Handbook of X-ray Photoelectron Spectroscopy

A Reference Book of Standard Spectra
for Identification and Interpretation of XPS Data

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Preface

X-ray Photoelectron Spectroscopy (XPS), also known as Electron Spectroscopy for Chemical Analysis (ESCA), is widely used to investigate the chemical composition of surfaces. The use of XPS in analytical laboratories throughout the world attests to the problem-solving capability of this technique. The ability to explore the first few atomic layers and assign chemical states to the detected atoms has shown XPS to be a powerful addition to any analytical laboratory.

A great deal of information has been published on the principles of the technique and the diverse range of applications for which it is used. Volumes of XPS spectra exist in the scientific literature, and international committees are establishing databases with reference spectra that will be made available to the general public. It is not the authors' intent to exclude these spectra or to ignore these databases. Rather the intent is to assemble a concise volume of standard spectra to aid in the identification of XPS data.

The previous version of this handbook, published in 1978, contained data acquired with a cylindrical mirror analyzer (CMA). Since that time, our XPS hardware has evolved. We currently use a spherical capacitance analyzer (SCA) in conjunction with improved detector technology and the choice of either a high-performance Al x-ray monochromator or an achromatic Mg/Al dual anode x-ray source. A 1992 version of this handbook was updated from the previous handbook with data acquired using our current SCA, which has a transmission function different from that of a CMA, and both monochromatic and achromatic x-ray sources. In addition, data are included from several elements not contained in the 1978 version of the handbook. The current 1995 version of the handbook is a reprint of the 1992 version which includes a few minor modifications. This handbook is meant to serve as a guide and reference work for the identification, quantification, calibration and interpretation of XPS spectra for users of Physical Electronics XPS systems equipped with SCAs and Omni Focus™ lenses. It is the authors' hope that this handbook will play a useful role in the practice of XPS.

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I. X-ray Photoelectron Spectroscopy

A. Introduction

X-ray Photoelectron Spectroscopy (XPS) was developed in the mid-1960s by Kai Siegbahn and his research group at the University of Uppsala, Sweden. The technique was first known by the acronym ESCA (Electron Spectroscopy for Chemical Analysis). The advent of commercial manufacturing of surface analysis equipment in the early 1970s enabled the placement of equipment in laboratories throughout the world. In 1981, Siegbahn was awarded the Nobel Prize for Physics for his work with XPS.

This handbook is meant to furnish the user with much of the information necessary to use XPS for diverse types of surface analysis. Information is provided on methods of sample preparation, data gathering, elemental identification, chemical state identification, quantitative calculation and elemental distribution.

Surface analysis by XPS involves irradiating a solid *in vacuo* with monoenergetic soft x-rays and analyzing the emitted electrons by energy. The spectrum is obtained as a plot of the number of detected electrons per energy interval versus their kinetic energy. Each element has a unique spectrum. The spectrum from a mixture of elements is approximately the sum of the peaks of the individual constituents. Because the mean free path of electrons in solids is very small, the detected electrons originate from only the top few atomic layers, making XPS a unique surface-sensitive technique for chemical analysis. Quantitative data can be obtained from peak heights or peak areas, and identification of chemical states often can be made from exact measurement of peak positions and separations, as well as from certain spectral features.

Included in this handbook are survey spectra, strong line spectra and x-ray excited Auger spectra for most of the elements and some of their compounds, in addition to plots and tables of energy shift data which aid in the identification of chemical states.

B. Principles of the Technique

Surface analysis by XPS is accomplished by irradiating a sample with monoenergetic soft x-rays and analyzing the energy of the detected electrons. Mg Kα (1253.6 eV), Al Kα (1486.6 eV), or monochromatic Al Kα (1486.7 eV) x-rays are usually used. These photons have limited penetrating power in a solid on the order of 1-10 micrometers. They interact with atoms in the surface region, causing electrons to be emitted by the photoelectric effect. The emitted electrons have measured kinetic energies given by:

$$KE = h\nu - BE - \phi_s \qquad (1)$$

where hν is the energy of the photon, BE is the binding energy of the atomic orbital from which the electron originates, and ϕ_s is the spectrometer work function.

The binding energy may be regarded as the energy difference between the initial and final states after the photoelectron has left the atom. Because there is a variety of possible final states of the ions from each type of atom, there is a corresponding variety of kinetic energies of the emitted electrons. Moreover, there is a different probability or cross-section for each final state. Relative binding energies and ionization cross-sections for an atom are shown schematically in Figure 1. The Fermi level corresponds to zero binding energy (by definition), and the depth beneath the Fermi level in the figure indicates the relative energy of the ion remaining after electron emission, or the binding energy of the electron. The line lengths indicate the relative probabilities of the various ionization processes. The p, d and f levels become split upon ionization, leading to vacancies in the $p_{1/2}$, $p_{3/2}$, $d_{3/2}$, $d_{5/2}$, $f_{5/2}$ and $f_{7/2}$. The spin-orbit splitting ratio is 1:2 for p levels, 2:3 for d levels and 3:4 for f levels. As an example, the spin-orbit splitting of the Si 2p is shown in Figure 2.

Because each element has a unique set of binding energies, XPS can be used to identify and determine the concentration of the elements in the surface. Variations in the elemental binding energies (the chemical shifts) arise from differences in the

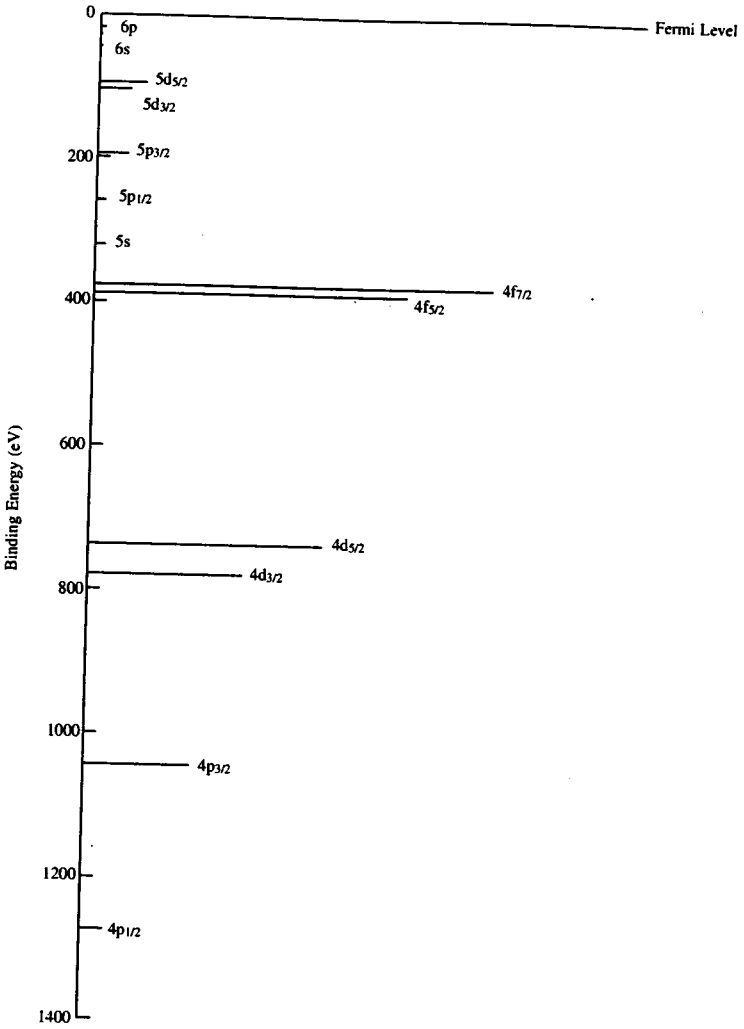


Figure 1. Relative binding energies and ionization cross-sections for U. The binding energy is proportional to the distance below the line indicating the Fermi level, and the ionization cross-section is proportional to the length of the line.

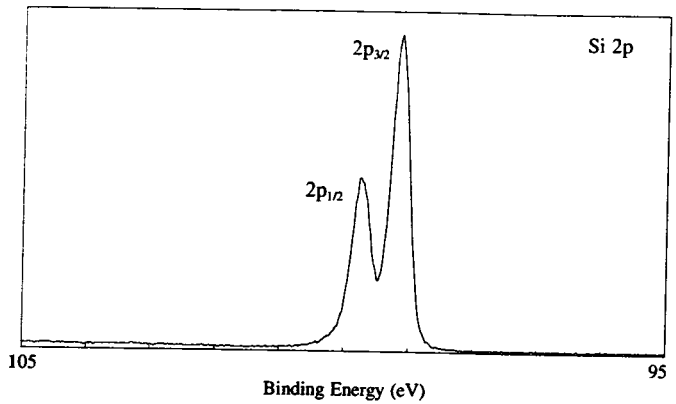


Figure 2. High-resolution spectrum of single-crystal Si showing the spin-orbit splitting of the 2p level.

chemical potential and polarizability of compounds. These chemical shifts can be used to identify the chemical state of the materials being analyzed.

In addition to photoelectrons emitted in the photoelectric process, Auger electrons may be emitted because of relaxation of the excited ions remaining after photoemission. This Auger electron emission occurs roughly 10^{-14} seconds after the photoelectric event. The competing emission of a fluorescent x-ray photon is a minor process in this energy range. In the Auger process (Figure 3), an outer electron falls into the inner orbital vacancy, and a second electron is simultaneously emitted, carrying off the excess energy. The Auger electron possesses kinetic energy equal to the difference between the energy of the initial ion and the doubly charged final ion, and is independent of the mode of the initial ionization. Thus, photoionization normally leads to two emitted electrons — a photoelectron and an Auger electron. The sum of the kinetic energies of the electrons emitted cannot exceed the energy of the ionizing photons.

Probabilities of electron interaction with matter far exceed those of the photons, so while the path length of the photons is of the order of micrometers, that of the electrons is of the order of tens of angstroms. Thus, while ionization occurs to a depth of a few

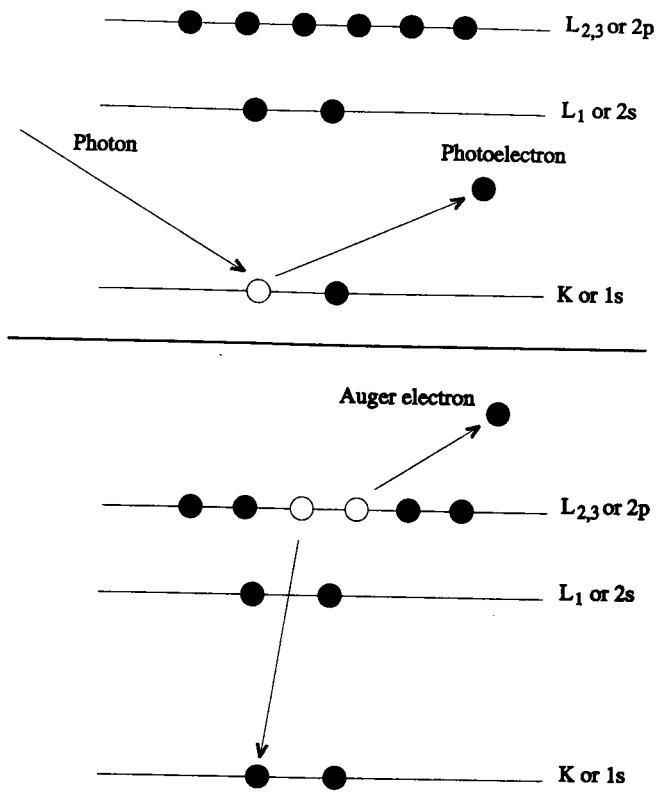


Figure 3. The XPS emission process (top) for a model atom. An incoming photon causes the ejection of the photoelectron. The relaxation process (bottom) for a model atom resulting in the emission of a $KL_{23}L_{23}$ electron. The simultaneous two-electron coulombic rearrangement results in a final state with two electron vacancies.

micrometers, only those electrons that originate within tens of angstroms below the solid surface can leave the surface without energy loss. These electrons which leave the surface without energy loss produce the peaks in the spectra and are the most useful. The electrons that undergo inelastic loss processes before emerging form the background. Calculations of the inelastic mean free paths of electrons in various materials are shown in Figure 4.

The electrons leaving the sample are detected by an electron spectrometer according to their kinetic energy. The analyzer is usually operated as an energy window, referred to as the pass energy, accepting only those electrons having an energy within the range of this window. To maintain a constant energy resolution, the pass energy is fixed. Incoming electrons are adjusted to the pass energy before entering the energy analyzer. Scanning for different energies is accomplished by applying a variable electrostatic field before the analyzer. This retardation voltage may be varied from zero up to and beyond the photon energy. Electrons are detected as discrete events, and the number of electrons for a given detection time and energy is stored and displayed.

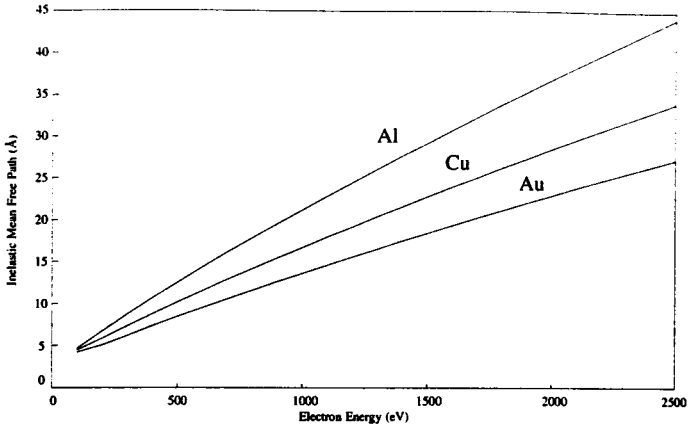


Figure 4. Calculated inelastic electron mean free paths in various metals from the method of S. Tanuma, C.J. Powell and D.R. Penn, *Surf. Interface Anal.* 17, 911 (1991).

C. Preparing and Mounting Samples

In the majority of XPS applications, sample preparation and mounting are not critical. Typically, the sample is mechanically attached to the specimen mount, and analysis is begun with the sample in the as-received condition. Additional sample preparation is discouraged in many cases because any preparation might modify the surface composition. For those samples where special preparation or mounting cannot be avoided, the following techniques are recommended.

1. Removing Volatile Material

Ordinarily, volatile material is removed from the sample before analysis. In exceptional cases, when the volatile layer is of interest, the sample may be cooled for analysis. The cooling must be to a sufficiently low temperature to guarantee that the volatile element is not warmed to evaporation by any heat load that the analysis conditions may impart.

Removal of unwanted volatile materials is usually accomplished by long-term pumping in a separate vacuum system or by washing with a suitable solvent. Use freshly distilled solvent to avoid contamination by high boiling point impurities within the solvent. Choice of the solvent can be critical. Hexane or other light hydrocarbon solvents are probably least likely to alter the surface, providing the solvent properties are satisfactory. Samples may also be washed efficiently in a Soxhlett extractor using a suitable solvent.

2. Removing Nonvolatile Organic Contaminants

When the nature of an organic contaminant is not of interest or when a contaminant obscures underlying material that is of interest, the contaminant may be removed with appropriate organic solvents. As with volatile materials, the choice of solvent can be critical.

3. Surface Etching

Ion sputter-etching or other erosion techniques, such as the use of an oxygen plasma on organic materials (see Section E.5.a.(3), p. 27), may be used to remove surface contaminants. This technique is particularly useful when removing adventitious hydrocarbons from the sample or when the native oxides, formed by exposure to the atmosphere, are not of interest.

Argon ion etching is commonly used to obtain information on composition as a function of the exposure time to ion etching. Calibration of the sputter rates can be used to convert sputter time to information on depth into the specimen. Because sputtering may cause changes in the surface chemistry, identification of the changes in chemical states with depth may not reflect the true composition.

4. Abrasion

Abrasion of a surface can be done without significant contamination by using a laboratory wipe, a cork, a file or a knife blade. This may cause local heating, and reaction with environmental gases may occur (e.g., oxidation in air and formation of nitrides in nitrogen). To prevent oxidation of more active materials, perform abrasion in an inert atmosphere such as a glove box. The abraded material should then be transferred to the ultra-high vacuum (UHV) chamber in a sealed vessel to preserve the clean surface.

5. Fracturing and Scraping

With proper equipment, many materials can be fractured or scraped within the test chamber under UHV conditions. While this obviates contamination by reaction with atmospheric gases, attention must be given to unexpected results which might occur. Fracturing might occur along the grain boundaries which may not be representative of the bulk material. Scraping can cover hard material with soft material when the sample is multiphase.

6. Grinding to Powder

If spectra characteristic of bulk composition are desired, samples may be ground to a powder in a mortar. Protection of the fresh surfaces from the atmosphere is required. When grinding samples, localized high temperatures can be produced, so grinding should be done slowly to minimize heat-induced chemical changes at the newly created surfaces. The mortar should be well cleaned before reuse.

7. Mounting Powders for Analysis

There are a number of methods which can be used to mount powders for analysis. Perhaps the most widely used method is dusting the powder onto a polymer-based adhesive tape with a camel-hair brush. The powder must be dusted across the surface carefully and lightly, with no wiping strokes. Some researchers shun organic tape for UHV work, but others have successfully used certain types of tape in the 10^{-10} Torr range.

Alternative methods for mounting powders include pressing the powder into indium or other soft foils, supporting the powder on a metallic mesh, pressing the powder into pellets or simply depositing the powder by gravity. With the foil method, the powder is pressed between two pieces of pure foil. The pieces are then separated, and one of them is mounted for analysis. Success with this technique has been varied. Sometimes bare foil remains exposed and, if the sample is an insulator, parts of the powder can charge differently. Differential charging can also be a problem when a metallic mesh is used to support the powder. If a press is used to form the powder into a pellet of workable dimensions, a press with hard and extremely clean working surfaces should be used. Gravity can effectively hold some materials in place, particularly if a shallow well or depression is cut in the surface of the sample mount. Allowing a liquid suspension of the powder to dry on the specimen holder is an effective way of producing a

uniform layer. With these methods, care must be taken in pump-down to ensure that gas evolution does not disturb the sample. A throttled roughing valve is especially effective.

D. Experimental Procedure

1. Technique for Obtaining Spectra

All spectra in this handbook were obtained using a PHI Model 5600 MultiTechnique system. A schematic diagram of the apparatus (Figure 5) illustrates the relationship of major components, including the electron energy analyzer, the x-ray source, and the ion gun used for sputter-etching. The Model 10-360 Electron Energy Analyzer incorporated into the 5600 is an SCA, and the input lens to the analyzer is an Omni Focus III lens. The excitation sources used were a Model 10-550 x-ray source with a Model 10-410 monochromator and a Model 04-548 dual-anode source which was used with a magnesium anode. All of the spectra in the handbook were taken with the x-ray source operating at 400 W (15 kV - 27 mA). The specimens were analyzed at an electron take-off angle of 70°, measured with respect to the surface plane. The monochromatic x-ray source is located perpendicular to the analyzer axis, and the standard x-ray source is located at 54.7° relative to the analyzer axis.

In the PHI Model 5600 MultiTechnique system, energy distribution, energy resolution and analysis area are all a function of the analyzer. For all of the spectra in this handbook, the spectrometer was operated in a standard mode. The Omni Focus III lens was used to scan the spectrum while the SCA was operated at a constant pass energy. This resulted in constant resolution (ΔE) across the entire energy spectrum. The size of the analysis area was defined by the aperture selection of the Omni Focus III lens. Analyzer energy resolution ($\Delta E/E$) was determined by the choice of pass energy and the selected aperture. All of the spectra in this handbook were obtained using an 800 μm diameter analysis area.

All of the spectra in this handbook were recorded and stored using the PHI *ACCESS*™ data system. The instrument was calibrated daily, and the calibration was checked several times each day during data acquisition. The analyzer work function was determined assuming the binding energy of the Au $4f_{7/2}$ peak to be 84.0 eV. All survey spectra scans were taken at a pass energy of 58.7 eV. The narrow scans of strong lines were, in most cases, just wide enough to encompass the peak(s) of interest and were obtained with a pass energy of 23.5 eV. A lower pass energy may show more structure for some materials. The narrow spectra were necessary to accurately determine the energy, shape and spin-orbit splitting of the strong lines. On insulating samples, a high-resolution spectrum was taken of the adventitious hydrocarbon on the surface of the sample to use as a reference for charge correction. The generally accepted binding energy for adventitious carbon is 284.8 eV.

The samples analyzed to obtain the spectra in this handbook are standard materials of known composition. Metal foils and polycrystalline materials with large surface areas were mechanically fastened to the specimen mount. Powder samples were ground with a mortar and pestle to expose fresh surfaces and were dusted onto adhesive tape. Most elemental standards were sputter-etched immediately prior to analysis to remove surface contamination. Most compounds, however, were ground or cleaved, and the freshly exposed surface was analyzed

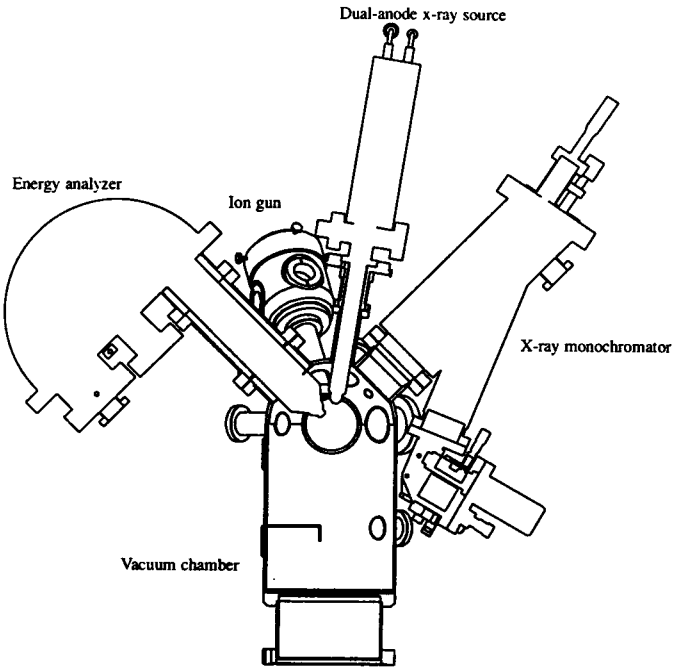


Figure 5. A schematic diagram of the PHI Model 5600 MultiTechnique system.

without etching in order to avoid possible changes in surface chemistry. Ne, Xe and Kr were implanted in graphite and Ar in silicon via ion implantation to unknown concentrations prior to analysis.

2. Instrument Calibration

To ensure the accuracy of the data presented in this handbook, the instrument used to obtain the data was calibrated regularly throughout the data-gathering process. The best way to check calibration, and the method used here, is to record suitable lines from a known, conducting specimen. Typically, the Au 4f or Cu 2p and 3p lines are used. The lines should be recorded with a narrow sweep width in the range of 5-10 eV, and a pass energy of 23.5 eV or less (corresponding to the pass energy normally used for high resolution scans) should be used.

There is general agreement on accurate values of Cu, Au and Ag standard line energies. The values in Table 1 are recommended for clean Au, Ag and Cu:

Table 1. Reference Binding Energies (eV)

	Al Kα	Mg Kα
Cu 3p	75.14	75.13
Au $4f_{7/2}$	83.98	84.00
Ag $3d_{5/2}$	368.26	368.27
Cu L_3MM	567.96	334.94
Cu $2p_{3/2}$	932.67	932.66
Ag M_4NN	1128.78	895.75

from M. P. Seah *Surf. Interface Anal.* **14**, 488 (1989)

Because the $2p_{3/2}$ and $3p_{3/2}$ photoelectron peak energies of Cu are widely separated in energy, measurement of these peak binding energies provides a quick and simple means of checking the accuracy of the binding energy scale. Utilizing all of the above standard energies establishes the linearity of the energy scale and its position, i.e., the location of the Fermi level.

3. Programming Scans for an Unknown Sample

For a typical XPS investigation where the surface composition is unknown, a broad scan survey spectrum should be obtained first to identify the elements present. Once the elemental composition has been determined, narrower detailed scans of selected peaks can be used for a more comprehensive picture of the chemical composition. This is the procedure that has been followed in compiling data for this handbook, even though specimen composition was known prior to analysis.

a. Survey Scans. Most elements have major photoelectron peaks below 1100 eV, and a scan range from 1100-0 eV binding energy is usually sufficient to

identify all detectable elements. The spectra in this handbook were recorded with a scan range of 1400-0 eV (Al excitation) or 1200-0 eV (Mg excitation) binding energy. In an unknown sample, if specific elements are suspected at low concentrations, their standard spectra should be consulted before programming the survey scan. If the strongest line occurs above 1100 eV binding energy, the scan range can be modified accordingly.

An analyzer pass energy of 187 eV, in conjunction with the appropriate aperture, is recommended for survey scans with the PHI Model 5600 MultiTechnique system. These settings result in adequate resolution for elemental identification and produce very high signal intensities, minimizing data acquisition time and maximizing elemental detectability.

b. Detail Scans. For purposes of chemical state identification, for quantitative analysis of minor components and for peak deconvolution or other mathematical manipulations of the data, detail scans must be obtained for precise peak location and for accurate registration of line shapes. There are some logical rules for this programming.

(1) Scans should be wide enough to encompass the background on both sides of the region of interest, yet with small enough step sizes to permit determination of the exact peak position. Sufficient scanning must be done within the time limits of the analysis in order to obtain good counting statistics.

(2) Peaks from any species thought to be radiation-sensitive or transient should be run first. Otherwise, any convenient order may be chosen.

(3) No clear guidelines can be given on the maximum duration of data gathering on any one sample. It should be recognized, however, that chemical states have vastly varying degrees of radiation sensitivity and that for any one set of irradiation conditions, there exists for many samples a condition beyond which it is impractical to attempt gathering data.

(4) With the PHI Model 5600 MultiTechnique system, an analyzer pass energy of 23 eV is normally used for routine detail scans. Where higher energy resolution is needed, lower pass energies can be utilized. For example, the sputter-cleaned Si 2p on p. 56, taken at 23 eV pass energy, can be compared to the chemically etched Si 2p shown in Figure 2 (p. 11).

E. Data Interpretation

1. The Nature of the Spectrum

a. General Features. The spectrum is displayed as a plot of the number of electrons versus electron binding energy in a fixed, small energy interval. The position on the kinetic energy scale equal to the photon excitation energy minus the spectrometer work function corresponds to a binding energy of 0 eV with reference to the Fermi level (Equation 1, p. 10). Therefore, a binding energy scale with 0 at that point and increasing to the left is customarily used.

The spectra in this handbook are typical for the various elements. The well-defined peaks are due to electrons

which have not suffered an inelastic energy loss emerging from the sample. Electrons that have lost energy increase the level of the background at binding energies higher than the peak energy. The background is continuous because the energy loss processes are random and multiple. The background in the Mg Kα induced spectra is larger than the background in the monochromated Al Kα induced spectra because of excitation by Bremsstrahlung radiation of the non-monochromated light.

The "noise" in the spectrum is not instrumental in origin but is the consequence of the collection of single electrons as counts randomly spaced in time. The standard deviation for counts collected in any channel is equal to the square root of the counts so that the percent standard deviation is $100/(\text{counts})^{1/2}$. The signal-to-noise ratio is then proportional to the square root of the counting time. The background level upon which the peak is superimposed is a characteristic of the specimen, the excitation source and the transmission characteristics of the instrument.

b. Types of Lines. Several types of peaks are observed in XPS spectra. Some are fundamental to the technique and are always observed. Others are dependent upon the exact physical and chemical nature of the sample. A third type is the result of instrumental effects. The following describes the various spectral features that are likely to be encountered:

(1) Photoelectron Lines. The most intense photoelectron lines are relatively symmetrical and are typically the narrowest lines observed in the spectra. Photoelectron lines of pure metals can, however, exhibit considerable asymmetry due to coupling with conduction electrons. Peak width is a convolution of the natural line width (the lifetime of the "hole" resulting from the photoionization process), the width of the x-ray line which created the photelectron line and the instrumental contribution to the observed line width. Less intense photoelectron lines at higher binding energies are usually wider by 1-4 eV than the lines at lower binding energies. All of the photoelectron lines of insulating solids are of the order of 0.5 eV wider than photoelectron lines of conductors. The approximate binding energies of all photoelectron lines detectable by Al or Mg radiation are cataloged in Appendices G and H.

(2) Auger Lines. These are groups of lines in rather complex patterns. There are four main Auger series observable in XPS. They are the KLL, LMM, MNN and NOO series, identified by specifying the initial and final vacancies in the Auger transition. The KLL series, for example, includes those processes with an initial vacancy in the K shell and final double vacancy in the L shell. The symbol V (e.g., KVV) indicates that the final vacancies are in valence levels. The KLL series has, theoretically, nine lines, and others have still more. Because Auger lines have kinetic energies which are independent of the ionizing radiation, they appear on a binding energy plot to be in different positions when ionizing photons of different energies (i.e., different x-ray sources) are used. Core-type Auger lines (with final vacancies deeper than the valence levels) usually have at least one component of intensity similar to the most intense photoelectron line. Positions of the more prominent Auger components are cataloged along with the photoelectron peaks in Appendices G and H.

(3) X-ray Satellites. The x-ray emission spectrum from a nonmonochromatic source used for irradiation exhibits not only the characteristic x-ray but also some minor x-ray components at higher photon energies. For each photoelectron peak that results from the routinely used Mg and Al Kα x-

ray photons, there is a family of minor peaks at lower binding energies, with intensity and spacing characteristic of the x-ray anode material. The pattern of such satellites for Mg and Al is shown in Table 2. A resultant spectrum using Mg x-rays is shown in Figure 6.

Table 2. X-ray Satellite Energies and Intensities

	$\alpha_{1,2}$	α_3	α_4	α_5	α_6	β
Mg displacement, eV	0	8.4	10.1	17.6	20.6	48.7
relative height	100	8.0	4.1	0.6	0.5	0.5
Al displacement, eV	0	9.8	11.8	20.1	23.4	69.7
relative height	100	6.4	3.2	0.4	0.3	0.6

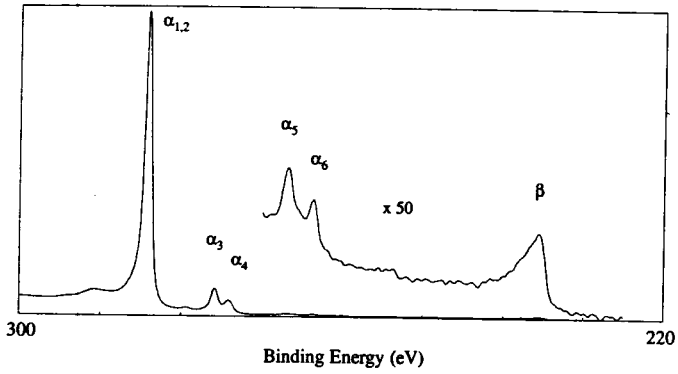


Figure 6. Mg x-ray satellites observed in the C 1s spectrum of graphite.

(4) X-ray Ghost Lines. Occasionally, x-radiation from an element other than the x-ray source anode material impinges upon the sample, resulting in small peaks corresponding to the most intense spectral peaks but displaced by a characteristic energy interval. These lines may result from Mg impurity in the Al anode or vice versa, Cu from the anode base structure, oxidation of the anode, or generation of x-ray photons in the Al foil x-ray window. On occasion, such lines can originate via generation of x-rays within the sample itself. This last possibility is rare because the probability of x-ray emission is low relative to Auger electron emission. Nevertheless, such minor lines can be puzzling. Table 3 indicates where such peaks are most likely to occur relative to the most intense photoelectron lines. Because such ghost lines rarely appear with nonmonochromatic x-ray sources and are not possible with monochromatic x-ray sources, they should not be considered in line identification until all other possibilities are excluded.

Table 3. Displacement of X-ray Ghost Lines (eV)

Contaminating Radiation	Anode Material Mg	Al
O (Kα)	728.7	961.7
Cu (Lα)	323.9	556.9
Mg (Kα)	—	233.0
Al (Kα)	-233.0	—

(5) Shake-Up Lines. Not all photoelectric processes are simple ones which lead to the formation of ions in the ground state, but there is a finite probability that the ion will be left in an excited state a few electron volts above the ground state. In this event, the kinetic energy of the emitted photoelectron is reduced, with the difference corresponding to the energy difference between the ground state and the excited state. This results in the formation of a satellite peak a few electron volts lower in kinetic energy (higher in binding energy) than the main peak. For example, the characteristic shake-up line for carbon in aromatic compounds, a shake-up process involving the energy of the $\pi \rightarrow \pi^*$ transition, is shown in Figure 7.

In some cases, most often with paramagnetic compounds, the intensity of the shake-up satellite may

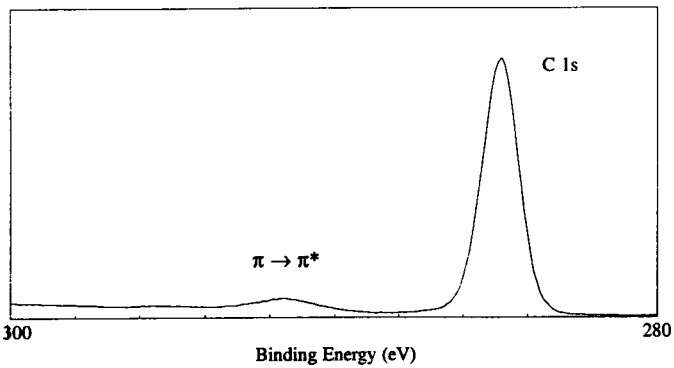


Figure 7. The π bond shake-up satellite for C 1s in polystyrene. The peak is about 6.7 eV higher than the main photopeak.

approach that of the main line. More than one satellite of a principal photoelectron line can also be observed, as shown in Figure 8. The occurrence of such lines is sometimes also apparent in Auger spectral contours (Figure 9). The displacements and relative intensities of shake-up satellites can sometimes be useful in identifying the chemical state of an element, as discussed in Section E.3.d. (p. 24).

(6) Multiplet Splitting. Emission of an electron from a core level of an atom that itself has a spin (unpaired electrons in valence levels) can create a vacancy in two or more ways. The coupling of the new unpaired electron left after photoemission from an s-type orbital with other unpaired electrons in the atom can create an ion with several possible final state configurations and as many energies. This results in a photoelectron line which is split asymmetrically into several components similar to the one shown in Figure 10.

Multiplet splitting also occurs in the ionization of p levels, but the result is more complex and subtle. In favorable cases, it results in an apparent slight

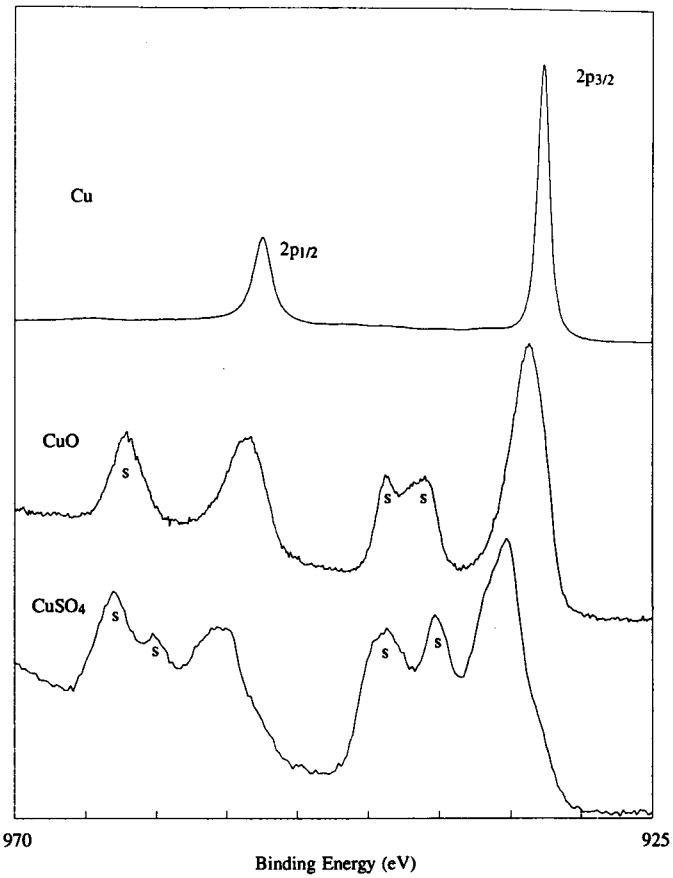


Figure 8. Examples of shake-up lines (s) of the copper 2p observed in copper compounds.

increase in the spin doublet separation, evidenced in the separation of the $2p_{1/2}$ and $2p_{3/2}$ lines in first-row transition metals, and in the generation of a less easily noticed asymmetry in the line shape of the components. Often such effects on the p doublet are obscured by shake-up lines.

(7) Energy Loss Lines. With some materials, there is an enhanced probability for loss of a specific

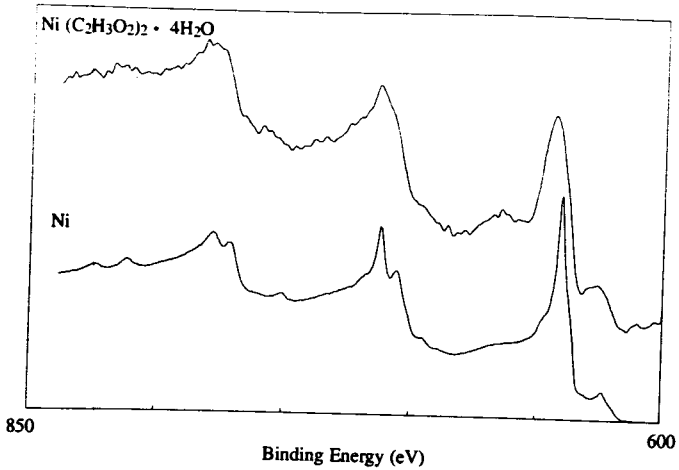


Figure 9. Examples of the effects of chemical states on Auger line shapes in nickel compounds.

amount of energy due to interaction between the photoelectron and other electrons in the surface region of the sample (Figure 11). The energy loss phenomenon produces a distinct and rather sharp hump 20-25 eV above the binding energy of the parent line. Under certain conditions of spectral display, energy loss lines can cause confusion. Such phenomena in insulators are rarely sharper than that shown in Figure 11 and are usually much more muted. They are different in each solid medium.

With metals, the effect is often much more dramatic, as indicated by the loss lines for aluminum shown in Figure 12. Energy loss to the conduction electrons occurs in well-defined quanta characteristic of each metal. These plasmons arise from group oscillations of the conduction electrons. The photoelectron line, or the Auger line, is successively mirrored at intervals of higher binding energy with reduced intensity. The energy

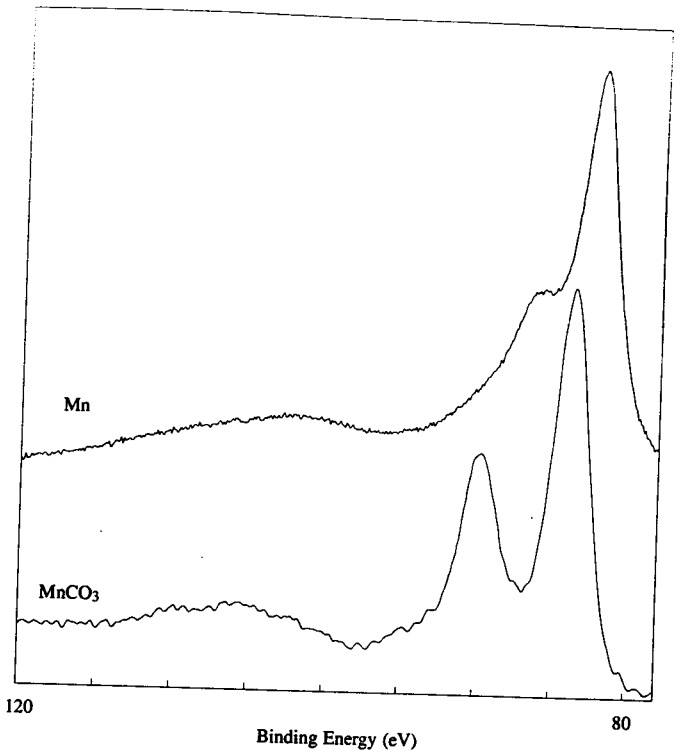


Figure 10. Multiplet splitting of the Mn 3s.

interval between the primary peak and the loss peak is called the plasmon energy. The so-called bulk plasmons are the more prominent of these lines. A second series, the surface plasmons, exists at energy intervals determined approximately by dividing the bulk plasmon energy by the square root of two. The effect is not easily observed in nonconductors, nor is it prominent in all conductors. Plasmon lines are especially prominent in the Groups Ia and IIa metal spectra in this handbook.

(8) Valence Lines and Bands. Lines of low intensity occur in the low binding energy region of the

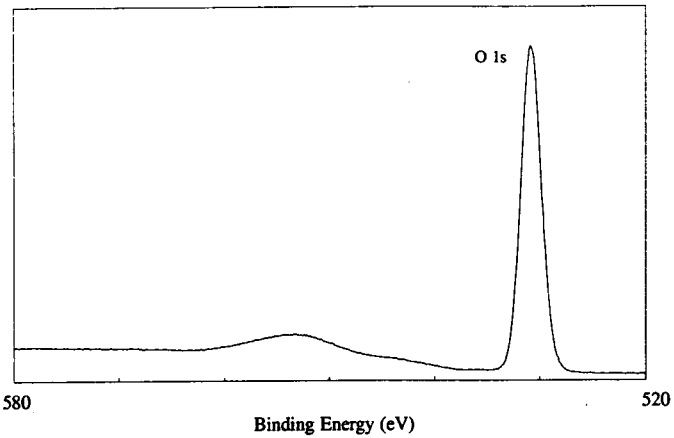


Figure 11. Energy loss envelope from the O 1s line in Al_2O_3 (sapphire).

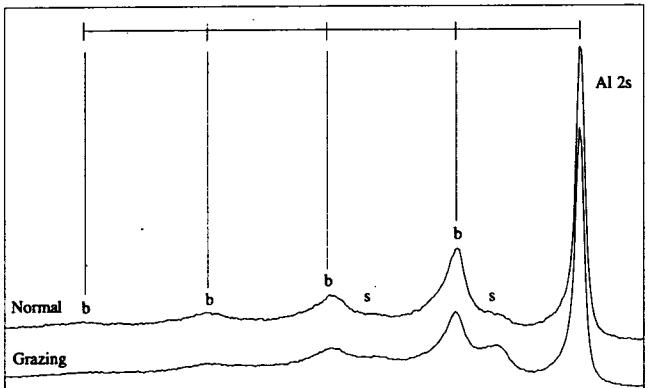


Figure 12. Surface (s) and bulk (b) plasmon lines associated with the Al 2s at normal and grazing take-off angles.

spectrum between the Fermi level and 10-20 eV binding energy. These lines are produced by photoelectron emission from molecular orbitals and from solid state energy bands. Differences between insulators and conductors are especially noted by the absence or presence of electrons from conduction bands at the Fermi level. Valence bands may also be used to distinguish between materials where the core level XPS photoelectron lines are quite similar in shape and position. Appendix D contains valence band spectra of several materials.

2. Line Identification

In general, interpretation of the XPS spectrum is most readily accomplished first by identifying the lines that are almost always present (specifically those of C and O), then by identifying major lines and associated weaker lines, and lastly by identifying the remaining weak lines. Most modern, commercially available spectrometers have peak identification algorithms within their data reduction packages. Poor signal-to-noise of the data or database limitations may require manual identification of some peaks. The following step-by-step procedure simplifies the data interpretation task and minimizes data ambiguities.

Step 1. The C 1s, O 1s, C (KLL) and O (KLL) lines are usually prominent in any spectrum. Identify these lines first along with all derived x-ray satellites and energy loss envelopes.

Step 2. Identify other intense lines (Appendix J) present in the spectrum, then label any related satellites and other less intense spectral lines associated with those elements. The energy positions of the less intense lines are noted in the line position table with the spectra. Keep in mind that some lines may be interfered with by more intense, overlapping lines from other elements. The most serious interferences by the C and O lines, for example, are Ru 3d by C 1s, V 2p and Sb 3d by O 1s, I (MNN) and Cr (LMM) by O (KLL), and Ru (MNN) by C (KLL).

Step 3. Identify any remaining minor lines. In doing this, assume they are the most intense lines of an unknown element. If not, they should already have been identified in the previous steps. Again, keep in mind possible line interferences. Small lines that seem unidentifiable can be ghost lines. Use Table 3 (p. 18) to check for the more intense parent photoelectron lines.

Step 4. Check the conclusions by noting the spin doublets for p, d and f lines. They should have the right separation (cf. spin orbit splitting for individual elements and Appendices G and H) and should be in the correct intensity ratio. The ratio for p lines should be about 1:2, d lines 2:3 and f lines 3:4. P lines, especially 4p lines, may be less than 1:2.

3. Chemical State Identification

The identification of chemical states primarily depends on the accurate determination of line energies. To determine line energies accurately, the voltage scale of the instrument must be precisely calibrated (cf. Section D.2., p. 15), a line with a narrow sweep range must be recorded with good statistics (of the order of several thousand counts-per-channel above background), and accurate correction must be made for static charge if the sample is an insulator.

a. Determining Static Charge on Insulators. During analysis, insulating samples tend to acquire a steady-state charge of as much as several volts. This steady-state charge is a balance between electron loss from the surface by emission and electron gain by conduction or by acquisition of slow or thermal electrons from the vacuum. The steady-state charge, usually positive, can be minimized with an adjacent neutralizer or flood gun. It is often advantageous to do this to reduce differential charging and sharpen the spectral lines.

A serious problem is exactly determining the extent of charging. Any positive charging retards outgoing electrons and tends to make the peaks appear at higher binding energies, whereas excessive charge compensation can make the peaks shift to lower binding energies. The following are four methods which are usually valid for charge correction on insulating samples:

(1) Measurement of the position of the C 1s line from adventitious hydrocarbon nearly always present on samples introduced from the laboratory environment or from the glove box. This line, on unsputtered inert metals such as Au or Cu, appears at 284.8 eV, so any shift from this value can be taken as a measure of the static charge. At this time, it is not known whether a reproducible line position exists for C remaining on the surface after ion beam etching.

(2) The use of an internal standard, such as a hydrocarbon moiety of a polymer sample. For the study of supported catalysts or similar materials, one can adopt a suitable value for a constituent of the support and use that to interrelate binding energies of different samples. One must be certain that treatments of the various samples are not so different that the inherent binding energies of support constituents are changed.

(3) The use of a normally insulating sample so thin that it effectively does not insulate. This can be assumed if the spectrum of the underlying conductor appears in good intensity and if line positions are not affected by changes in electron flux from the charge neutralizer.

(4) For the study of insulating polymer films, binding energies of the C functional groups may also be determined by applying a small amount of poly(dimethyl siloxane) solution (10^{-6} M) to the sample surface and charge reference to the Si 2p of the silicone (at about 102.1 eV).

Some precautions should be kept in mind. If the sample is heterogeneous on even a micrometer scale, particles of different materials can be charged to different extents, and interpretation of the spectrum is complicated accordingly. One cannot physically mix a conducting standard like Au or graphite of micron dimensions with a powder and validly use the Au or graphite line in order to correct for static charge. Differential charging can be minimized to a great extent by using a flood source of low-energy electrons.

b. Photoelectron Line Chemical Shifts and Separations. An important advantage of XPS is its ability to obtain information on chemical states from the variations in binding energies, or chemical shifts, of the photoelectron lines. While many attempts have been made to calculate chemical shifts and absolute binding energies, the factors involved (especially in the solid state) are imperfectly understood, and one must rely on experimental data from standard materials. The tables accompanying the spectra in this handbook record considerable data from the literature as well as data obtained specifically for this handbook. All literature data have been carefully evaluated to the instrumental calibration and static charge reference values given above and are, therefore, directly comparable.

