiF2	3 1	857.4	842.4	1699.8	WGR	79
		2p <sub>3</sub>	L <sub>3</sub> M <sub>45</sub> M <sub>45</sub>	α		
<b>COPPER</b>						
Cu	26 3	932.67	918.65	1851.32	AnSe	84
Al2Cu		933.9	918.0	1851.9	FKWF	77
CuP2		932.4			NSDU	75
Cu2S	7 1	932.4			NSSP	80
CuS	6 1	932.3			Brio	80
CuFeS2	2	932.0			Brio	80
CuAl2O4	2	934.7			SLFH	85
Cu2O	14	932.4	916.8	1849.4	THC	83
CuO	16 1	933.8	917.9	1851.7	WRDM	79
CuCl	5	932.4	915.6	1848.0	GaWi	77
CuCl2	7 3	934.4	915.5	1849.9	GaWi	77
CuF2	5 2	936.1	916.0	1852.1	GaWi	77
<b>ZINC</b>						
Zn	13 2	1021.70	992.10	2013.80	Evan	85
ZnP2		1020.9			NSDU	75
ZnTe		1021.6	991.3	2012.9	HFV	77
ZnSe		1022.0	989.5	2011.5	HFV	77
ZnS	3	1021.6	989.7	2011.3	GaWi	77
ZnO	11 2	1022.1	987.7	2009.8	GaWi	77
ZnI2	2	1022.5	988.7	2011.2	GaWi	77
ZnBr2	2	1023.4	987.3	2010.7	Wagn	75
ZnSO4	2	1023.0	986.2	2009.2	StHe8	4a
ZnF2	2	1021.8	986.2	2008.0	GaWi	77
		3d	L <sub>3</sub> M <sub>45</sub> M <sub>45</sub>	α		
<b>GALLIUM</b>						
Ga	7	18.7	1068.1	1086.8	WRDM	79
GaAs	14 1	19.3	1066.3	1085.6	MINN	78
GaP	7	19.3	1065.6	1084.9	NIMN	78
GaN		19.54	1064.5	1084.05	HeMa	80
AlGaAs		19.0			TAYL	82
Ga2Se3	2	19.7	1065.6	1085.3	ITI	82
Ga2O3	6	20.5	1062.4	1082.9	ITI	82
<b>GERMANIUM</b>						
Ge	9	29.15	1145.2	1174.35	WRDM	79
GeAs2		29.7			HKMP	74
GeTe	2	30.0	1144.8	1174.8	SFS	77
GeSe3		31.2	1141.7	1172.9	Ueno	83
GeSe	2	31.7	1142.9	1173.6	Ueno	83
GeS		30.5	1143.7	1174.2	SFS	77
GeO2		32.7	1137.7	1170.4	Wagn	82
Ph4Ge		31.2			HWVV	74
Na2GeF6		33.3	1135.7	1169.0	Wagn	82

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TABLE 5. A subset of values for photoelectron binding energies and Auger kinetic energies for all the elements – Continued

		Values in Chemical State				
		Values in Error ( 0.5 eV)				
		3d	L <sub>3</sub> M <sub>45</sub> M <sub>45</sub>	α		Ref. (median)
<b>ARSENIC</b>						
As	12	41.5	1225.0	1266.5		BWWI 76
NbAs		40.8	1226.0	1266.8		BWWI 76
AlAs	2	41.0				Tayl 82
AlGaAs		41.0				Tayl 82
GaAs	16	41.2	1225.0	1266.2		Tayl 82
As <sub>2</sub> Sc <sub>3</sub>	6 1	43.0	1223.3	1266.3		BWWI 76
As <sub>2</sub> S <sub>3</sub>		43.4	1222.0	1265.5		BWWI 76
As <sub>2</sub> O <sub>3</sub>	9 3	44.9	1218.7	1263.6		Tayl 82
As <sub>2</sub> O <sub>5</sub>	4	46.1	1217.4	1263.6		BWWI 76
NaAsO <sub>2</sub>	2	44.3	1219.6	1263.9		Tayl 82
AsI <sub>3</sub>		43.5	1222.9	1266.4		BWWI 76
AsBr <sub>3</sub>		45.3	1218.1	1263.4		BWWI 76
Ph <sub>3</sub> AsS	2	44.1	1220.0	1264.1		BWWI 76
Ph <sub>3</sub> As	4	42.76				HVV 79
KAsF <sub>6</sub>		47.8	1213.8	1261.6		WGR 79
<b>SELENIUM</b>						
Se	18 4	55.2				CIKT 85
As <sub>2</sub> Se <sub>3</sub>	6	54.9				UeOd 82
GeSe <sub>2</sub>	3	54.5				UeOd 82
Ga <sub>2</sub> Se <sub>3</sub>	3	54.6				ITI 82
CuInSe <sub>2</sub>	2	53.8				CIKT 85
PbSe	2	53.4				SFS 77
H <sub>2</sub> SeO <sub>3</sub>		59.0	1301.0	1360.0		BWI 81
H <sub>2</sub> SeO <sub>4</sub>		61.0	1298.1	1359.1		BWI 81
SeO <sub>2</sub>	4	58.8	1301.6	1360.4		BWI 81
Ph <sub>2</sub> Se		55.8	1304.0	1359.8		BWI 81
Ph <sub>2</sub> Se <sub>2</sub>		55.8	1304.3	1360.1		BWI 81
Ph <sub>2</sub> SeO		57.6	1301.9	1359.5		BWI 81
<b>BROMINE</b>						
CsBr	4 1	68.3				NSBM 80
RbBr		68.4				MVS 73
KBr	3	68.7				WaTa 80
NaBr	2	68.8				ShIg 78
LiBr		68.9	1389.1	1458.1		Wagn 78
KBrO <sub>3</sub>		74.8	1384.4	1459.2		Wagn 78
PbBr <sub>2</sub>	2	68.7				Nefe 82
K <sub>2</sub> PtBr <sub>4</sub>	3	69.3				NSBM 80
K <sub>2</sub> PtBr <sub>6</sub>	2	69.2				NSBM 80
Ni(NH <sub>3</sub> ) <sub>6</sub> Br <sub>2</sub>		68.7				NZB 78
<b>KRYPTON</b>						
		<b>3p<sub>3</sub></b>				
Kr in Ag		207.6				CiHa 74
Kr in Cu		207.3				CiHa 74
<b>RUBIDIUM</b>						
		<b>3d<sub>5</sub></b>				
Rb		112.0				EbSi 79
RbCl		110.1				NSMN 74
<b>STRONTIUM</b>						
Sr		134.4				VaVe 80
SrO		135.3				VaVe 80
SrMoO <sub>4</sub>		133.5				NFS 82
SrRh <sub>2</sub> O <sub>4</sub>		133.0				NFS 82
SrF <sub>2</sub>		133.75				WRDM 79