Because occasional line interferences do occur, it is sometimes necessary to use a line other than the most intense one in the spectrum. Chemical shifts of a minor line are within 0.2 eV of the chemical shift of the primary line. However, exceptional separations can occur in paramagnetic materials because of multiplet splitting. Separations of photoelectron lines can be determined approximately from the line position tables in Appendices G and H.

c. Auger Line Chemical Shifts and the Auger Parameter. Core-type Auger lines (transitions ending with double vacancies below the valence levels) usually have at least one component that is narrow and intense, often nearly as intense as the strongest photoelectron line (cf. spectra for F, Na, As, In, Te and Pb). There are four core Auger groups that can be generated by Mg or Al x-rays: the KLL (Na, Mg); the LMM (Cu, Zn, Ga, Ge, As, Se); the MNN (Ag, Cd, In, Sn, Sb, Te, I, Xe, Cs, Ba); and NOO (Th, U). The MNN lines in the rare earths, while accessible, are very broad because of multiplet splitting and shake-up phenomena with most of the compounds. Valence-type Auger lines (final states with vacancies in valence levels) — such as those for O and F (KLL); Mn, Fe, Co and Ni (LMM); and Ru, Rh and Pd (MNN) — can be intense and are, therefore, also useful. Chemical shifts occur with Auger lines as well as with photoelectron lines. The chemical shifts are different from those of the photoelectron lines, but they are often more pronounced. This can be very useful for identifying chemical states, especially in combination with photoelectron chemical shift data. If data for the various chemical states of an element are plotted with the binding energy of the photoelectron line on the abscissa and the kinetic energy of the Auger line on the ordinate, a two-dimensional chemical state plot can be obtained. Such plots are in Appendix A for F, Na, Al, Si, S, Cu, Zn, As, Se, Ag, Cd, In, Sn and Te.

With chemical states displayed in two dimensions, the Auger parameter method becomes more powerful as a tool for identifying the chemical components than using photoelectron chemical shifts alone. In the format adopted for this handbook, the kinetic energy of the Auger line is plotted against the binding energy of the photoelectron line, with the latter plotted in the -x direction (kinetic energy is still, implicitly, +x). The kinetic energy of the Auger electron, referred to the Fermi level, is easily calculated by subtracting from the photon energy the position of the Auger line on the binding energy scale.

With this arrangement, each diagonal line represents all values of equal sums of Auger kinetic energy and

photoelectron binding energy. The Auger parameter, α, is defined as,

$$\alpha = KE_A - KE_P = BE_P - BE_A \qquad (2)$$

or as the difference in binding energy between the photoelectron and Auger lines. This difference can be accurately determined because static charge corrections cancel. With all kinetic and binding energies referenced to the Fermi level, and recalling that:

$$KE = h\nu - BE \qquad (3)$$

then...

$$KE_A + BE_P = h\nu + \alpha \qquad (4)$$

or the sum of the kinetic energy of the Auger line and the binding energy of the photoelectric line equals the Auger parameter plus the photon energy. A plot showing Auger kinetic energy versus photoelectron binding energy then becomes independent of the photon energy.

In general, polarizable materials, especially conductive materials, have a high Auger parameter, while insulating compounds have a lower Auger parameter.

d. Chemical Information from Satellite Lines and Peak Shapes

(1) Shake-up Lines. These satellite lines have intensities and separations from the parent photoelectron line that are unique to each chemical state (Figure 8, p. 19). Some Auger lines also exhibit radical changes with chemical state that reflect these processes (Figure 9, p. 20). With transition elements and rare earths, the absence of shake-up satellites is usually characteristic of the elemental or diamagnetic states. Prominent shake-up patterns typically occur with paramagnetic states. Table 4 is a guide to some expected paramagnetic states.

Table 4. General Guide to Paramagnetic Species

Multiplet splitting and shake-up lines are generally expected in the paramagnetic states below:

Atomic No.	Paramagnetic States	Diamagnetic States
22	Ti(II) Ti(III)	Ti(IV)
23	V(II), V(III), V(IV)	V(V)
24	Cr(II), Cr(III), Cr(IV), Cr(V)	Cr(VI)
25	Mn(II), Mn(III), Mn(IV), Mn(V)	Mn(VII)
26	Fe(II), Fe(III)	$K_4Fe(CN)_6$, $Fe(CO)_4Br_2$
27	Co(II), Co(III)	CoB, $Co(NO_2)_3NH_3)_3$, $K_3Co(CN)_6$, $Co(NH_3)_6Cl_3$
28	Ni(II)	$K_2Ni(CN)_4$, square planar complexes
29	Cu(II)	Cu(I)
42	Mo(IV), Mo(V)	Mo(VI), MoS_2, $K_4Mo(CN)_8$
44	Ru(III), Ru(IV), Ru(V)	Ru(II)
47	Ag(II)	Ag(I)
58	Ce(III)	Ce(IV)
59-70	Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb compounds	
74	W(IV), W(V)	W(VI), WO_2, WCl_4, WC, $K_4W(CN)_8$
75	Re(II), Re(III), Re(IV), Re(V), Re(VI)	Re(VII), ReO_3
76	Os(III), Os(IV), Os(V)	Os(II), Os(VI), Os(VIII)
77	Ir(IV)	Ir(III)
92	U(III), U(IV)	U(VI)

(2) Multiplet Splitting. On occasion, the multiplet splitting phenomenon can also be helpful in identifying chemical states. The 3s lines in the first series of transition metals, for example, exhibit separations characteristic of each paramagnetic chemical state. The 3s line, however, is weak and therefore is not often useful analytically. The 2p doublet separation is also affected by multiplet splitting, and the lines are more intense. The effect becomes very evident with Co compounds where the separation varies up to 1 eV. When first-row transition metal compounds are under study, it is

useful to accurately record these line separations and make comparisons with model compounds.

(3) Auger Line Shape. Valence-type Auger transitions form final-state ions with vacancies in molecular orbitals. The distribution of the group of lines is strongly affected, therefore, by the nature of the molecular orbitals in the different chemical states. Although little has yet been tabulated on this subject, the spectroscopist should bear in mind the possible utility of Auger line shapes.

4. Quantitative Analysis

For many XPS investigations, it is important to determine the relative concentrations of the various constituents. Methods have been developed for quantifying the XPS measurement utilizing peak area and peak height sensitivity factors. The method which utilizes peak area sensitivity factors typically is the more accurate and is discussed below. This approach is satisfactory for quantitative work. For transition metal spectra with prominent shake-up lines, it is best to include the entire 2p region when measuring peak area.

For a sample that is homogeneous in the analysis volume, the number of photoelectrons per second in a specific spectra peak is given by:

$$I = nf\sigma\theta y\lambda AT \qquad (5)$$

where n is the number of atoms of the element per cm^3 of the sample, f is the x-ray flux in photons/cm^2-sec, σ is the photoelectric cross-section for the atomic orbital of interest in cm^2, θ is an angular efficiency factor for the instrumental arrangement based on the angle between the photon path and detected electron, y is the efficiency in the photoelectric process for formation of photoelectrons of the normal photoelectron energy, λ is the mean free path of the photoelectrons in the sample, A is the area of the sample from which photoelectrons are detected, and T is the detection efficiency for electrons emitted from the sample. From Equation 5:

$$n = I/f\sigma\theta y\lambda AT \qquad (6)$$

The denominator in Equation 6 can be defined as the atomic sensitivity factor, S. If we consider a strong line from each of two elements, then:

$$\frac{n_1}{n_2} = \frac{I_1/S_1}{I_2/S_2} \qquad (7)$$

This expression may be used for all homogeneous samples if the ratio S_1/S_2 is matrix-independent for all materials. It is certainly true that such quantities as σ and λ vary somewhat from material to material (especially λ), but the ratio of each of the two quantities σ_1/σ_2 and λ_1/λ_2 remains nearly constant. Thus, for any spectrometer, it is possible to develop a set of relative values of S for all of the elements. Multiple sets of values may be necessary for instruments with multiple x-ray sources at different angles relative to the analyzer.

A general expression for determining the atom fraction of any constituent in a sample, C_x, can be written as an extension of Equation 7:

$$C_x = \frac{n_x}{\sum n_i} = \frac{I_x/S_x}{\sum I_i/S_i} \qquad (8)$$

Values of S based on peak area measurements are indicated in Appendices E and F. The values of S in the appendices are based on empirical data (C.D. Wagner et al. *Surf. Interface Anal.* **3**, 211 (1981)) which have been corrected for the transmission function of the spectrometer. The values in the appendix are only valid for and should only be applied when the electron energy analyzer used has the transmission characteristics of the SCA supplied by Physical Electronics. An example of the application of Equation 8 to analysis of a

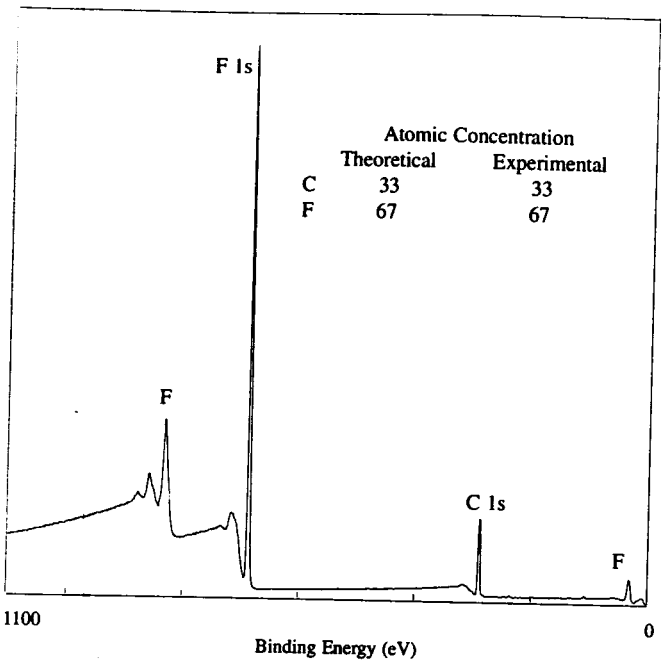


Figure 13. Quantitative analysis of poly(tetrafluoroethylene).

sample of known composition, poly(tetrafluoroethylene), is shown in Figure 13.

The use of atomic sensitivity factors in the manner described will normally furnish semiquantitative results (within 10-20%), except in the following situations:

a. The technique cannot be applied rigorously to heterogeneous samples. It can be useful with heterogeneous samples in measuring the relative number of atoms detected, but one must be conscious that the microscopic character of the heterogeneous system influences the quantitative results. Moreover, an overlying contamination layer has the effect of diminishing the intensity of high binding energy peaks more than that of low binding energy peaks.

b. Transition metals, especially of the first series, have widely varying and low values of y, whereas y for the other elements is rather uniform at about 0.8 eV. Thus, a value of S determined on one chemical state for a transition metal may not be valid for another chemical state. This effect can be minimized by including shake-up peaks in the area measurement.

c. When peak interferences occur, alternative lines must sometimes be used. The ratios of spin doublets (except 4p) are rather uniform, and the weaker of the pair can often be substituted. The spectra of the elements should be consulted, but caution must be exercised because the spectra of the elements themselves can be different from the spectra of their compounds.

d. Occasionally, an x-ray satellite from an intense photoelectron line interferes with measurement of a weak component. A mathematical approach can then be used to subtract the x-ray satellite before the measurement.

For quantitative work, check the spectrometer operation frequently to ensure that analyzer response is constant and optimum. A useful test is the recording of the three widely spaced spectral lines from Cu. Measurement of the peak height in counts-per-second should be made on 20-volt-wide scans of the $2p_{3/2}$, LMM Auger and 3p lines. Maintenance of such records makes it easy to notice if an instrument change occurs that would affect quantitative analysis.

5. Determining Element Location

a. Depth. There are four methods of obtaining information on the depth of an element in the sample. The first two methods described below utilize the characteristics of the spectrum itself but provide limited information. The third provides more detailed information but is attended by certain problems. The fourth utilizes measurements at two or more electron escape angles.

(1) The presence or absence of an energy loss peak or envelope indicates whether the emitting atoms are in the bulk or at the surface. Because electrons from surface atoms do not traverse the bulk, peaks from the surface atoms are symmetrical above level baselines on both sides, and the energy loss peak is absent. For a homogeneous sample, peaks from all elements will have similar inelastic loss structures.

(2) Elements whose spectra exhibit photoelectron lines widely spaced in kinetic energy can be approximately located by noting the intensity ratio of the lines. In the energy range above approximately 100 eV, electrons moving through a solid with lower kinetic energy are attenuated more strongly than those with higher kinetic energy. Thus, for a surface species, the low kinetic energy component will be relatively stronger than the high kinetic energy component, compared to that observed in the pure material. The data for homogeneous bulk solids can be compared with intensity ratios observed on unknowns to determine qualitatively the distribution of the element in the sample. Suitable elements include Na and Mg (1s and 2s); Zn, Ga, Ge and As ($2p_{3/2}$ and 3d); and Cd, In, Sn, Sb, Te, I, Cs and Ba ($3p_{3/2}$ and 4d or $3d_{5/2}$ and 4d).

When the element is in a bulk homogeneous layer beneath a thin contaminating layer, the characteristic intensity ratio is modified in the opposite direction. Thus, for a pair of lines from subsurface species, the low kinetic energy line will be attenuated more than the high kinetic energy line, distorting the characteristic intensity ratio. By observing such intensity ratios and comparing them with the pure bulk elements, it is possible to deduce whether the observed lines are from predominantly surface-, subsurface- or homogeneously distributed material.

(3) Depth profiling can be accomplished using controlled erosion of the surface by ion sputtering. Table 5 lists some data on sputter rates as a general guide. One can use this technique on organic materials, but few data are available for calibration. Chemical states are often changed by the sputter technique, but useful information on elemental distribution can still be obtained.

Table 5. Relative Sputter Rates at 4 kV.

Target	Sputter Rate
Ta_2O_5	1.00
Si	0.90
SiO_2	0.85
Pt	2.20
Cr	1.40
Al	0.95
Au	4.10

Another useful method of controlled erosion, especially of organic materials, is reaction with oxygen atoms from a plasma. This technique may also change the chemical states in the affected surface. Further, because the elements differ in their rates of reaction with oxygen atoms, the rate of removal of surface materials will be sample dependent.

(4) In XPS studies, the sample-mounting angle is not usually critical, though it does have some effect on the spectra. Very shallow electron take-off angles accentuate the spectrum of any component segregated on the surface, whereas a sample mounted at an angle normal to the analyzer axis minimizes the contribution from such a component. This effect can be used to estimate the depth of layers on or in the surface. This effect is not limited to flat surfaces, because angular dependence is even observed with powders, though the effects are muted. The spectrometer used to obtain the spectra presented in this handbook in-

tegrates the signal over only a narrow range of take-off angles.

It is possible to change the angle between the plane of the sample surface and the angle of entrance to the analyzer. At 90° with respect to the surface plane, the signal from the bulk is maximized relative to that from the surface layer. At small angles, the signal from the surface becomes greatly enhanced, relative to that from the bulk. The location of an element can thus be deduced by noting how the magnitude of its spectral peaks changes with sample orientation in relation to those from other elements. The analysis depth may be estimated by $d = \lambda \sin\theta$, where d is the analysis depth of the overlayer, λ is the inelastic mean free path, and θ is the take-off angle of the analyzed electrons.

Physical Electronics SCAs permit angle-dependent studies by simply varying the angle of the sample surface with respect to the input lens of the analyzer. The magnification of the lens determines the half-angle acceptance of the analyzer. An example of the information that can be gained through the use of this capability is shown in Figure 14. Data were obtained at normal (near 90°) and grazing (near 15°) take-off angles from a silicon sample with a thin silicon oxide overlayer. The observed intensity ratio of oxidized to elemental Si is much greater at the low take-off angle.

b. Surface Distribution. Many XPS systems have the capability to obtain data from areas as small as 30 μm in diameter using lens defined areas. Alternately, analysis areas of < 10 μm can be achieved with a scanning focused photo beam. These relatively high lateral resolutions allow for the acquisition of XPS maps which show both elemental and chemical state information.

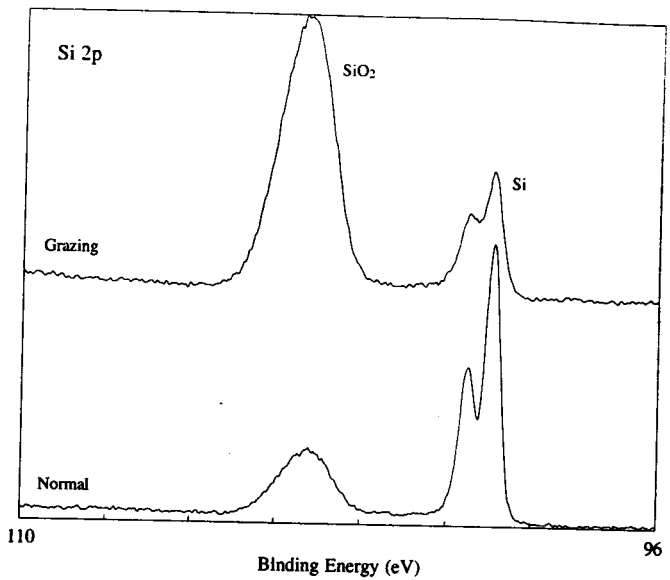


Figure 14. An example of the enhanced surface sensitivity achieved by varying the electron take-off angle. A thin oxide on silicon is enhanced at the low take-off angle.

c. Insulating Domains on a Conductor. The occurrence of steady-state charging of an insulator during analysis sometimes has useful consequences. Microscopic insulating domains on a conductor reach their own steady-state charge, while the conductor remains at spectrometer potential. Thus, an element in the same chemical state in both phases will exhibit two peaks. If a change is made in the supply of low-energy electrons which stabilize the charge (as from the neutralizer filament) or if a bias is applied to the conductor, the spectral peaks from the insulating phase will move relative to those from the conducting phase. For such heterogeneous systems, this can be an extremely useful technique. It makes it possible to determine whether the elements that contribute to the overall spectrum are in the conducting phase, the insulating phase or both.

F. How to Use this Handbook

1. Qualitative Analysis

Elemental and chemical identification of sample constituents can be performed by combining the information in the survey spectra with the binding energy tables of Appendices G, H and J.

a. Identify all major photoelectron peaks by using the line position tables in Appendix J.

b. Compare the elemental identifications with the elemental survey spectra to see that line positions and relative intensities are consistent. Also note the positions of the Auger electron peaks.

c. Review Section E (pp. 16-28) to account for fine structures such as energy loss lines, shake-up peaks, satellite lines, etc., not identified in the handbook spectra or energy tables.

d. Identify any remaining peaks assuming they are intense photoelectron or Auger lines using Appendices G or H.

e. Chemical state identification can be determined from high resolution spectra of the strongest photoelectron and sharpest Auger lines.

(1) Correct binding energies for static charging of insulators. When applicable, charge reference the binding energy scale to the C 1s photoelectron peak at 284.8 eV.

(2) Determine the chemical state from the measured shifts in the photoelectron binding energies by comparing the binding energy to the charts with the standard spectra and with the tabulated data in Appendix B.

(3) As suggested above, much about the chemical state can be learned from the magnitude and position of shake-up lines as well as from the energy and shape of valence Auger lines.

(4) For the elements F, Na, Al, Si, S, Cu, Zn, As, Se, Ag, Cd, In, Sn and Te, the Auger parameter tables in Appendix A may prove useful. The Auger line positions may be converted to kinetic energy by subtracting from the photon energy (Al = 1486.6 eV, Mg = 1253.6 eV). Note the location of the points for Auger kinetic energy and photoelectron binding energy on the respective elemental plot. Proximity of the experimental points to those of recorded chemical states should be considered probable identification. Note that experimental error is much greater along the Auger parameter grid than normal to the grid lines.

2. Quantification

The atomic sensitivity factors presented in Appendices E and F are applicable to the Physical Electronics Model 10-360 SCA and the Omni Focus III lens. A simplified expression to determine the atomic concentration of any element is given by Equation 8 (p. 25). However, the accuracy is limited by the assumptions made in Section E.4. (p. 25).

II. Standard XPS Spectra of the Elements

Standard Spectra of the Elements

This section of the handbook contains survey spectra of 81 elements, high resolution spectra of the most useful photoelectron lines, a chart of binding energies for each of the observed photoelectron and major Auger electron peaks, and a photoelectron chemical state binding energy chart for each of the elements. Used in combination with the appendices, the survey spectra aid in elemental identification, while the high-resolution spectra and binding energy data aid in the identification of chemical states.

Survey Spectra

The survey data include all of the lines which are normally useful. For most elements, the survey data were acquired with both a monochromatic Al x-ray source and a nonmonochromatic Mg x-ray source. When survey spectra for two compounds are presented, the monochromatic source is used for both. The photon source for each survey is noted on the survey. The photoelectron and Auger lines for the element of interest are identified. Lines which occur due to other elements are only designated by the elemental symbol, and x-ray satellites and energy loss lines are not noted. For many elements, the Auger peaks are presented in expanded form.

The ordinate is left undesignated, but the general contours and intensity ratios of the spectra are typical of measurements made using a Physical Electronics Model 10-360 SCA with an Omni Focus lens.

High-Resolution Spectra

The high-resolution spectra of the most useful photoelectron peaks are presented. Unless otherwise noted, the high-resolution data were acquired using the same photon source as the survey on the same page. The binding energy of the main line is noted and when appropriate, the spin orbit separation (Δ) is given. The lines from insulators were charge-corrected to adventitious hydrocarbon at 284.8 eV.

The spectra of the inert gas atoms implanted in graphite or silicon deserve special mention. The high-resolution data often show an asymmetric peak shape or a second resolvable peak when a single symmetric peak is expected. The intensity of the second, high binding energy peak is dependent on the implantation energy and is diminished at lower energies. The spectra are of inert gas atoms implanted at 4 kV.

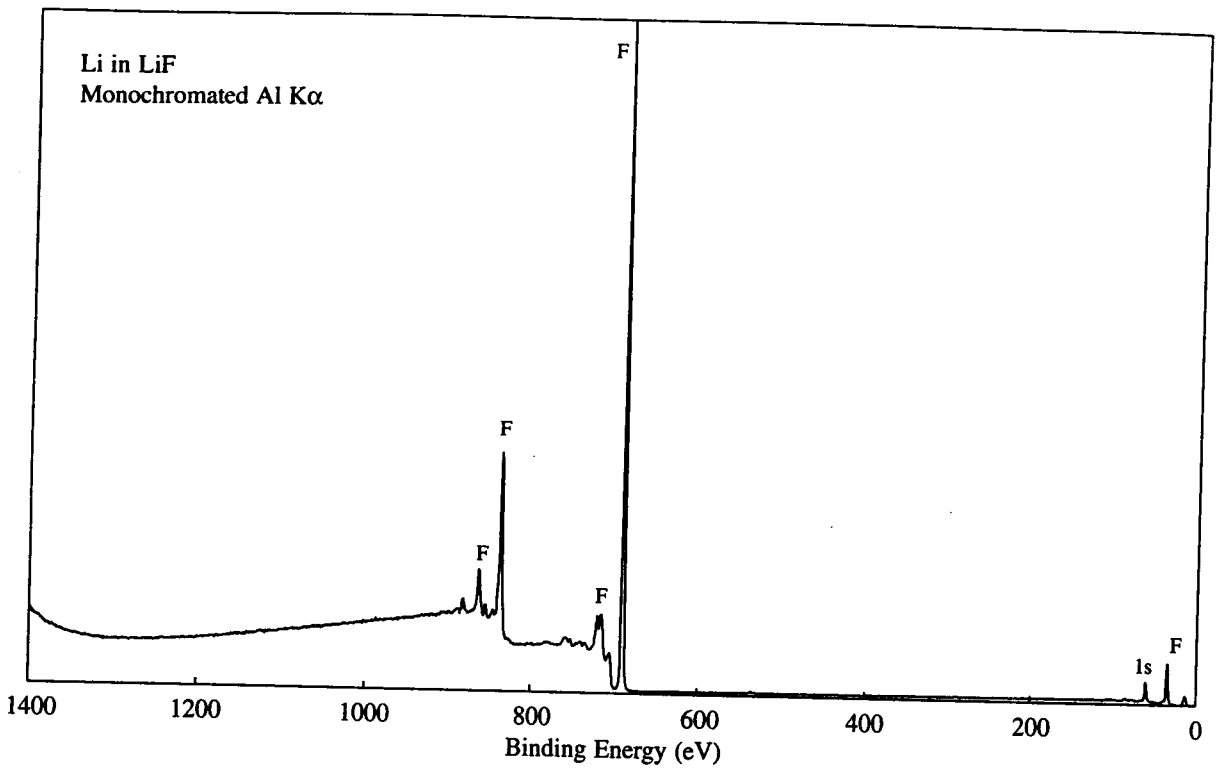
Photoelectron and Auger Electron Line Position Tables

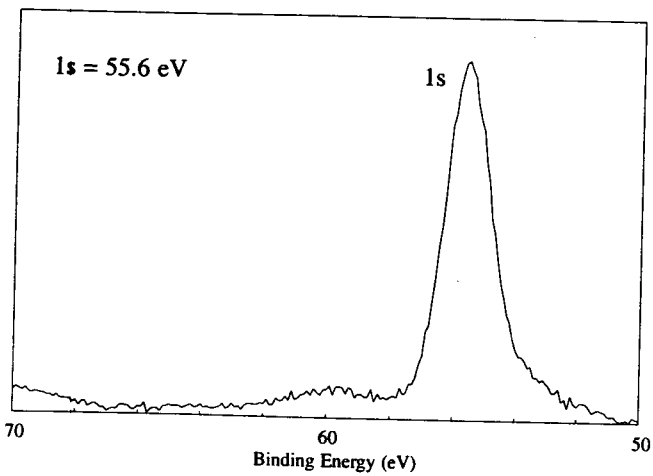
The photoelectron and Auger line position tables reflect the energies of the elemental peaks observed in this handbook. For oxidized or reduced species, the measured values may differ by a few electron volts.

Chemical State Binding Energy Tables

The binding energy tables have been constructed to reflect the general changes in binding energy with change in oxidation state or chemical environment. A more extensive listing with specific binding energy values for more than 1500 compounds is presented in Appendix B.

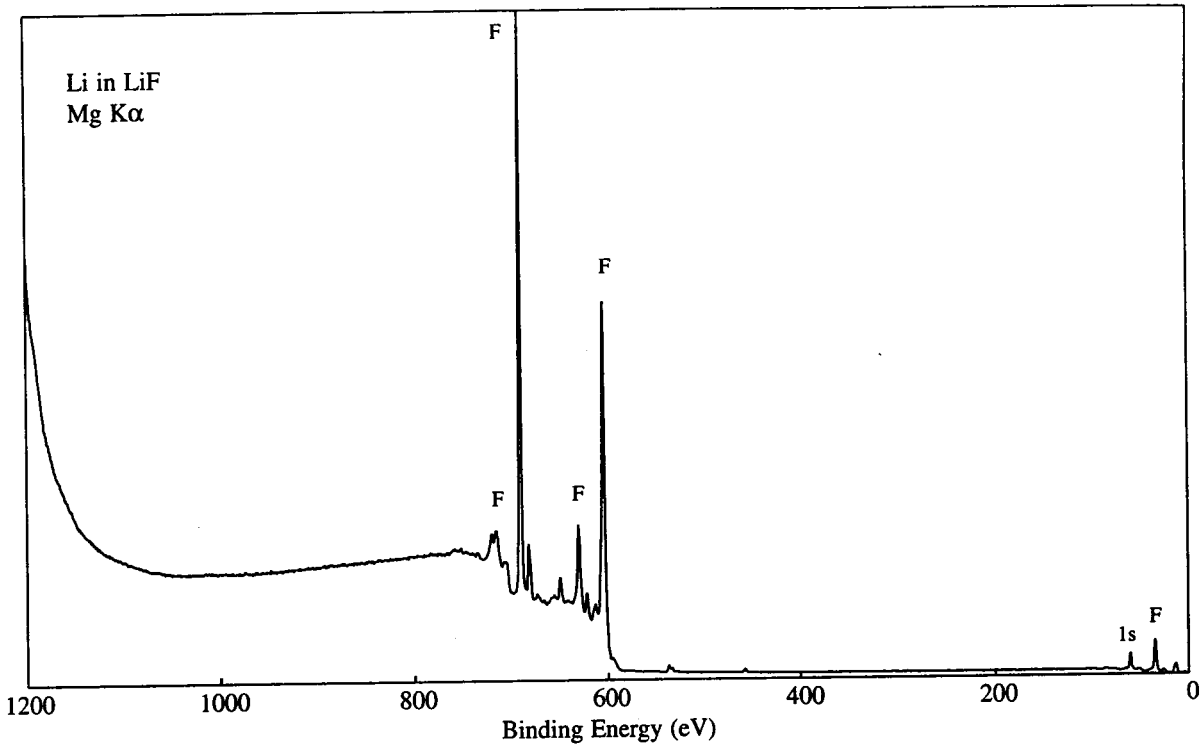
Abbreviations in the chemical state database are as follows: acac = acetyl acetonate; metallocene = metal $(C_5H_5)_2$; Bu = butyl; Et = ethyl; Me = methyl; Ph = phenyl; OAc = acetate.

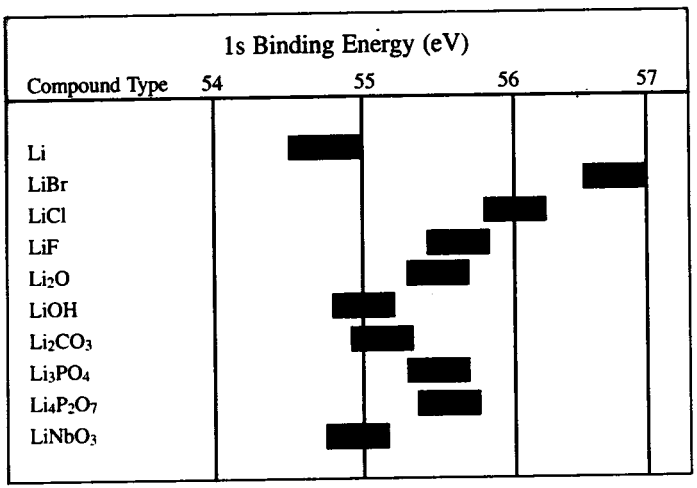


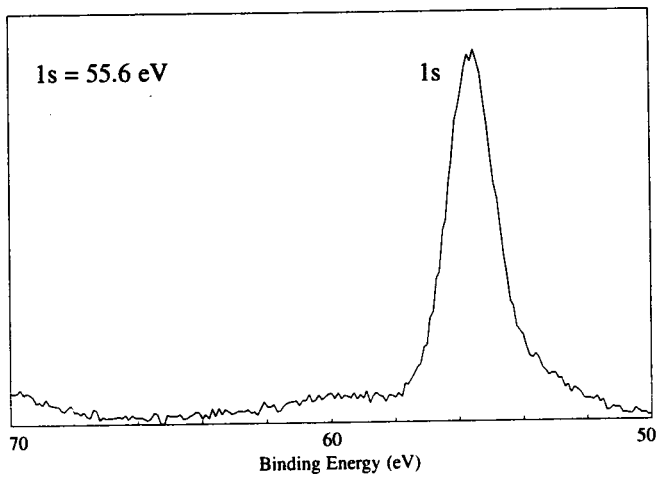


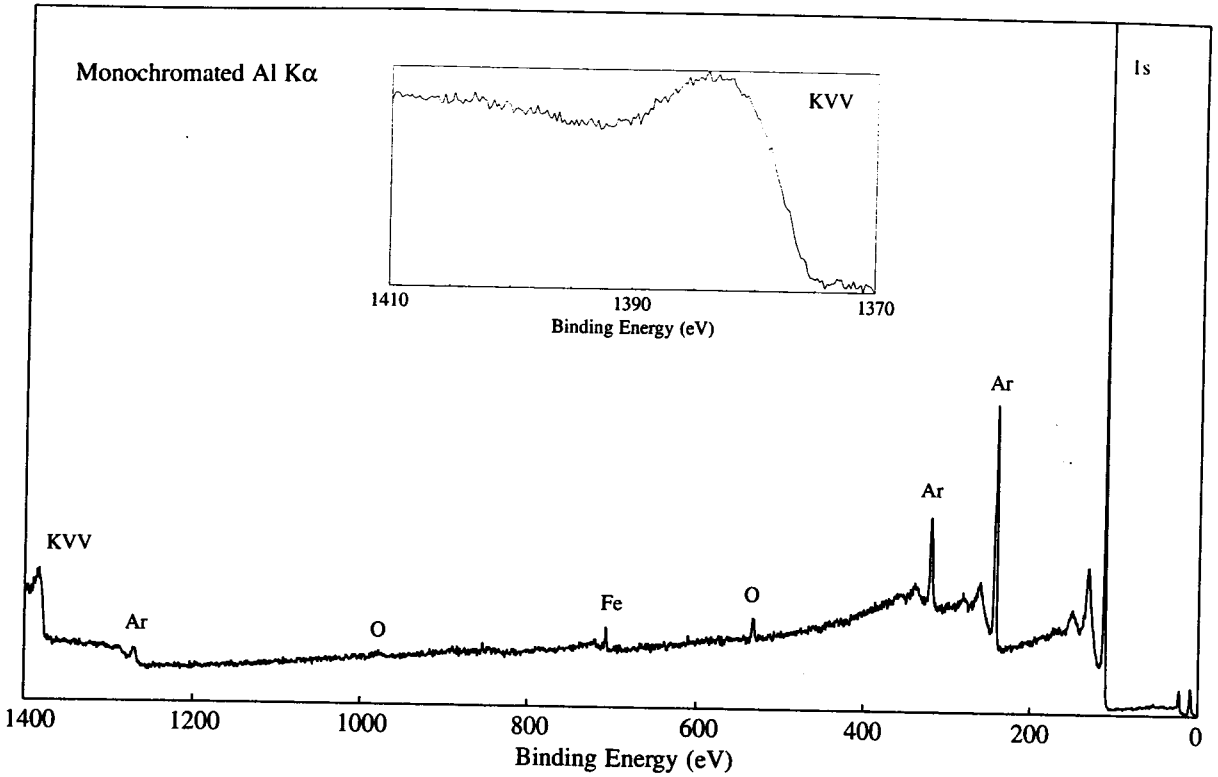
Line Positions (eV)

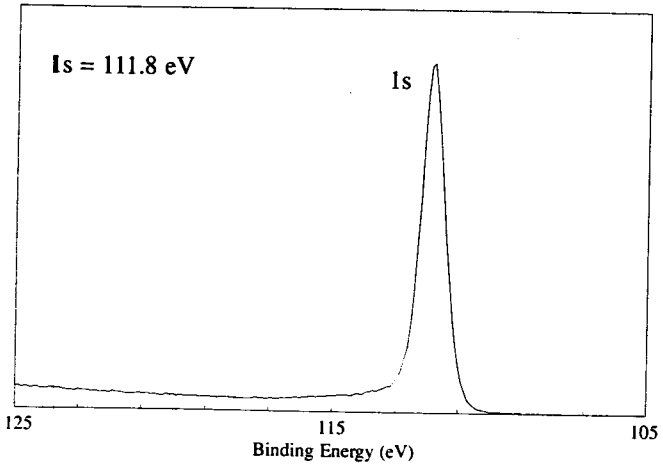
Photoelectron Lines
1s
56


Li in LiF
Mg Kα
F
F
F
F
1s
F
1200
1000
800
600
400
200
0
Binding Energy (eV)


1s Binding Energy (eV)
Compound Type
54
55
56
57
Li
LiBr
LiCl
LiF
Li2O
LiOH
Li2CO3
Li3PO4
Li4P2O7
LiNbO3


1s = 55.6 eV
1s
70
60
50
Binding Energy (eV)





Line Positions (eV)

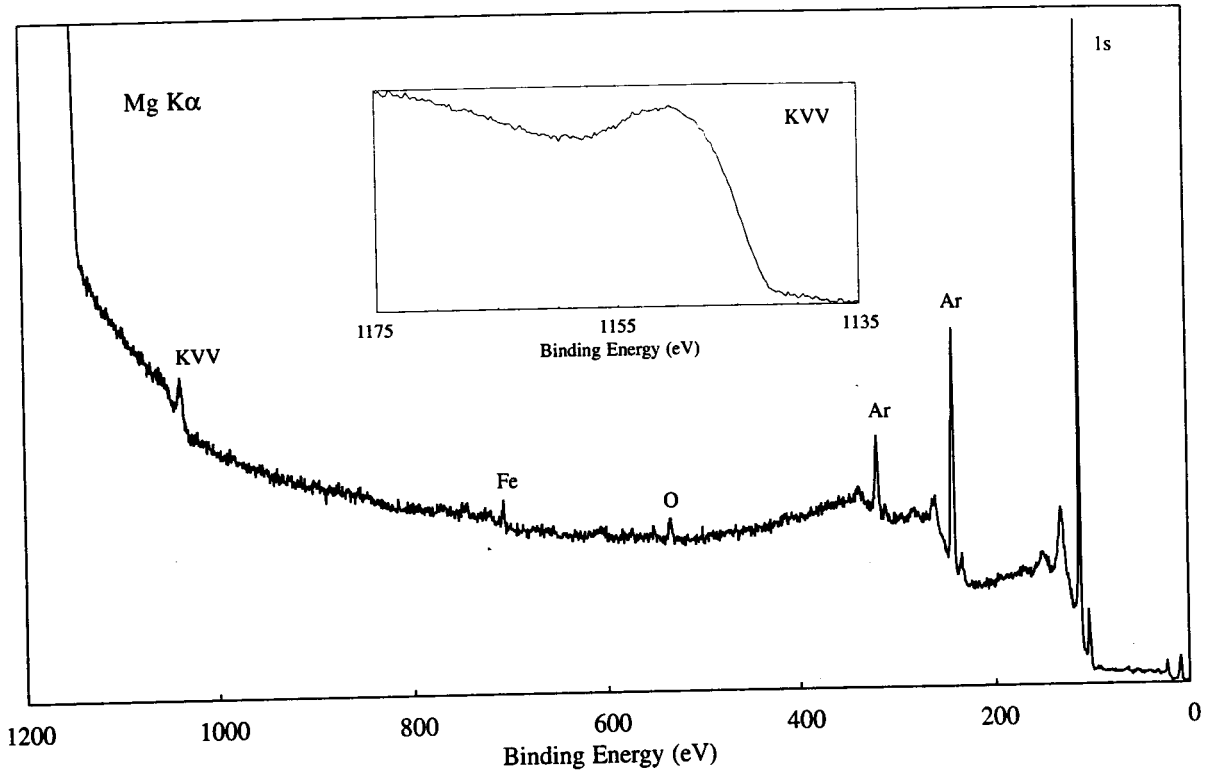
Photoelectron Lines

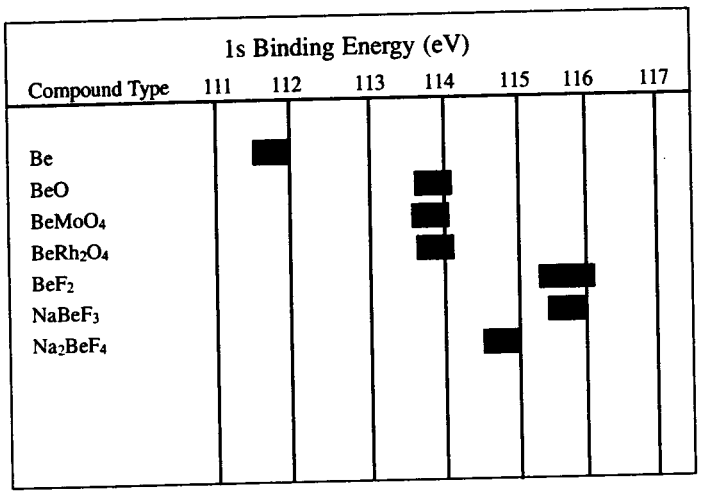
1s
112

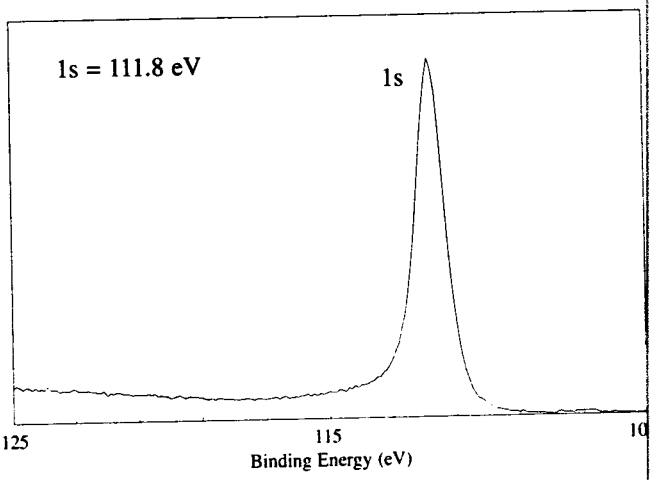
Auger Lines

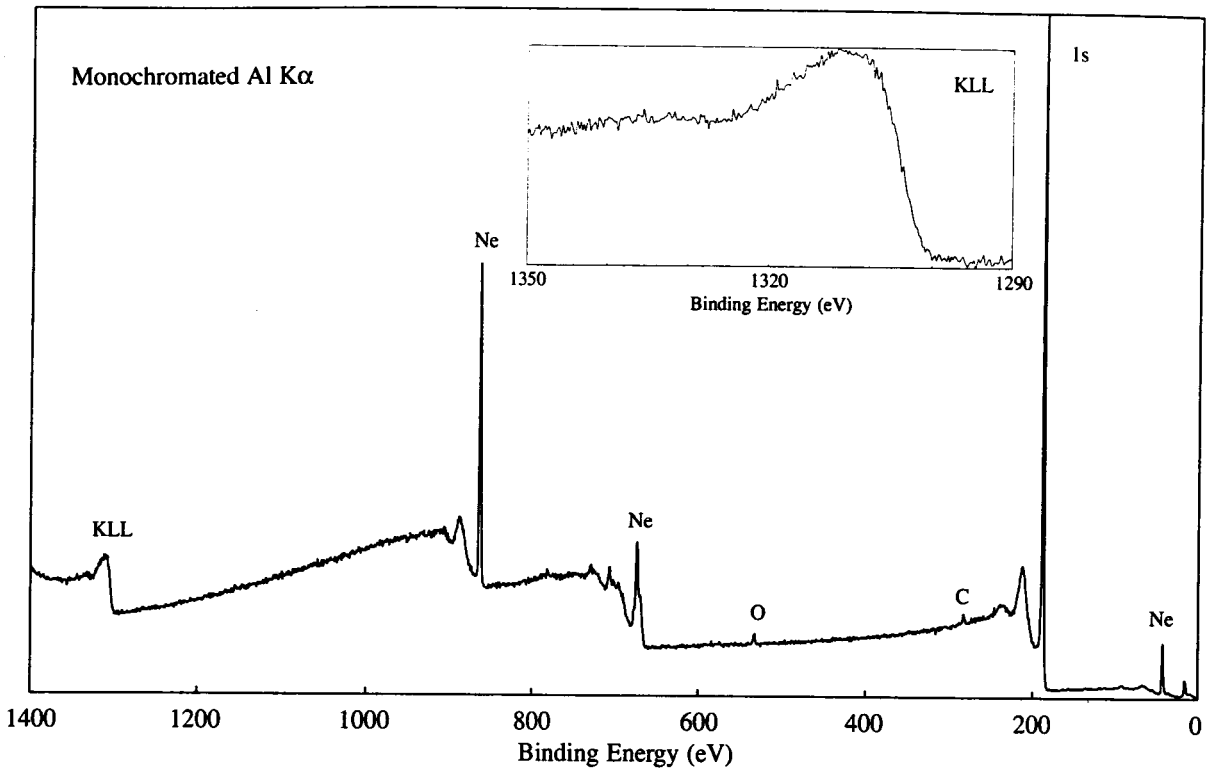
KVV	
1384	(Al)
1151	(Mg)

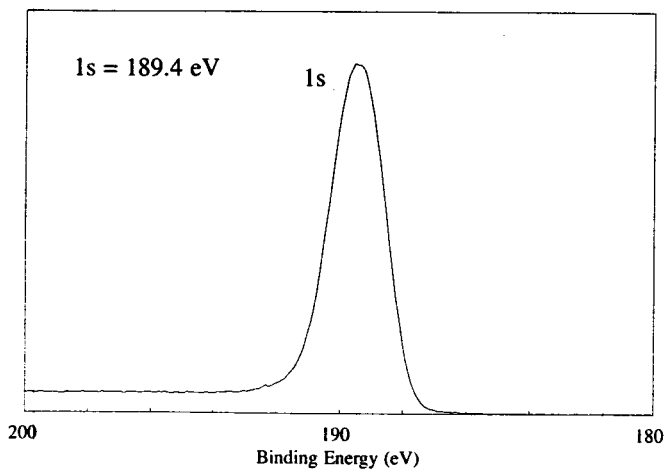
Beryllium Be
Atomic Number 4











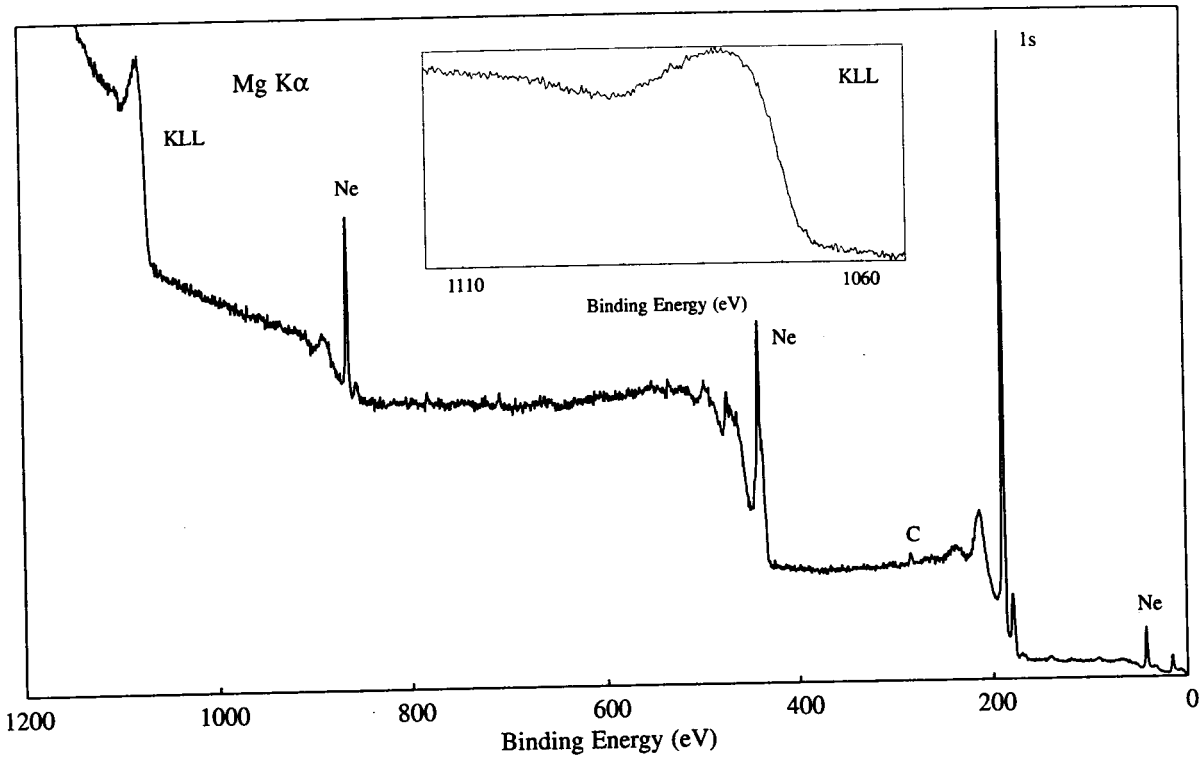
Line Positions (eV)