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TABLE 5. A subset of values for photoelectron binding energies and Auger kinetic energies for all the elements – Continued

		Values in Chemical State				
		Values in Error ( 0.5 eV)				
		3d	L <sub>3</sub> M <sub>45</sub> M <sub>45</sub>	α	Ref.	
					(median)	
<b>YTTRIUM</b>						
Y		155.8			NyMa	80
YH <sub>3</sub>		157.7			FuSc	84
Y <sub>2</sub> O <sub>3</sub>	4 1	157.0			UIY	84
Y <sub>2</sub> (C <sub>2</sub> O <sub>4</sub> ) <sub>3</sub>		159.7			UIY	84
Y <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>		160.0			UIY	84
<b>ZIRCONIUM</b>						
Zr	5	178.79			NyMa	80
ZrCr <sub>2</sub>		178.4			RKOS	84
ZrCr <sub>2</sub> H <sub>4</sub>		179.5			RKOS	84
ZrH <sub>2</sub>		178.8			CoMa	75
ZrO <sub>2</sub>	4 1	182.2			NGDS	75
ZrF <sub>4</sub>		185.3			NKBP	73
K <sub>2</sub> ZrF <sub>6</sub>		184.2			NKBP	73
<b>NIOBIUM</b>						
Nb	10 2	202.26			NyMa	80
NbN		203.8			Bahl	75
NbSe <sub>4</sub>		203.4			Bahl	75
NbO	4 2	203.7			Bahl	75
NbO <sub>2</sub>	5 2	205.7			Bahl	75
Nb <sub>2</sub> O <sub>5</sub>	12 4	207.6			NFS	82
NbI <sub>5</sub>		207.1			GSS	84
NbBr <sub>5</sub>		207.1			MSC	73
NbCl <sub>5</sub>		208.0			MSC	73
KNbO <sub>3</sub>		206.5			MSC	73
K <sub>2</sub> NbF <sub>7</sub>		209.4			MSC	73
<b>MOLYBDENUM</b>						
		3d <sub>5</sub>	M <sub>5</sub> VV	α		
Mo	14 3	227.9	222.8	450.7	WaTa	80
MoB <sub>2</sub>		227.9			MECC	73
Mo <sub>2</sub> C		227.8			BrWh	78
MoS <sub>2</sub>	8 2	229.0			ZMTB	80
MoO <sub>2</sub>	12 4	229.6			FIMa	82
MoO <sub>3</sub>	17 2	232.8			FIMa	82
Al <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub>	3	232.7			ZMTB	80
CoMoO <sub>4</sub>	5 3	233.1			PCLH	76
InMo <sub>6</sub> S <sub>8</sub>		227.9			MAS	85
Na <sub>2</sub> MoO <sub>4</sub>	4	232.0			NFS	82
MoCl <sub>5</sub>	2	231.0			GrMa	75
<b>RUTHENIUM</b>						
Ru	8 1	280.02			NyMa	80
RuO <sub>2</sub>	5 2	280.9			McGi	82
RuO <sub>3</sub>		282.5			KiWi	74
RuO <sub>4</sub>		283.3			KiWi	74
RuCl <sub>3</sub>		281.8			Folk	73
BaRuO <sub>4</sub>		284.2			OGB	80

# THE NIST X-RAY PHOTOELECTRON SPECTROSCOPY (XPS) DATABASE

TABLE 5. A subset of values for photoelectron binding energies and Auger kinetic energies for all the elements – Continued

		Values in Chemical State Values in Error ( 0.5 eV)				
		3d <sub>5</sub>	M <sub>5</sub> VV	α		Ref. (median)
<b>RHODIUM</b>						
Rh	8 2	307.2	301.3	608.5		WRDM 79
Rh <sub>2</sub> S <sub>3</sub>		308.8				GiDi 84
Rh <sub>2</sub> O <sub>3</sub>	3	308.7				NFS 82
RhCl <sub>3</sub>	2	310.2				AnSc 81
RhI <sub>3</sub>	2	308.6				Nefe 78
Na <sub>3</sub> RhCl <sub>6</sub>		310.0	297.7	607.7		WGR 79
KRhO <sub>2</sub>		308.5				NFS 82
Rh <sub>2</sub> MoO <sub>6</sub>		309.2				NFS 82
RhCl <sub>3</sub> ·3H <sub>2</sub> O	6	310.0				FMPS 85
Rh <sub>6</sub> (CO) <sub>16</sub>		308.8				AWH 81
K <sub>3</sub> Rh(NO <sub>2</sub> ) <sub>6</sub>		310.5				SNMK 78
K <sub>3</sub> Rh(NO <sub>3</sub> ) <sub>6</sub>	3	311.1				SNMK 78
ClRh(PPh <sub>3</sub> ) <sub>3</sub>	4 1	307.6				OIIT 79
K <sub>3</sub> RhCl <sub>6</sub>	3	309.8				SNMK 78
K <sub>3</sub> RhF <sub>6</sub>		312.2				SNMK 78
<b>PALLADIUM</b>						
		3d <sub>5</sub>	M <sub>4</sub> M <sub>45</sub> M <sub>45</sub>	α		
Pd	21 3	335.1	327.8	662.9		WRDM 79
Al <sub>3</sub> Pd		337.7				HFBZ 82
LaPd		336.4				HFBZ 82
Pd <sub>2</sub> Si		336.8				GGM 82
PdO		336.3				KGW 74
PdO <sub>2</sub>		337.9				KGW 74
PdCl <sub>2</sub>	4	337.8				CKJT 85
K <sub>2</sub> Pd(NO <sub>2</sub> ) <sub>4</sub>	2	338.8				NZMP 73
K <sub>2</sub> PdBr <sub>4</sub>	2	337.7				NZMP 73
K <sub>2</sub> PdCl <sub>4</sub>	3	337.9	323.1	661.0		WGR 79
K <sub>2</sub> PdCl <sub>6</sub>	3	340.3				Nefe 78
Pd(NH <sub>3</sub> ) <sub>4</sub> Cl <sub>2</sub>		338.4	323.8	662.2		WGR 79
Pd(PPh <sub>3</sub> ) <sub>4</sub>		335.1	324.4	659.5		WGR 79
<b>SILVER</b>						
		3d <sub>5</sub>	M <sub>4</sub> M <sub>45</sub> M <sub>45</sub>	α		
Ag	16	368.28	357.84	726.12		AnSe 84
AlAg <sub>2</sub>		368.7	357.7	726.4		FKWF 77
CuAgSe		367.8	357.3*	725.1		RRD 78
Ag <sub>2</sub> Se		367.8	357.4*	725.2		RRD 78
Ag <sub>2</sub> S		367.1	357.2*	725.3		RRD 78
Ag <sub>2</sub> O	4 1	367.8	356.7*	724.5		GaWi 77
AgO	4 1	367.4	356.6*	724.0		GaWi 77
AgI		368.0	356.1*	724.1		GaWi 77
AgF		367.7	355.3*	723.0		GaWi 77
AgF <sub>2</sub>		367.3	355.6*	722.9		GaWi 77
*6.0 eV added to value for M <sub>5</sub> N <sub>45</sub> N <sub>45</sub> to give value for M <sub>4</sub> N <sub>45</sub> N <sub>45</sub> .						
<b>CADMIUM</b>						
		3d <sub>5</sub>	M <sub>4</sub> N <sub>45</sub> N <sub>45</sub>	α		
Cd	8 2	405.0	384.0*	789.0		GaWi 77
CdTe	9	405.2	382.4	787.6		Pola 82
CdSe	2	405.0	381.7	786.7		Pola 82
CdS	7	405.3	381.3*	786.6		GaWi 77
CdO	7	404.2	382.4*	786.6		GaWi 77
Cd(OH) <sub>2</sub>	2	405.1	380.0	785.1		WGR 79
CdSO <sub>4</sub>		405.4				RVJK 85
CdCO <sub>3</sub>		405.1				HGW 75
CdI <sub>2</sub>	3	405.4	381.2*	786.6		GaWi 77
CdCl <sub>2</sub>		406.1				SATD 73
CdF <sub>2</sub>	5	405.9	379.0*	784.9		GaWi 77
*6.8 eV added to value for M <sub>5</sub> N <sub>45</sub> N <sub>45</sub> to give value for M <sub>4</sub> N <sub>45</sub> N <sub>45</sub> .						

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TABLE 5. A subset of values for photoelectron binding energies and Auger kinetic energies for all the elements – Continued

		Values in Chemical State					
		Values in Error ( 0.5 eV)					
		3d <sub>5</sub>	M <sub>4</sub> N <sub>45</sub> N <sub>45</sub>	α	4d <sub>5</sub>	Ref.	
						(median)	
<b>INDIUM</b>							
In	17 4	443.84	410.41	854.25	16.76	PVVA	79
InSb	2	444.3				VaGr	81
InP	6 1	444.6	408.0	852.6		Bert	81
In <sub>2</sub> Se <sub>3</sub>	3 1	444.5	408.0	852.5		CIKT	85
CuInSe <sub>2</sub>	2	444.1	408.6	852.7		CIKT	85
In <sub>2</sub> S <sub>3</sub>	2	444.7	407.3	852.0		WGR	79
InMo <sub>6</sub> S <sub>8</sub>		444.4				MAS	85
In <sub>2</sub> O <sub>3</sub>	10 4	444.4	406.4	850.8		Bert	81
InI <sub>3</sub>	3 1	445.8	405.8	851.6		Wagn	77
InBr <sub>3</sub>	3 1	446.0	404.8	850.8		Wagn	77
InCl <sub>3</sub>	3 1	445.9				FHT	77
InF <sub>3</sub>	2	446.2	403.7	849.9		Wagn	75
(NH <sub>4</sub> ) <sub>3</sub> InF <sub>6</sub>		445.6	404.1	849.7		Wagn	77
*7.6 eV added to value for M <sub>5</sub> N <sub>45</sub> N <sub>45</sub> to give value for M <sub>4</sub> N <sub>45</sub> N <sub>45</sub> .							
		3d <sub>5</sub>	M <sub>4</sub> N <sub>45</sub> N <sub>45</sub>	α			
<b>TIN</b>							
Sn	17	484.87	437.27	922.7		PVVA	79
SnTe		485.6				SFS	77
SnSe		485.7				SFS	77
SnS	3 1	485.6	435.7	921.3		Wagn	75
SnO	6 2	486.9				WVV	79
SnO <sub>2</sub>	11	486.6	432.6	919.2		LAK	77
Me <sub>3</sub> SnF		486.7				WVV	79
Ph <sub>4</sub> Sn	4	486.3				MoVa	73
SnBr <sub>2</sub>		486.9				GZF	73
SnCl <sub>2</sub>	2	486.7				WVV	79
SnF <sub>2</sub>	3	487.4				Shut	80
SnF <sub>4</sub>	2	488.2				Shut	80
NaSnF <sub>3</sub>		487.4	430.8	918.2		Wagn	75
<b>ANTIMONY</b>							
Sb	8 1	528.2	464.5	992.7		VaTr	79
Na <sub>3</sub> Sb				990.6		BaGa	80
AlSb		528.6				MSV	73
InSb		528.0				VaGr	81
Sb <sub>2</sub> S <sub>3</sub>	4 1	529.5	462.1	991.6		Wagn	75
Sb <sub>2</sub> S <sub>5</sub>	2	529.3	462.2	991.5		Wagn	75
Sb <sub>2</sub> O <sub>3</sub>	2	530.0	459.7	989.7		Wagn	75
SbI <sub>3</sub>		530.4				MSV	73
SbCl <sub>5</sub>		530.9				MSV	73
Ph <sub>3</sub> Sb		528.9				BCH	75
Ph <sub>3</sub> SbS		528.7				BCH	75
SbF <sub>3</sub>		531.7				MSV	73
KSbF <sub>6</sub>		532.9	454.4	987.3		WGR	75



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TABLE 5. A subset of values for photoelectron binding energies and Auger kinetic energies for all the elements – Continued