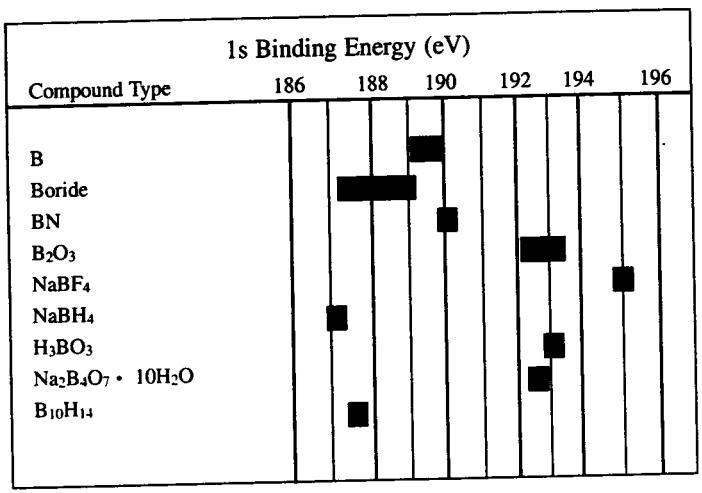
Photoelectron Lines

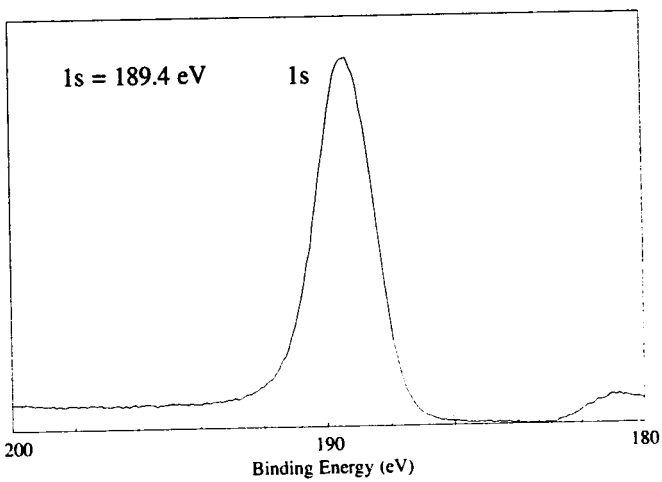
1s
189

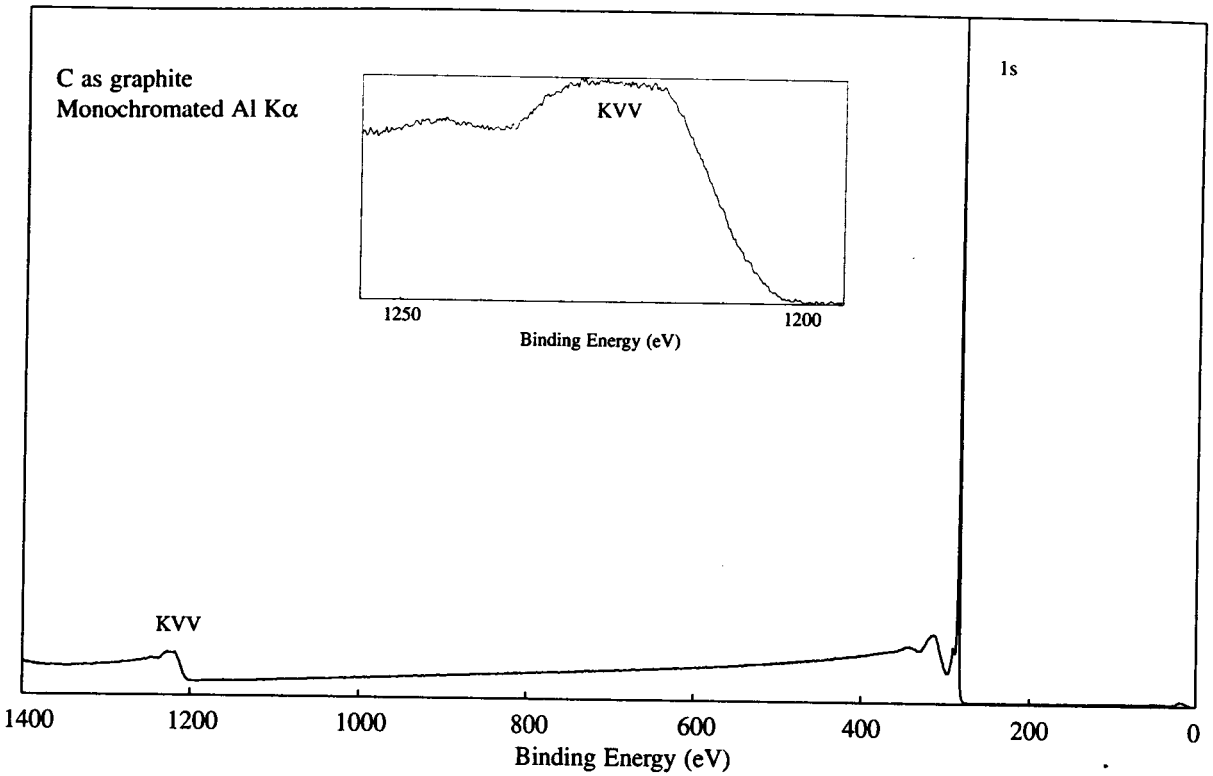
Auger Lines

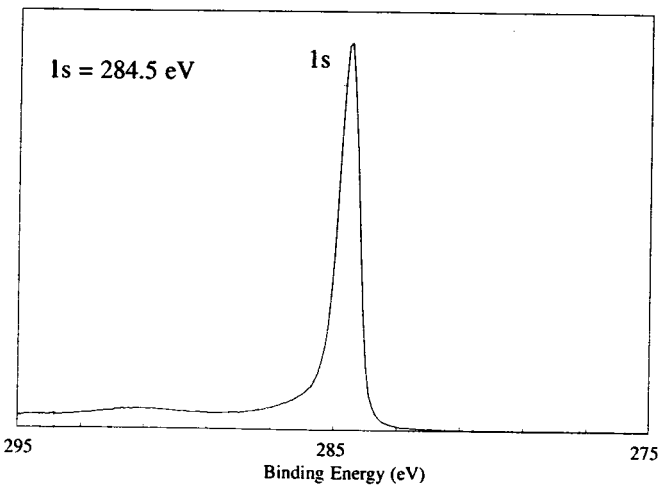
KLL	
1310	(Al)
1077	(Mg)


Mg Kα
KLL
Ne
KLL
1110
1060
Binding Energy (eV)
1s
Ne
C
Ne
1200
1000
800
600
400
200
0
Binding Energy (eV)


1s Binding Energy (eV)
Compound Type
186
188
190
192
194
196
B
Boride
BN
B_2O_3
$NaBF_4$
$NaBH_4$
H_3BO_3
$Na_2B_4O_7 \cdot 10H_2O$
$B_{10}H_{14}$


1s = 189.4 eV
1s
200
190
180
Binding Energy (eV)





Line Positions (eV)

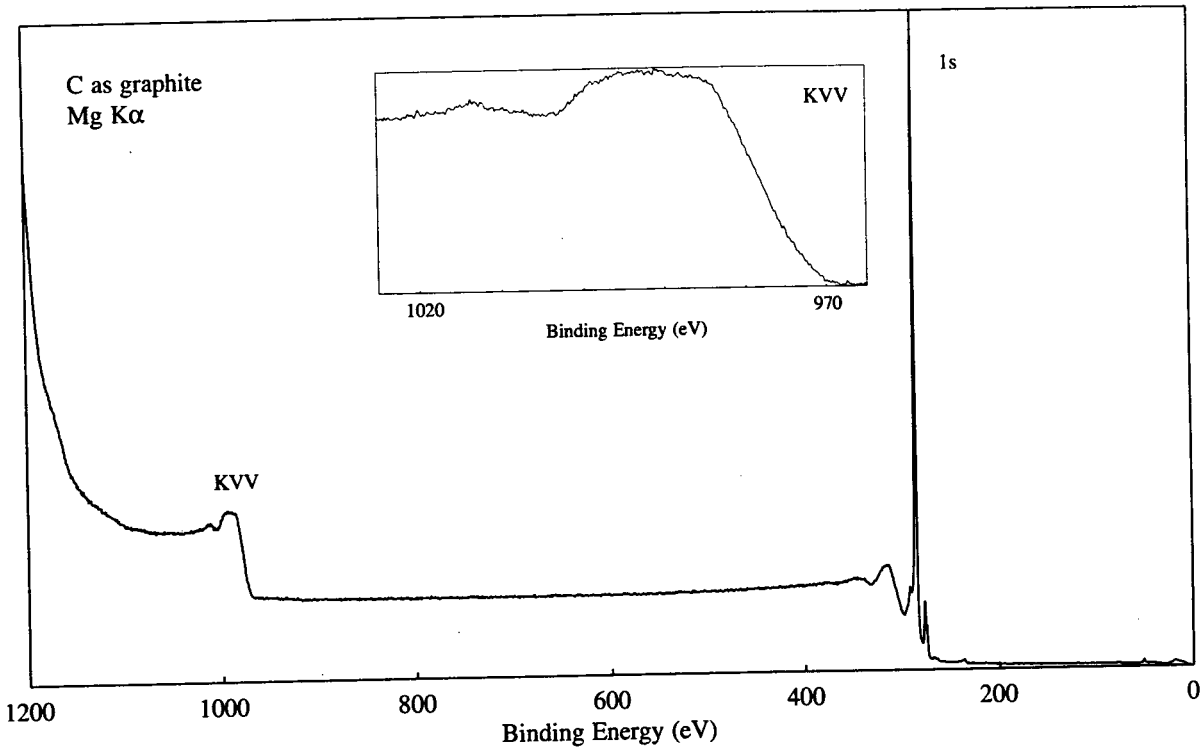
Photoelectron Lines

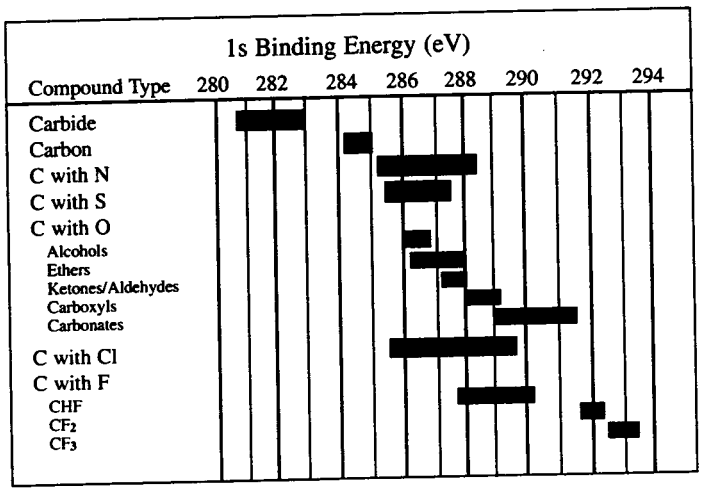
1s
285

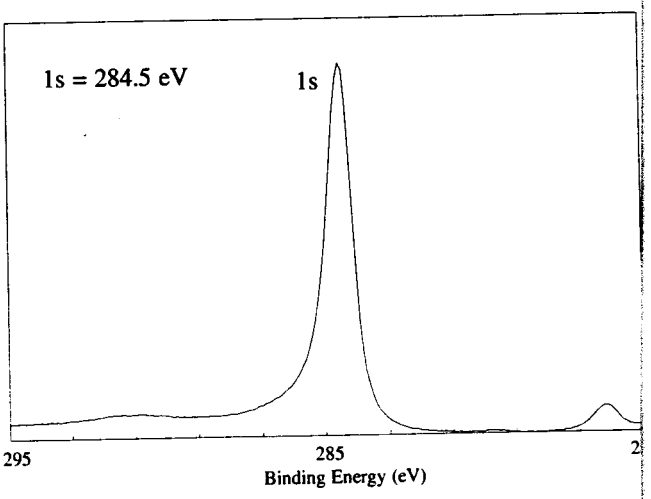
Auger Lines

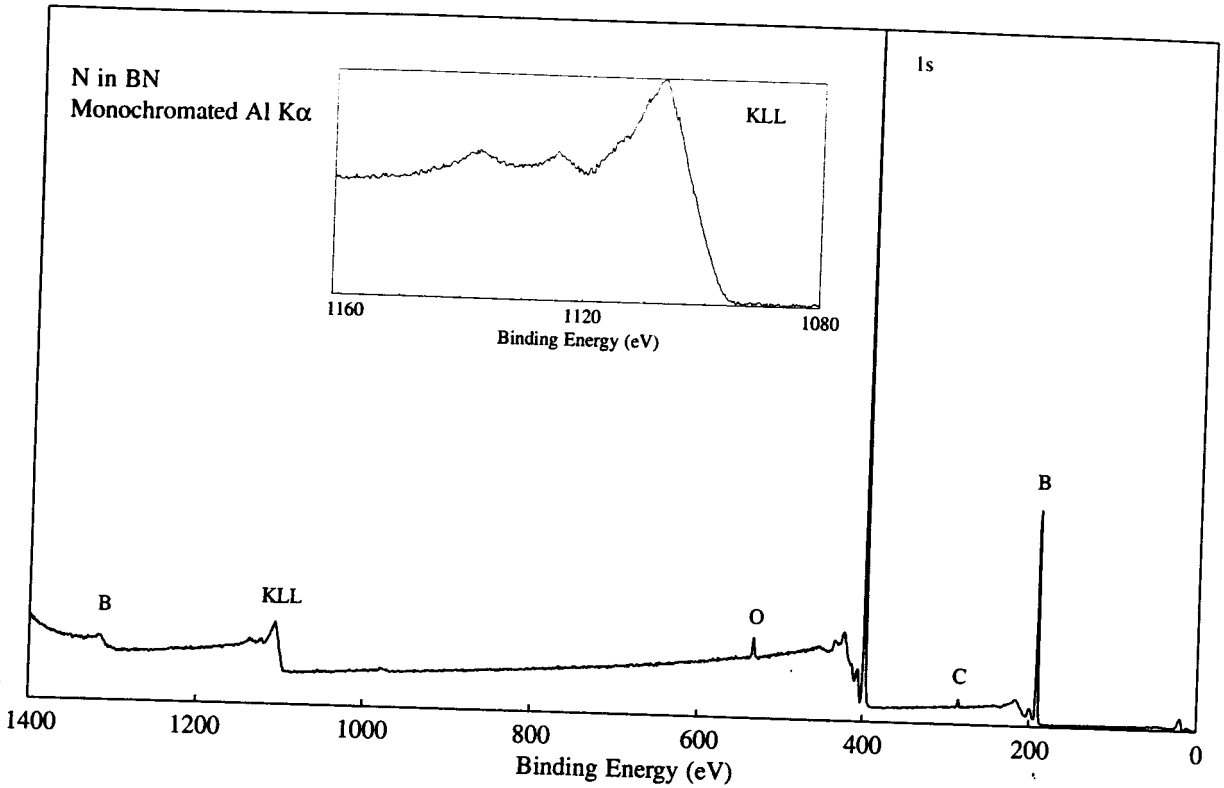
KVV	
1223	(Al)
990	(Mg)

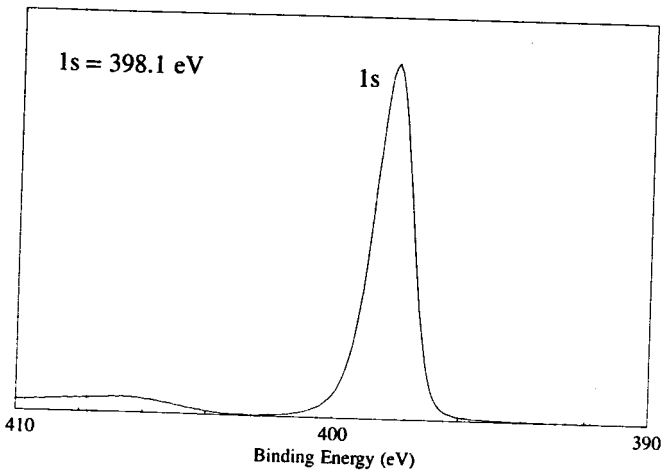
Carbon
Atomic Number C









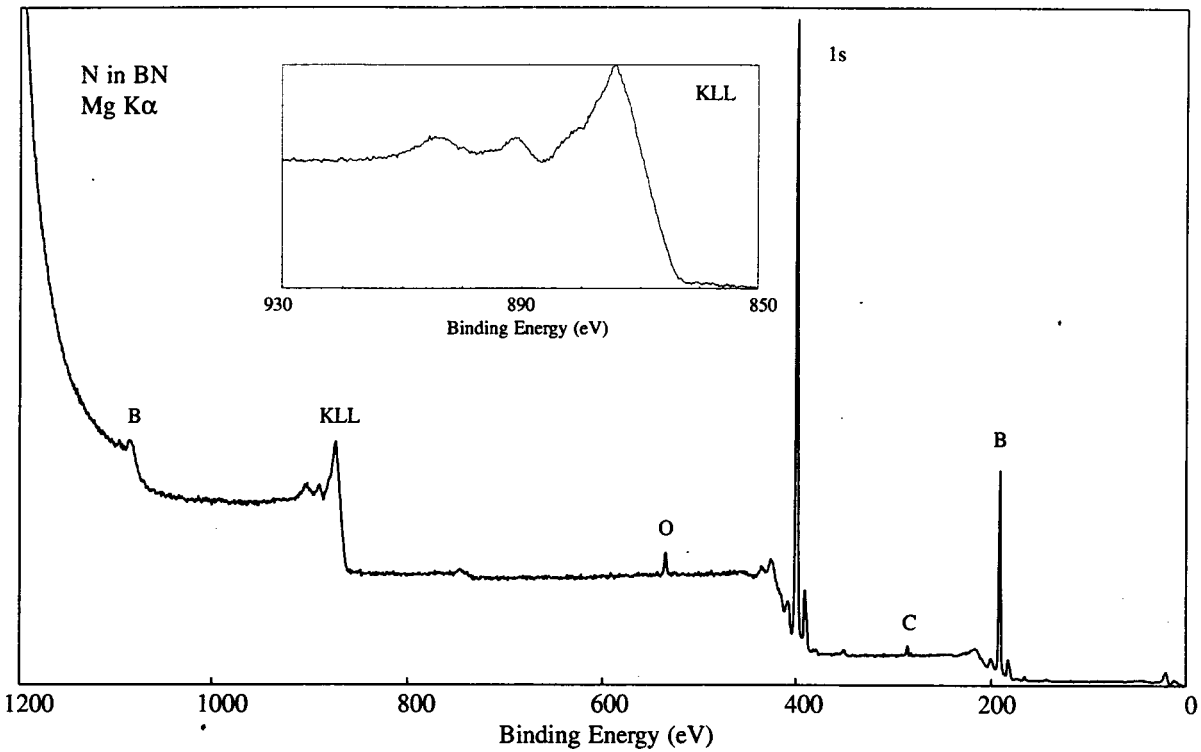


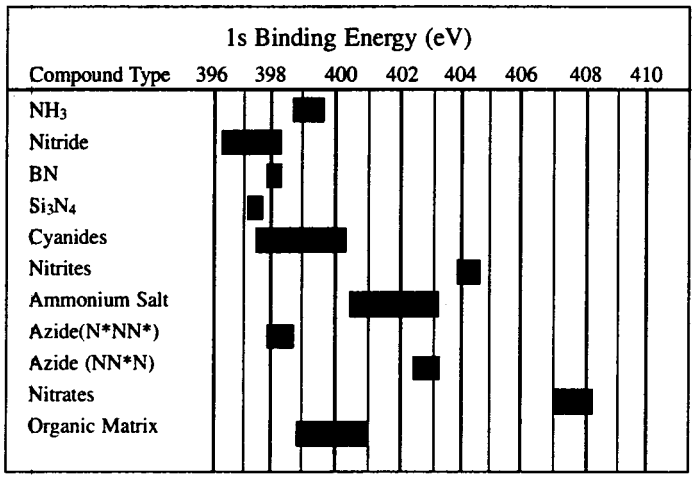
Line Positions (eV)

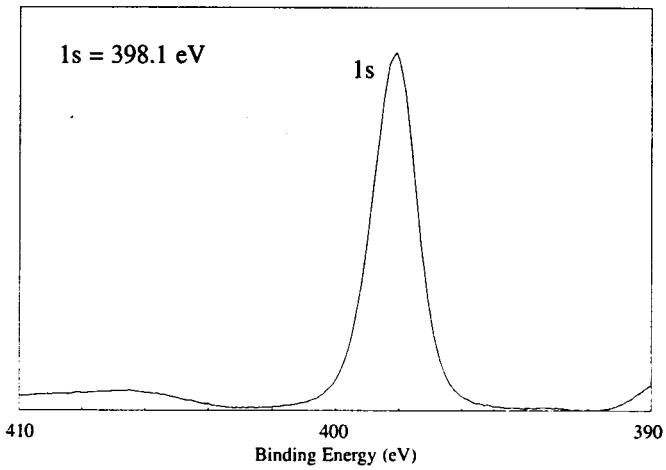
Photoelectron Lines	
1s	
398	

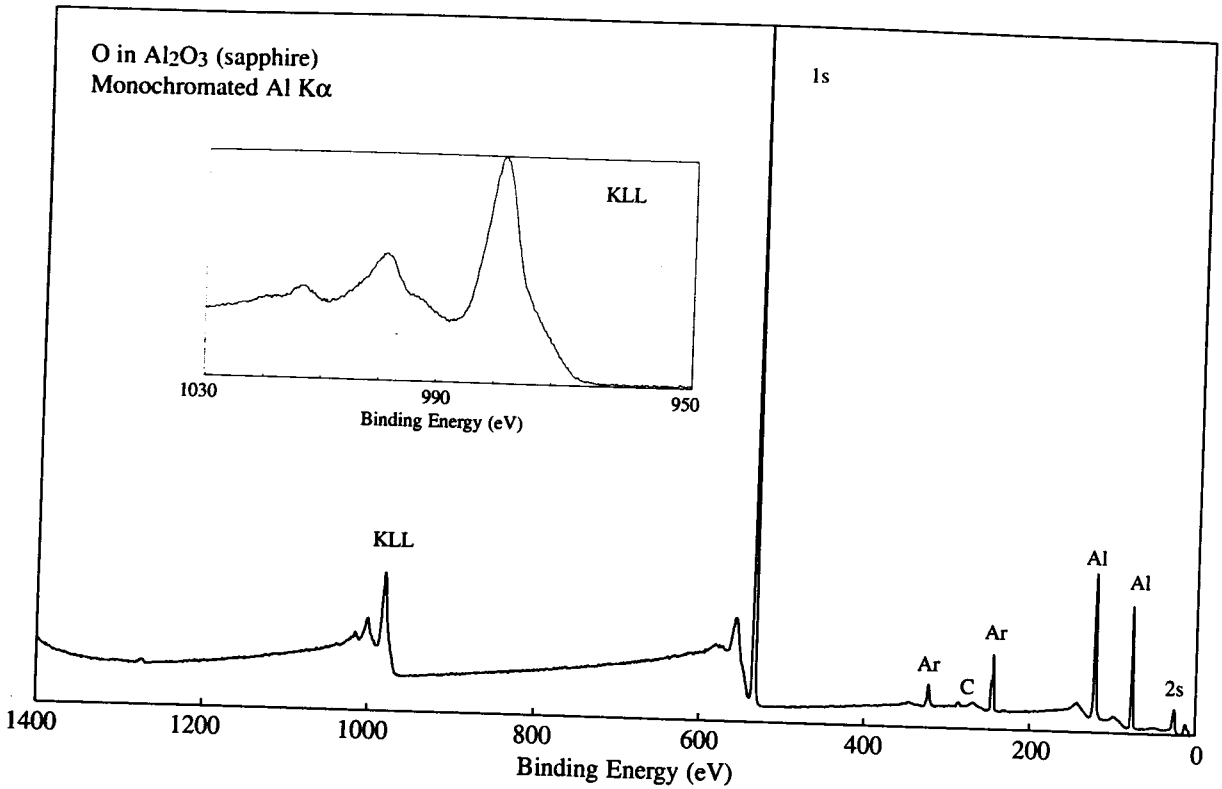
Auger Lines		
KLL		
1107	(Al)	
874	(Mg)	

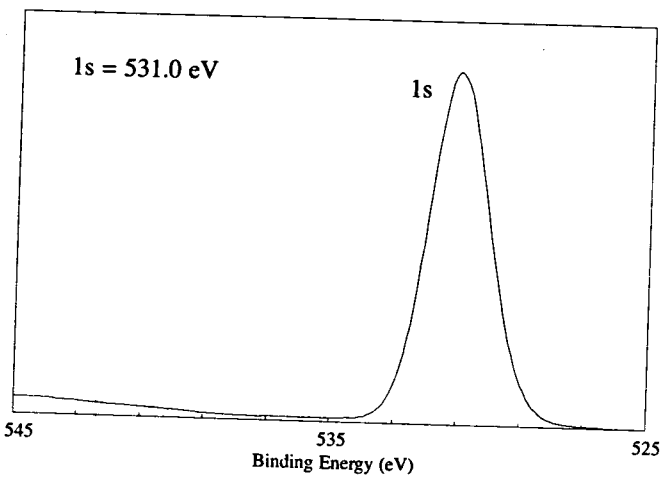
Nitrogen N
Atomic Number 7











Line Positions (eV)

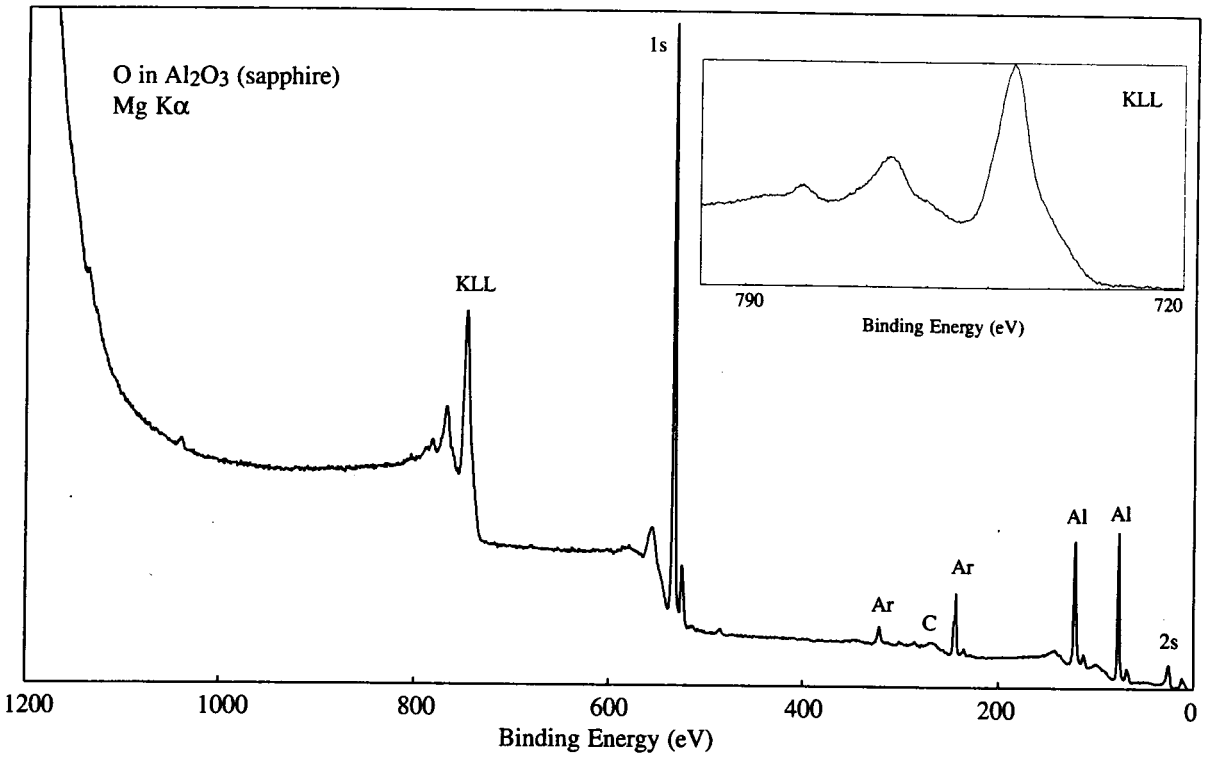
Photoelectron Lines

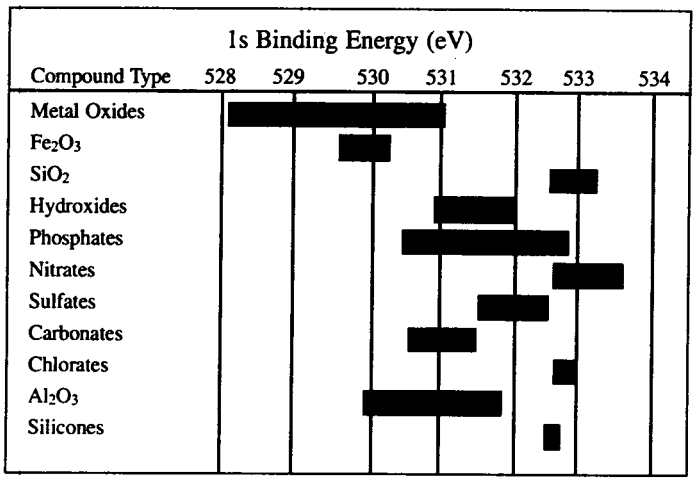
1s	2s
531.	23

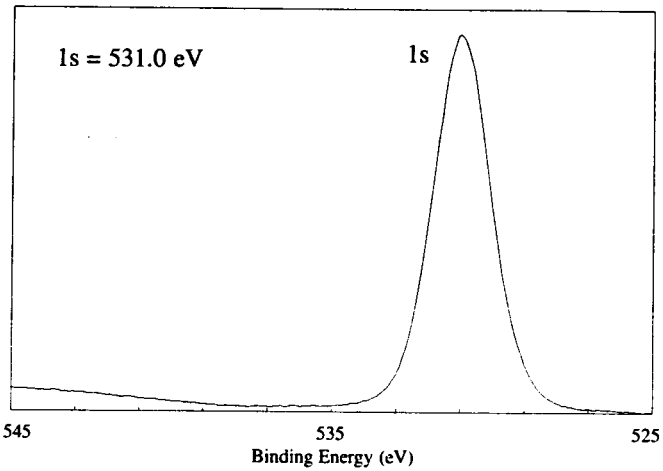
Auger Lines

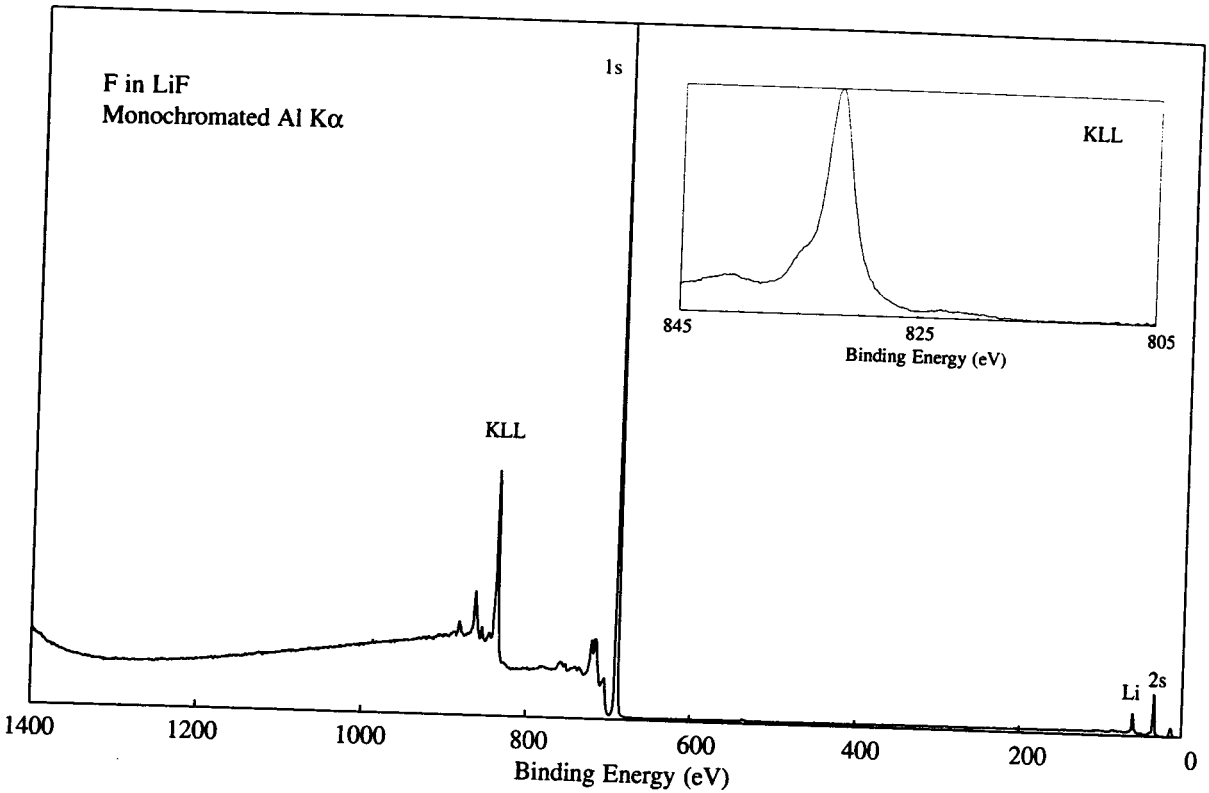
KL_1L_1	KL_1L_{23}	$KL_{23}L_{23}$	
1013	999	978	(Al)
780	766	745	(Mg)

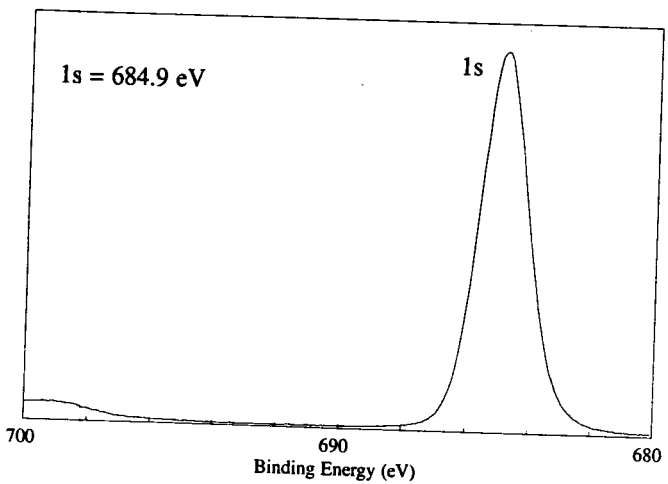
Oxygen O
Atomic Number 8











Line Positions (eV)

Photoelectron Lines

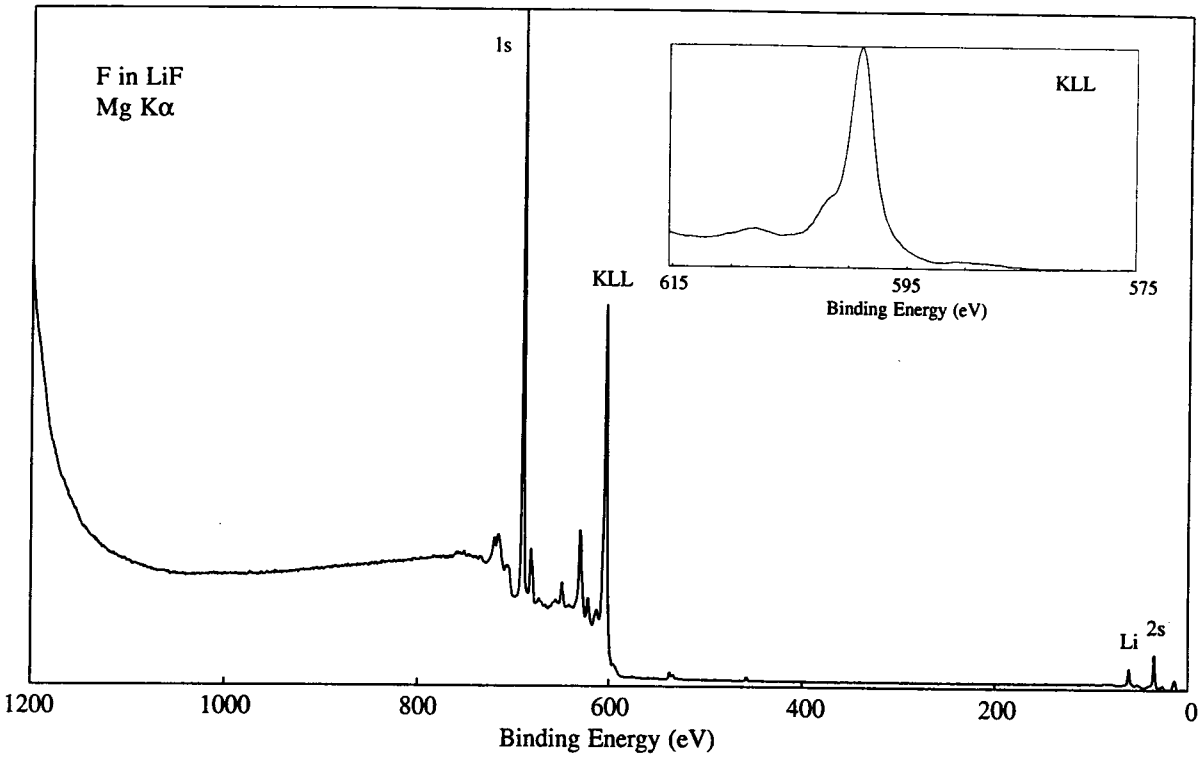
1s	2s
685	30

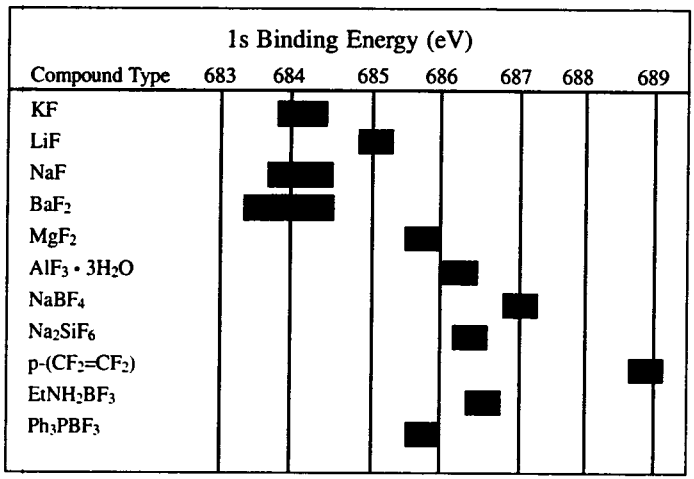
Auger Lines

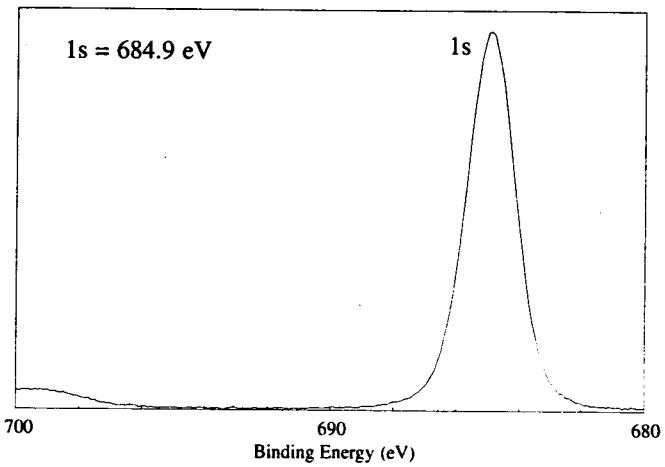
KL_1L_1	KL_1L_{23}	$KL_{23}L_{23}$	
877	858	832	(Al)
644	625	599	(Mg)

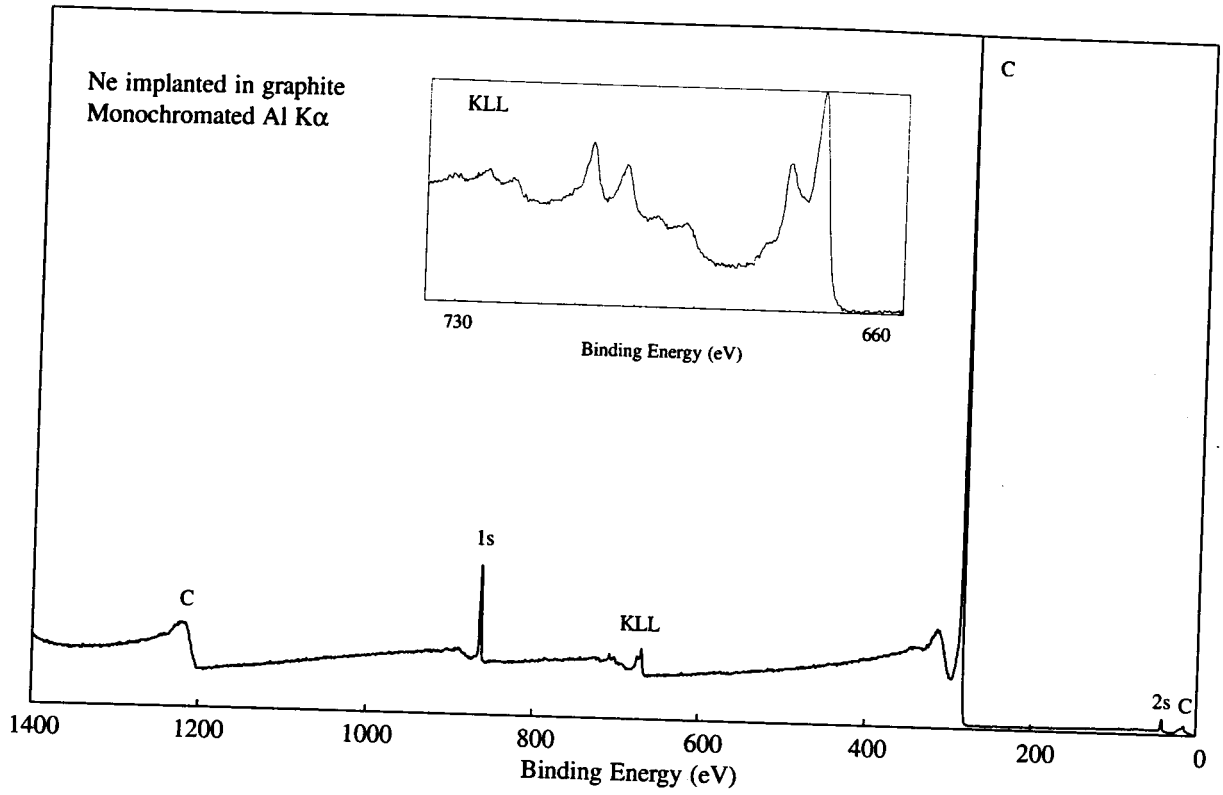
Fluorine F

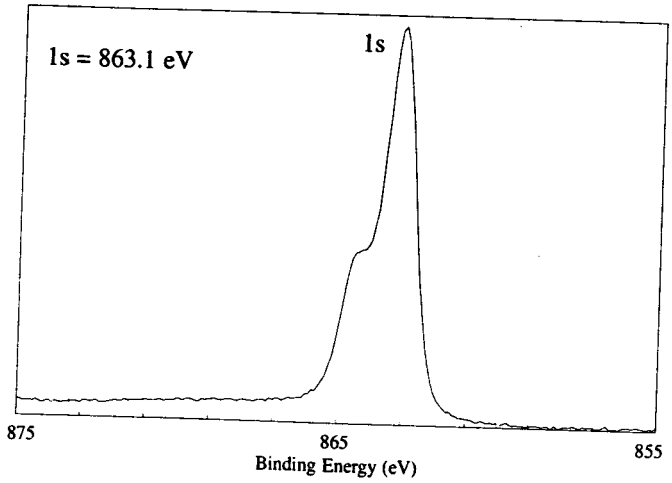
Atomic Number 9











Line Positions (eV)