		Values in Chemical State				Ref. (median)
		Values in Error ( 0.5 eV)				
		3d <sub>5</sub>	M <sub>4</sub> N <sub>45</sub> N <sub>45</sub>	α	4d <sub>5</sub>	
<b>TELLURIUM</b>						
Te	17 4	572.85	492.13	1064.98	40.26	PVVA 79
SnTe		572.3				SFS 77
PbTe		572.0				SFS 77
CdTe	8	572.7	490.8	1063.5		Pola 82
Ga <sub>2</sub> Te <sub>3</sub>		572.4	40.3			TIWB 72
GeTe		572.7	40.2			SFS 77
GeTe <sub>3</sub> As		572.5				HKMP 74
TeO <sub>2</sub>	6	576.1	487.1	1063.2	43.4	BWI 77
TeO <sub>3</sub>	2 1	577.3	485.5	1062.8	44.6	BWI 77
Te(OH) <sub>6</sub>		577.1	485.1	1062.2	45.0	BWI 77
Na <sub>2</sub> TeO <sub>4</sub>		576.8	485.5	1062.3		Wagn 75
TeI <sub>4</sub>		575.8	43.8			BWI 77
TeBr <sub>4</sub>		576.7	487.3	1064.0	44.0	BWI 77
TeCl <sub>4</sub>		576.9	486.1	1063.0	44.3	BWI 77
(NH <sub>4</sub> ) <sub>2</sub> TeCl <sub>6</sub>		576.9	486.4	1063.3	45.3	BWI 77
Ph <sub>2</sub> Te <sub>2</sub>		573.9	488.5	1062.4	42.8	BWI 77
Ph <sub>2</sub> TeCl <sub>2</sub>		576.2	486.3	1062.5	43.8	BWI 77
		3d <sub>5</sub>	M <sub>4</sub> N <sub>45</sub> N <sub>45</sub>	α		
<b>IODINE</b>						
I <sub>2</sub>	2	619.9	519.0	1138.9		DMKK 84
UI <sub>3</sub>		620.3	517.3	1137.6		DMKK 84
LiI	2 1	619.7	517.0	1136.7		WRDM 79
NaI	2	618.4				Sher 76
NiI <sub>2</sub>		619.0	518.8*	1137.8		GaWi 77
AgI		619.4	518.3*	1137.7		GaWi 77
NbI <sub>4</sub>			620.0			GSS 84
HIO <sub>3</sub>		623.1				Sher 76
NaIO <sub>3</sub>		623.5				Sher 76
NaIO <sub>4</sub>		624.0				Sher 76
ICl		621.5				Sher 76
ICl <sub>3</sub>		622.5				Sher 76
I <sub>2</sub> O <sub>5</sub>		623.3				Sher 76
*11.5 eV added to value for M <sub>5</sub> N <sub>45</sub> N <sub>45</sub> to provide value for M <sub>4</sub> N <sub>45</sub> N <sub>45</sub> .						
<b>XENON</b>						
Xe (implanted in graphite)		669.65	545.2	1214.85		WRDM 79
Xe (implanted in Ag)		669.6				CiHa 74
Na <sub>4</sub> XeO <sub>6</sub>		674.1	541.4	1215.5		Wagn 77
		3d <sub>5</sub>	M <sub>4</sub> N <sub>45</sub> N <sub>45</sub>	α	4d <sub>5</sub>	
<b>CESIUM</b>						
Cs	2	726.3			77.5	EbSi 79
CsN <sub>3</sub>		723.6				SGRS 72
Cs <sub>2</sub> O	2 1				77.6	EbSi 79
CsOH		724.15	568.7	1292.85		WRDM 79
Cs <sub>2</sub> SO <sub>4</sub>		723.9	568.4	1292.3		Wagn 77
Cs <sub>3</sub> PO <sub>4</sub>		723.9				MVS 73
CsI		723.9				MVS 73
CsCl	2	724.0				NSMN 74
CsClO <sub>4</sub>		724.2				MVS 73
CsF		724.0				MVS 73

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TABLE 5. A subset of values for photoelectron binding energies and Auger kinetic energies for all the elements – Continued

		Values in Chemical State					
		Values in Error ( 0.5 eV)					
		3d <sub>5</sub>	M <sub>4</sub> N <sub>45</sub> N <sub>45</sub>	α	4d <sub>5</sub>	Ref.	
						(median)	
<b>BARIUM</b>							
Ba	4 1	780.6	601.0	1381.6	90.2	KoGr	85
BaH <sub>2</sub>		782.0				FMUK	77
BaS		779.8				SiWo	80
BaO	4 1	779.9	598.0	1377.9	89.8	KoGr	85
BaCO <sub>3</sub>		779.9				CLSW	83
Ba(NO <sub>3</sub> ) <sub>2</sub>		780.7				CLSW	83
BaSO <sub>4</sub>	4 1	780.8	596.1	1376.9		Wagn	77
BaCrO <sub>4</sub>		778.9				ACHT	73
BaF <sub>2</sub>		781.7	594.9	1376.6		SeSo	84
		<b>3d<sub>5</sub></b>			<b>4d<sub>5</sub></b>		
<b>LANTHANUM</b>							
La	2	835.9				SOS	82
LaH <sub>2</sub>		837.2				SOS	82
LaH <sub>3</sub>	2	838.8				SOS	82
La <sub>2</sub> O <sub>3</sub>	4 2	834.8			102.1	UIY	84
La <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>		837.4			104.4	UIY	84
La <sub>2</sub> (C <sub>2</sub> O <sub>4</sub> ) <sub>3</sub>		837.2			104.6	UIY	84
LaCrO <sub>3</sub>		833.0			101.7	HoTh	80
<b>CERIUM</b>							
Ce	3 1	883.9				SOS	82
CeAl <sub>2</sub>		883.5			109.1	LFBC	80
CePd <sub>3</sub>		884.3				LFBC	80
CeH <sub>2</sub>		885.8				SOS	82
CeH <sub>3</sub>	2	886.0				SOS	82
CeSe		884.3				LFBC	80
CeO <sub>2</sub>	4 1	881.93				BFCB	83
<b>PRASEODYMIUM</b>							
Pr		932.0				FuOs	84
PrH <sub>2</sub>		933.2				FuOs	84
PrH <sub>3</sub>		934.2				FuOs	84
Pr <sub>2</sub> O <sub>3</sub>	2	933.6			116.1	SaRa	80
PrO <sub>2</sub>		935.3			116.2	SaRa	80
Pr <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>		936.1			116.8	UIY	84
Pr <sub>2</sub> (C <sub>2</sub> O <sub>4</sub> ) <sub>3</sub>		935.8			116.8	UIY	84
<b>NEODYMIUM</b>							
Nd <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>		984.9			122.5	UIY	84
Nd <sub>2</sub> (C <sub>2</sub> O <sub>4</sub> ) <sub>3</sub>		984.7			122.1	UIY	84
<b>PROMETHIUM</b>							
PmCl <sub>3</sub>		1033.5			128.3	MNTB	70
<b>SAMARIUM</b>							
Sm		1081.2				DKMB	76
Sm <sub>2</sub> O <sub>3</sub>		1084.3			131.0	UIY	84
Sm <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>		1085.6			132.9	UIY	84
Sm <sub>2</sub> (C <sub>2</sub> O <sub>4</sub> ) <sub>3</sub>		1085.5			132.8	UIY	84
<b>EUROPIUM</b>							
Eu					128.4	NNBF	68
Eu <sub>2</sub> O <sub>3</sub>		1135.6			135.6	UIY	84
Eu <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>		1137.9			137.5	UIY	84
Eu <sub>2</sub> (C <sub>2</sub> O <sub>4</sub> ) <sub>3</sub>		1136.4			135.1	UIY	84
<b>GADOLINIUM</b>							
Gd					141.7	TeLe	79
Gd <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>		1190.0			143.8	UIY	84
Gd <sub>2</sub> (C <sub>2</sub> O <sub>4</sub> ) <sub>3</sub>		1189.8			144.4	UIY	84

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TABLE 5. A subset of values for photoelectron binding energies and Auger kinetic energies for all the elements — Continued

		Values in Chemical State				
		Values in Error ( 0.5 eV)				
		3d <sub>s</sub>		4d <sub>s</sub>	Ref.	
					(median)	
<b>TERBIUM</b>						
Tb <sub>2</sub> O <sub>3</sub>		1241.5		148.7	SaRa	80
TbO <sub>2</sub>		1241.4		149.2	SaRa	80
Tb <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>				150.5	UIY	84
Tb <sub>2</sub> (C <sub>2</sub> O <sub>4</sub> ) <sub>3</sub>				150.9	UIY	84
<b>DYSPROSIUM</b>						
Dy <sub>2</sub> O <sub>3</sub>		1298.9			SaRa	80
Dy <sub>2</sub> O <sub>3</sub>				155.8	UIY	84
Dy <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>				156.5	UIY	84
Dy <sub>2</sub> (C <sub>2</sub> O <sub>4</sub> ) <sub>3</sub>				156.0	UIY	84
<b>HOLMIUM</b>						
Ho <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>				162.8	UIY	84
Ho <sub>2</sub> (C <sub>2</sub> O <sub>4</sub> ) <sub>3</sub>				163.3	UIY	84
<b>ERBIUM</b>						
Er <sub>2</sub> O <sub>3</sub>				168.8	UIY	84
Er <sub>2</sub> (C <sub>2</sub> O <sub>4</sub> ) <sub>3</sub>				170.7	UIY	84
<b>THULIUM</b>						
Tm <sub>2</sub> O <sub>3</sub>				176.6	UIY	84
Tm <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>				178.3	UIY	84
Tm <sub>2</sub> (C <sub>2</sub> O <sub>4</sub> ) <sub>3</sub>				178.3	UIY	84
<b>YTTERBIUM</b>						
Yb	4 2			183.0	PLNW	77
Yb <sub>2</sub> O <sub>3</sub>				185.2	UIY	84
Yb <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>				187.3	UIY	84
Yb <sub>2</sub> (C <sub>2</sub> O <sub>4</sub> ) <sub>3</sub>				187.3	UIY	84
<b>LUTETIUM</b>						
Lu	3			196.6	PLNW	77
Lu <sub>2</sub> O <sub>3</sub>	4 1			196.5	UIY	84
Lu <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>				198.5	UIY	84
Lu <sub>2</sub> (C <sub>2</sub> O <sub>4</sub> ) <sub>3</sub>				198.7	UIY	84
<b>HAFNIUM</b>						
		4f		4d <sub>s</sub>		
Hf	2	14.23		211.5	NBM	80
HfO <sub>2</sub>		16.7		213.0	SaRa	80
<b>TANTALUM</b>						
		4f <sub>7</sub>	M <sub>5</sub> N <sub>67</sub> N <sub>67</sub>	α	4d <sub>s</sub>	
Ta	4	21.9	1674.65	1696.6		WaTa 80
TaSi <sub>2</sub>		27.0			231.1	MSC 73
TaS <sub>2</sub>		26.7			230.8	MSC 73
Ta <sub>2</sub> O <sub>5</sub>	4	26.5			230.4	SaRa 80
KTaO <sub>3</sub>		25.9			229.8	MSC 73
TaBr <sub>5</sub>		26.9			231.2	MSC 73
TaCl <sub>5</sub>		27.3			231.0	MSC 73
TaF <sub>5</sub>		27.8			231.6	MSC 73
K <sub>2</sub> TaF <sub>7</sub>		29.4			234.9	NKSP 73

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TABLE 5. A subset of values for photoelectron binding energies and Auger kinetic energies for all the elements – Continued

		Values in Chemical State			Values in Error ( 0.5 eV)			
		4f <sub>7</sub>	M <sub>5</sub> N <sub>67</sub> N <sub>67</sub>	α	4d <sub>5</sub>	Ref.	(median)	
<b>TUNGSTEN</b>								
W	9	31.32			243.5	NBM		80
WC		31.5				CoRa		76
WS <sub>2</sub>		33.2	1727.8	1761.0		Wagn		75
WO <sub>2</sub>	8 3	32.7				CoRa		76
WO <sub>3</sub>	12 2	35.7				CoRa		76
Al <sub>2</sub> (WO <sub>4</sub> ) <sub>3</sub>	4 1	36.3				SMSB		81
Na <sub>2</sub> WO <sub>4</sub>		36.3	1722.0	1758.3		Wagn		75
H <sub>2</sub> WO <sub>4</sub>		36.1	1723.9	1760.0		Wagn		78
Li <sub>2</sub> WO <sub>4</sub>	2	36.0			247.6	MSC		73
CuWO <sub>4</sub>		36.1	1725.3	1761.4		Wagn		78
WBr <sub>5</sub>		36.3			247.6	MSC		73
WBr <sub>6</sub>		35.9			247.7	MSC		73
WCl <sub>4</sub>		34.9				GMW		85
WCl <sub>6</sub>		36.6				GMW		85
<b>RHENIUM</b>								
		4f <sub>7</sub>			4d <sub>5</sub>			
Re	8 1	40.46			260.5	BMNN		79
ReO <sub>2</sub>	3 1	43.2				KOAG		83
Re <sub>2</sub> O <sub>7</sub>		46.7				CDGV		80
K <sub>2</sub> ReO <sub>4</sub>		46.07				TCCW		85
NH <sub>4</sub> ReO <sub>4</sub>		46.2				KOAG		83
K <sub>2</sub> ReBr <sub>6</sub>		43.5				NSSK		80
K <sub>2</sub> ReCl <sub>6</sub>	3	44.0				NSSK		80
<b>OSMIUM</b>								
Os	4	50.7			278.5	BNMN		79
OsO <sub>2</sub>	2 1	52.0			280.1	SaRa		80
K <sub>2</sub> OsO <sub>4</sub>					283.6	SaRa		80
K <sub>2</sub> OsI <sub>6</sub>		51.9				Nefe		78
K <sub>2</sub> OsCl <sub>6</sub>	5 1	53.2				LZML		83
OsCl <sub>3</sub>		53.1				Nefe		78
K <sub>2</sub> OsO <sub>2</sub> (OH) <sub>4</sub>		55.2				Nefe		78
O <sub>6</sub> Os(C <sub>5</sub> H <sub>5</sub> N) <sub>4</sub>		53.8				LZML		83
Os(NH <sub>3</sub> ) <sub>5</sub> N <sub>2</sub> I <sub>2</sub>		50.9				Folk		73
<b>IRIDIUM</b>								
Ir	6	60.75			296.3	NBM		80
IrO <sub>2</sub>	2	62.0				Peuc		84
IrCl <sub>3</sub>		62.7				Folk		73
IrCl <sub>4</sub> (PEt <sub>3</sub> ) <sub>2</sub>		63.6				LeBr		72
IrClN <sub>2</sub> (PPh <sub>3</sub> ) <sub>2</sub>		60.7				Folk		73
K <sub>2</sub> IrBr <sub>6</sub>		62.6				Nefe		78
K <sub>2</sub> IrCl <sub>6</sub>	4 1	63.5				KSPB		76
K <sub>3</sub> IrBr <sub>6</sub>		61.8				Nefe		78
K <sub>3</sub> IrCl <sub>6</sub>		62.5				NBSN		77
K <sub>3</sub> Ir(CN) <sub>6</sub>		61.8				InFl		84