Photoelectron Lines

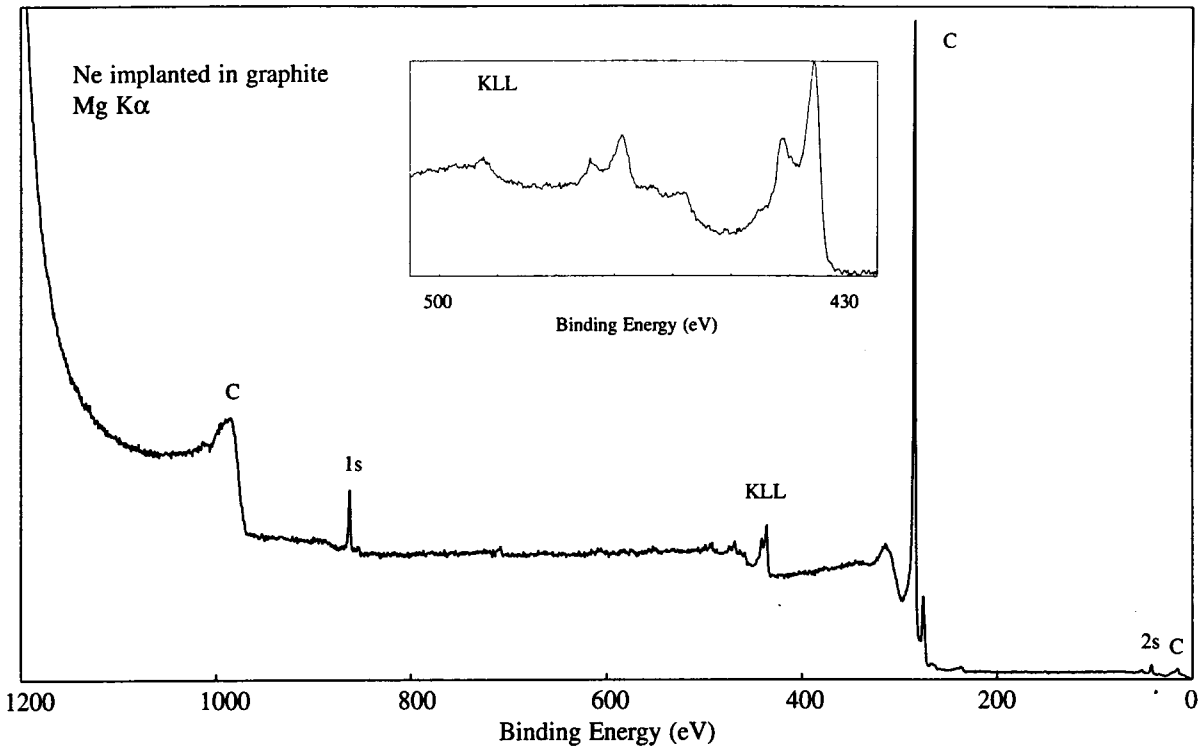
1s	2s	2p
863	41	14

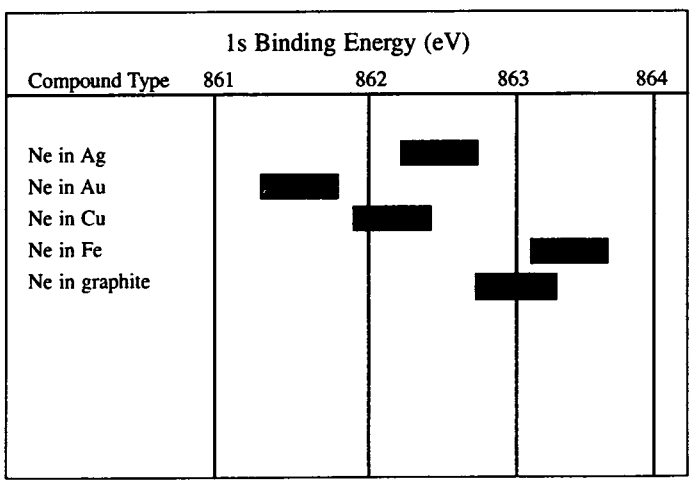
Auger Lines

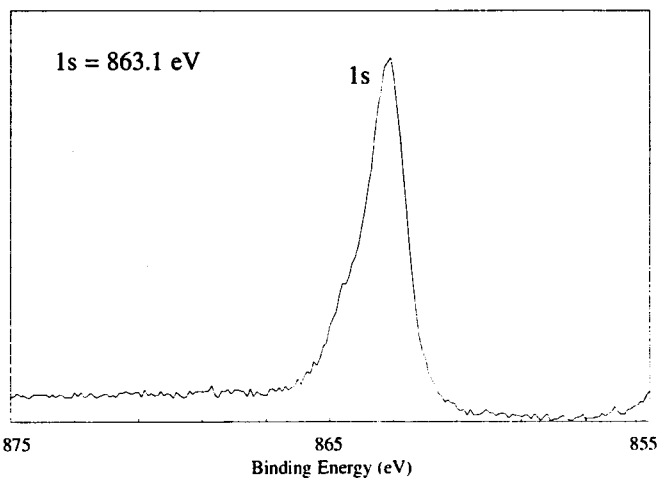
KL_1L_1	KL_1L_{23}	$KL_{23}L_{23}$	
725	702	669	(Al)
492	469	436	(Mg)

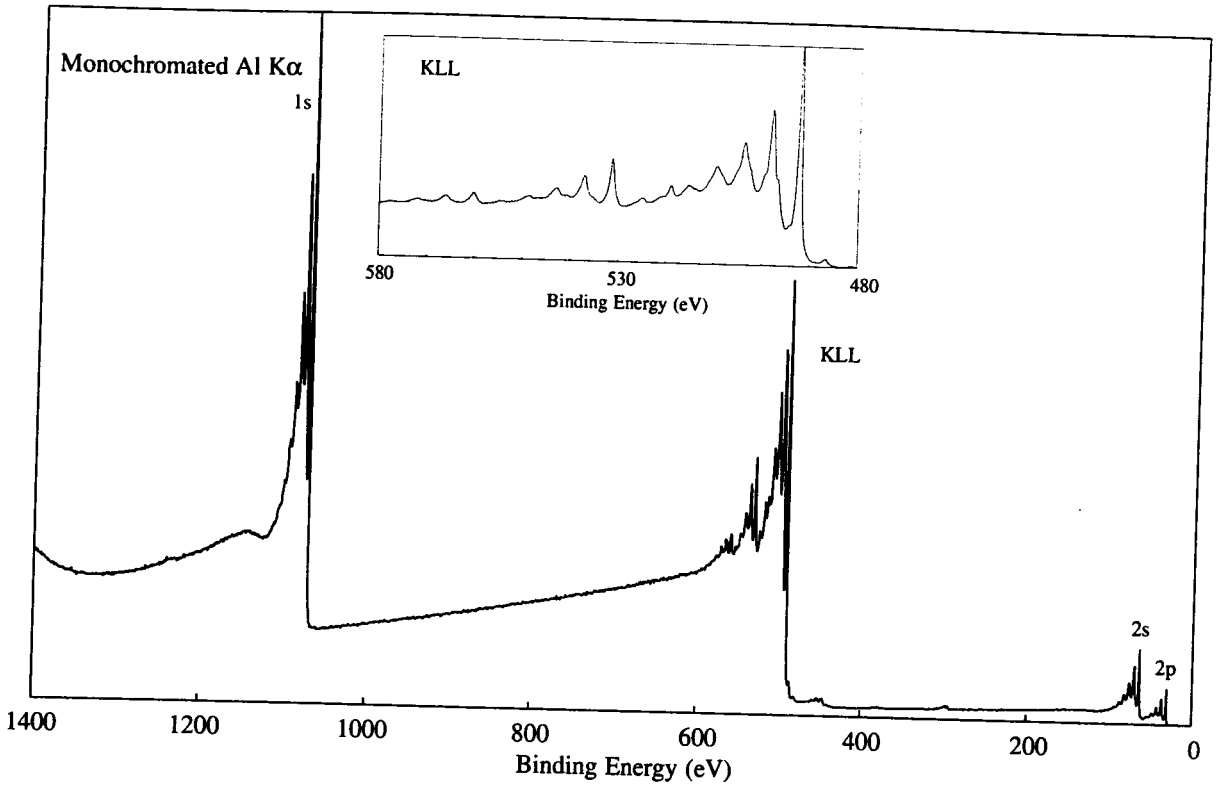
Neon Ne

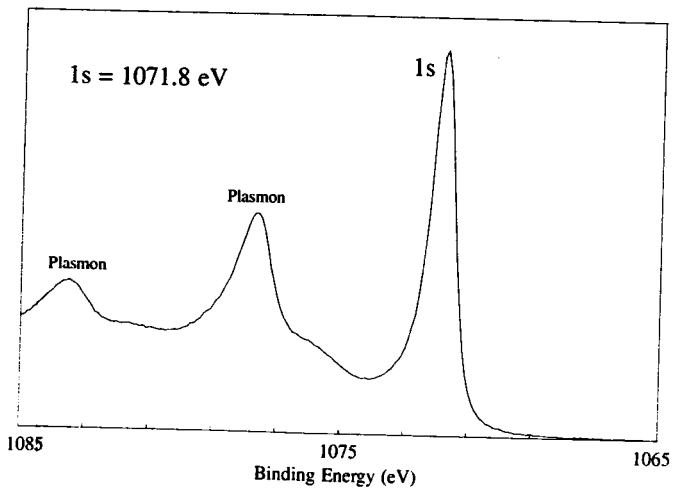
Atomic Number 10











Line Positions (eV)

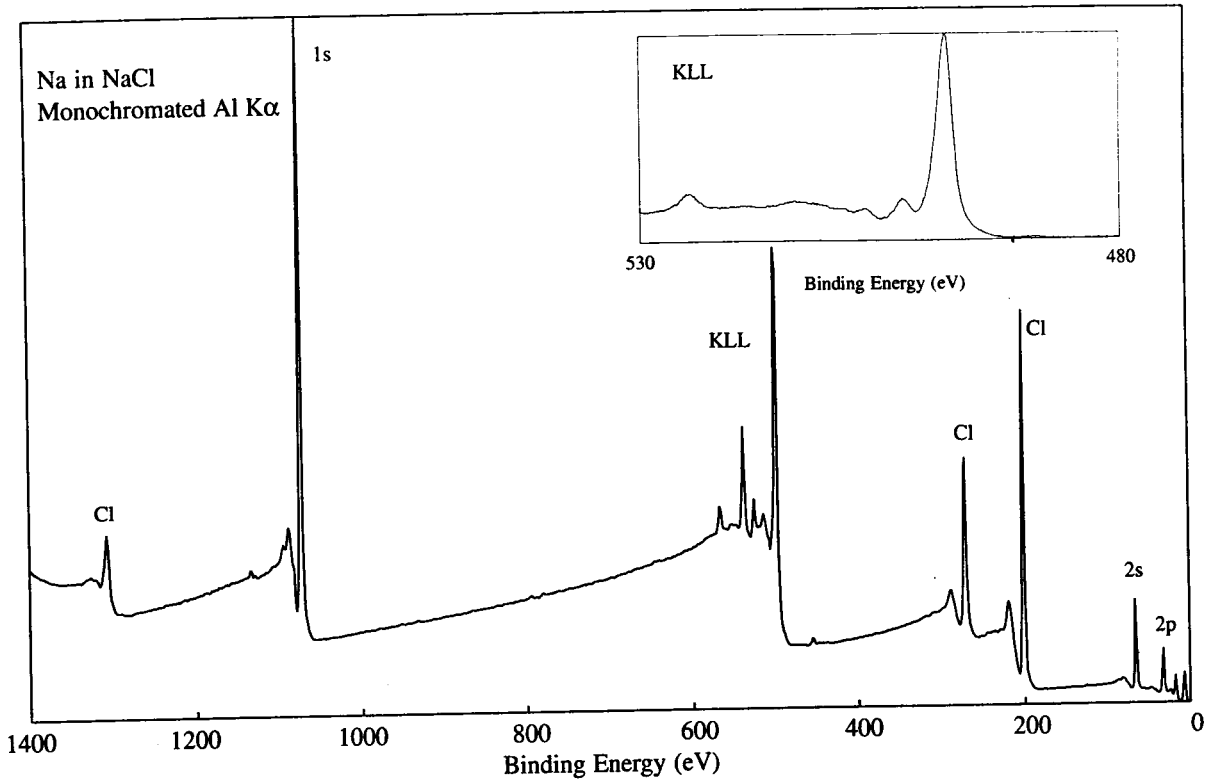
Photoelectron Lines

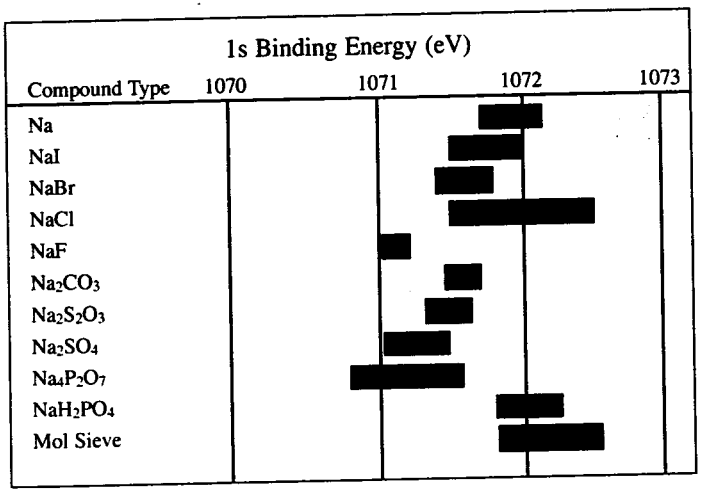
1s	2s	2p
1072	64	31

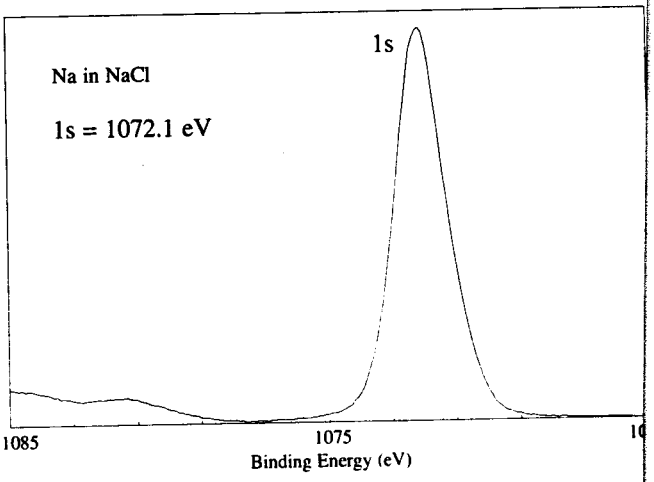
Auger Lines

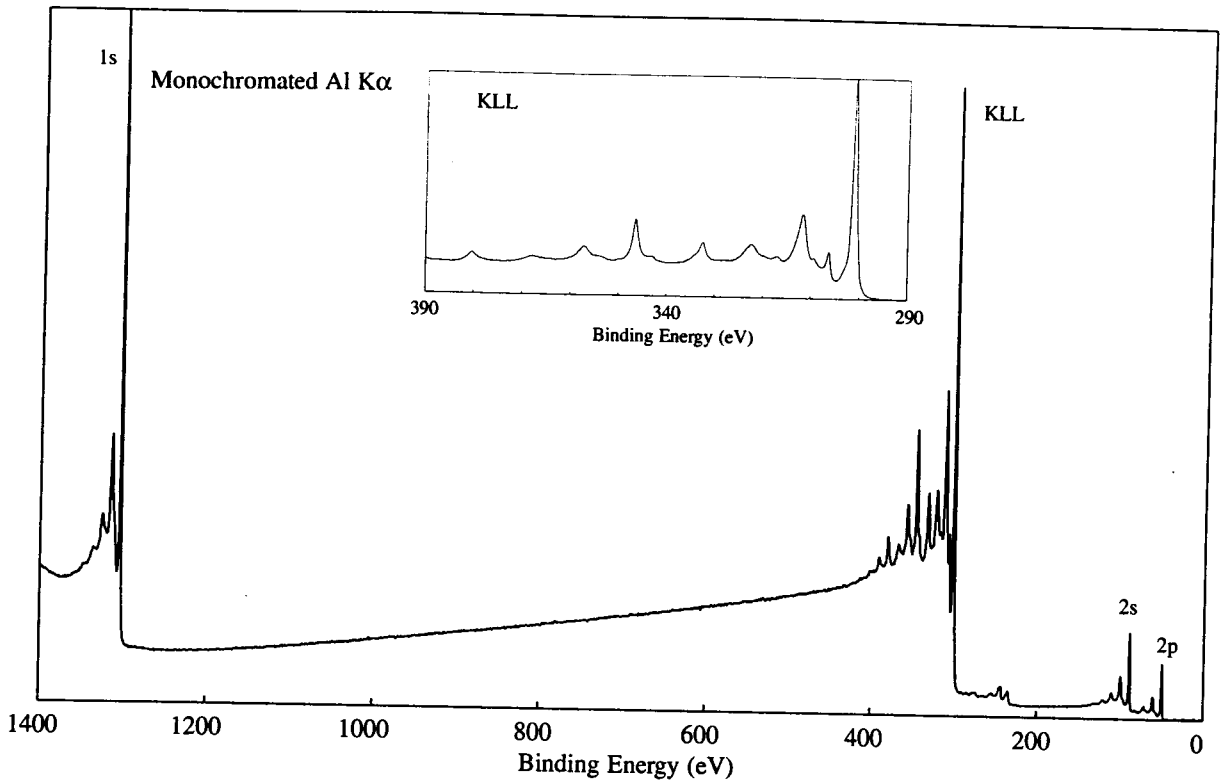
KL_1L_1	KL_1L_{23}	$KL_{23}L_{23}$	
561	532	493	(Al)
328	299	260	(Mg)

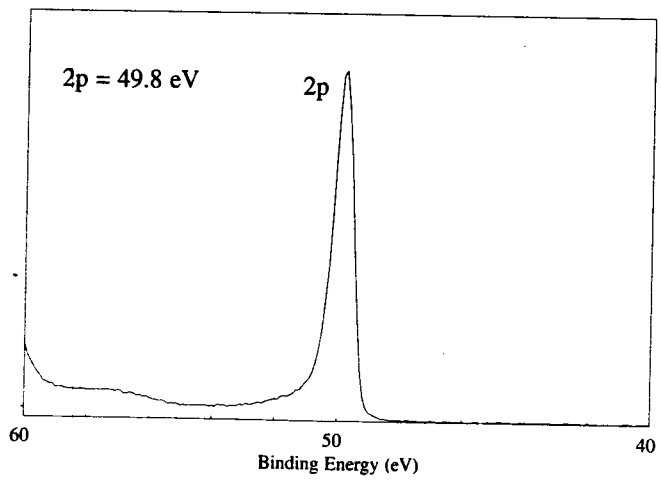
Sodium Na
Atomic Number 11











Line Positions (eV)

Photoelectron Lines

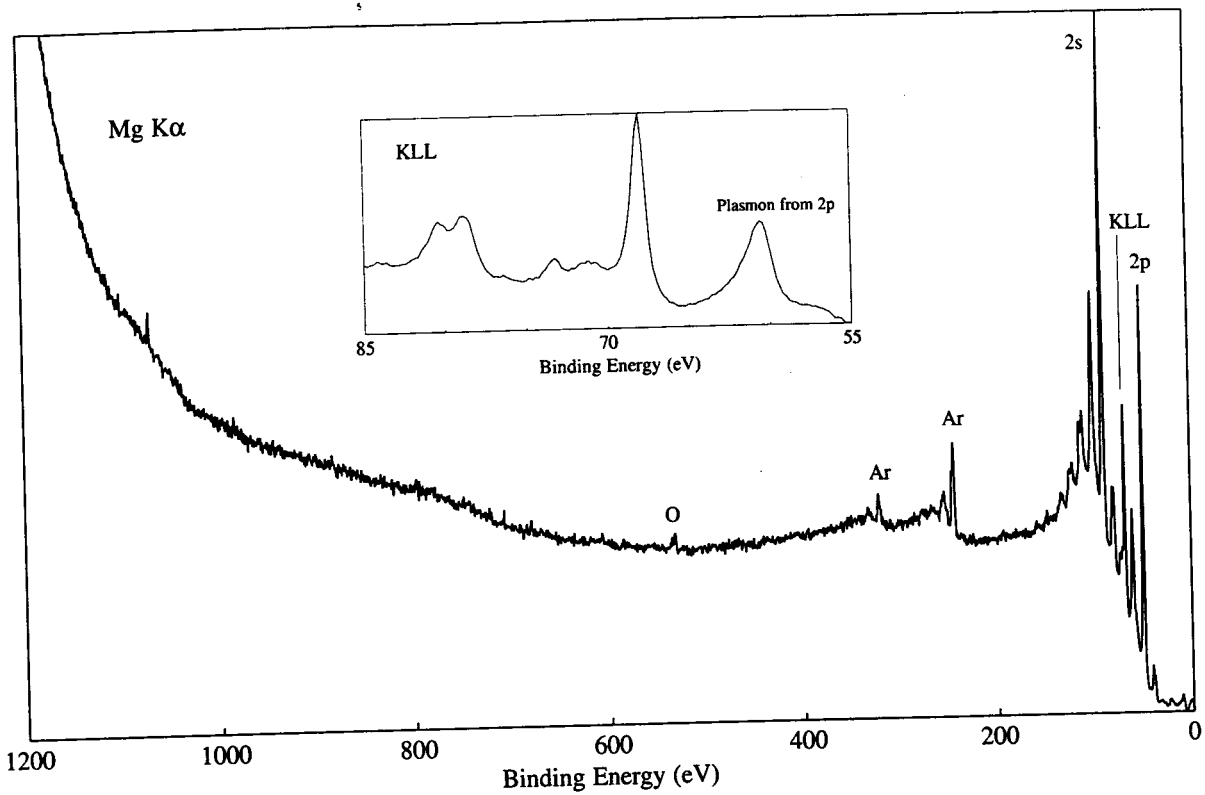
1s	2s	2p
1303	89	50

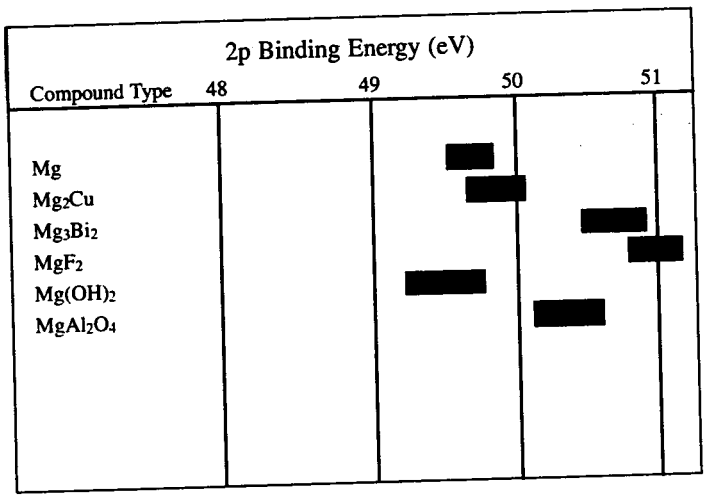
Auger Lines

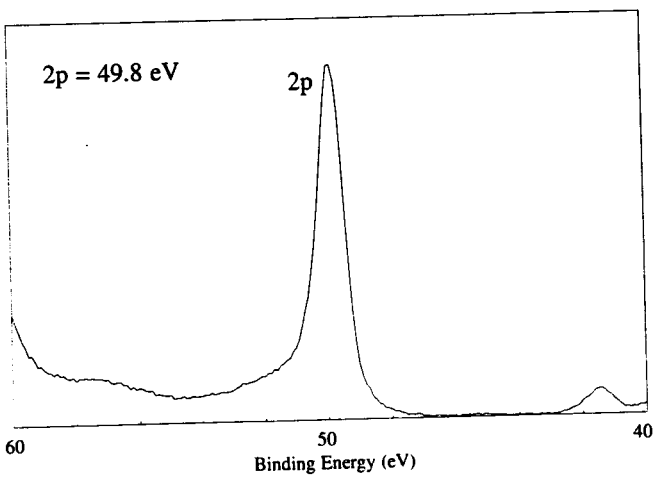
KL_1L_1	KL_1L_{23}	$KL_{23}L_{23}$	
381	347	301	(Al)
148	114	68	(Mg)

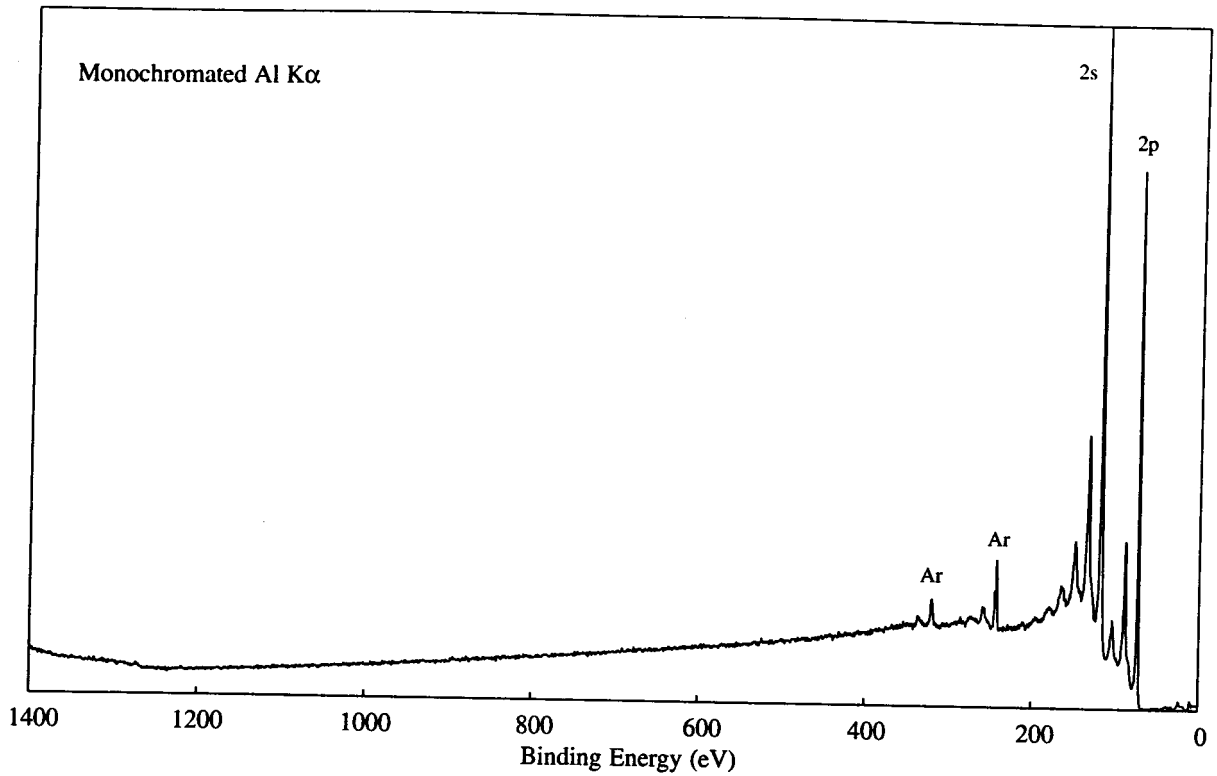
Magnesium Mg

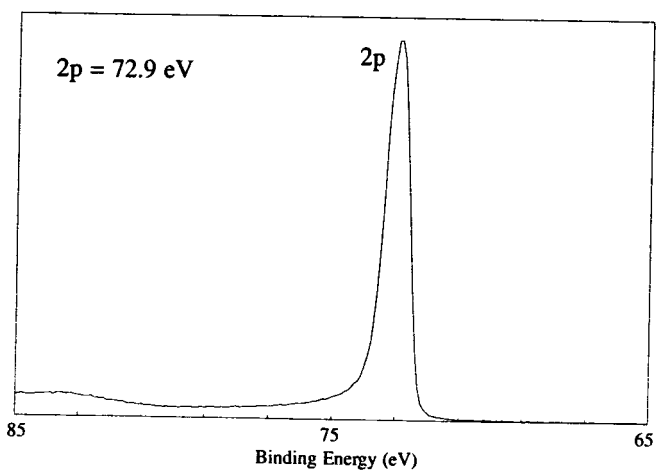
Atomic Number 12











Line Positions (eV)

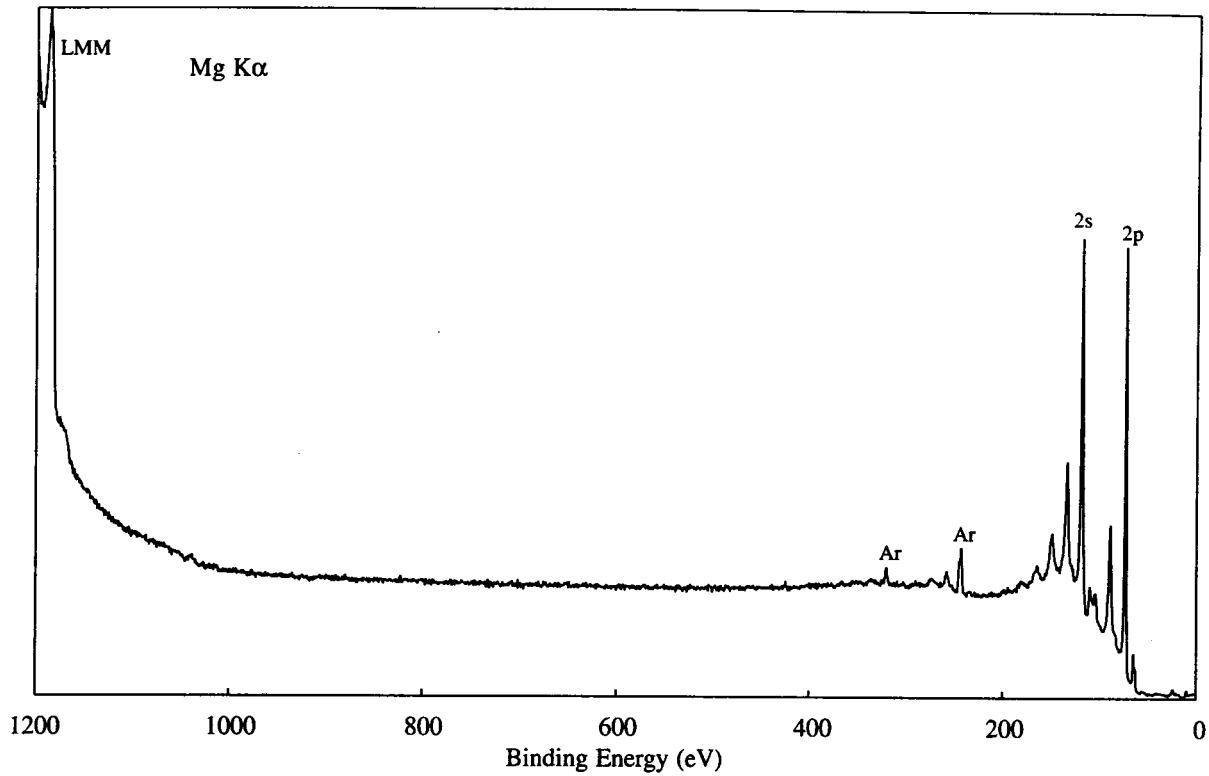
Photoelectron Lines

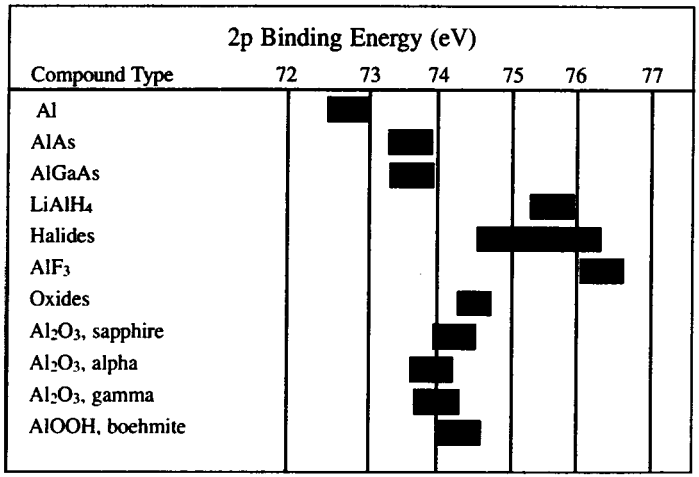
2s	2p
118	73

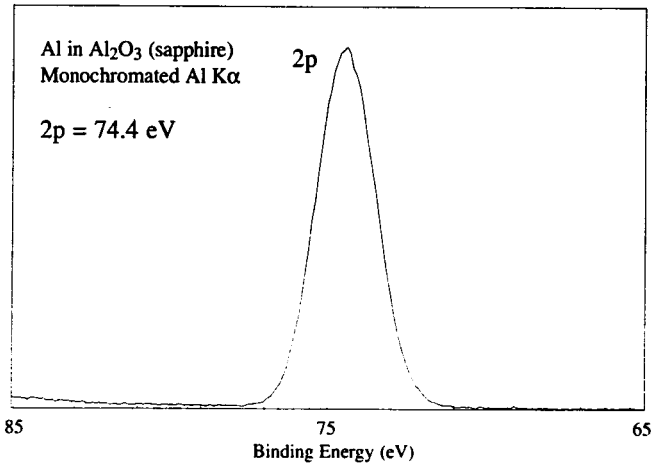
Auger Lines

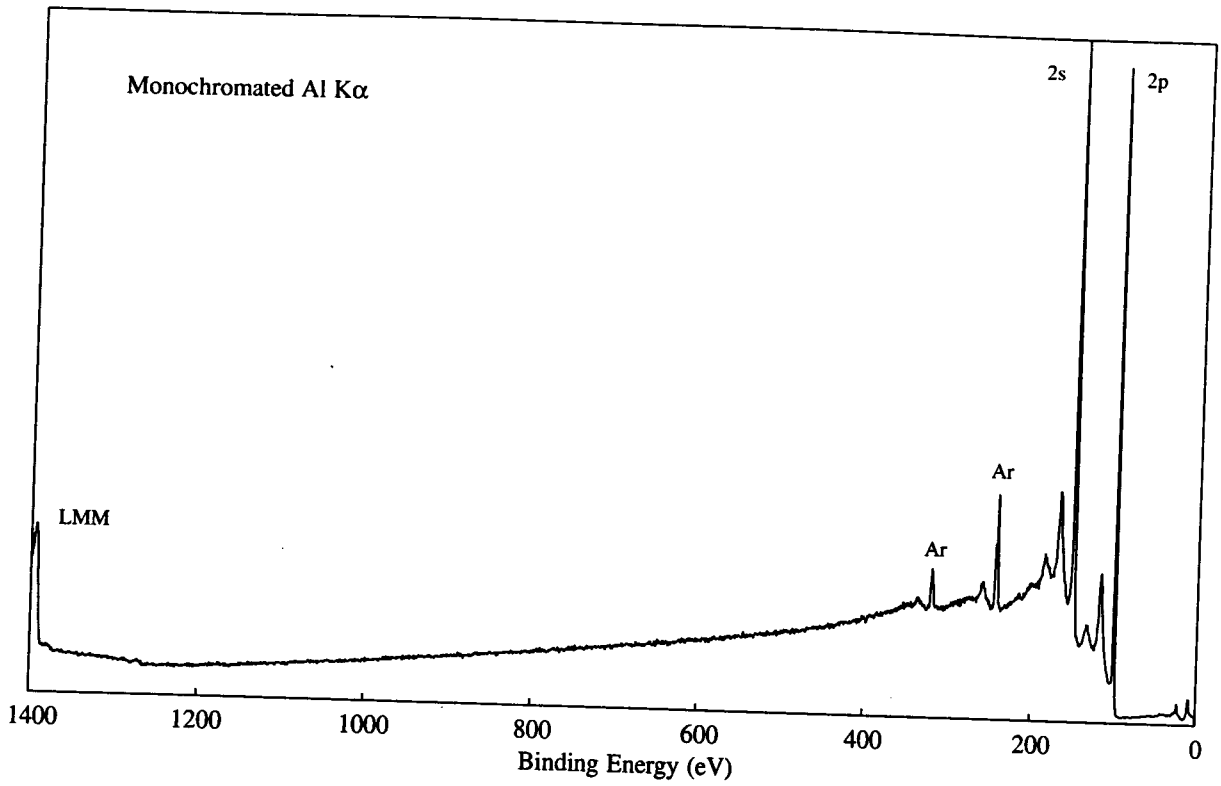
$L_{23}M_1M_{23}$	
1419	(Al)
1186	(Mg)

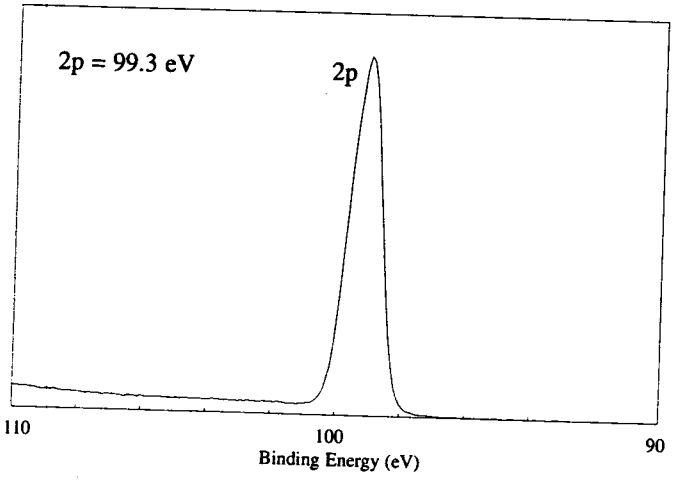
Aluminum Al
Atomic Number 13











Line Positions (eV)

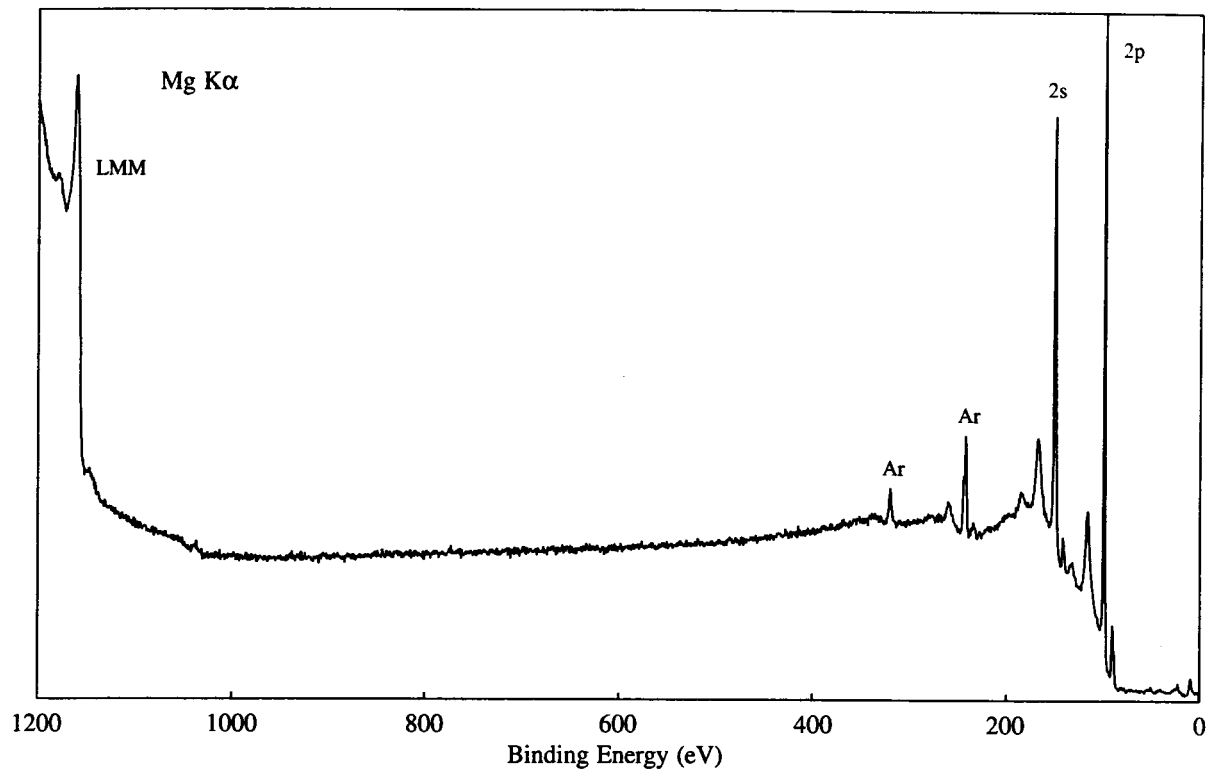
Photoelectron Lines

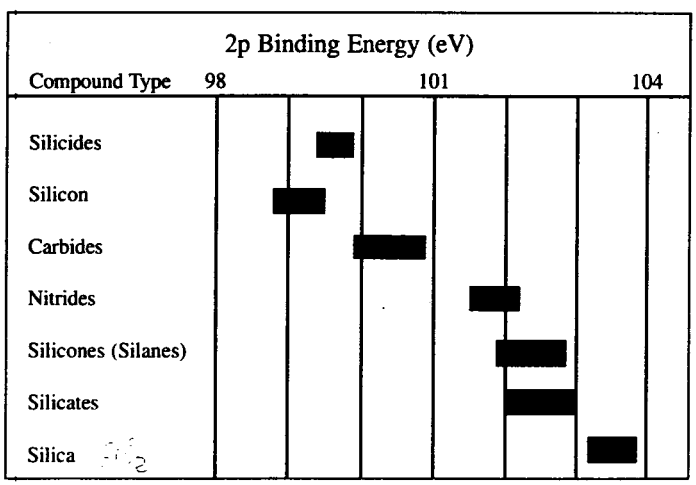
2s	2p
151	99

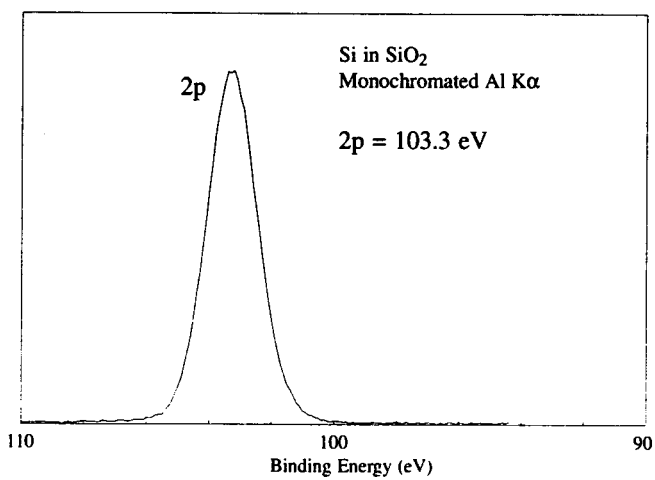
Auger Lines

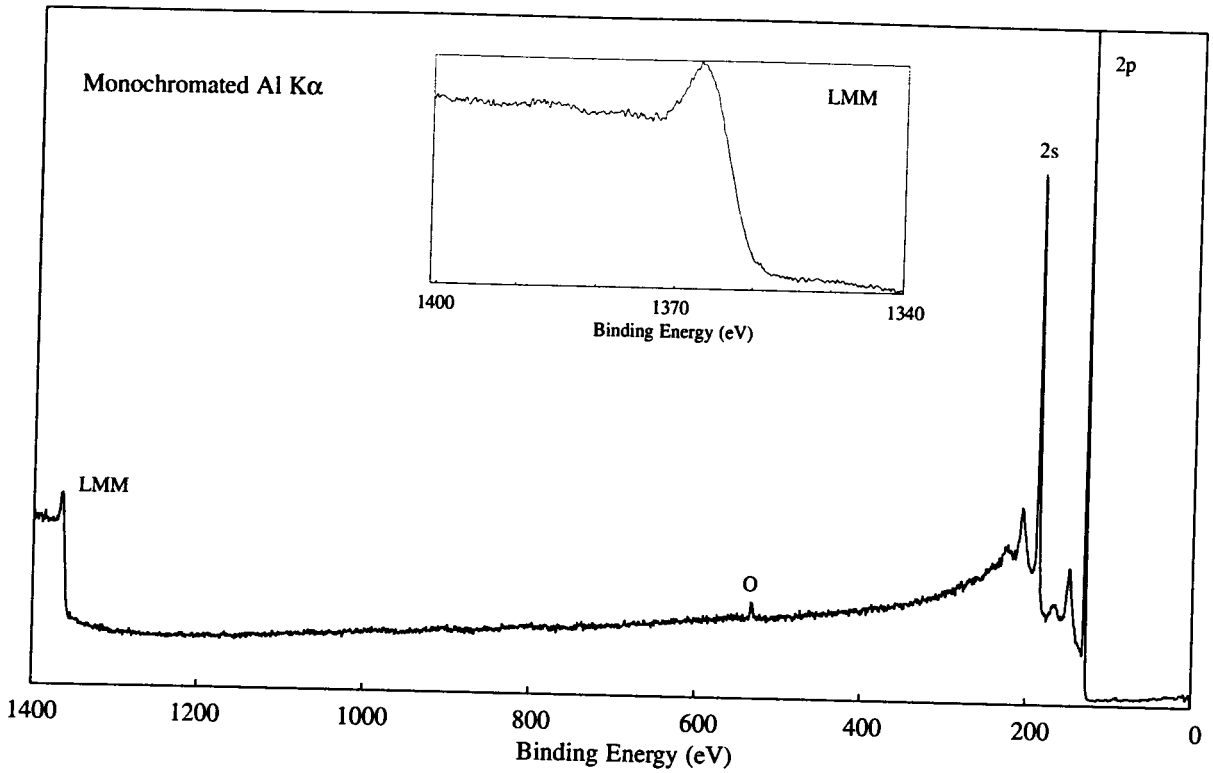
$L_{23}M_{23}M_{23}$

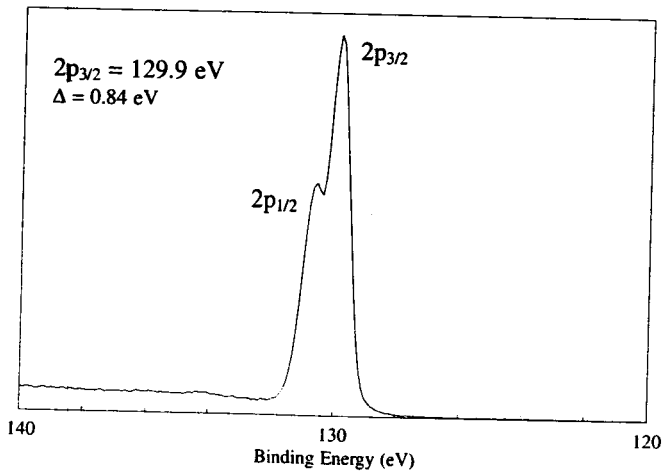
1394	(Al)
1161	(Mg)


Mg Kα
LMM
2p
2s
Ar
Ar
1200
1000
800
600
400
200
0
Binding Energy (eV)


2p Binding Energy (eV)
Compound Type
98
101
104
Silicides
Silicon
Carbides
Nitrides
Silicones (Silanes)
Silicates
Silica


Si in SiO2
Monochromated Al Kα
2p
2p = 103.3 eV
110
100
90
Binding Energy (eV)





Line Positions (eV)

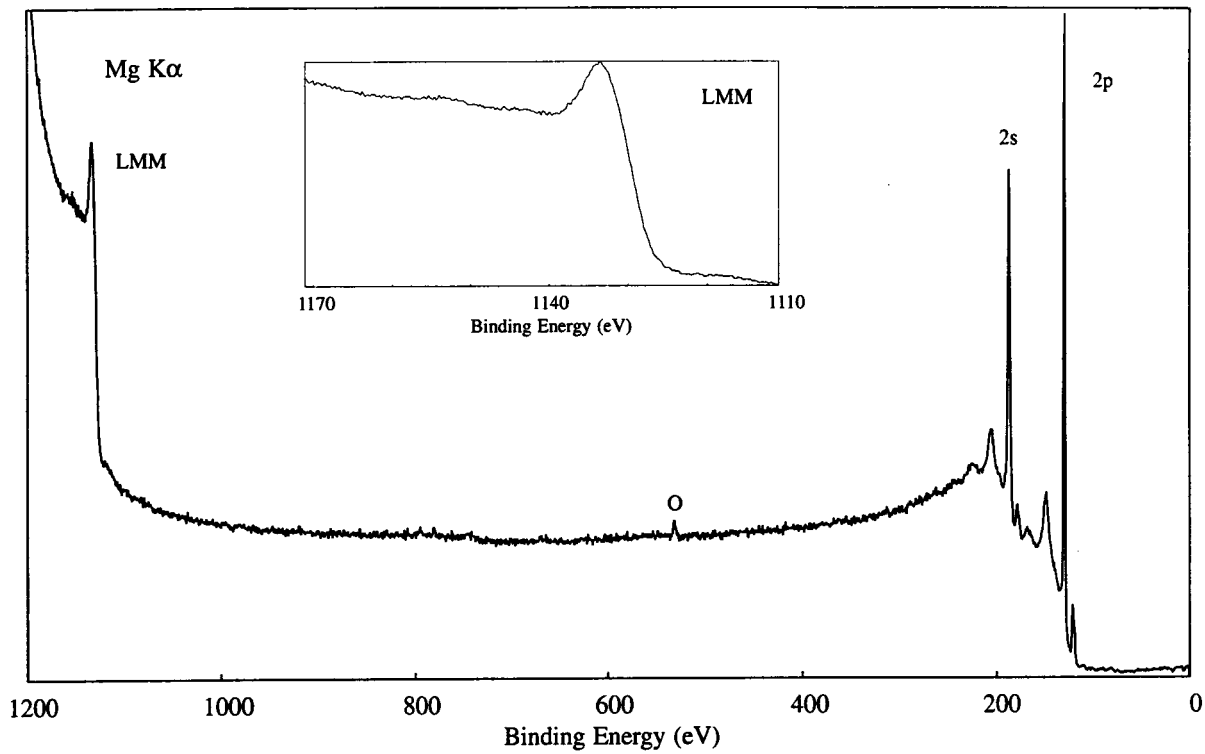
Photoelectron Lines

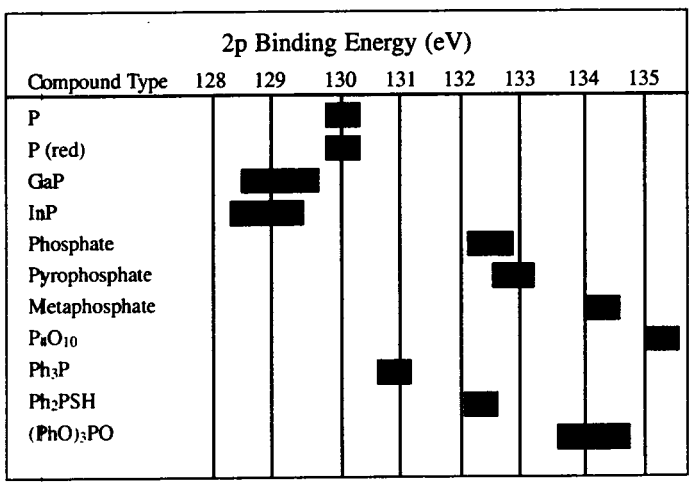
2s	$2p_{1/2}$	$2p_{3/2}$	3s
188	131	130	14