# THE NIST X-RAY PHOTOELECTRON SPECTROSCOPY (XPS) DATABASE

TABLE 5. A subset of values for photoelectron binding energies and Auger kinetic energies for all the elements – Continued

		Values in Chemical State					
		Values in Error ( 0.5 eV)					
		4f <sub>7</sub>			4d <sub>5</sub>	Ref.	
						(median)	
<b>PLATINUM</b>							
Pt	2	71.07			314.6	NBM	80
Pt	13	71.2				Wagn	75
PtSi		73.0				GGM	82
Pt2Si		72.5				GGM	82
PtO	3 1	74.2			317.3	EPCC	75
PtO2	4 2	75.0			318.1	EPCC	75
Pt(OH)2		72.6				HaWi	77
Pt(OH)4		74.6				PCB	84
Pt(OAc)2		73.8				RCMS	80
PtCl2		73.6			316.7	EPCC	75
PtCl4		75.5			318.6	EPCC	75
K2PtI6	2	73.4				NSBM	80
K2PtCl4	6 1	73.0			316.1	Wagn	75
K2PtCl6	6	75.5			318.6	NSBM	80
K2PtF6	2	77.6				NSBM	80
K2Pt(OH)6	2	75.1				NSBM	80
K2Pt(NO2)6	2	75.9				NSBM	80
Pt(NH3)6Cl4	2	76.3				NSBM	80
Pt(PPh3)3	2	71.4				Rigg	72
		4f <sub>7</sub>	M <sub>5</sub> N <sub>67</sub> N <sub>67</sub>	α	M <sub>4</sub> N <sub>67</sub> N <sub>67</sub>	4d <sub>5</sub>	
<b>GOLD</b>							
Au		83.97				VaTr	79
Au		84.1	2015.8	2099.9	69.8*	335.1	PEJ
Au	13	84.0	2015.7	2099.7	2101.6		WaTa
Au2O3		85.9					PLTD
(PPh3)AuCl	5	85.3					MBSG
(PPh3)2AuCl	2	85.2					MBSG
(PPh3)AuCl3	2	87.5					MBSG
(PPh3)AuI	2	85.4					BMCK
(PPh3)8Au9(NO3)3	3	85.0					BMZN
(PPh3)AuNO3	2	85.4					BMCK
(PPh3)4Au(ClO4)		85.0					MBSG
*Line N <sub>7</sub> VV.							
		4f <sub>7</sub>				4d <sub>5</sub>	
<b>MERCURY</b>							
Hg	4	99.9				359.3	SMBM
HgS		100.8					NSSP
HgO	2	100.8					NSSP
Hg3PO4		101.1					NSK
Hg2SO4		101.0					NSK
Hg2(NO3)2		101.2					NSK
Hg2I2		100.9					NSK
HgI2		100.7					SATD
Hg2Cl2		100.8					NSK
HgCl2		101.4					SATD
HgF2		101.2					SATD
Hg2C2O4		101.1					NSK
<b>THALLIUM</b>							
Tl	3	117.73				385.0	MBN
TlS		118.7				385.5	MSC
TlS3		118.7				385.3	MSC
Tl2O3		117.5				384.7	MSC
TlI		118.5				385.4	MSC
TlBr		119.2				386.1	MSC
TlCl		119.0				385.7	MSC
TlF		119.2				386.1	MSC

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TABLE 5. A subset of values for photoelectron binding energies and Auger kinetic energies for all the elements — Continued

		Values in Chemical State					Ref.	
		Values in Error ( 0.5 eV)					(median)	
		4f <sub>7</sub>	M <sub>5</sub> N <sub>67</sub> N <sub>67</sub>	α	M <sub>4</sub> N <sub>67</sub> N <sub>67</sub>	4d <sub>5</sub>		
<b>LEAD</b>								
Pb		136.78				412.0	NBM	80
Pb		137.0	2180.3	2317.3	2282.1		WaTa	80
		4f <sub>7</sub>	N <sub>6</sub> O <sub>45</sub> O <sub>45</sub>			4d <sub>5</sub>		
Pb	12	136.8	96.25	233.05			Pede	82
PbTe	2	137.25	95.45	232.7			Pede	82
PbSe	2	137.6	94.75	232.35			Pede	82
PbS	4	137.5	94.55	232.05			Pede	82
PbO	14	137.25	92.85	230.1			Pede	82
PbO <sub>2</sub>	6 1	137.4	93.05	230.45			Pede	82
Pb(OH) <sub>2</sub>	2	137.95	91.95	229.9			Pede	82
Pb(OAc) <sub>2</sub>	3	138.5	91.45	229.95			Pede	82
Pb(OAc) <sub>4</sub>		137.2					BeFl	80
PbSO <sub>4</sub>	4 2	140.0	90.1	230.1			Pede	82
PbSiO <sub>3</sub>		138.65	91.1	229.75			Pede	82
PbI <sub>2</sub>		138.35	93.35	231.7			Pede	82
PbCl <sub>2</sub>		138.9	92.1	231.0			Pede	82
PbF <sub>2</sub>		138.5	90.6	229.1			Pede	82
Pb(IO <sub>4</sub> ) <sub>2</sub>		138.2	92.7	230.9			Pede	82
Ph <sub>4</sub> Pb		138.2				413.3	MoVa	73
		4f <sub>7</sub>		5d <sub>5</sub>		4d <sub>5</sub>		
<b>BISMUTH</b>								
Bi	7	156.88				440.3	VaTr	79
Bi <sub>2</sub> Se <sub>3</sub>				25.0			TSH	84
Bi <sub>2</sub> S <sub>3</sub>		158.9					MSV	73
BiOCl		159.9					MSV	73
Bi <sub>2</sub> MoO <sub>6</sub>	2 1	159.6					VVS	85
NaBiO <sub>3</sub>		159.1					MSV	73
BiI <sub>3</sub>		159.3					MSV	73
BiF <sub>3</sub>		160.8					MSV	73
Ph <sub>3</sub> Bi				25.37			HVV	79
<b>THORIUM</b>								
Th	4	333.1		85.4		675.2	ScLa	81
ThO <sub>2</sub>		334.6		87.0		675.7	VLDH	77
Th(OAc) <sub>4</sub>				87.3			NMSI	74
Th <sub>3</sub> (PO <sub>4</sub> ) <sub>4</sub>				87.5			NMSI	74
ThCl <sub>4</sub>		335.7					ATT	83
ThCl <sub>4</sub>				86.2			NMSI	74
ThF <sub>4</sub>	2	336.9					ATT	83
ThF <sub>4</sub>				88.1			NMSI	74

## THE NIST X-RAY PHOTOELECTRON SPECTROSCOPY (XPS) DATABASE

TABLE 5. A subset of values for photoelectron binding energies and Auger kinetic energies for all the elements – Continued

		Values in Chemical State				
		Values in Error ( 0.5 eV)				
		4f <sub>7</sub>	5d <sub>5</sub>	4d <sub>5</sub>	Ref.	
					(median)	
<b>URANIUM</b>						
U	11 2	377.4	94.0	736.4	ScLa	81
UTe3		381.3			SNRS	76
USe		380.3			SNRS	76
USe3		379.1			SNRS	76
US		380.1			SNRS	76
US3		379.4			SNRS	76
UO2	10 1	380.2	97.0		FSL	85
U3O8	4	380.7	97.3		FSL	85
UO3	6	381.3	97.6		DBLG	83
UOBr2		380.4			TBVL	82
UOCl		380.0			TBVL	82
UOCl2		380.3			TBVL	82
UO2Br		380.5			TBVL	82
UO2Br2		381.1			TBVL	82
UO2F2	2	383.0			TBVL	82
U(SO4)2		381.6			Chad	73
UO2MoO4		381.0	97.5		FSL	85
UI3		379.0			DMKK	84
UBr4		379.9			TBVL	82
UCl3		378.3			TBVL	82
UCl4	2 1	380.2			TBVL	82
UF4	5	382.2			TBVL	82
UF6		384.9			TrRi	82
K2UF6		382.4			PMDS	77
<b>PLUTONIUM</b>						
Pu2O3	2	424.7			CCHB	81
PuO2	2	426.2			CCHB	81
<b>AMERICIUM</b>						
Am(OH)3		449.1	109.2	831.8	KrWu	72

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### Appendix A. Long References

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Appendix C. Figures

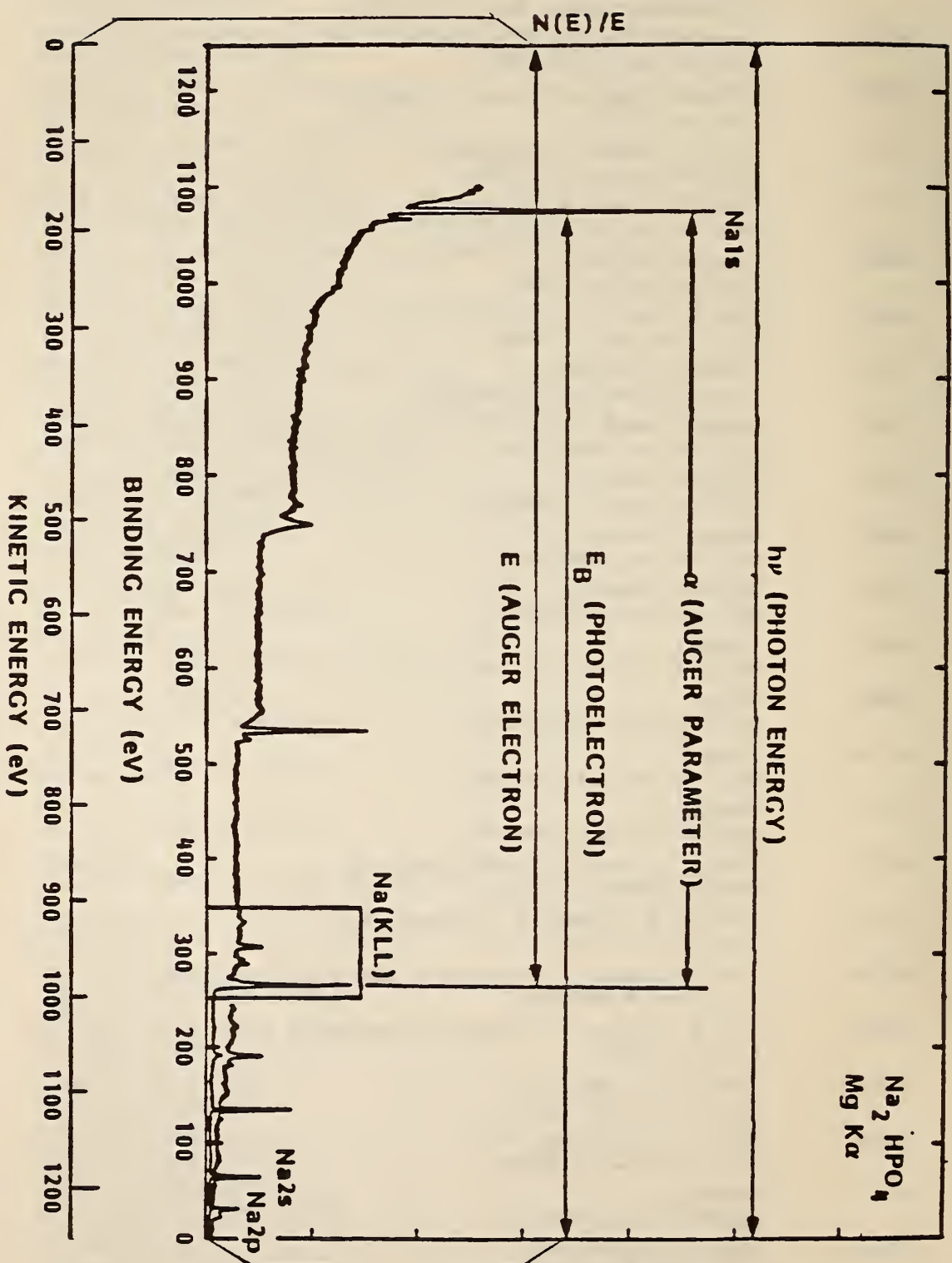


Figure 1. Spectrum of sodium hydrogen phosphate showing photoelectron line, Auger line, and Auger parameter ( $E + E_B \alpha + h\nu$ , modified).