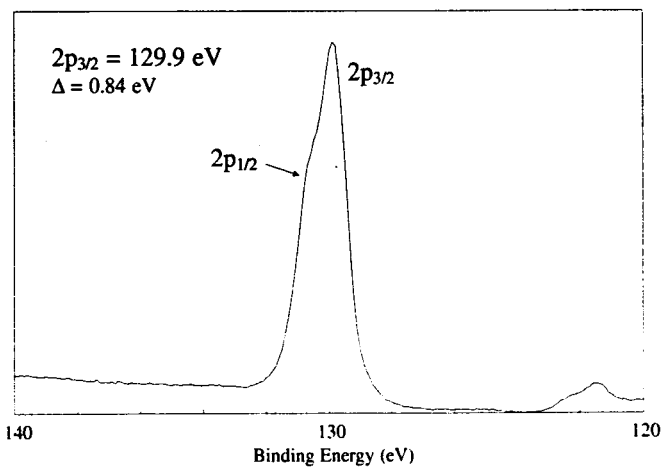
Auger Lines

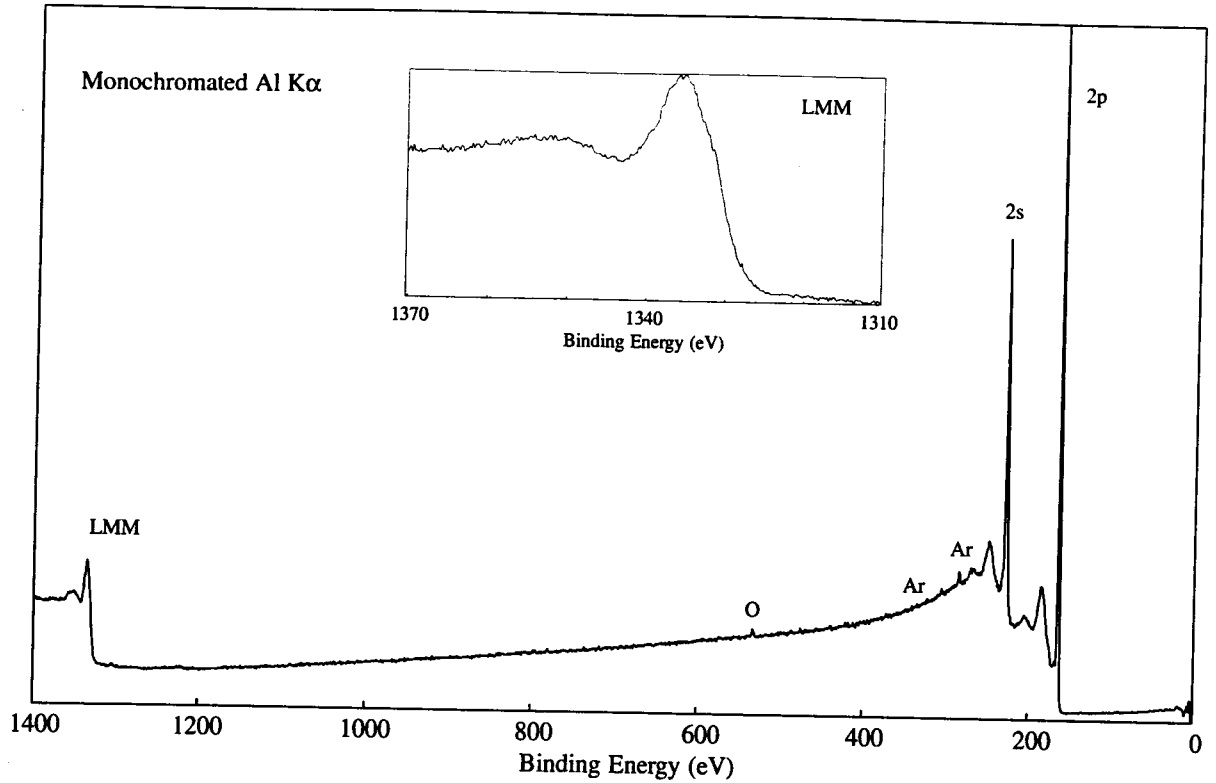
$L_{23}M_{23}M_{23}$

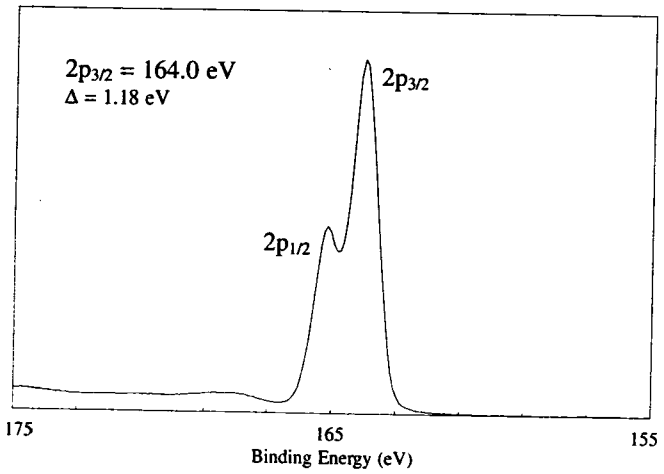
1367	(Al)
1134	(Mg)


Mg Kα
LMM
LMM
2p
2s
O
1170
1140
1110
Binding Energy (eV)
1200
1000
800
600
400
200
0
Binding Energy (eV)


2p Binding Energy (eV)
Compound Type
128
129
130
131
132
133
134
135
P
P (red)
GaP
InP
Phosphate
Pyrophosphate
Metaphosphate
P4O10
Ph3P
Ph2PSH
(PhO)3PO


2p3/2 = 129.9 eV
Δ = 0.84 eV
2p3/2
2p1/2
140
130
120
Binding Energy (eV)





Line Positions (eV)

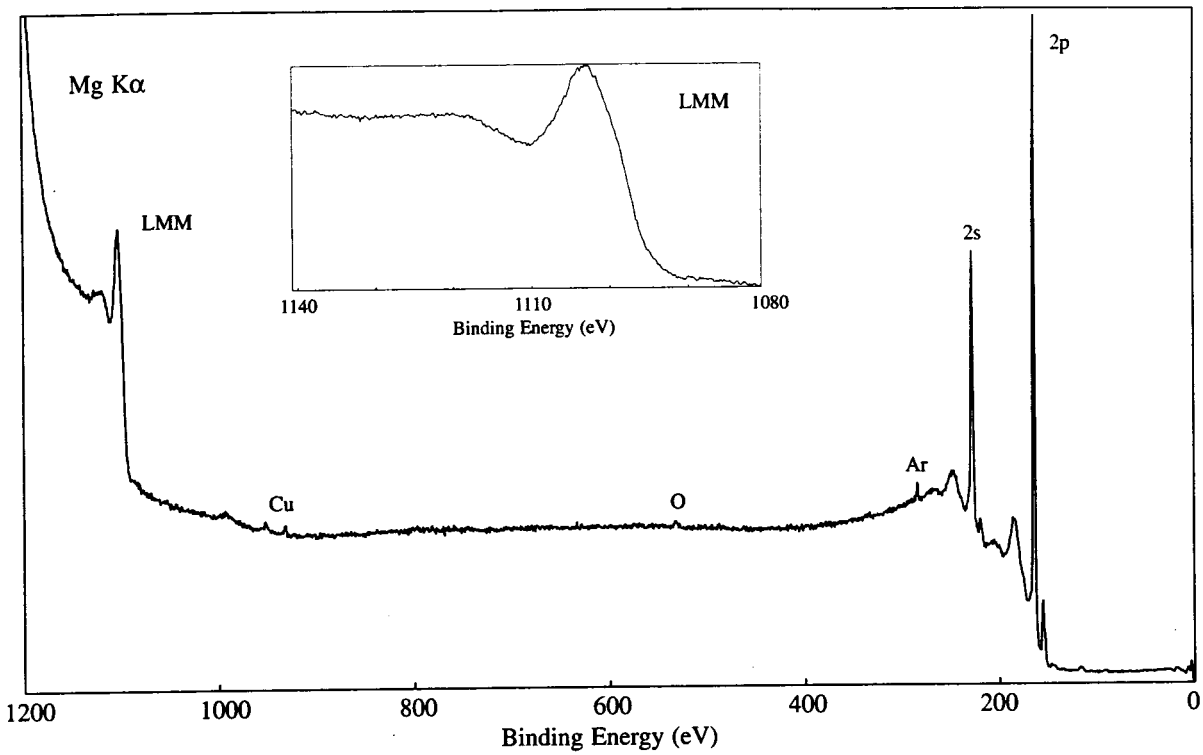
Photoelectron Lines

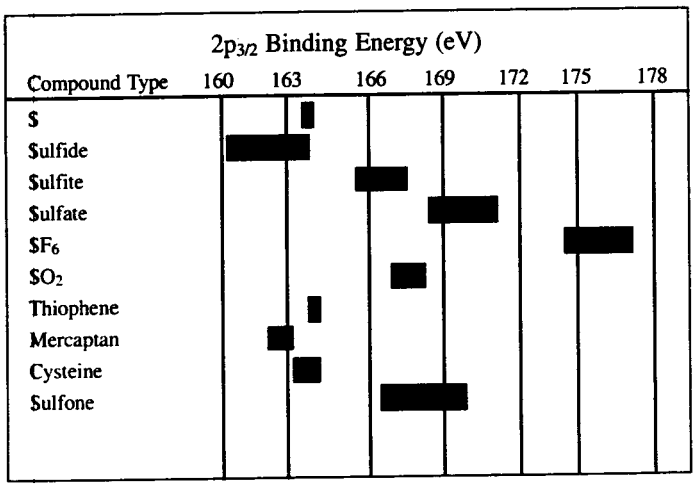
2s	$2p_{1/2}$	$2p_{3/2}$	3s
228	165	164	18

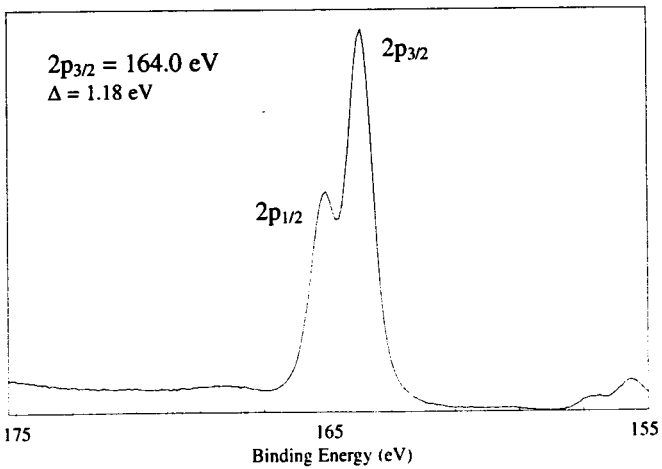
Auger Lines

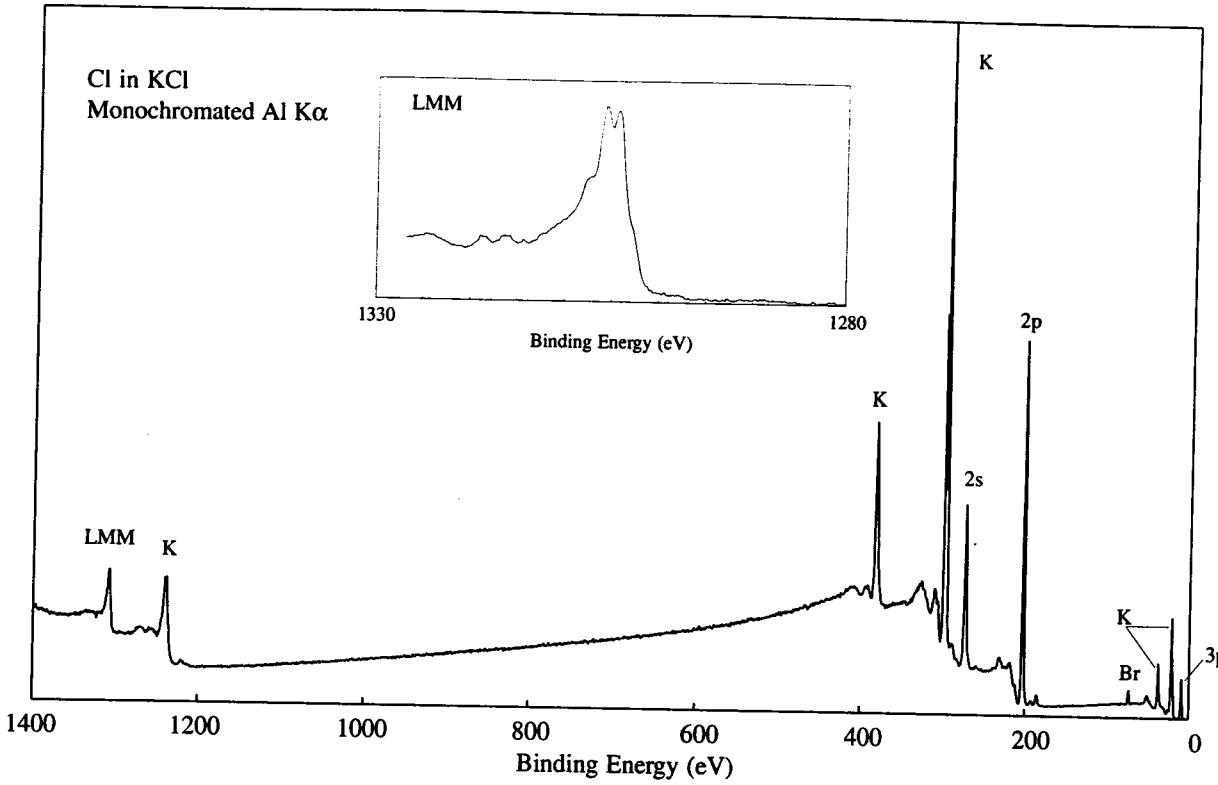
$L_{23}M_{23}M_{23}$

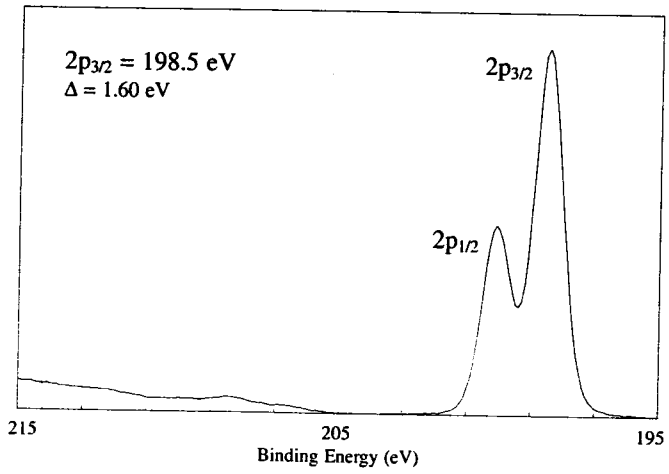
1336	(Al)
1103	(Mg)


Mg Kα
LMM
LMM
1140
1110
1080
Binding Energy (eV)
2p
2s
Ar
Cu
O
1200
1000
800
600
400
200
0
Binding Energy (eV)


2p3/2 Binding Energy (eV)
Compound Type
160
163
166
169
172
175
178
$
$ulfide
$ulfite
$ulfate
$F6
$O2
Thiophene
Mercaptan
Cysteine
$ulfone


2p3/2 = 164.0 eV
Δ = 1.18 eV
2p3/2
2p1/2
175
165
155
Binding Energy (eV)





Line Positions (eV)

Photoelectron Lines

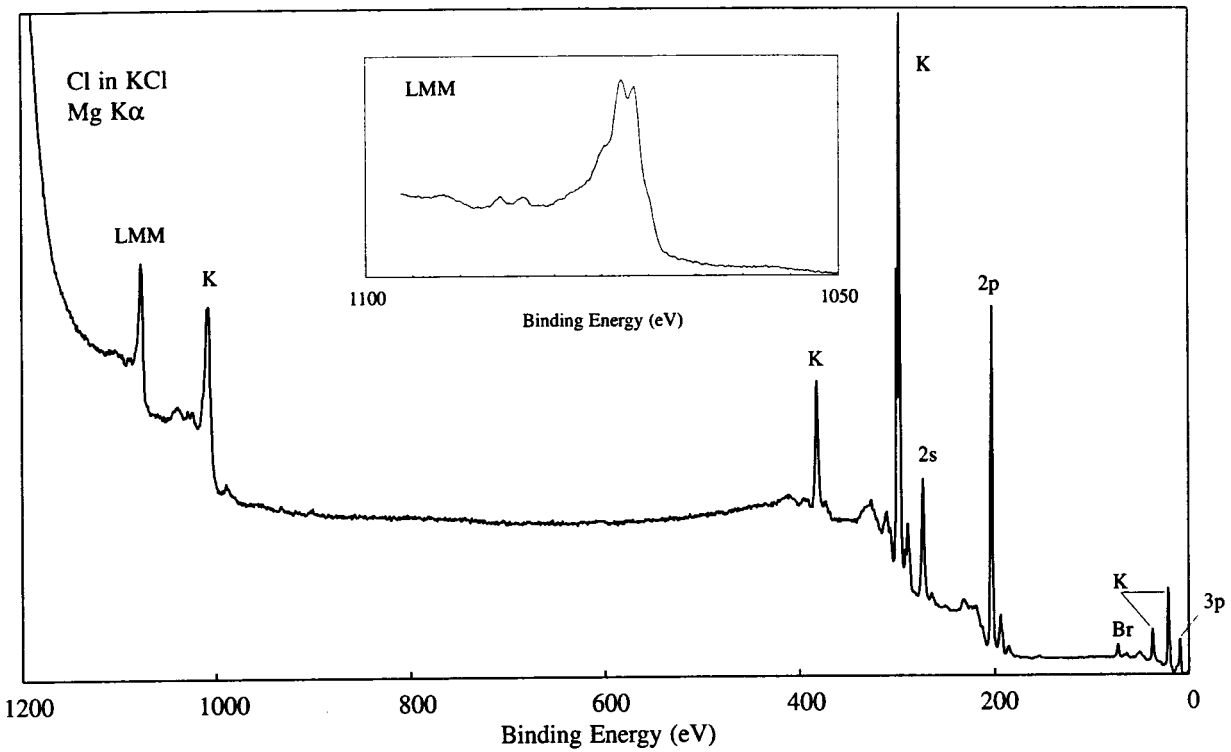
2s	2p1/2	2p3/2	3s	3p
271	201	199	17	6

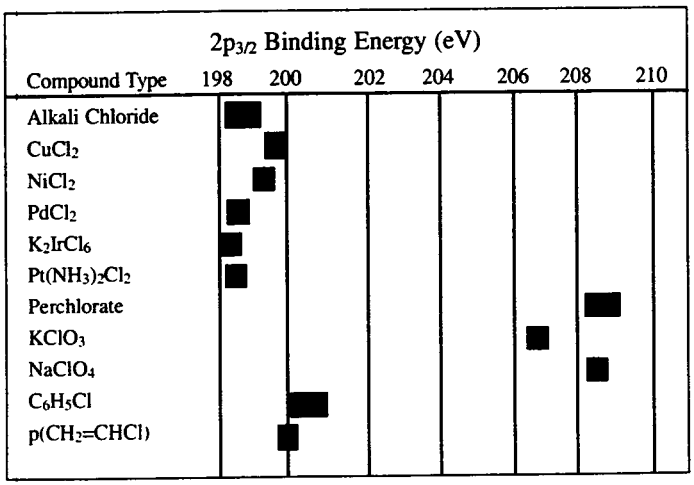
Auger Lines

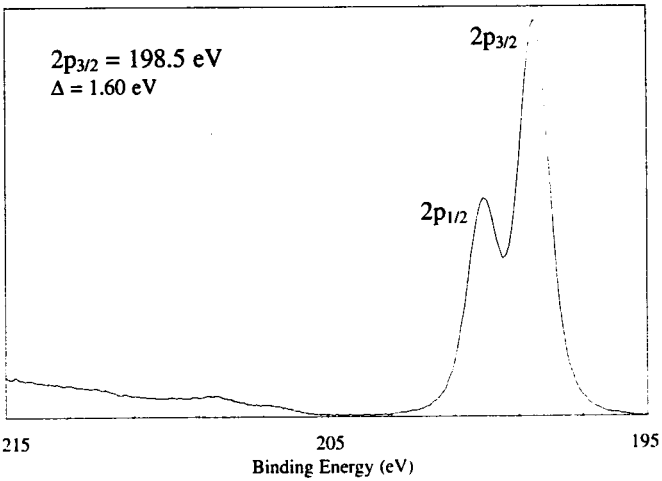
$L_{23}M_{23}M_{23}$

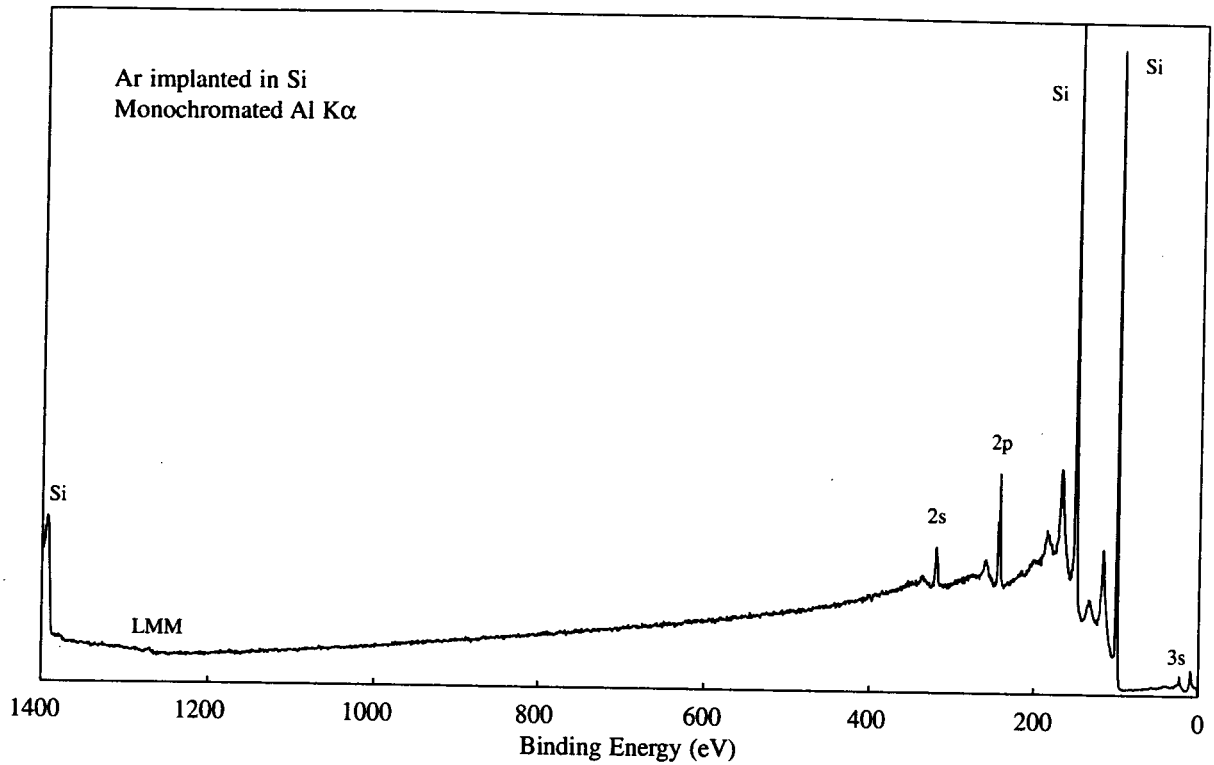
1304 (Al)
1071 (Mg)

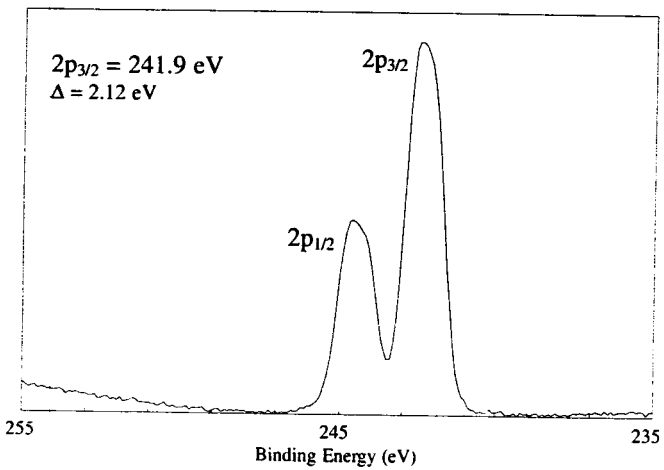
Chlorine Cl
Atomic Number 17











Line Positions (eV)

Photoelectron Lines

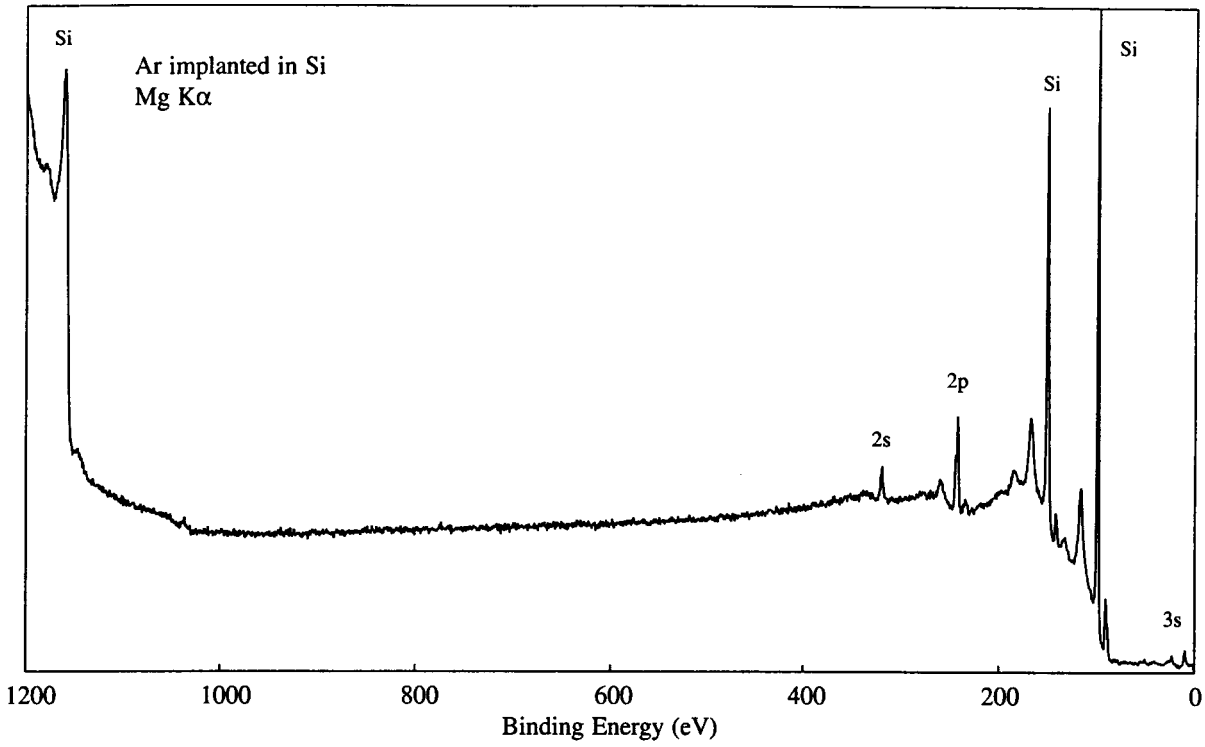
2s	2p1/2	2p3/2	3s
320	244	242	24

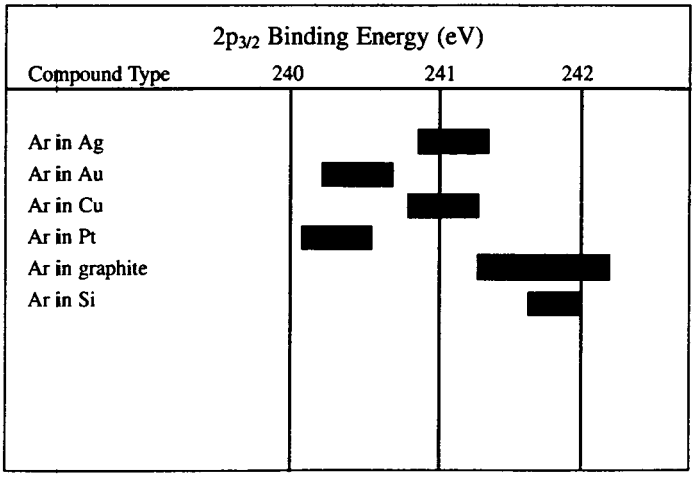
Auger Lines

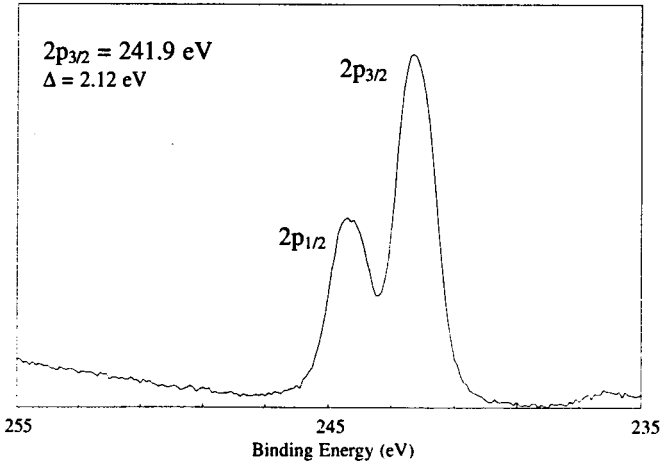
$L_{23}M_{23}M_{23}$

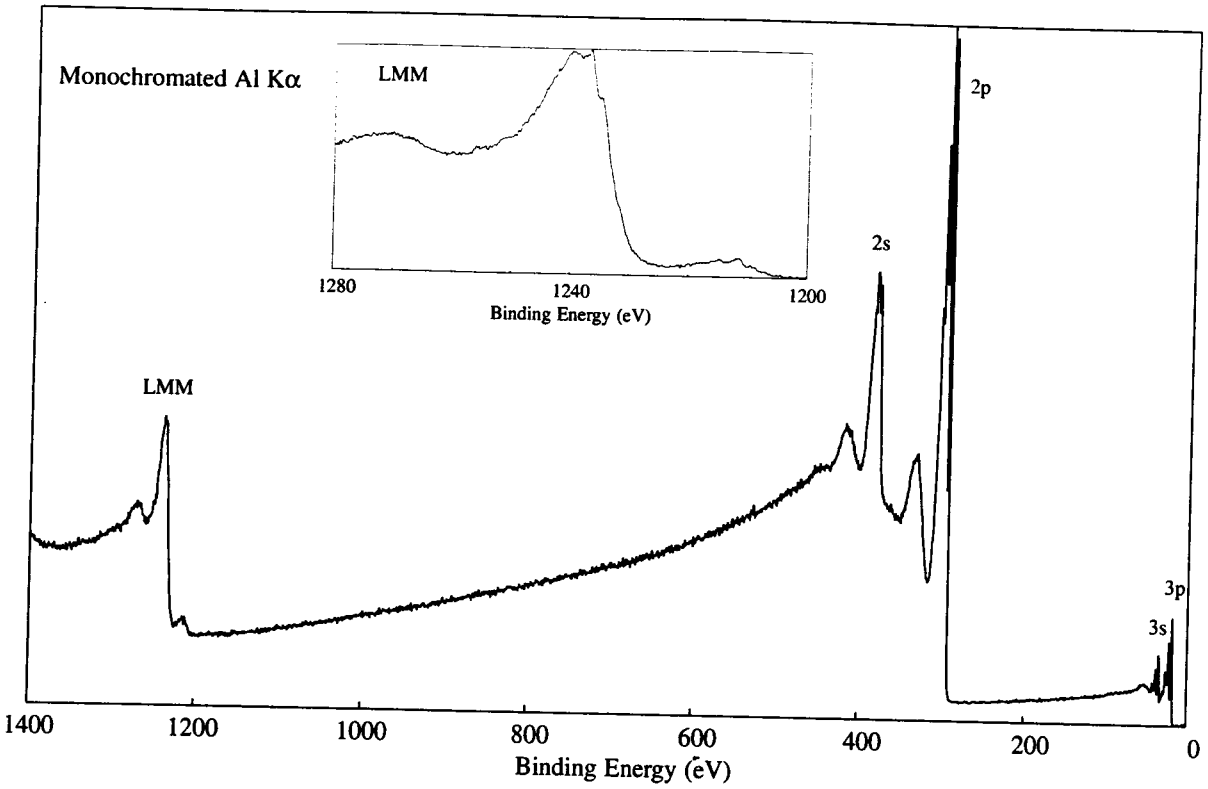
1272	(Al)
1039	(Mg)

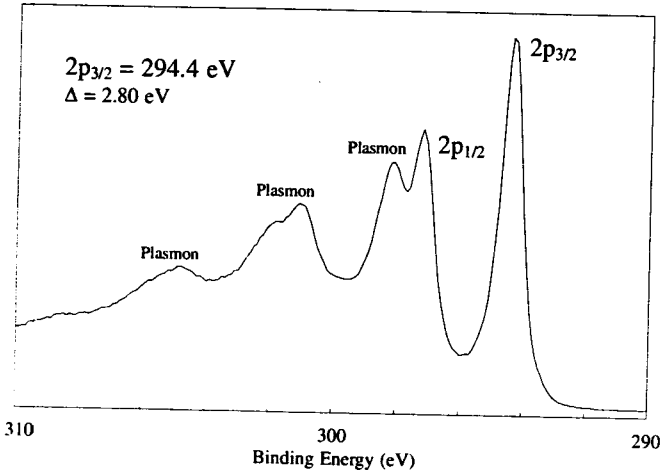
Argon Ar
Atomic Number 18











Line Positions (eV)

Photoelectron Lines

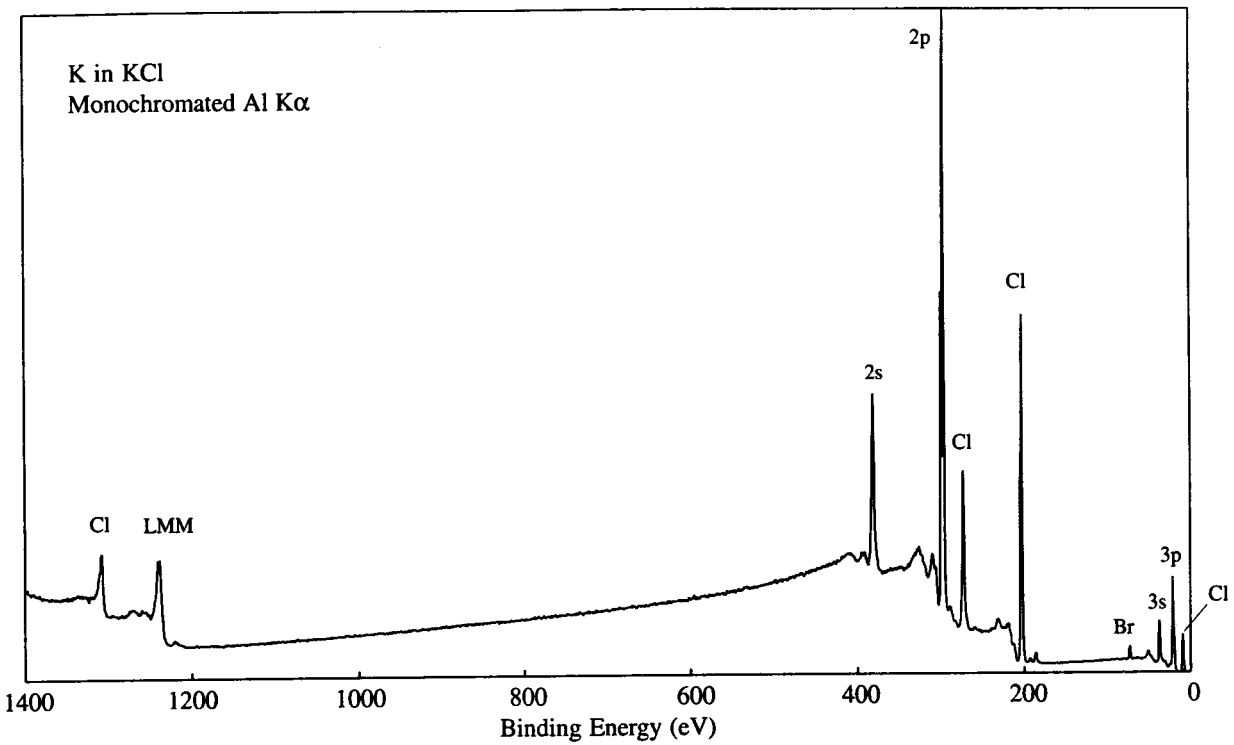
2s	$2p_{1/2}$	$2p_{3/2}$	3s	3p
380	297	294	35	19

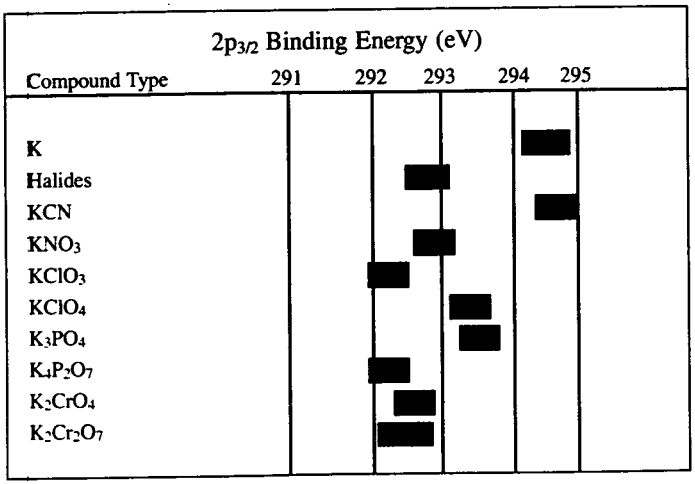
Auger Lines

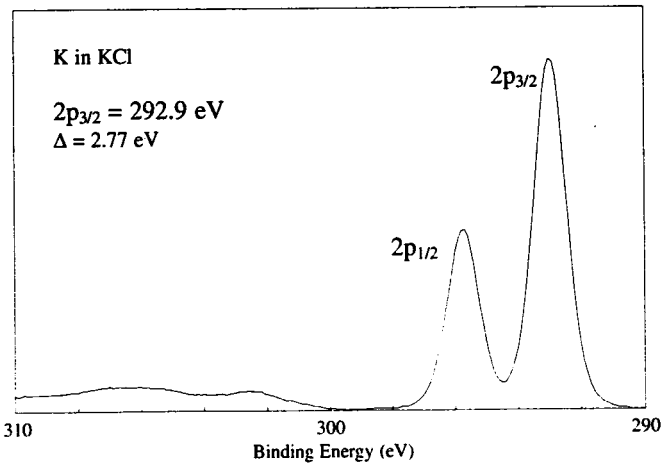
$L_{23}M_{23}M_{23}$

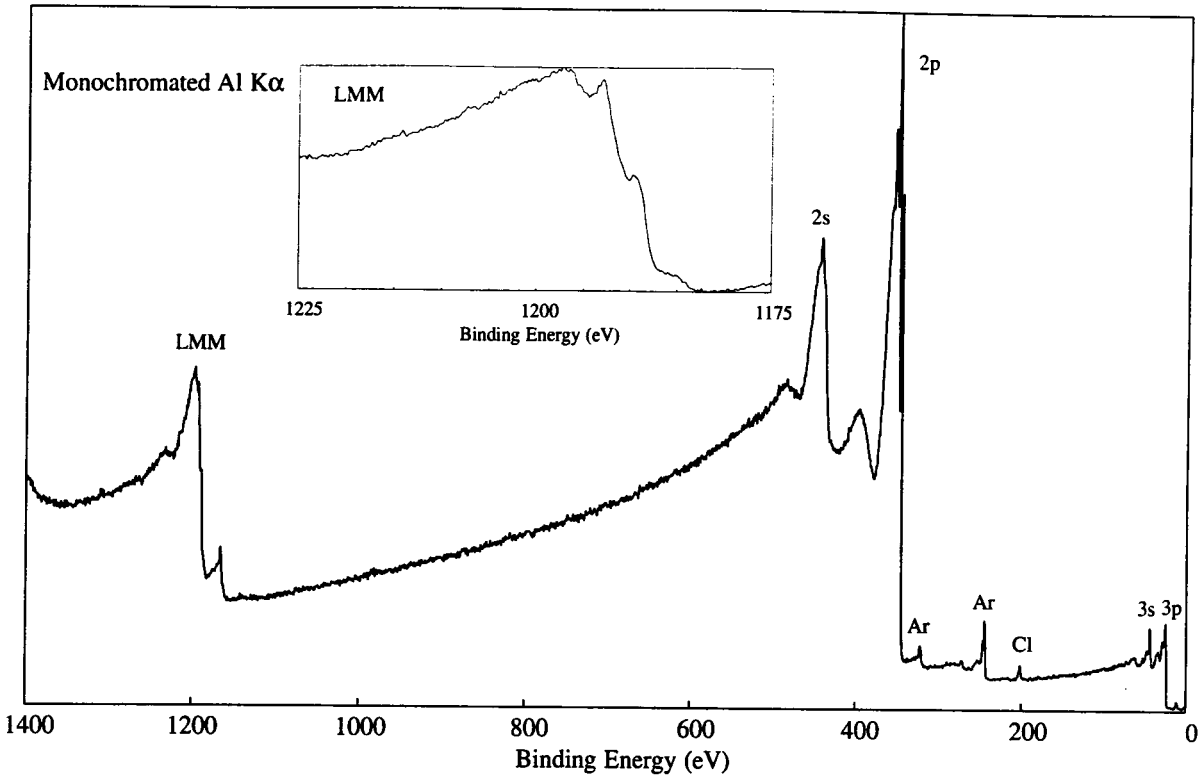
1239	(Al)
1006	(Mg)

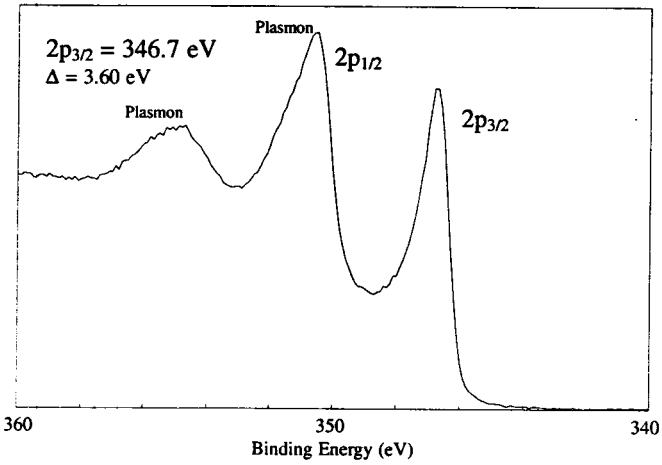
Potassium K
Atomic Number 19











Line Positions (eV)

Photoelectron Lines

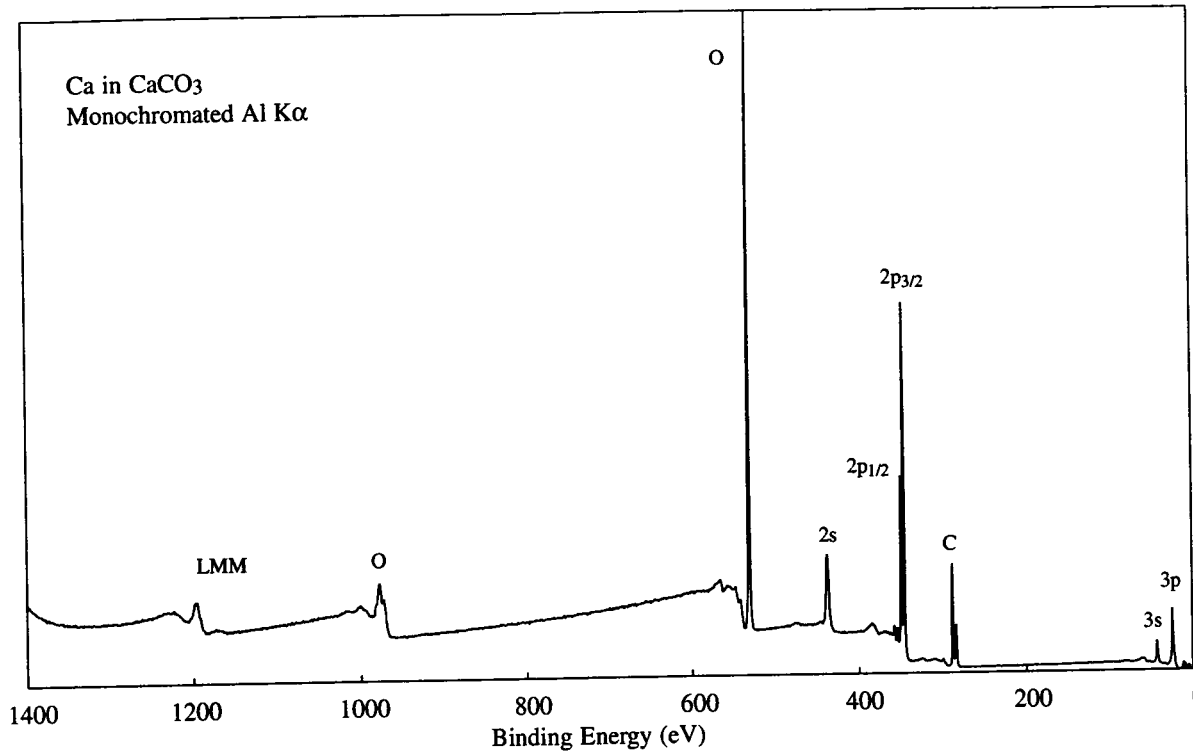
2s	$2p_{1/2}$	$2p_{3/2}$	3s	3p
440	351	347	45	26