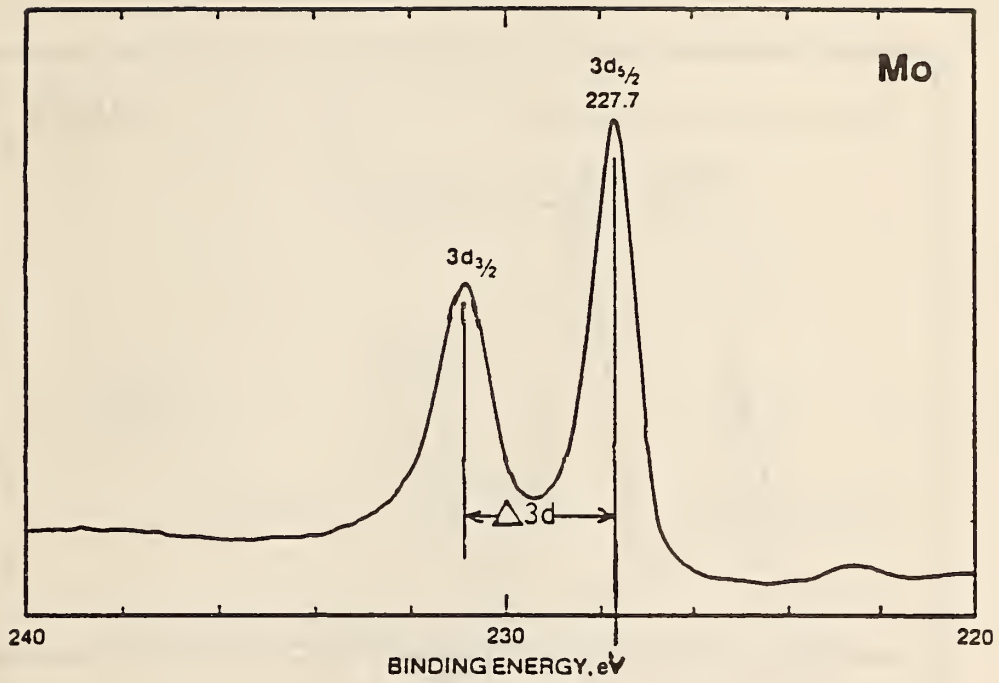


Figure 2. Doublet separation in photoelectron line.

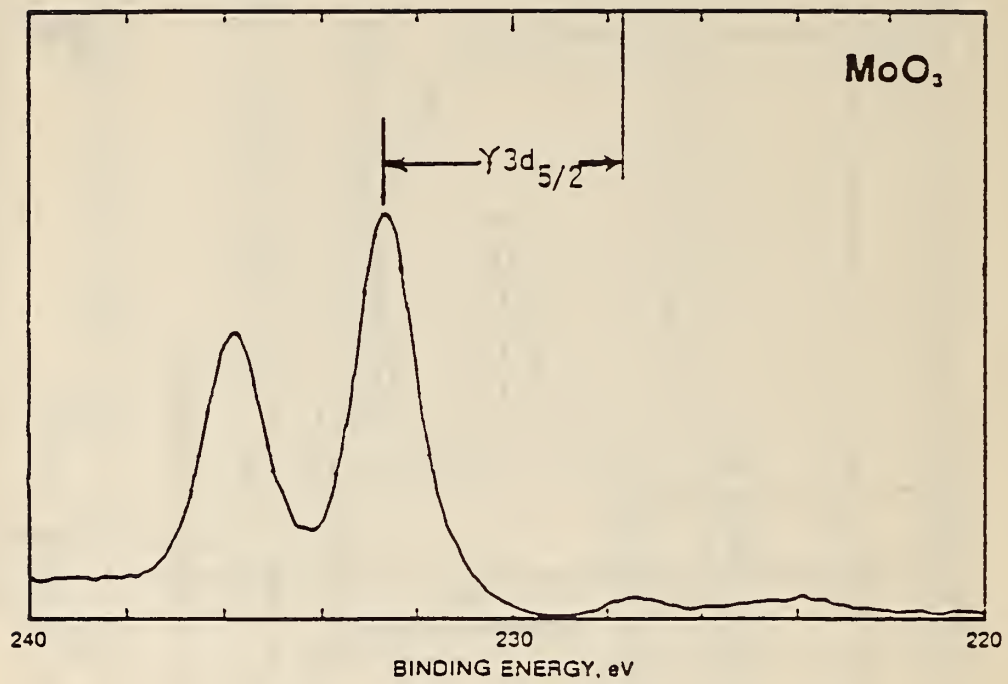


Figure 3. Chemical shift from elemental form.

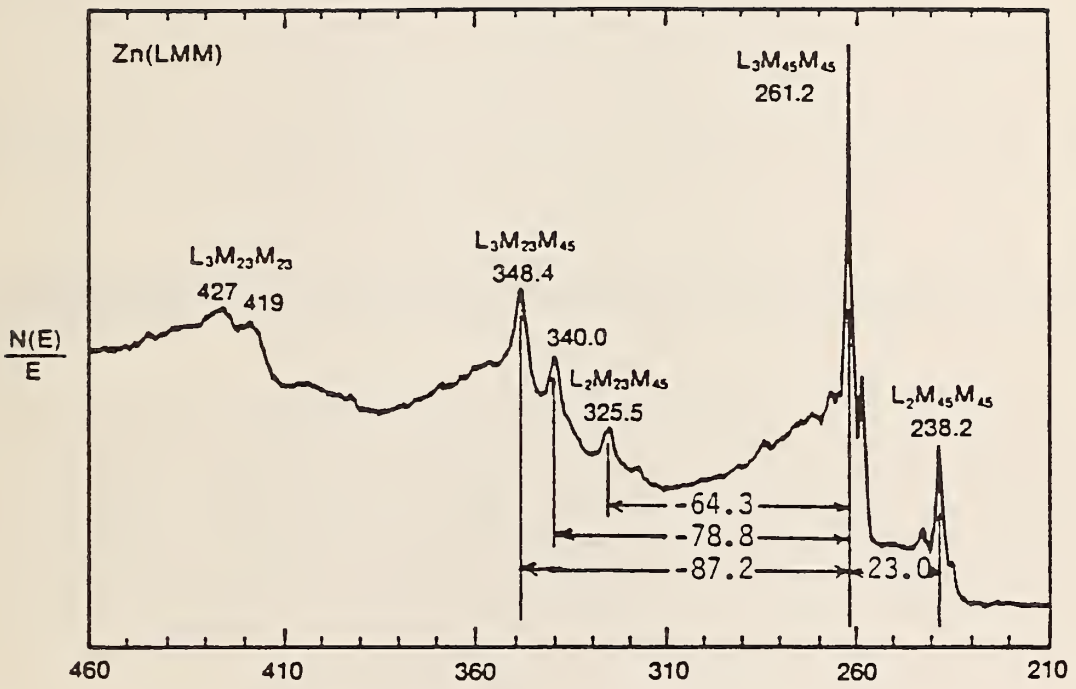


Figure 4. Separation from the sharpest Auger line.





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The technique known as XPS (X-Ray Photoelectron Spectroscopy) involves x-ray irradiation of surface samples under high vacuum. Electrons escaping from the samples are sorted and arranged to form a spectrum. A compilation of data for binding energy and kinetic energy of sample electrons from all elements has been collected. Depending on the nature of the chemical bond, the chemical shift can be as much as 10 eV. Over the past 6 years the author has indexed articles related to this subject area. The data bank contains a total of 13,200 records, from a total of 800 papers.

12. KEY WORDS (6 TO 12 ENTRIES; ALPHABETICAL ORDER; CAPITALIZE ONLY PROPER NAMES; AND SEPARATE KEY WORDS BY SEMICOLONS)

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