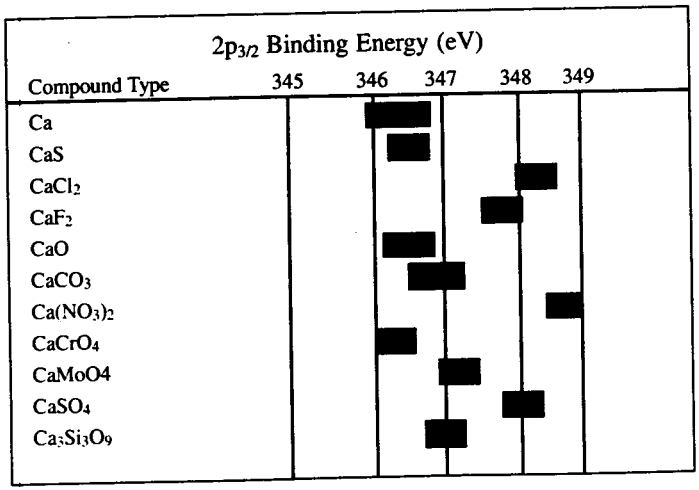
Auger Lines

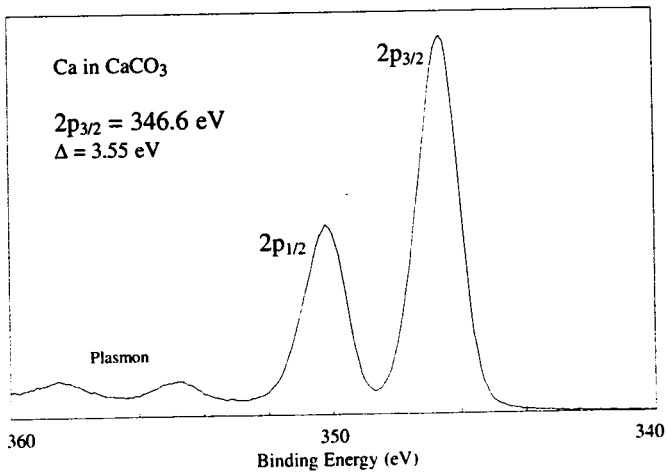
$L_{23}M_{23}M_{23}$

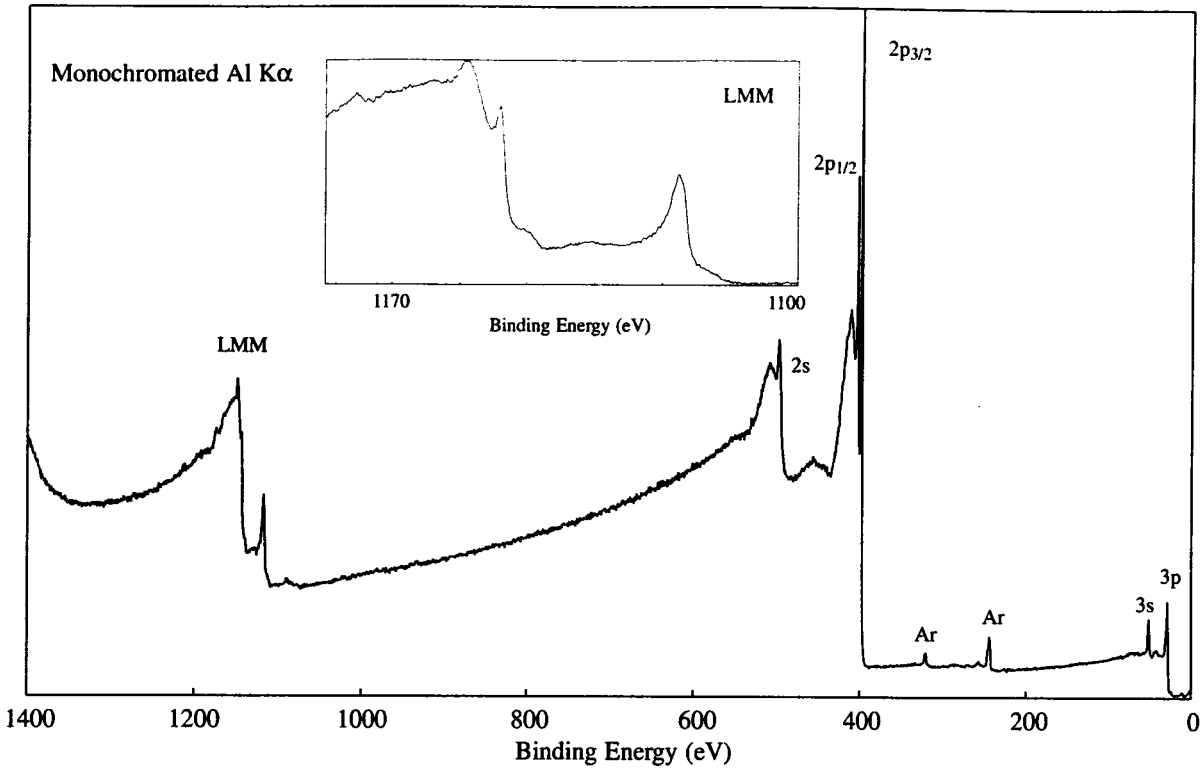
1197	(Al)
964	(Mg)

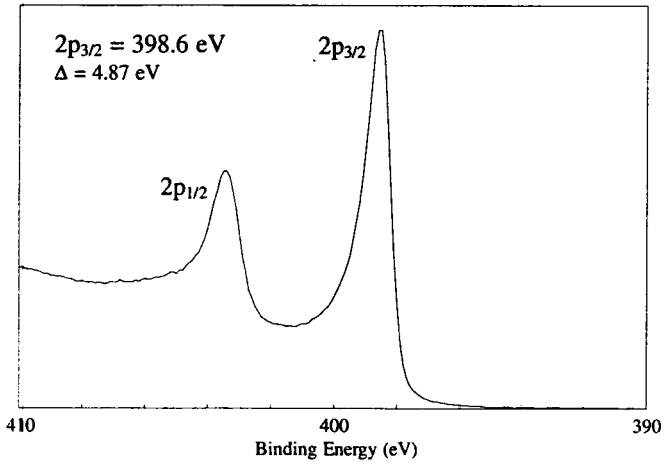
Calcium Ca
Atomic Number 20











Line Positions (eV)

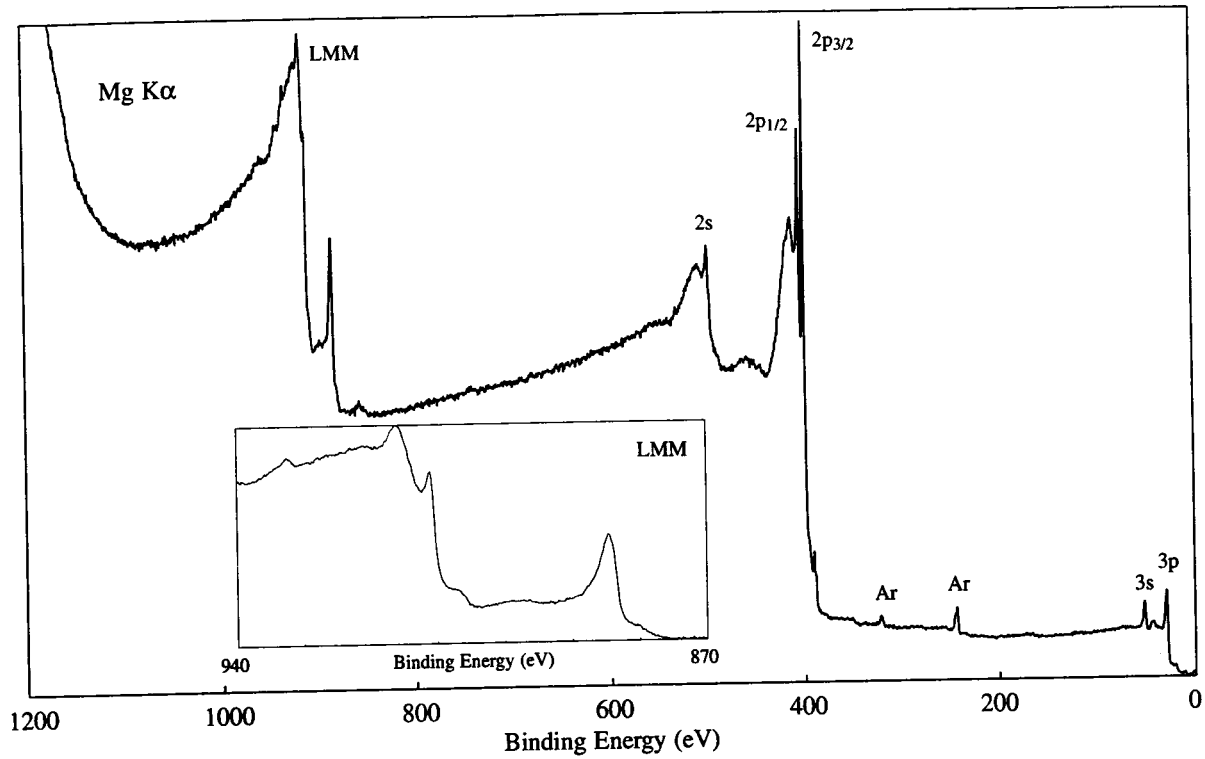
Photoelectron Lines

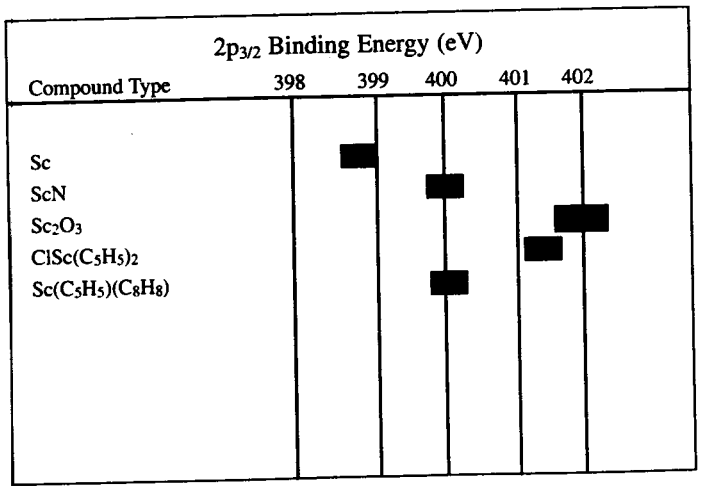
2s	2p1/2	2p3/2	3s	3p
499	404	399	51	29

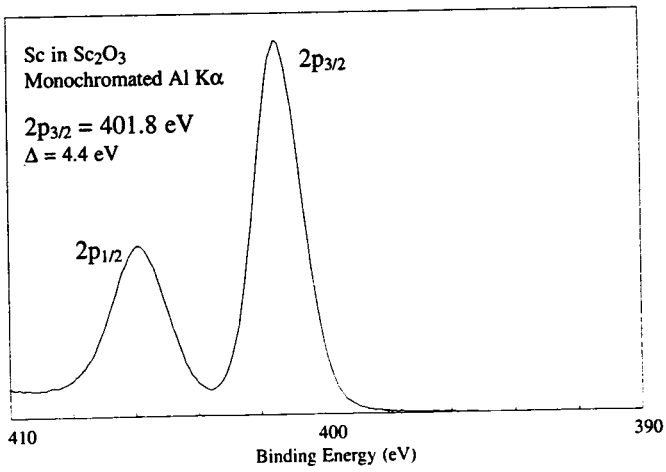
Auger Lines

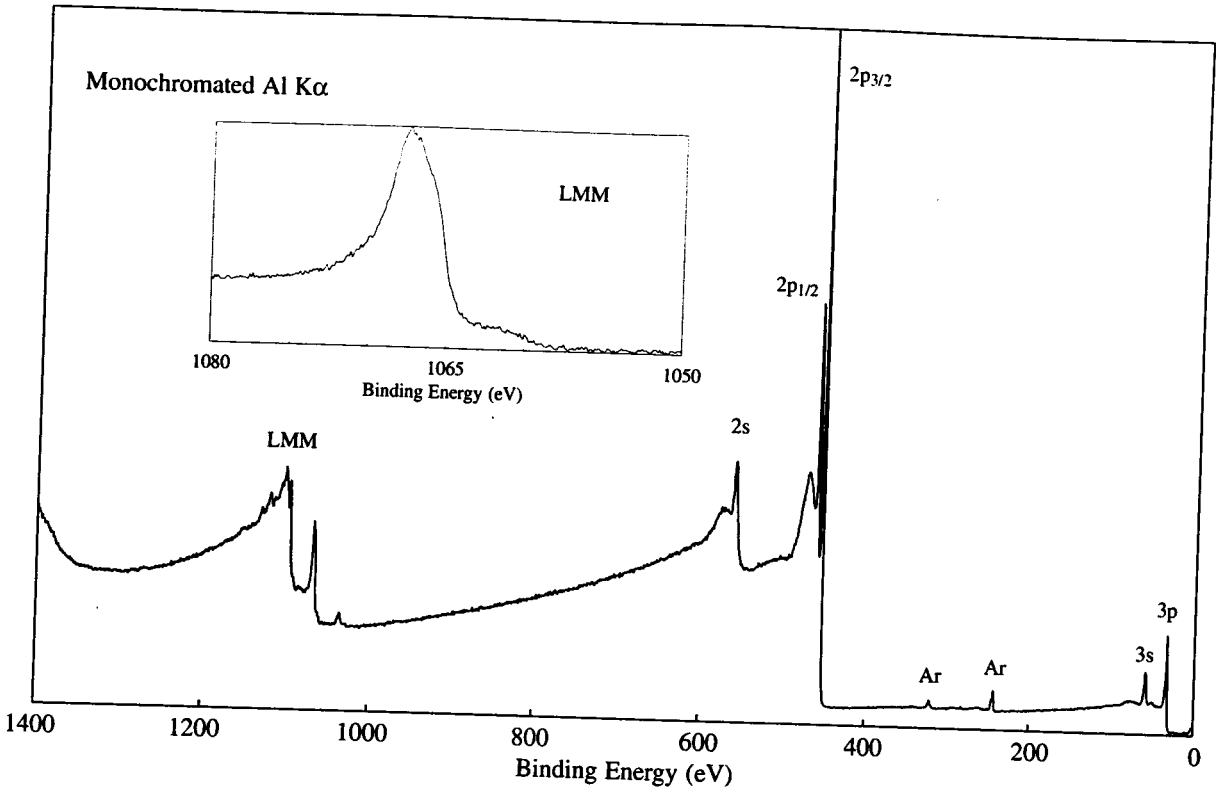
$LM_{23}M_{23}$	$L_3M_{23}M_{45}$ (^1P)	
1149	1118	(Al)
916	885	(Mg)

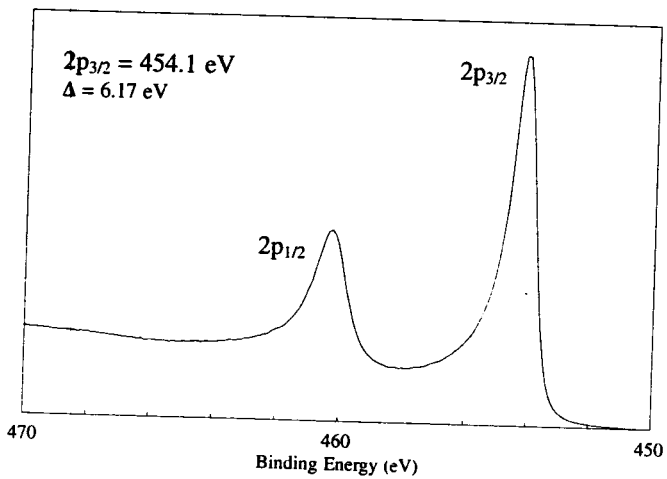
Scandium Sc
Atomic Number 21











Line Positions (eV)

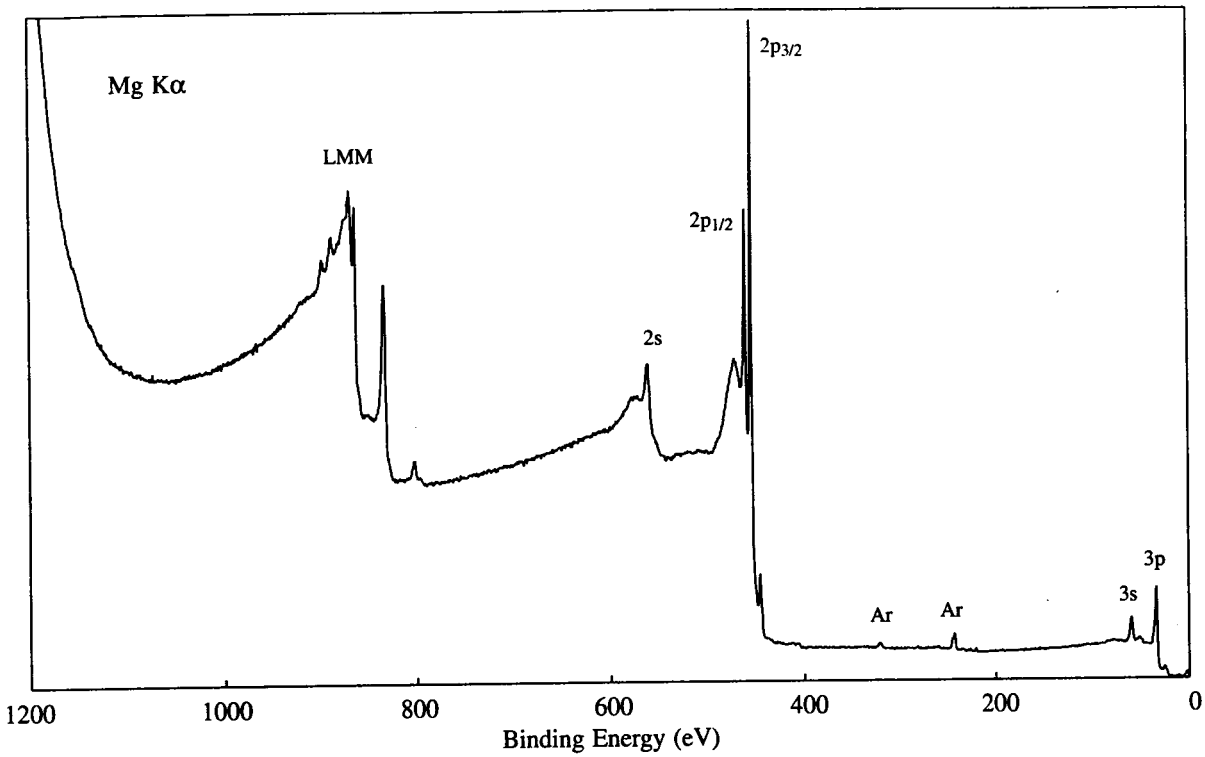
Photoelectron Lines

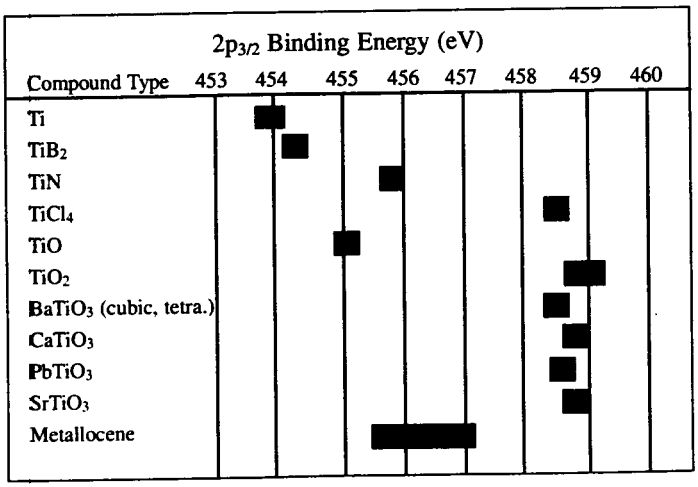
2s	2p1/2	2p3/2	3s	3p
561	460	454	59	33

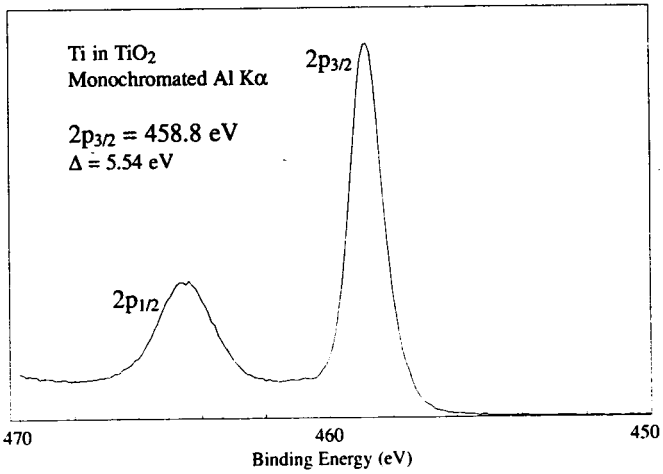
Auger Lines

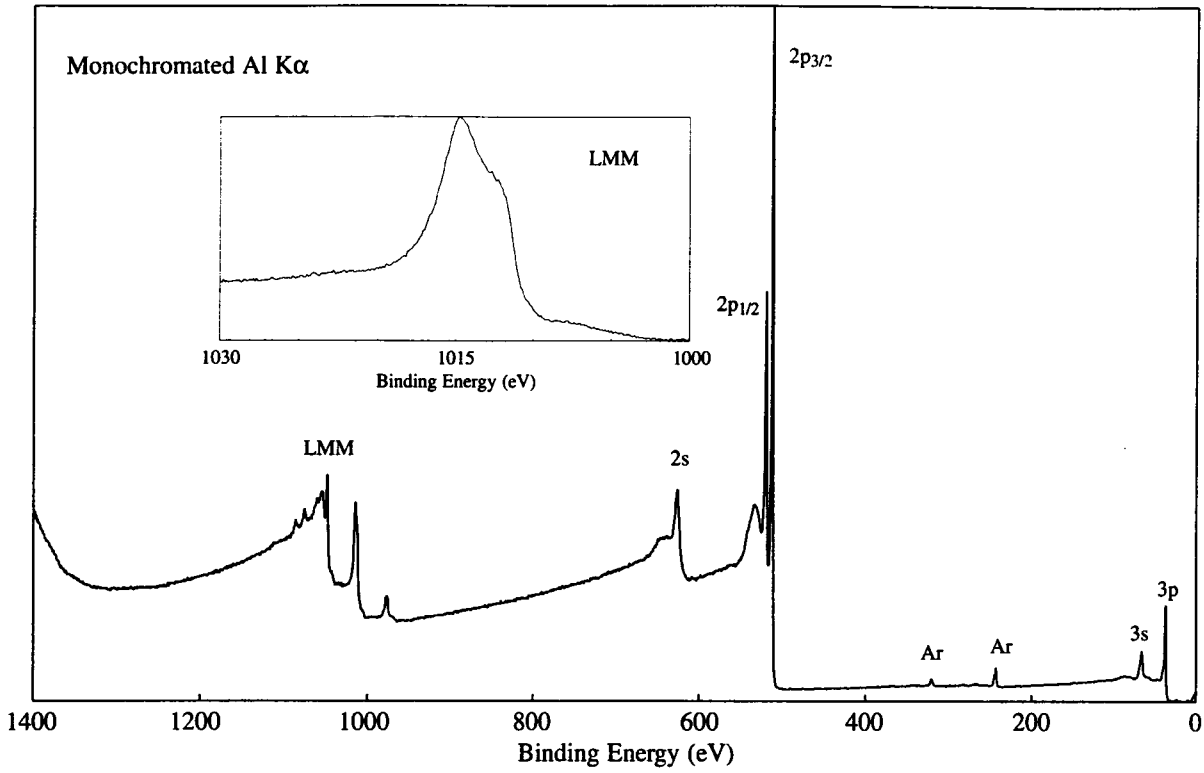
$LM_{23}M_{23}$	$L_3M_{23}M_{45}$ (^1P)	
1098	1068	(Al)
865	835	(Mg)

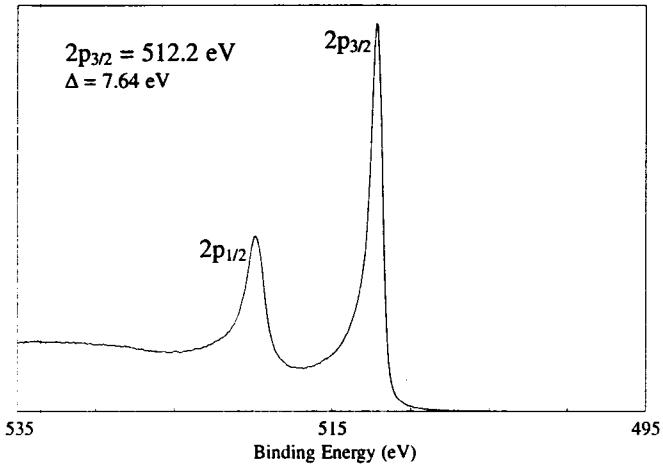
Titanium Ti
Atomic Number 22











Line Positions (eV)

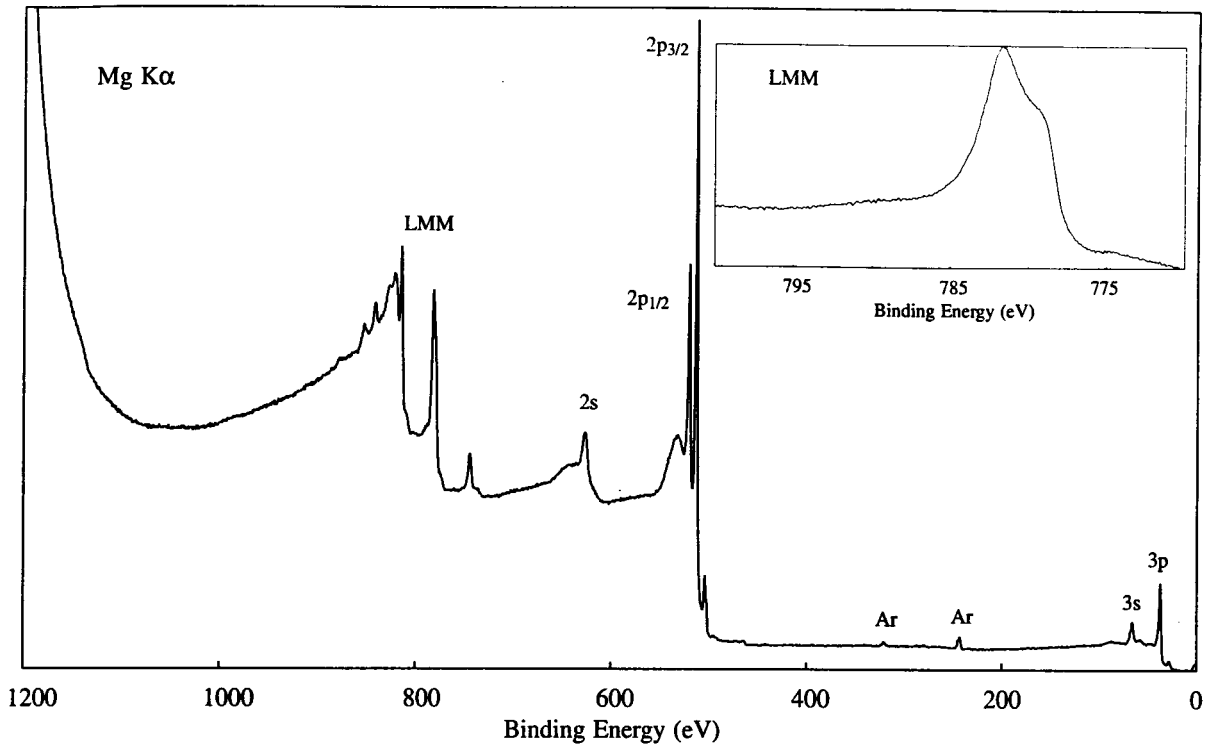
Photoelectron Lines

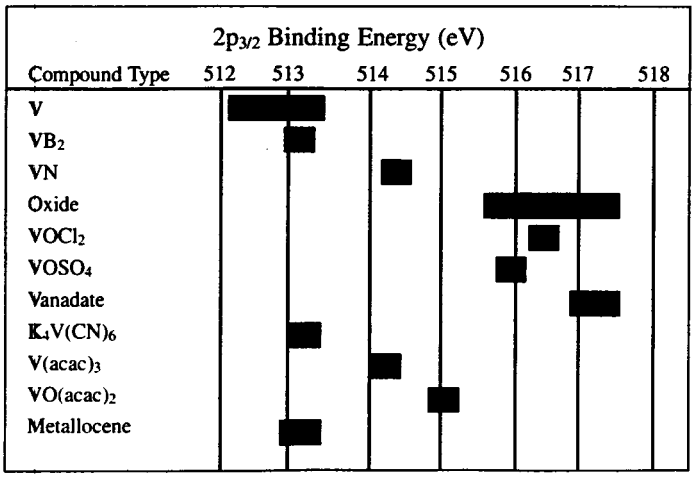
2s	$2p_{1/2}$	$2p_{3/2}$	3s	3p
627	520	512	66	37

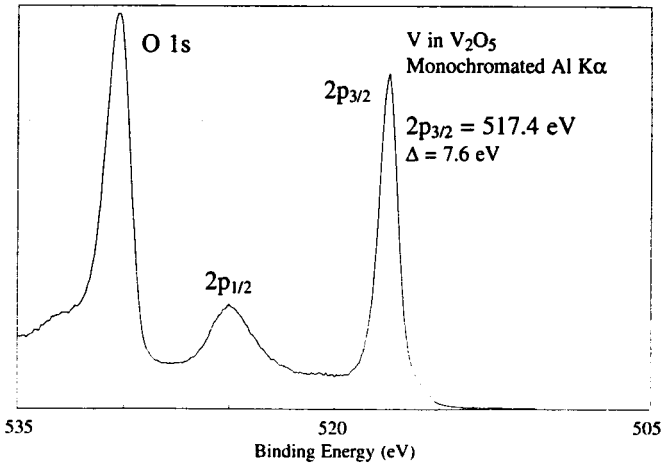
Auger Lines

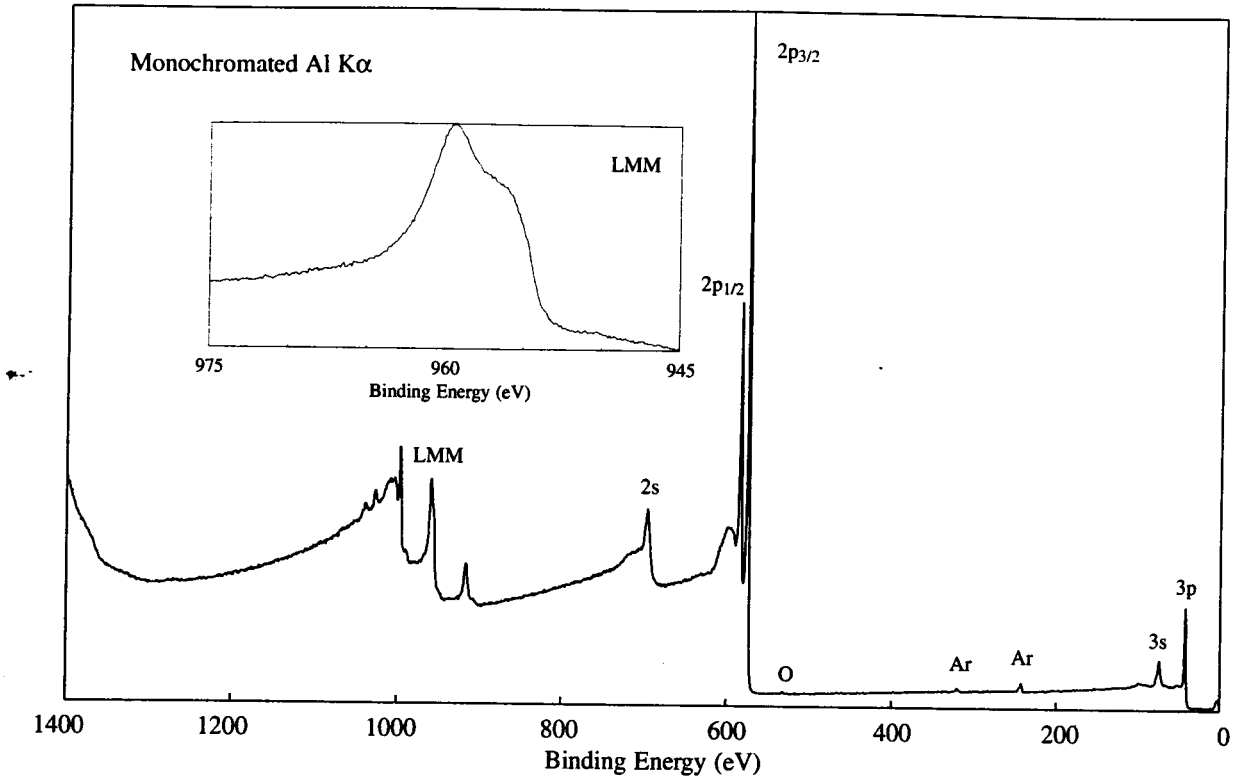
$L_{23}M_{23}M_{23}$	$L_3M_{23}M_{45}$ (^1P)	$L_3M_{45}M_{45}$	
1048	1014	977	(Al)
815	781	744	(Mg)

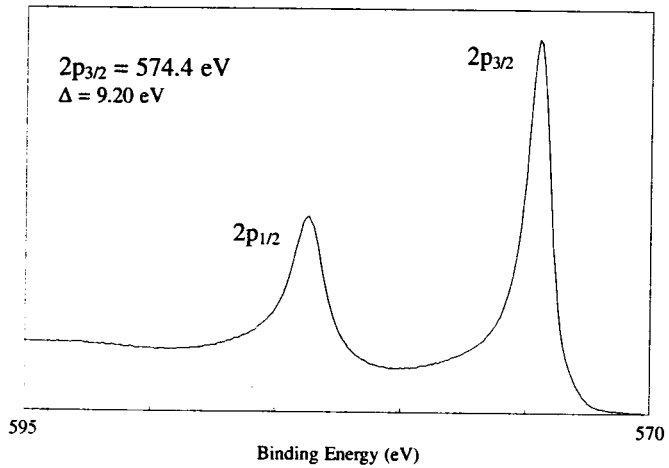
Vanadium V
Atomic Number 23











Line Positions (eV)

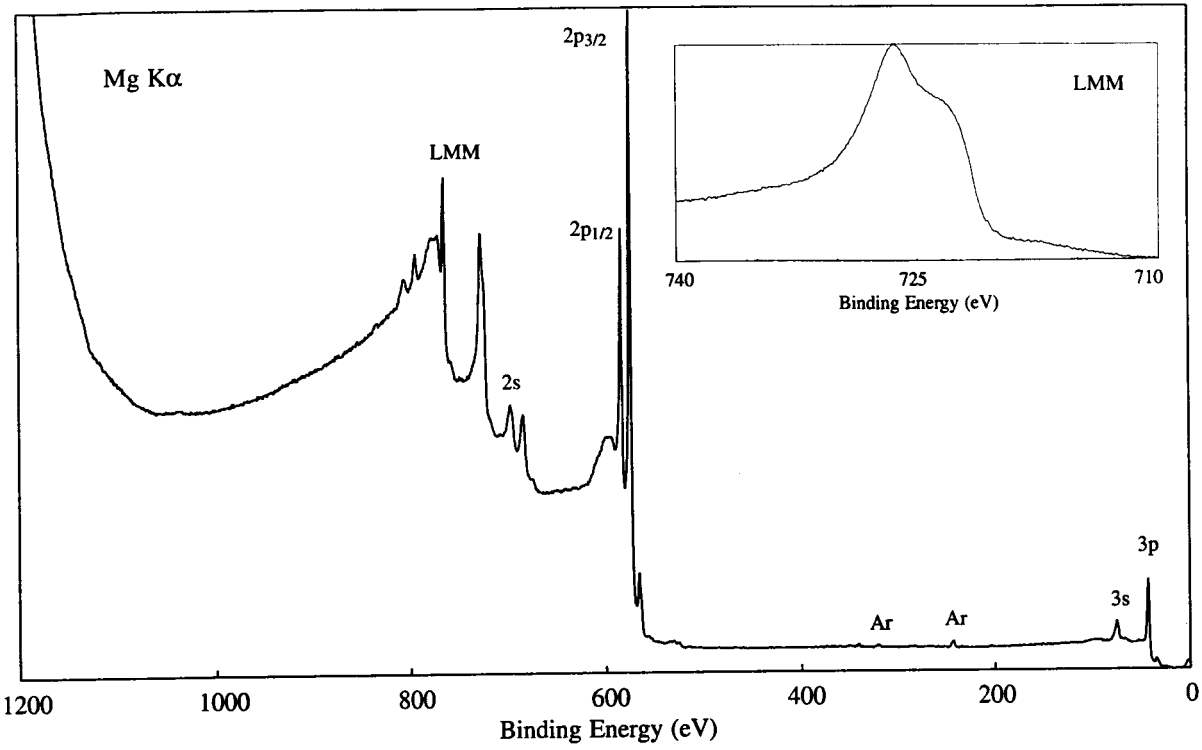
Photoelectron Lines

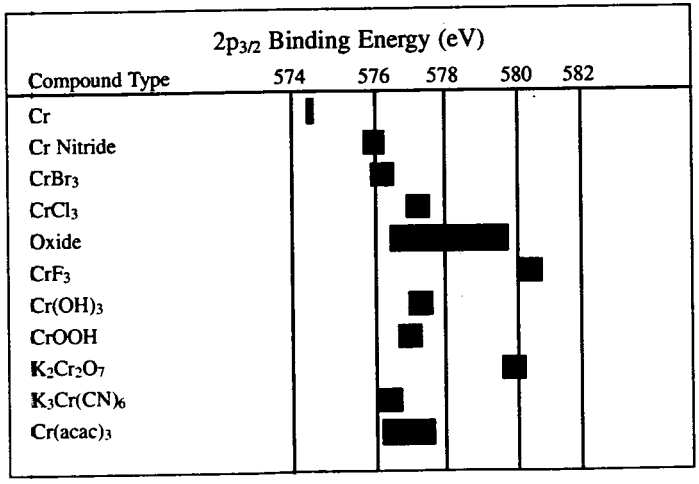
2s	$2p_{1/2}$	$2p_{3/2}$	3s	3p
696	583	574	75	43

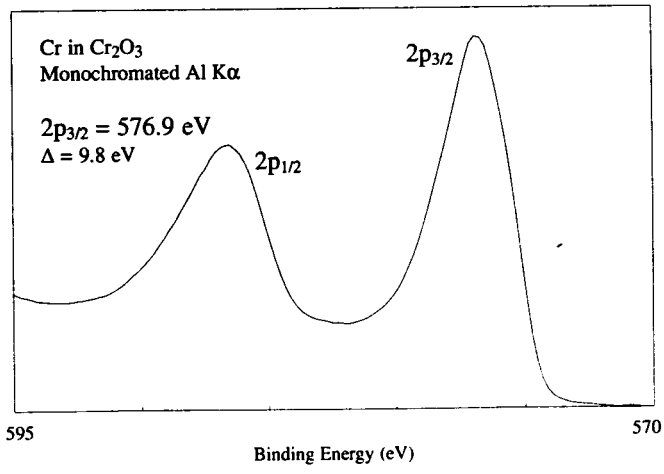
Auger Lines

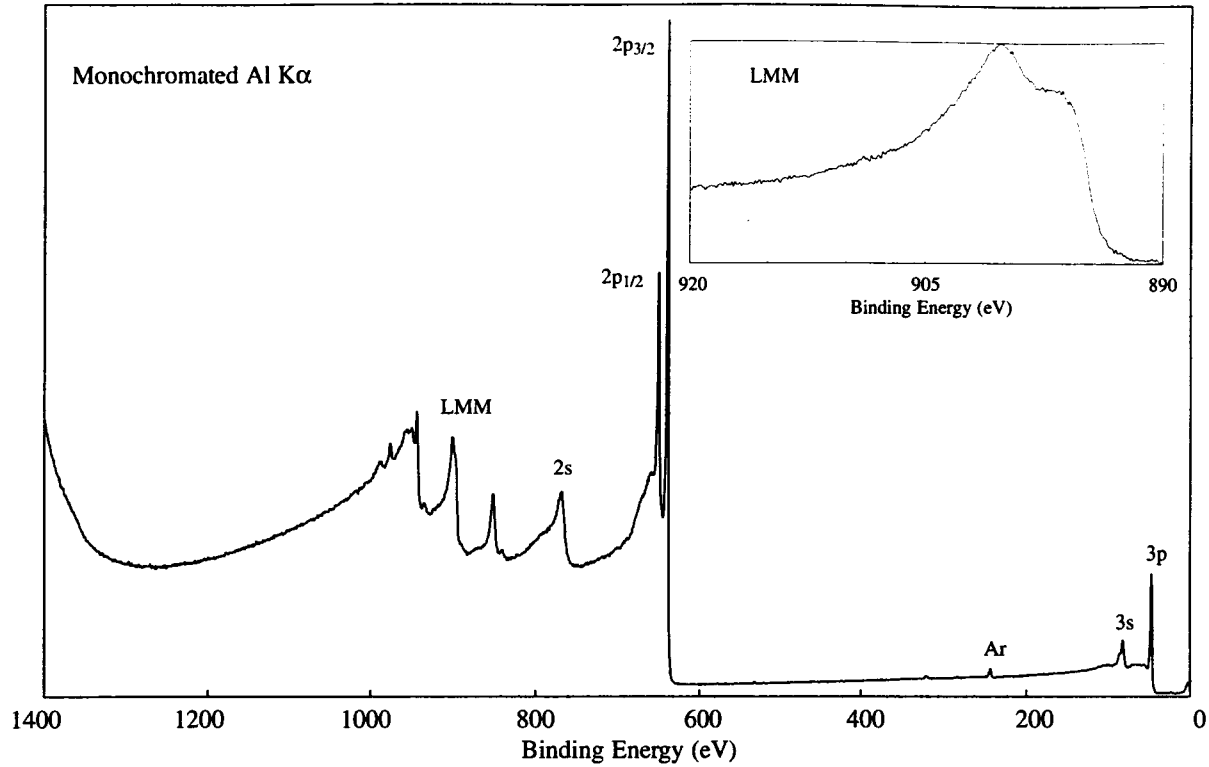
$L_{23}M_{23}M_{23}$	$L_3M_{23}M_{45}$ (^1P)	$L_3M_{45}M_{45}$	
997	959	917	(Al)
764	726	684	(Mg)

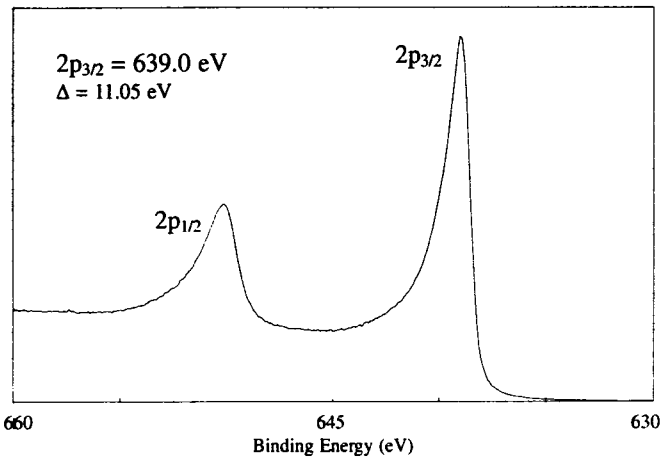
Chromium Cr
Atomic Number 24











Line Positions (eV)

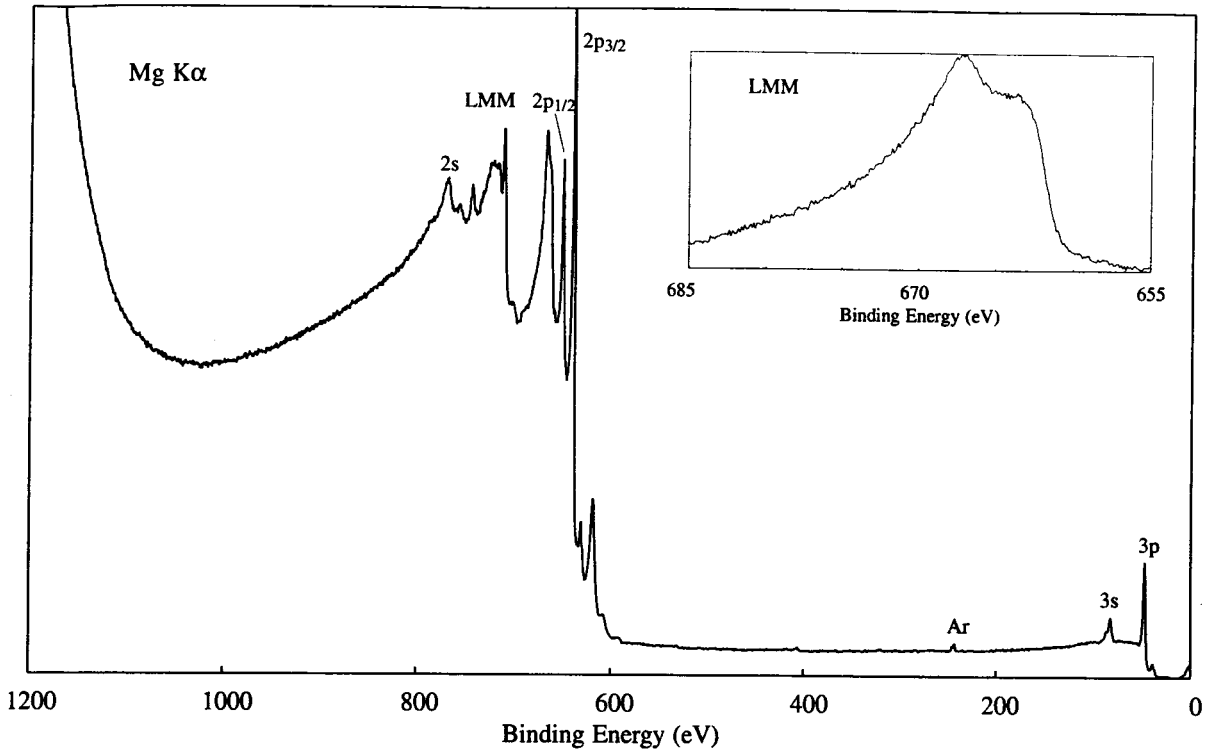
Photoelectron Lines

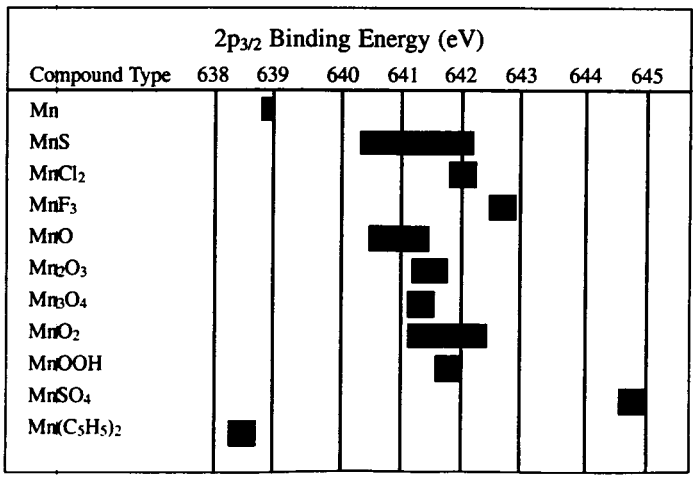
2s	2p1/2	2p3/2	3s	3p
769	650	639	83	48

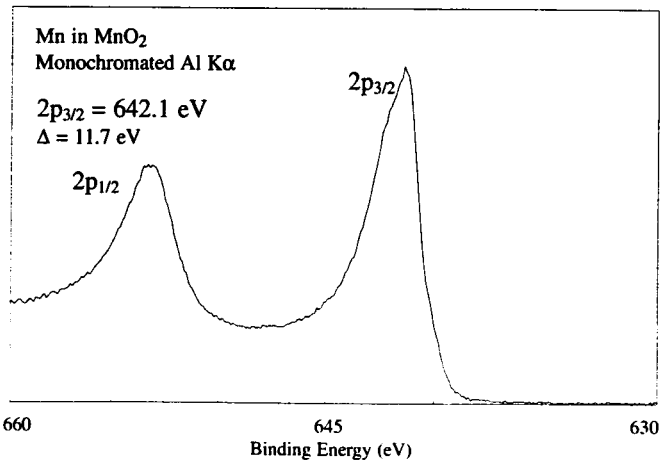
Auger Lines

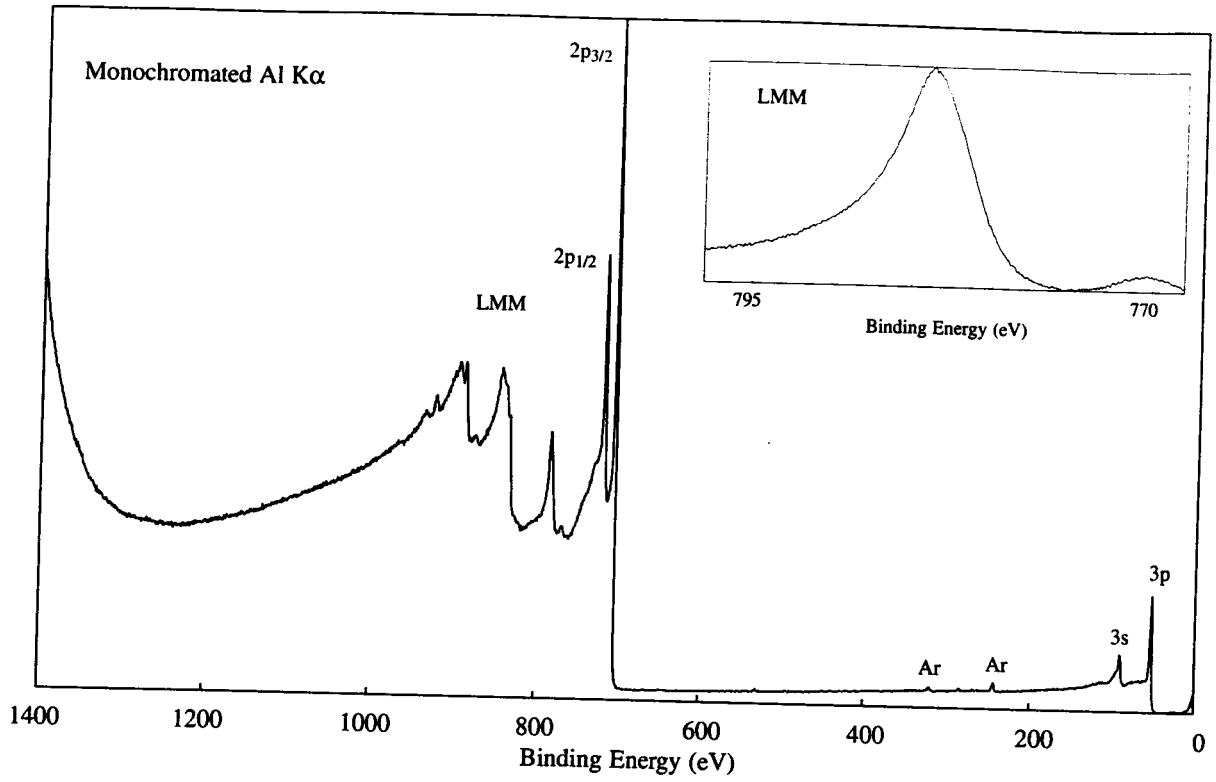
$L_{23}M_{23}M_{23}$	$L_3M_{23}M_{45}$	$L_3M_{45}M_{45}$	
944	900	852	(Al)
711	667	619	(Mg)

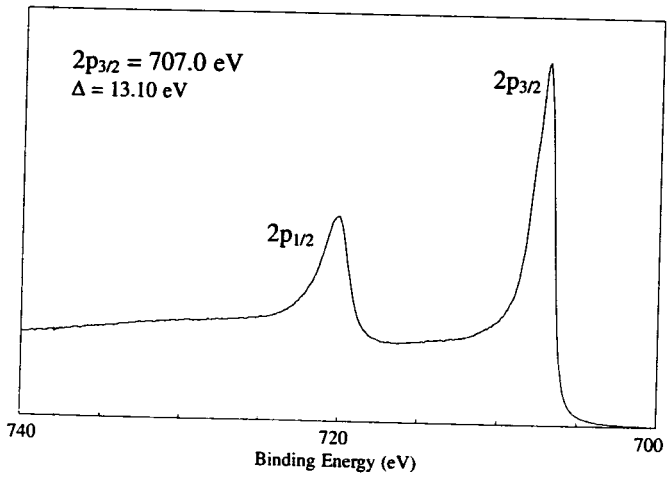
Manganese Mn
Atomic Number 25











Line Positions (eV)

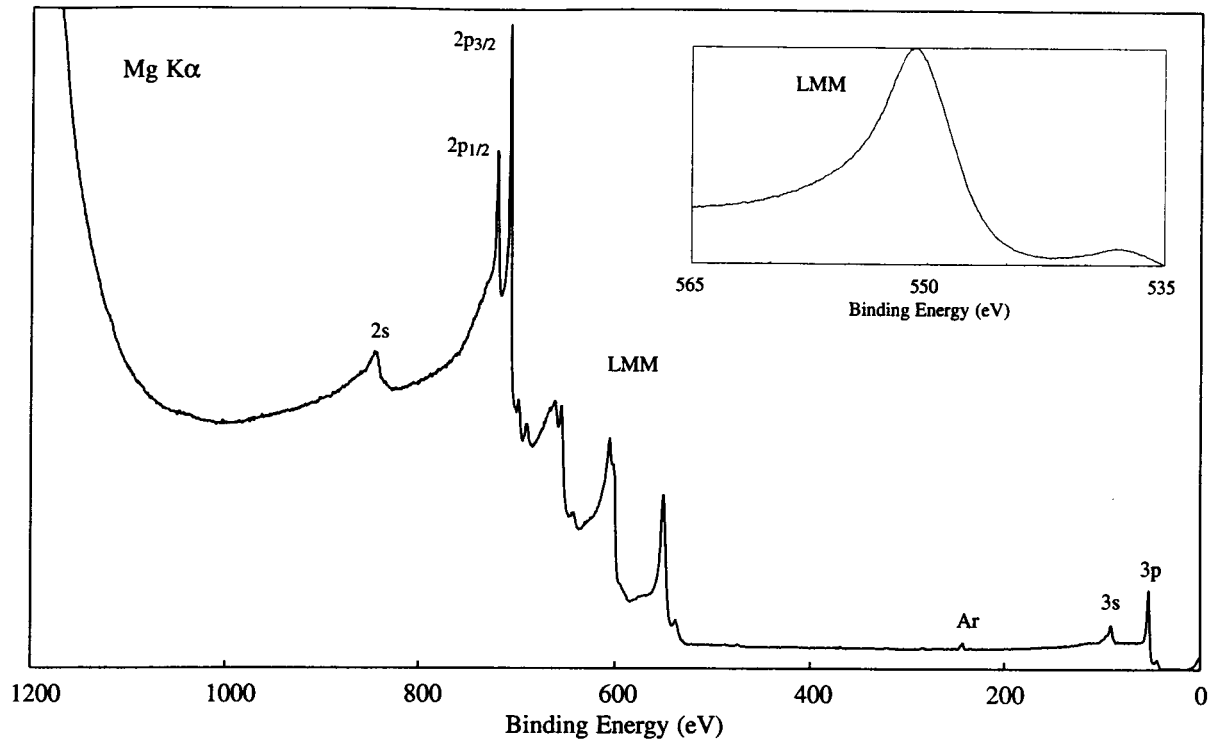
Photoelectron Lines

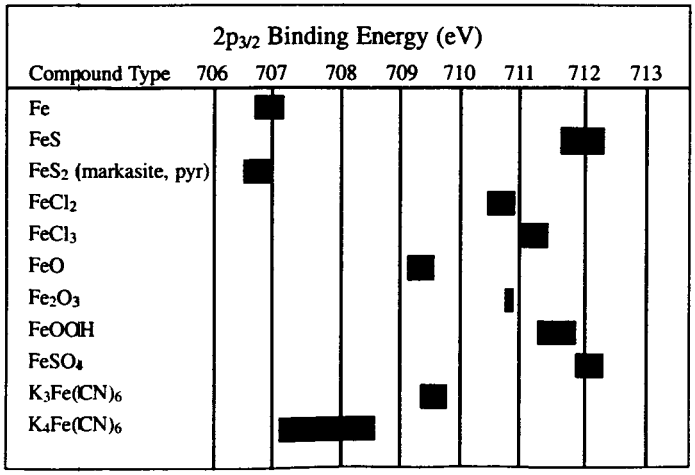
2s	2p1/2	2p3/2	3s	3p
845	720	707	92	53

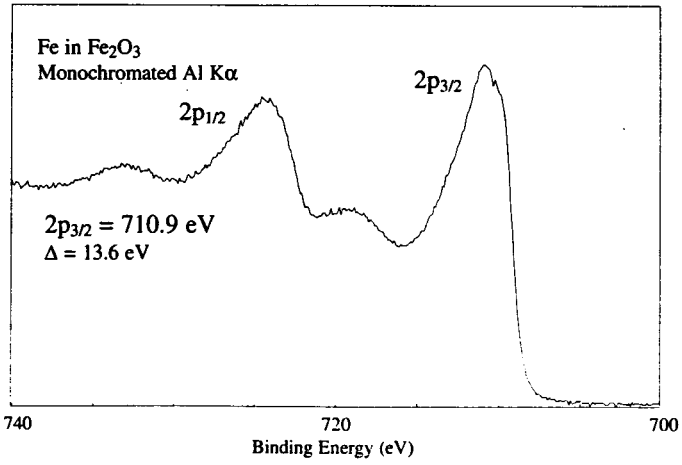
Auger Lines

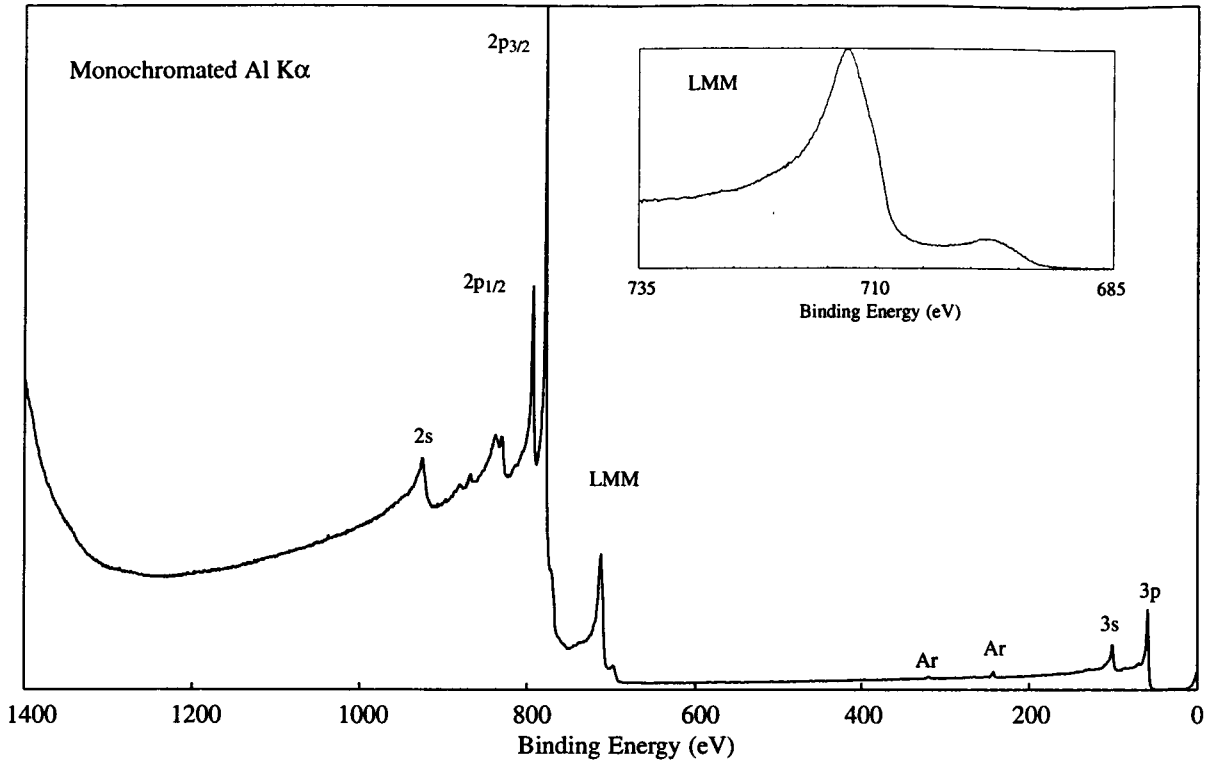
$LM_{23}M_{23}$	$L_3M_{23}M_{45}$ (^1P)	$L_3M_{45}M_{45}$	
888	839	784	(Al)
655	606	551	(Mg)

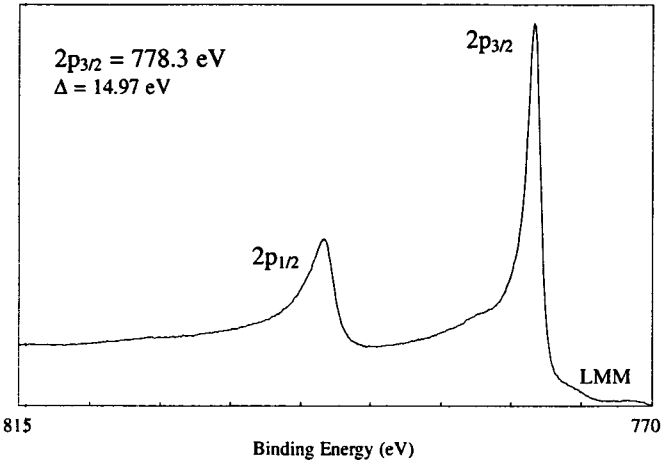
Iron Fe
Atomic Number 26











Line Positions (eV)

Photoelectron Lines

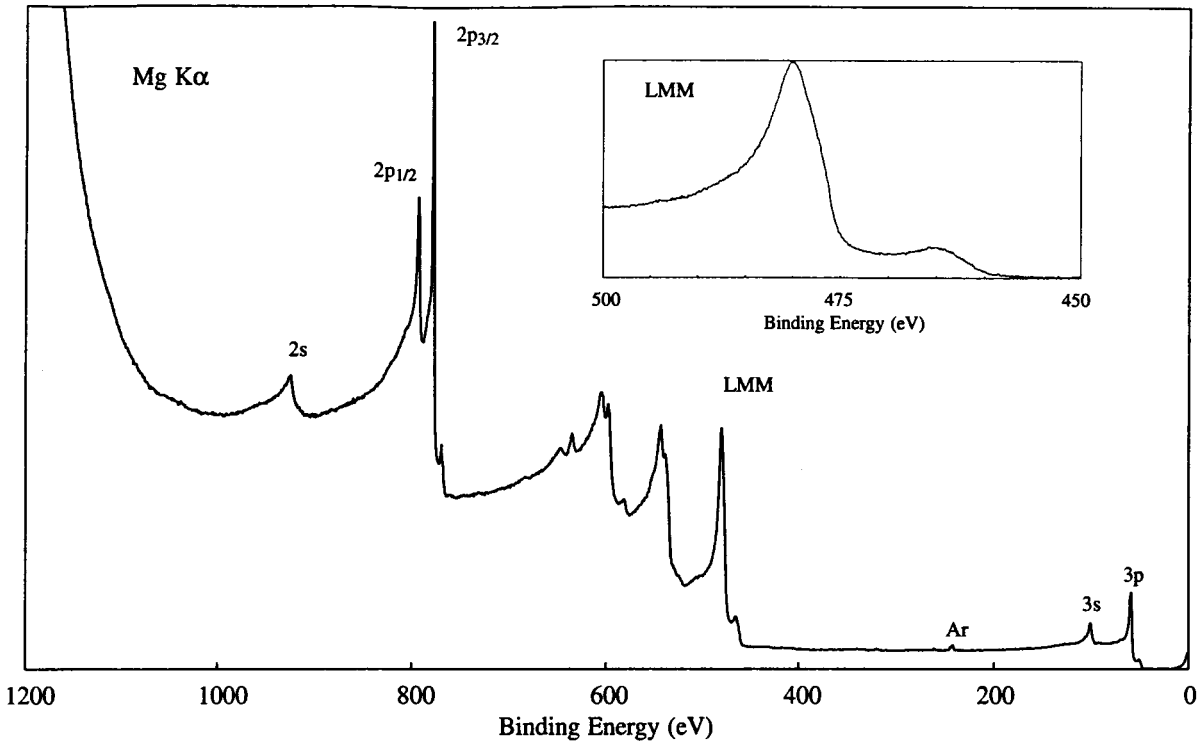
2s	2p1/2	2p3/2	3s	3p
925	793	778	101	60

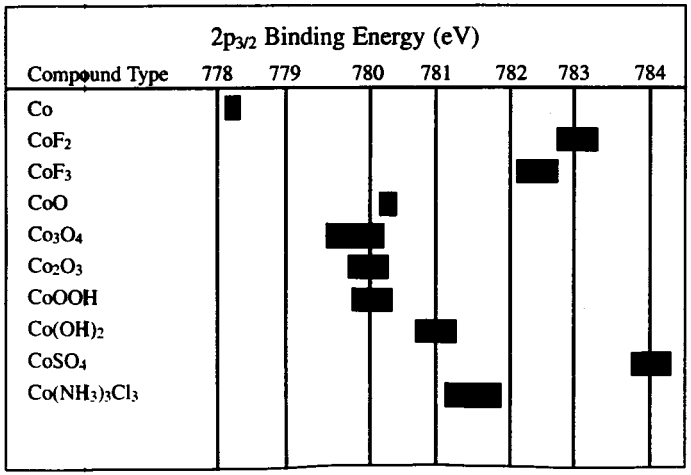
Auger Lines

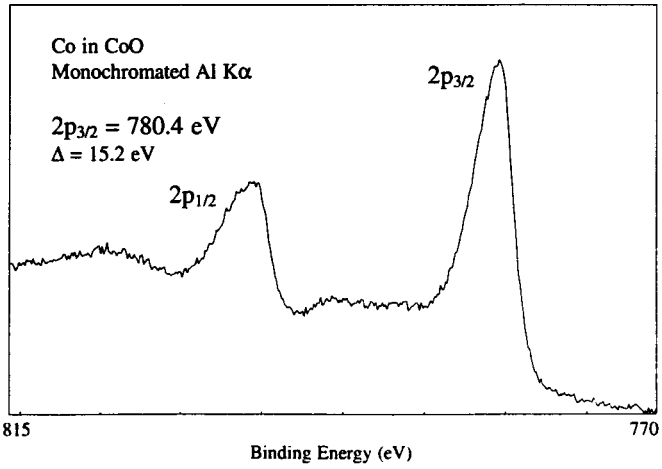
$L_3M_{23}M_{23}$	$L_2M_{23}M_{23}$	$L_3M_{23}M_{45}$ (^1P)	
838	831	777	(Al)
605	598	544	(Mg)

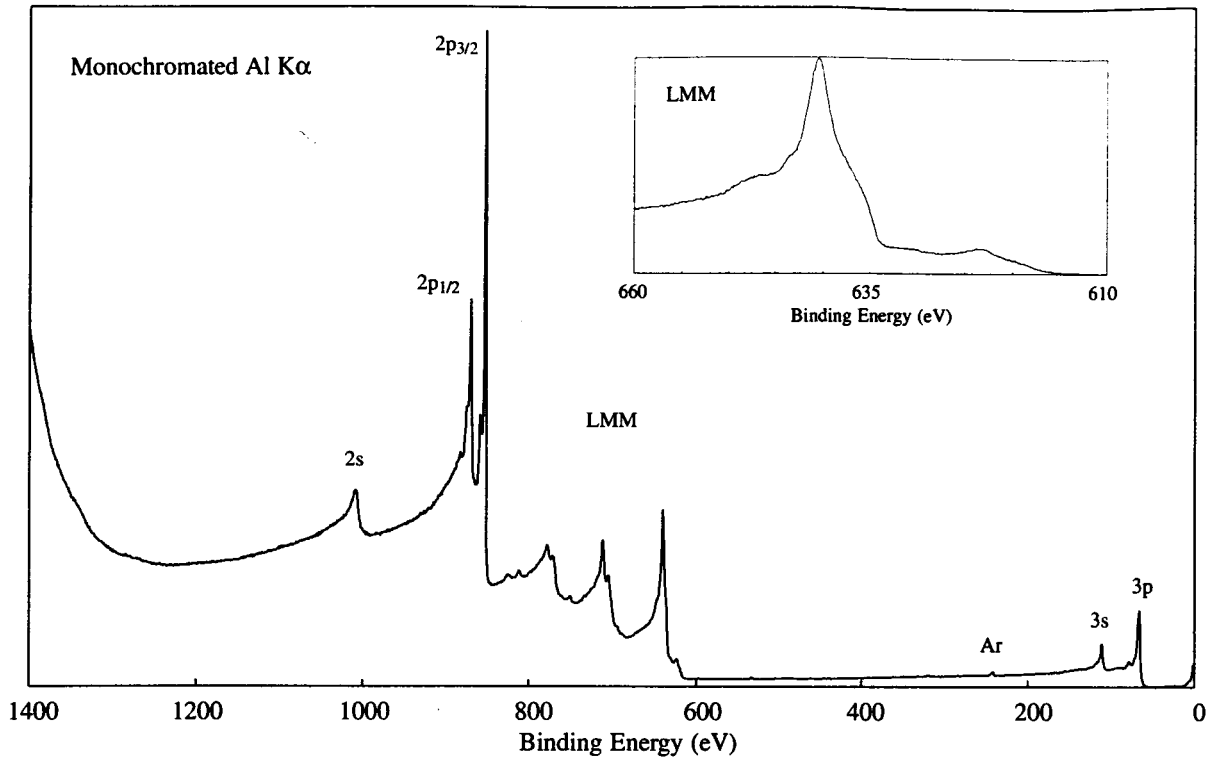
$L_3M_{23}M_{45}$ (^3P)	$L_2M_{23}M_{45}$ (^1P)	$L_3M_{45}M_{45}$	
771	713	698	(Al)
538	480	465	(Mg)

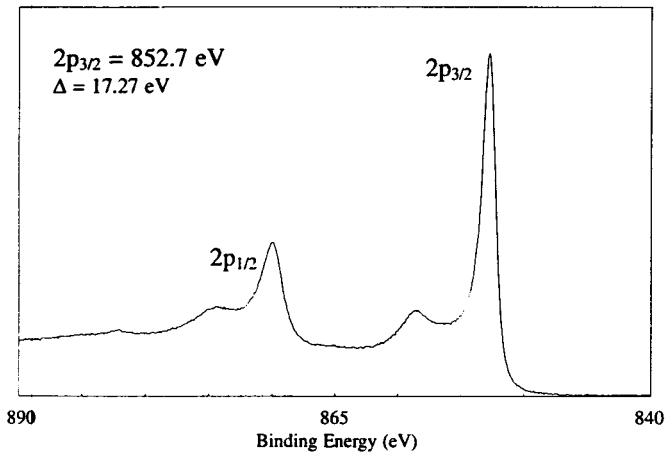
Cobalt Co
Atomic Number 27











Line Positions (eV)

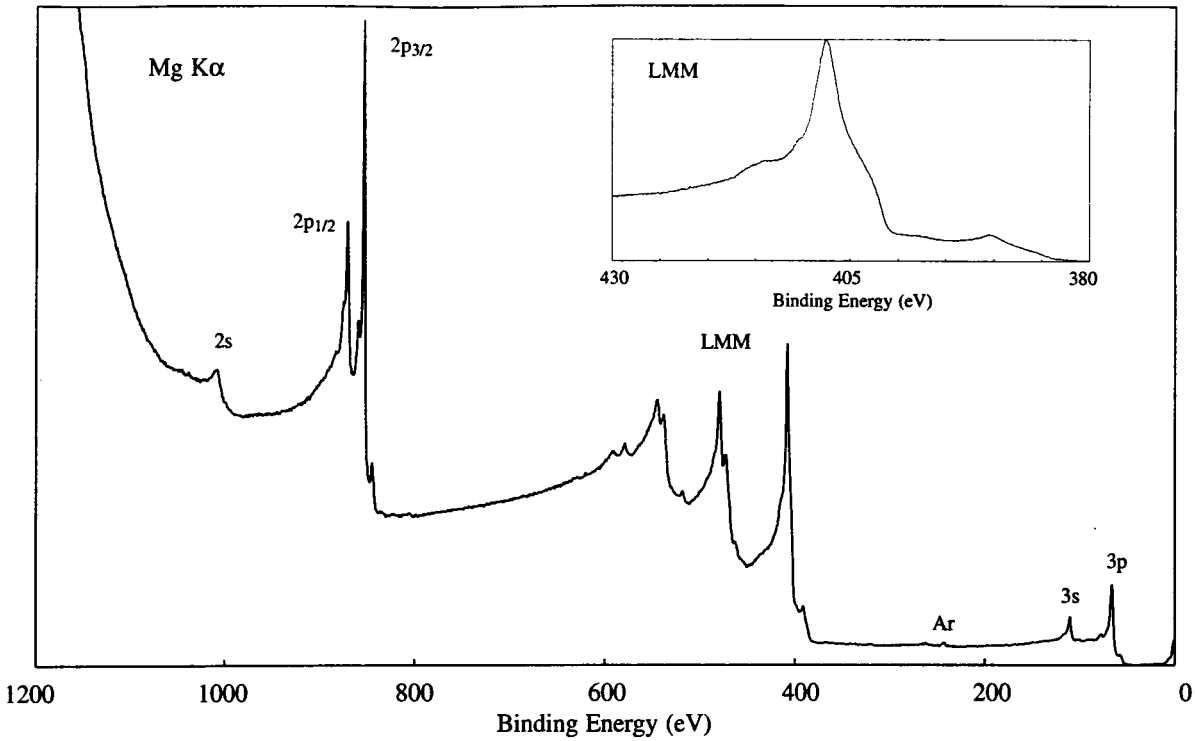
Photoelectron Lines

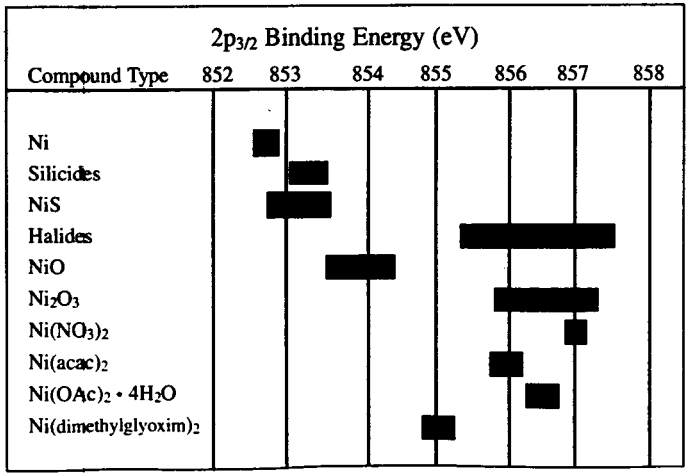
2s	2p1/2	2p3/2	3s	3p
1009	870	853	111	67

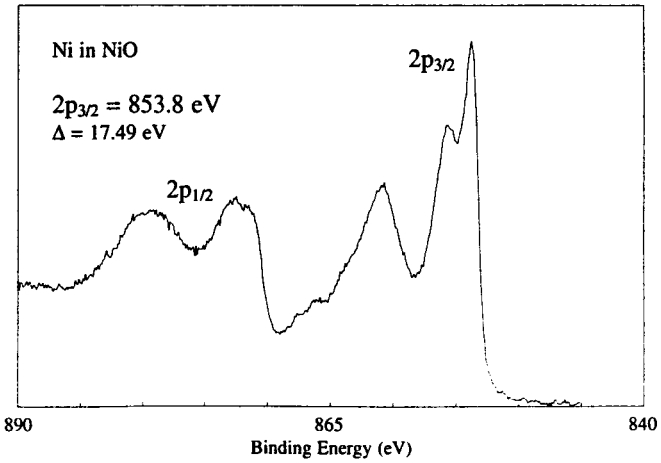
Auger Lines

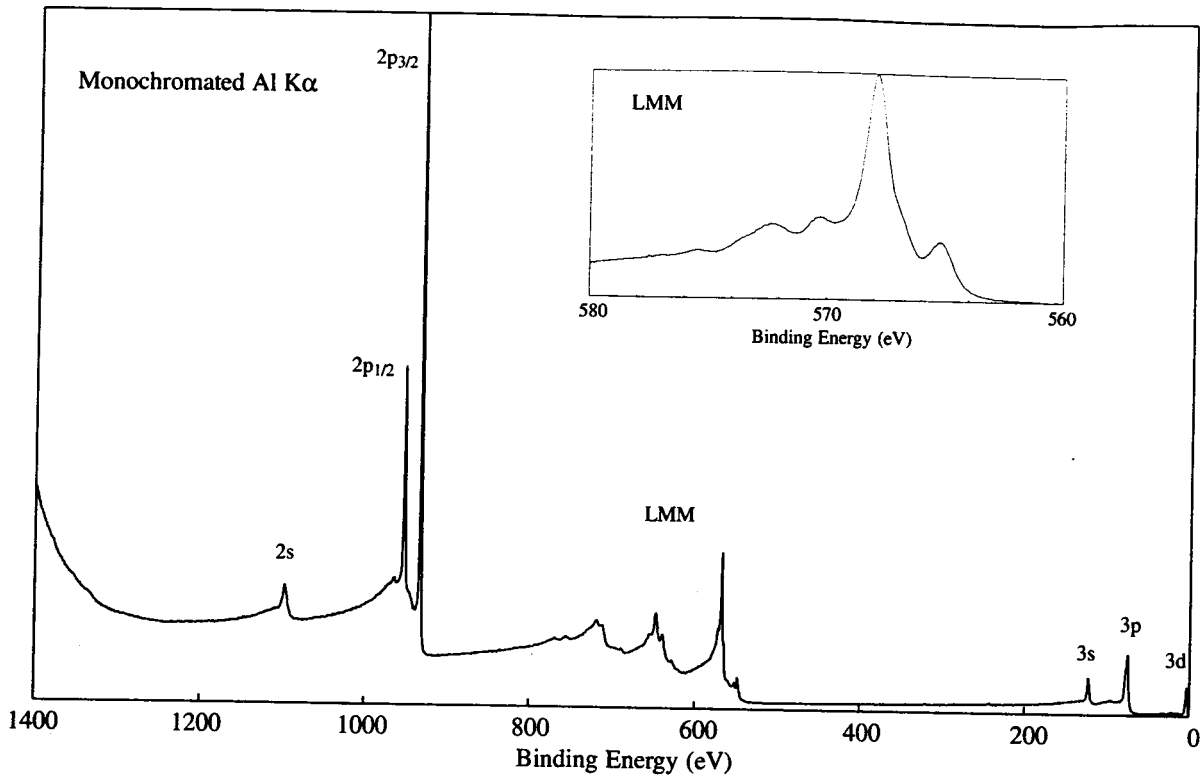
$L_3M_{23}M_{23}$	$L_2M_{23}M_{23}$	$L_3M_{23}M_{45}$ (^1P)	
778	772	712	
545	539	479	
$L_3M_{23}M_{45}$ (^3P)	$L_2M_{23}M_{45}$ (^1P)	$L_3M_{45}M_{45}$	
706	641	624	(Al)
473	408	391	(Mg)

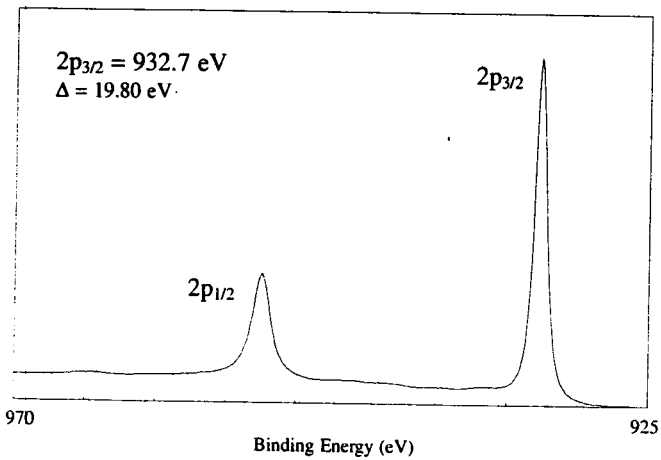
Nickel Ni
Atomic Number 28











Line Positions (eV)

Photoelectron Lines

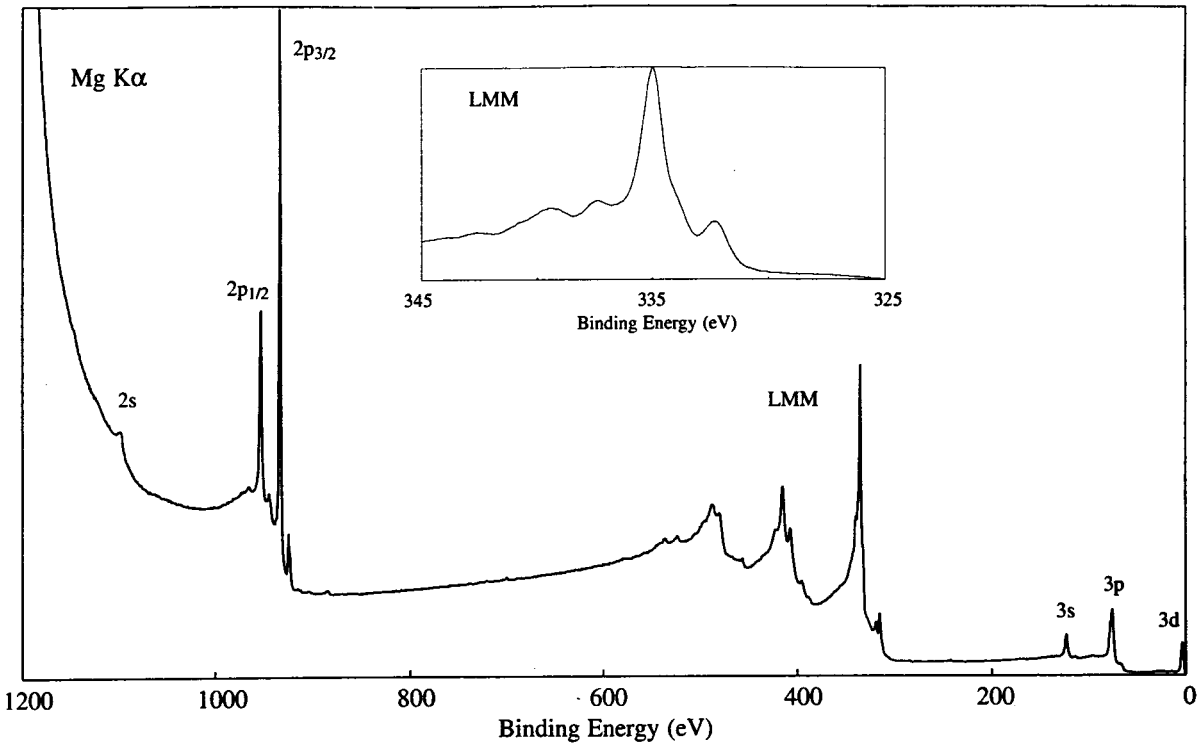
2s	2p1/2	2p3/2	3s	3p1/2	3p3/2
1097	953	933	123	77	75

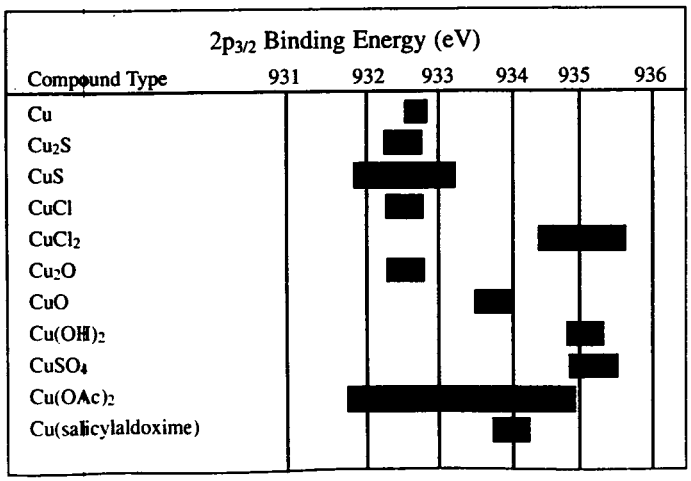
Auger Lines

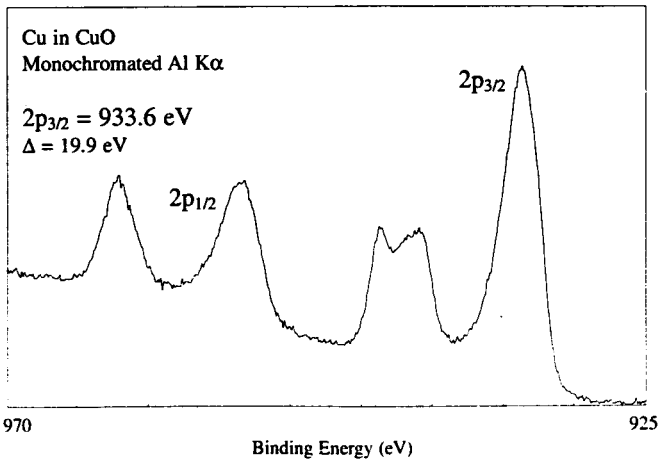
$L_3M_{23}M_{23}$	$L_2M_{23}M_{23}$	$L_3M_{23}M_{45}$ (^1P)	
719	712	648	(Al)
486	479	415	(Mg)

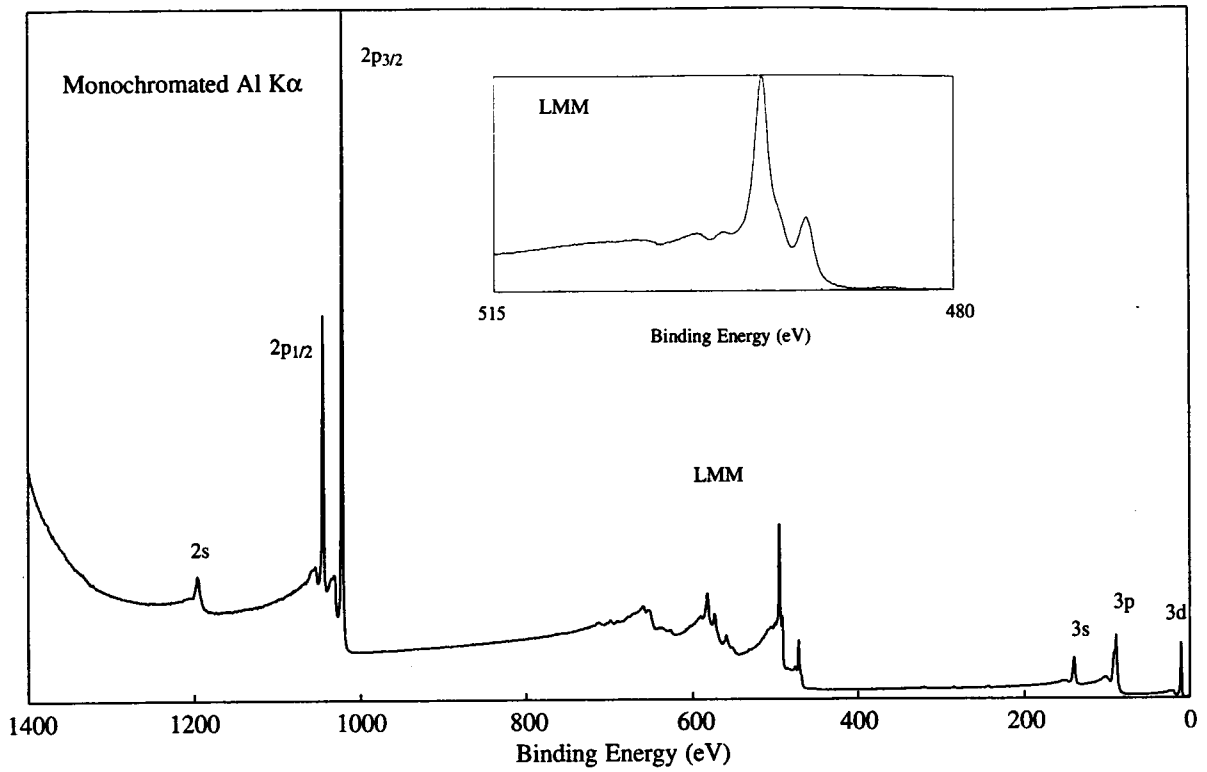
$L_3M_{23}M_{45}$ (^3P)	$L_2M_{23}M_{45}$ (^1P)	$L_3M_{45}M_{45}$	$L_2M_{45}M_{45}$	
640	628	568	548	(Al)
407	395	335	315	(Mg)

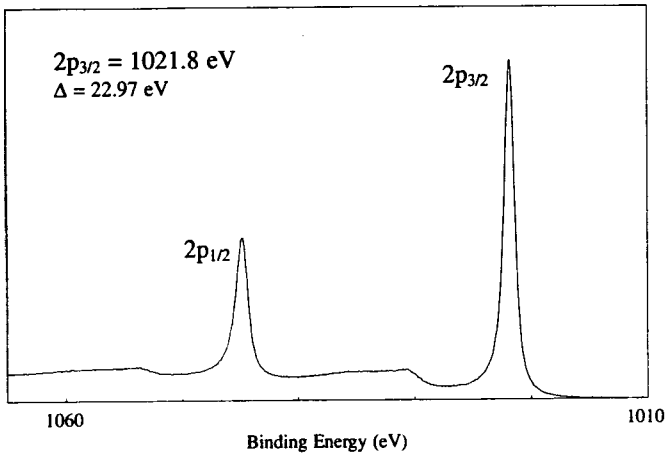
Copper Cu
Atomic Number 29











Line Positions (eV)

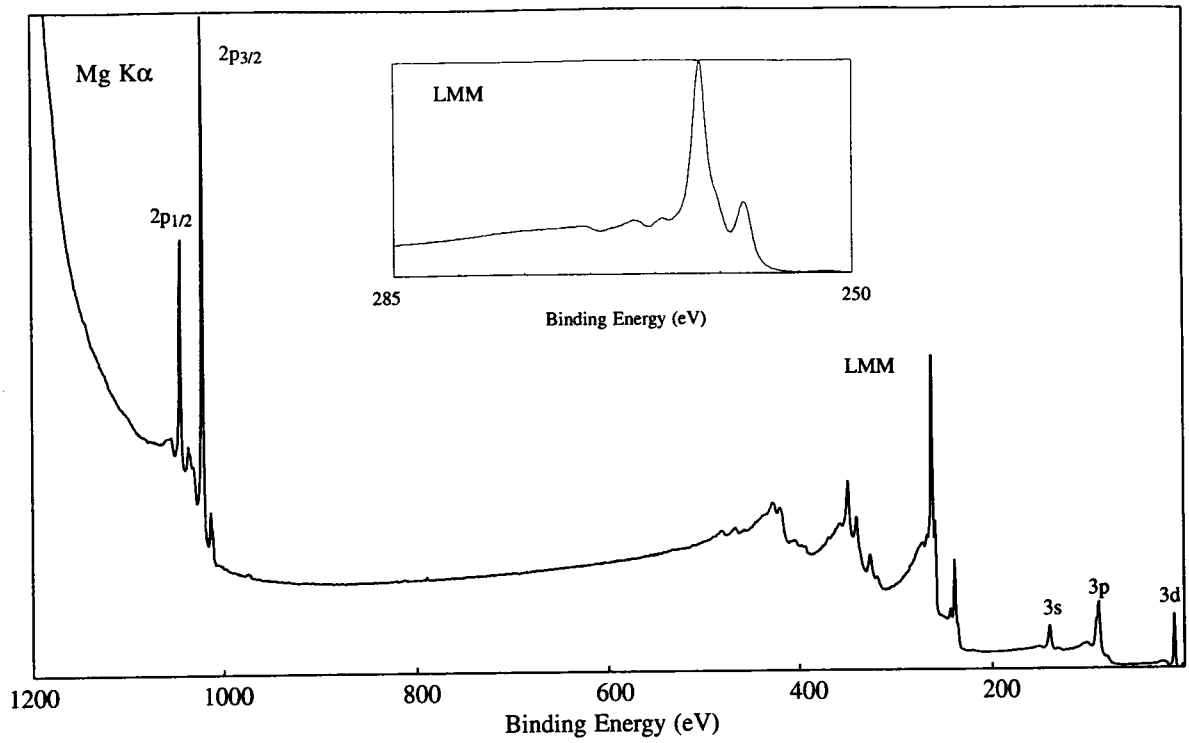
Photoelectron Lines

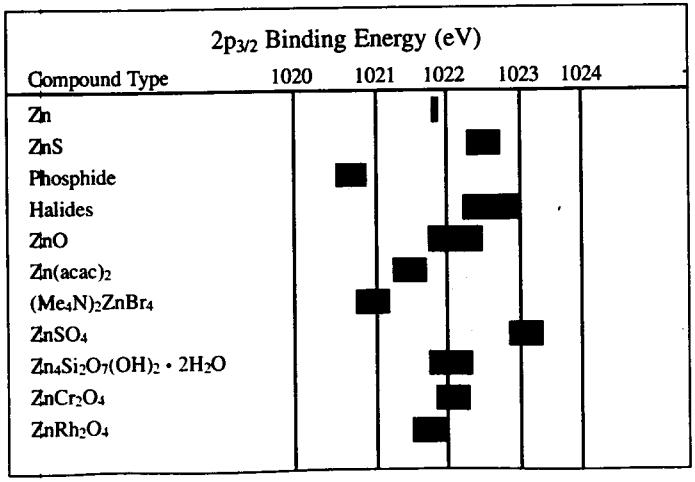
2s	2p1/2	2p3/2	3s	3p1/2	3p3/2	3d
1195	1045	1022	140	91	89	10

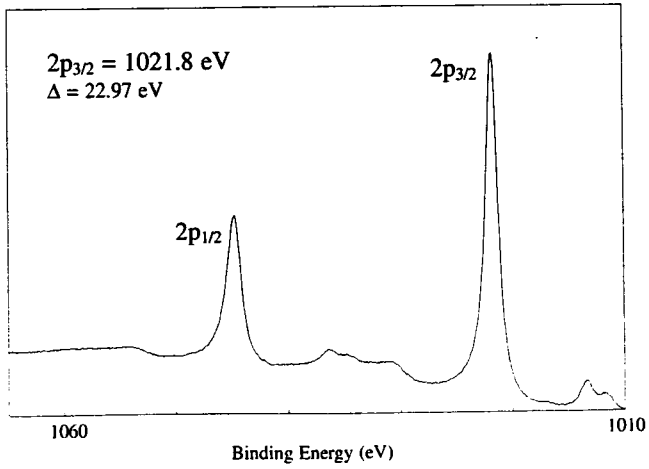
Auger Lines

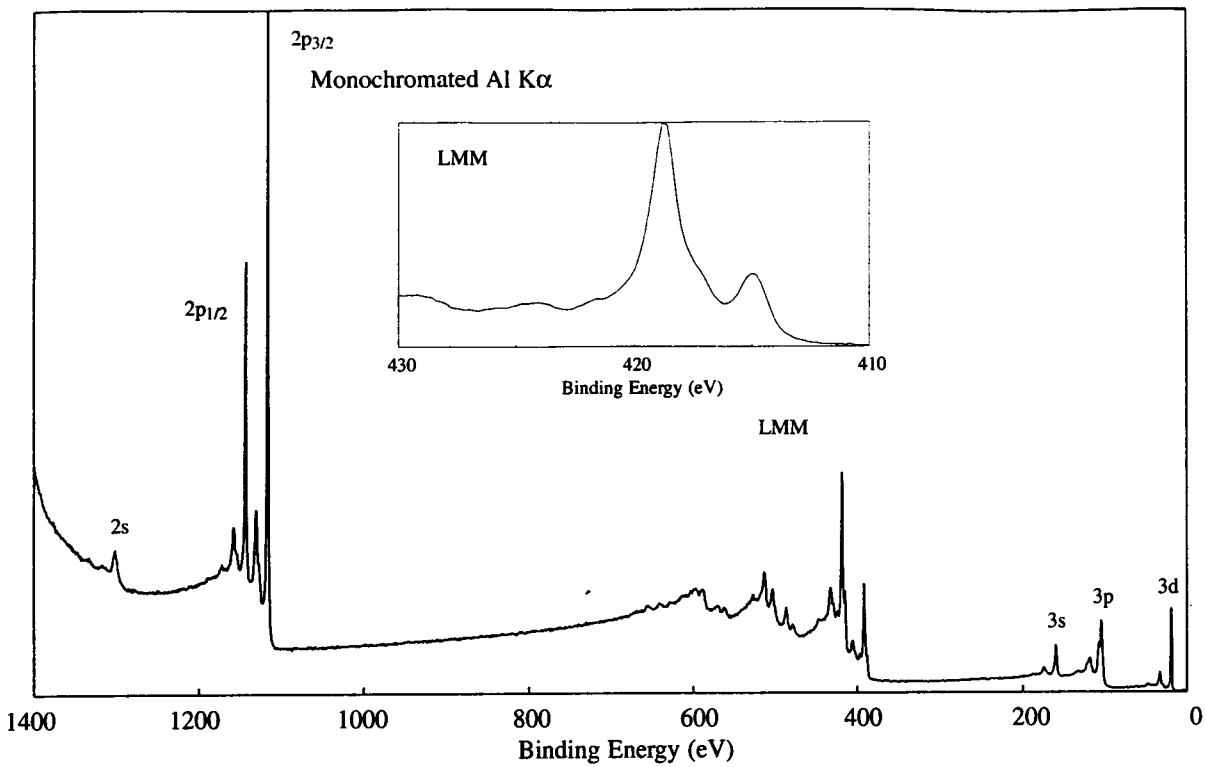
$L_3M_{23}M_{23}$	$L_2M_{23}M_{23}$	$L_3M_{23}M_{45}$ (^1P)	
660	652	582	(Al)
427	419	349	(Mg)

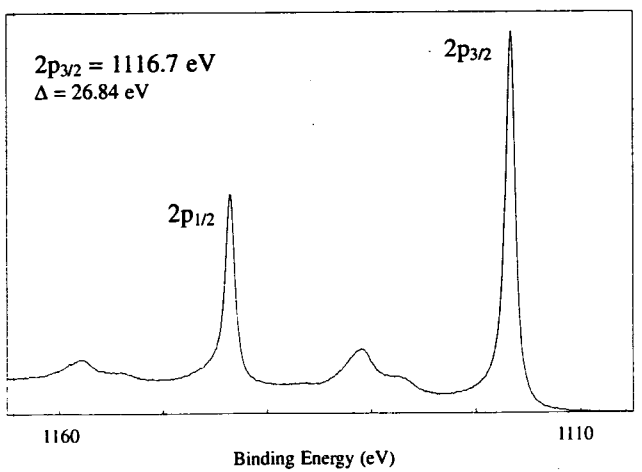
$L_3M_{23}M_{45}$ (^3P)	$L_2M_{23}M_{45}$ (^1P)	$L_3M_{45}M_{45}$	$L_2M_{45}M_{45}$	
573	559	495	472	(Al)
340	326	262	239	(Mg)


Mg Kα
2p3/2
2p1/2
LMM
285
250
Binding Energy (eV)
LMM
3s
3p
3d
1200
1000
800
600
400
200
0
Binding Energy (eV)


2p3/2 Binding Energy (eV)
Compound Type
1020
1021
1022
1023
1024
Zn
ZnS
Phosphide
Halides
ZnO
Zn(acac)2
(Me4N)2ZnBr4
ZnSO4
Zn4Si2O7(OH)2 • 2H2O
ZnCr2O4
ZnRh2O4


2p3/2 = 1021.8 eV
Δ = 22.97 eV
2p3/2
2p1/2
1060
1010
Binding Energy (eV)





Line Positions (eV)

Photoelectron Lines

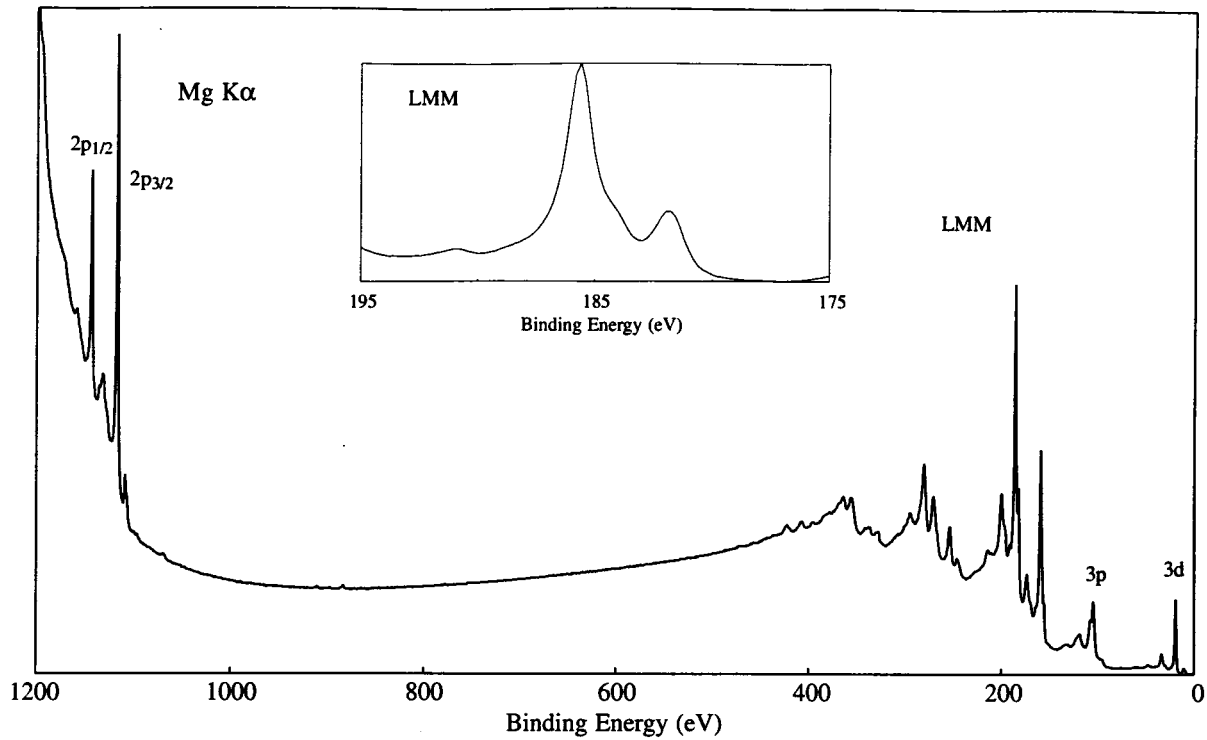
2s	2p1/2	2p3/2	3s	3p1/2	3p3/2	3d
1301	1144	1117	160	107	104	19

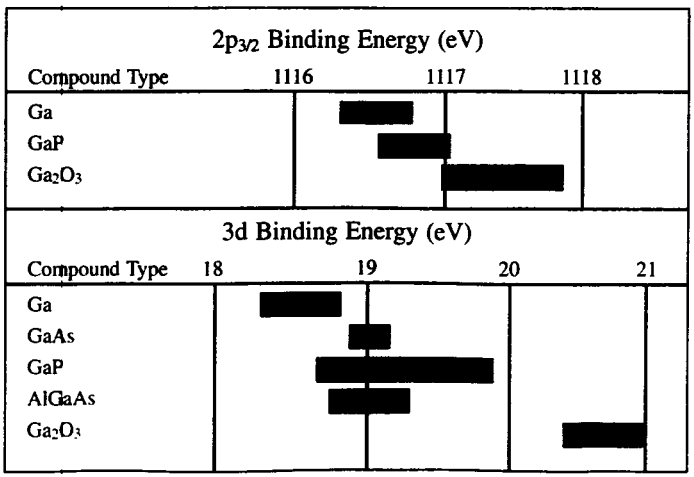
Auger Lines

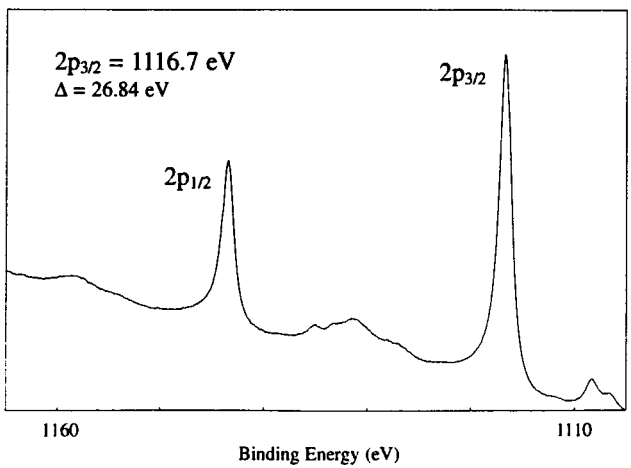
$L_3M_{23}M_{23}$	$L_2M_{23}M_{23}$	$L_3M_{23}M_{45}$ (^1P)	
597	589	514	(Al)
364	356	281	(Mg)

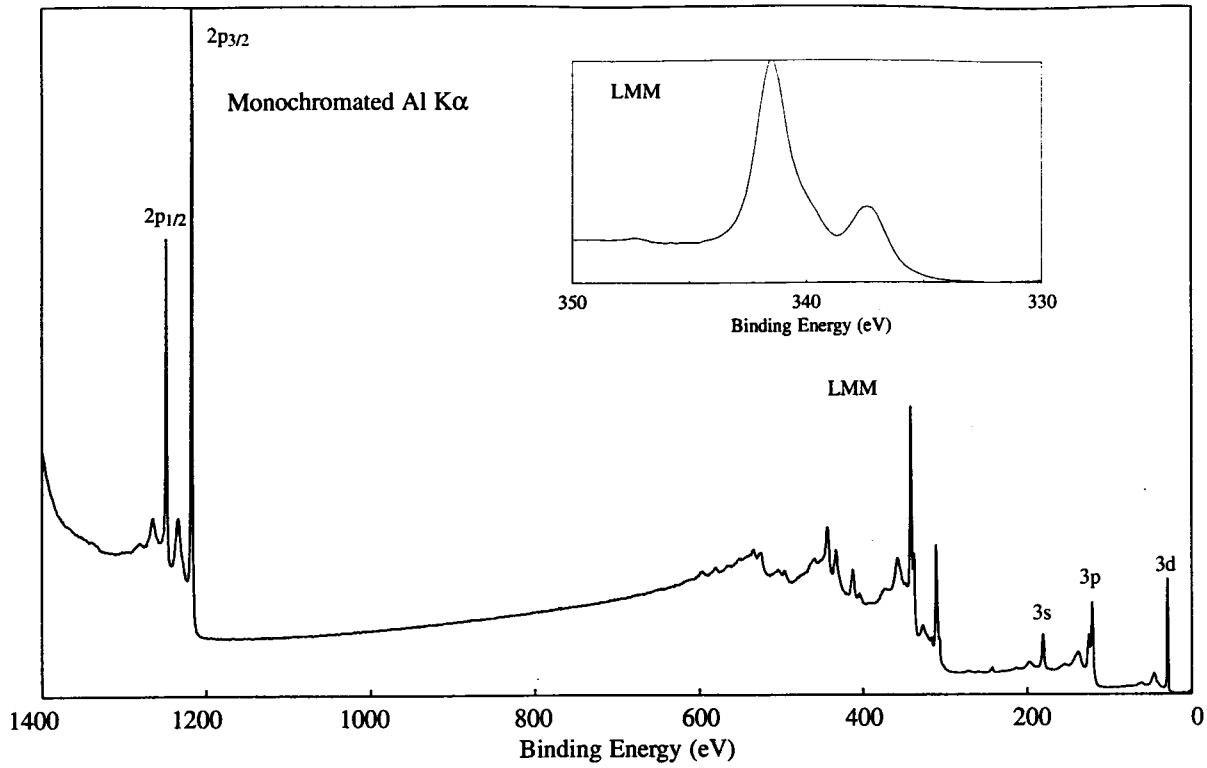
$L_3M_{23}M_{45}$ (^3P)	$L_2M_{23}M_{45}$ (^1P)	$L_3M_{45}M_{45}$	$L_2M_{45}M_{45}$	
504	487	419	392	(Al)
271	254	186	159	(Mg)

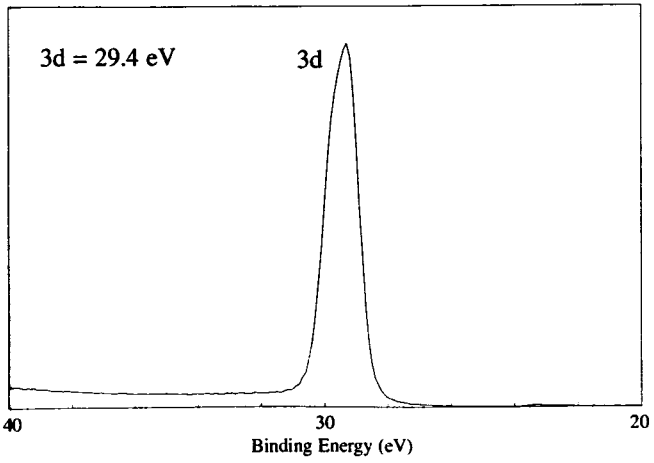
Gallium Ga
Atomic Number 31











Line Positions (eV)

Photoelectron Lines

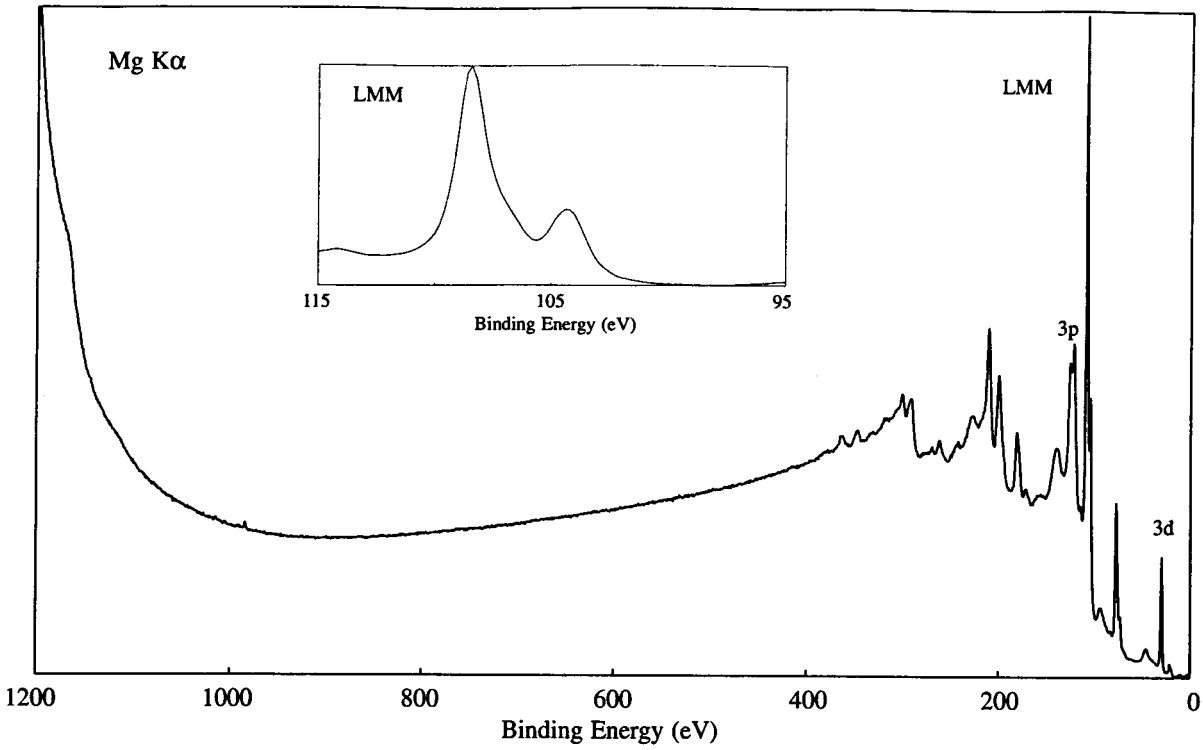
$2p_{1/2}$	$2p_{3/2}$	3s	$3p_{1/2}$	$3p_{3/2}$	3d
1248	1217	181	126	122	29

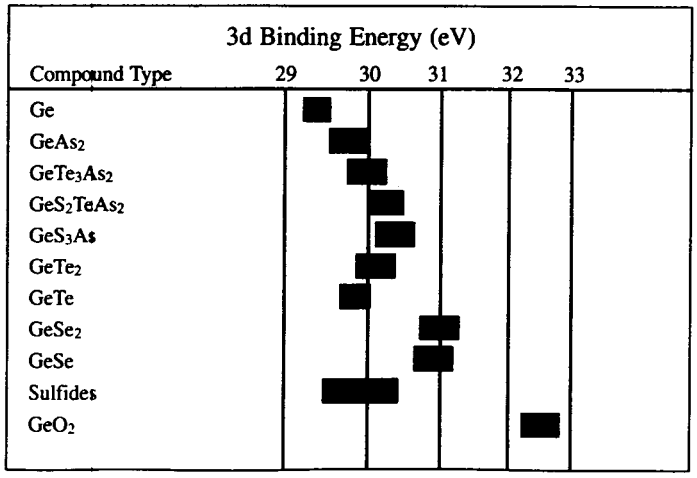
Auger Lines

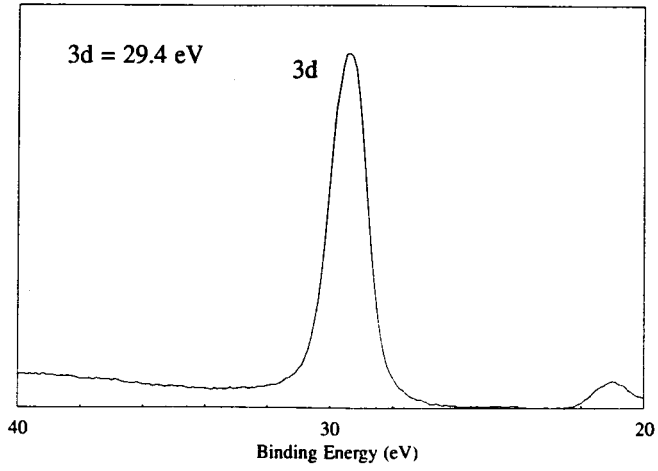
$L_3M_{23}M_{23}$	$L_2M_{23}M_{23}$	$L_3M_{23}M_{45}$ (^1P)	
534	525	444	(Al)
301	292	211	(Mg)

$L_3M_{23}M_{45}$ (^3P)	$L_2M_{23}M_{45}$ (^1P)	$L_3M_{45}M_{45}$	$L_2M_{45}M_{45}$	
433	412	342	310	(Al)
200	179	109	77	(Mg)

Germanium Ge
Atomic Number 32

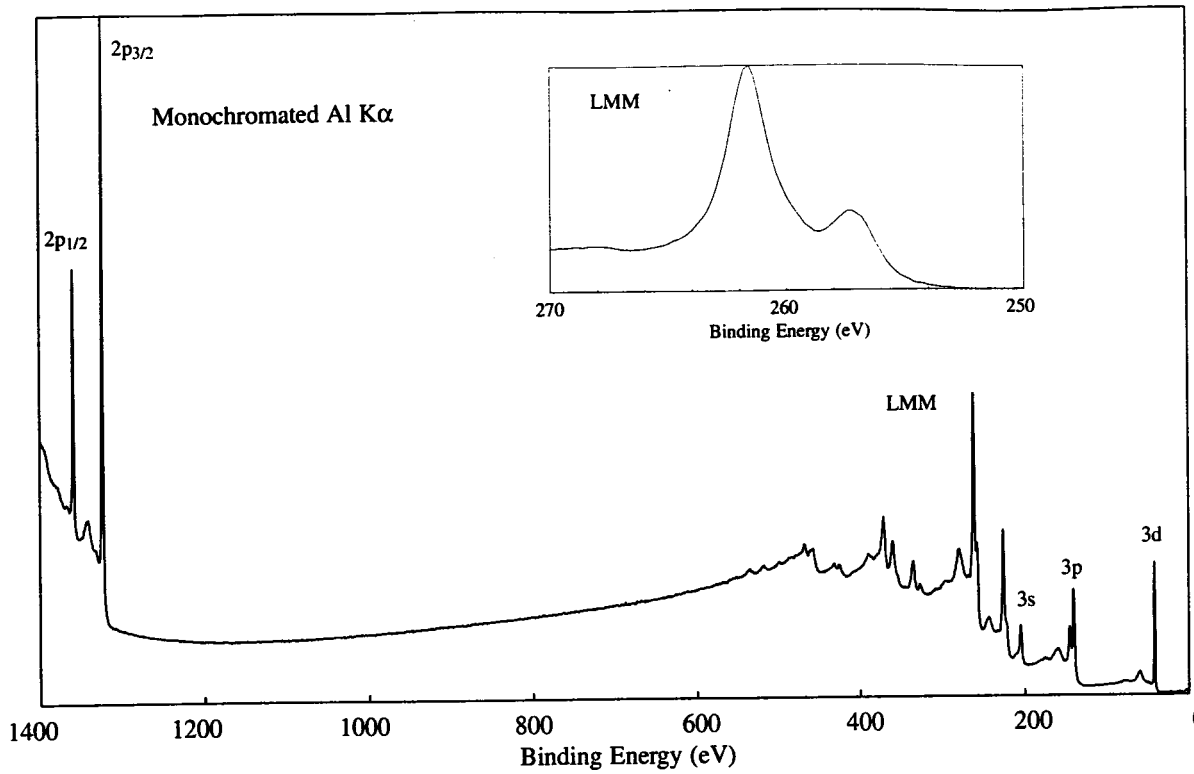


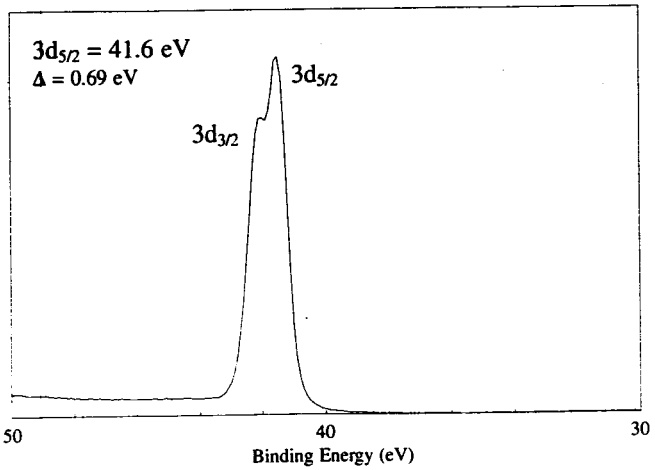




Arsenic As

Atomic Number 33





Line Positions (eV)

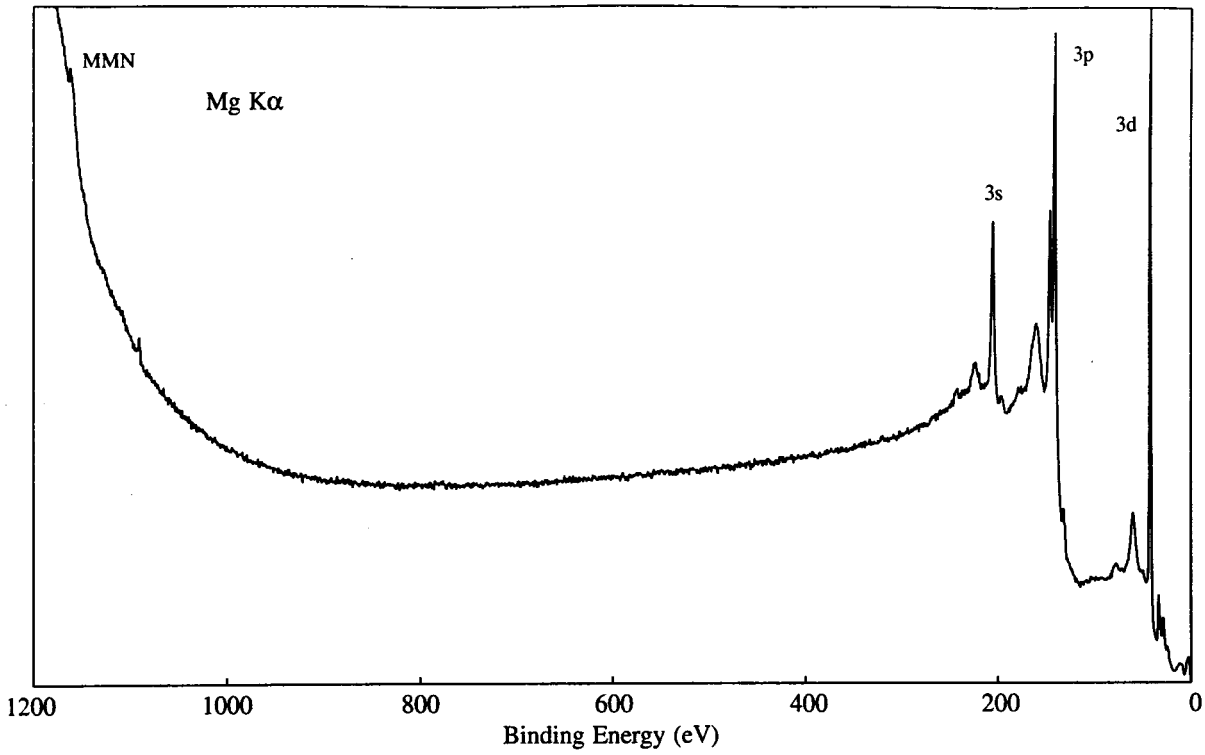
Photoelectron Lines

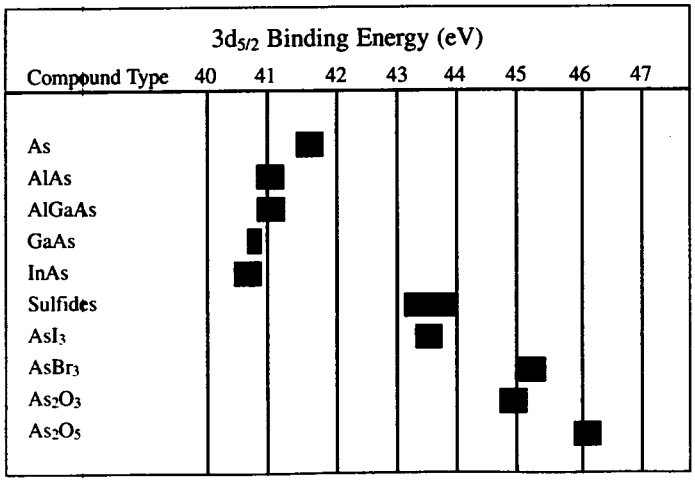
$2p_{1/2}$	$2p_{3/2}$	3s	$3p_{1/2}$	$3p_{3/2}$	$3d_{3/2}$	$3d_{5/2}$
1359	1324	205	146	141	43	42

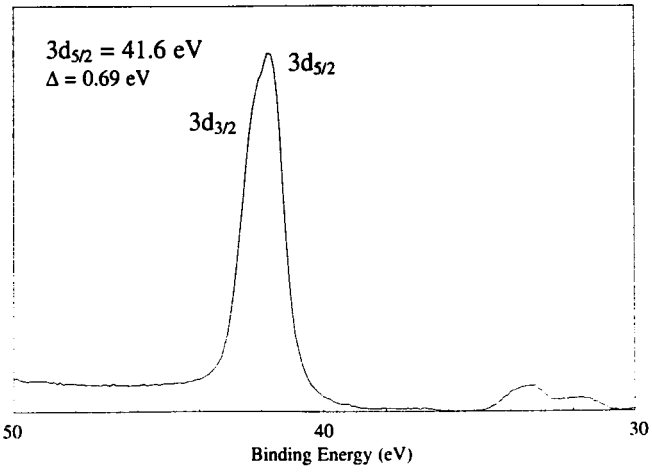
Auger Lines

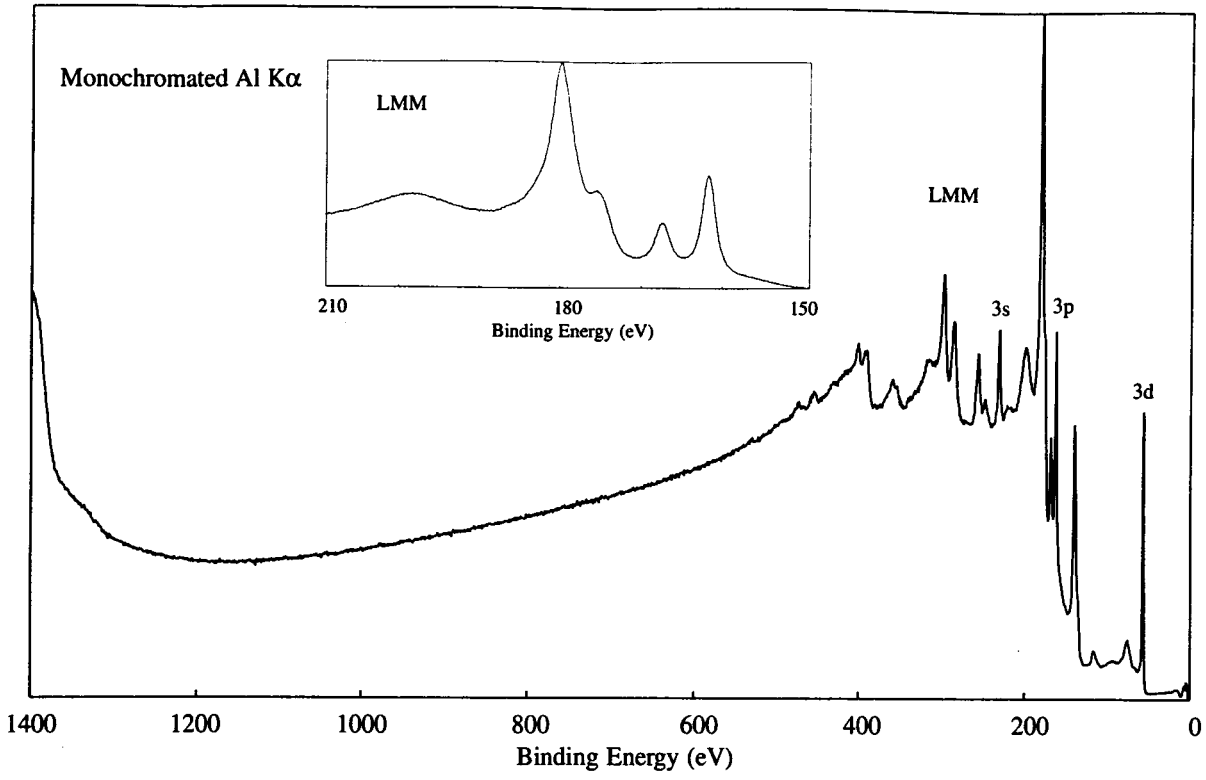
$L_3M_{23}M_{45}$ (^1P)	$L_3M_{23}M_{45}$ (^3P)		
371	360	(Al)	
$L_2M_{23}M_{45}$ (^1P)	$L_3M_{45}M_{45}$	$L_2M_{45}M_{45}$	
336	262	226	(Al)

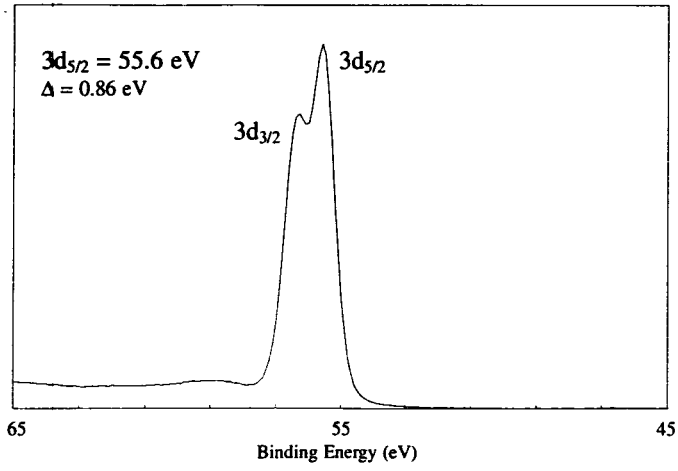
Arsenic As
Atomic Number 33











Line Positions (eV)

Photoelectron Lines

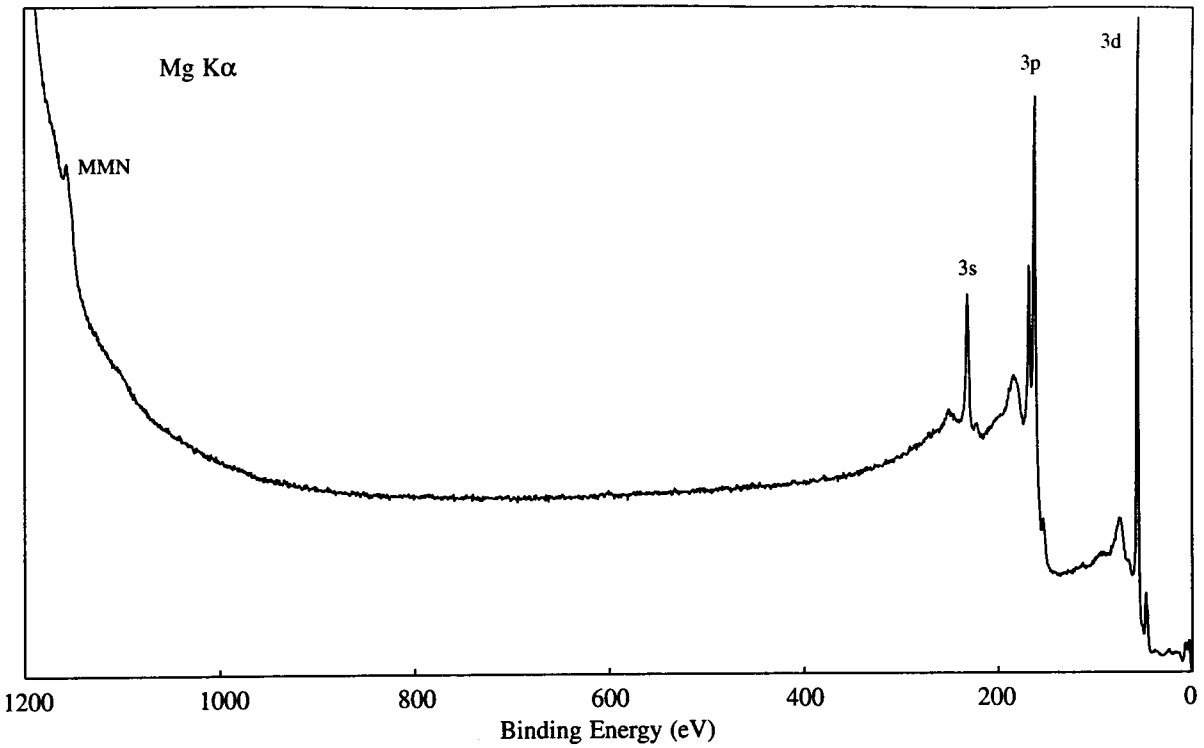
3s	3p1/2	3p3/2	3d3/2	3d5/2
232	169	163	57	56

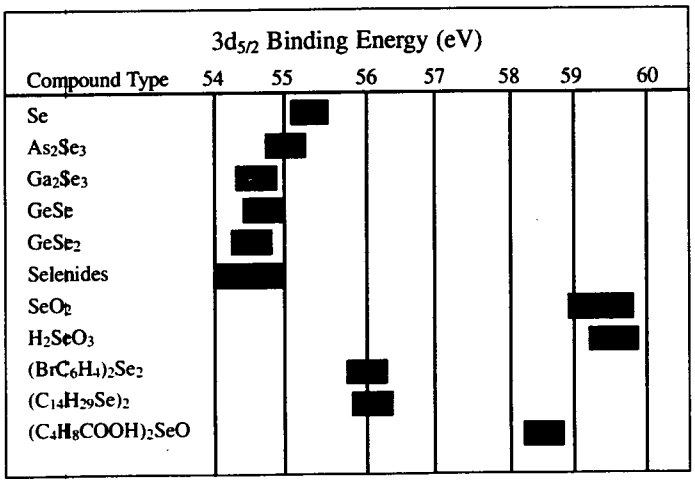
Auger Lines

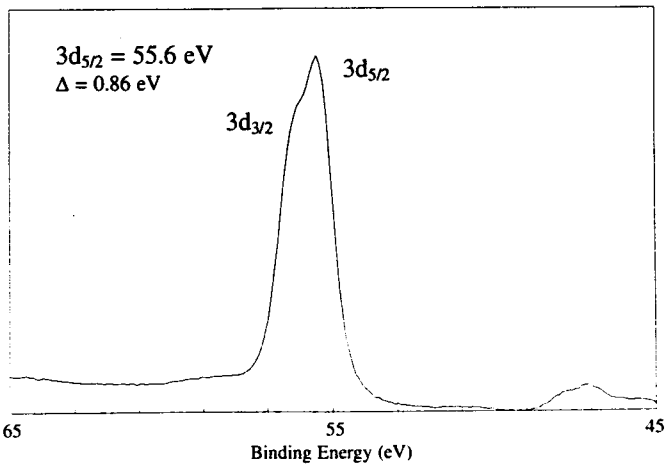
$L_3M_{23}M_{45}$ (^1P)		$L_3M_{23}M_{45}$ (^3P)	
299		287	(Al)
$L_2M_{23}M_{45}$ (^1P)	$L_3M_{45}M_{45}$	$L_2M_{45}M_{45}$	
257	181	140	(Al)

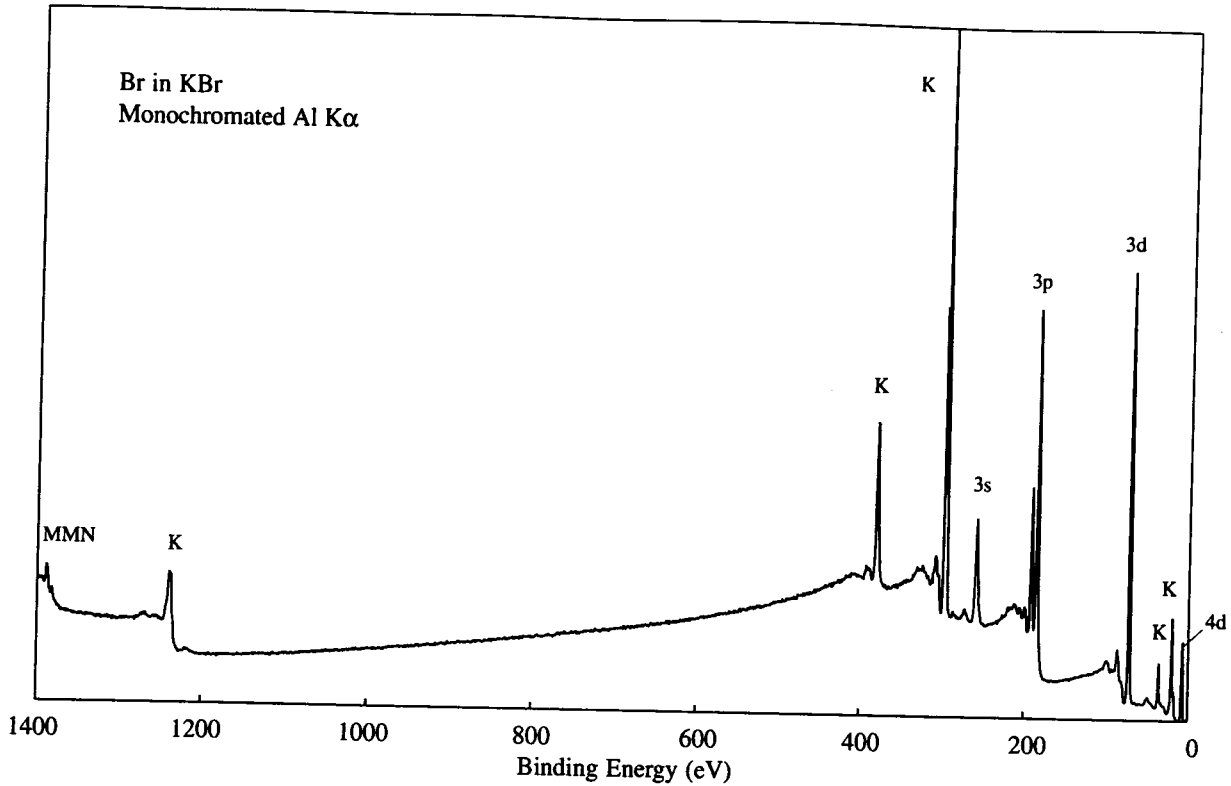
Selenium Se

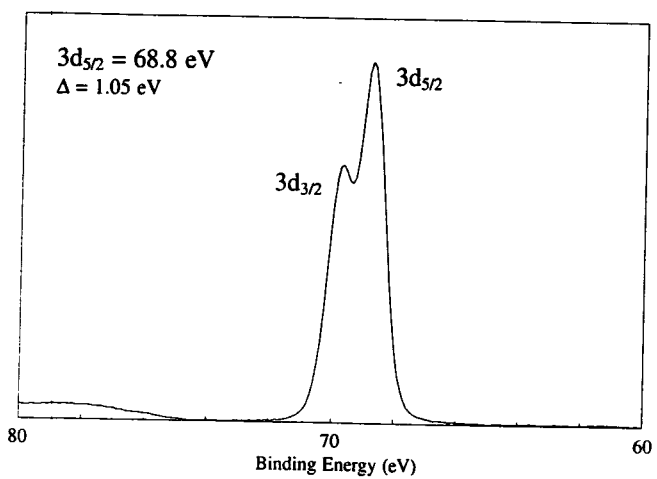
Atomic Number 34











Line Positions (eV)

Photoelectron Lines

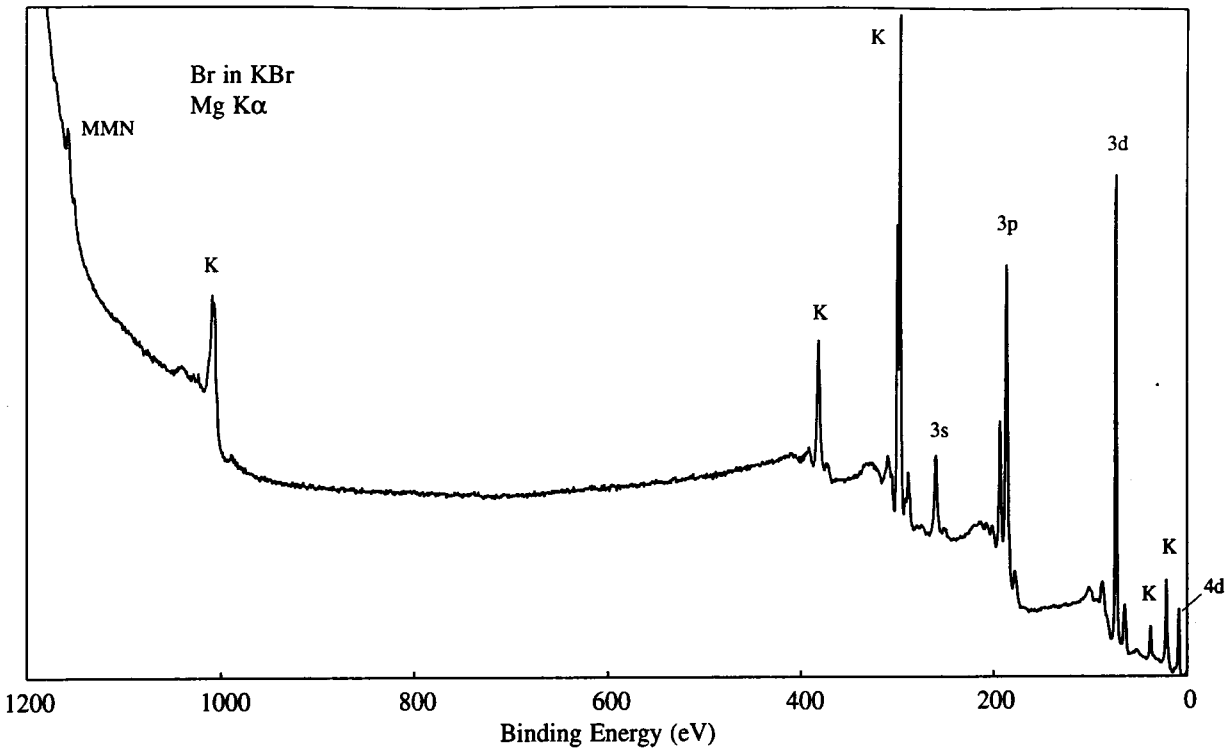
3s	3p1/2	3p3/2	3d3/2	3d5/2	4s	4d
256	189	182	70	69	15	5

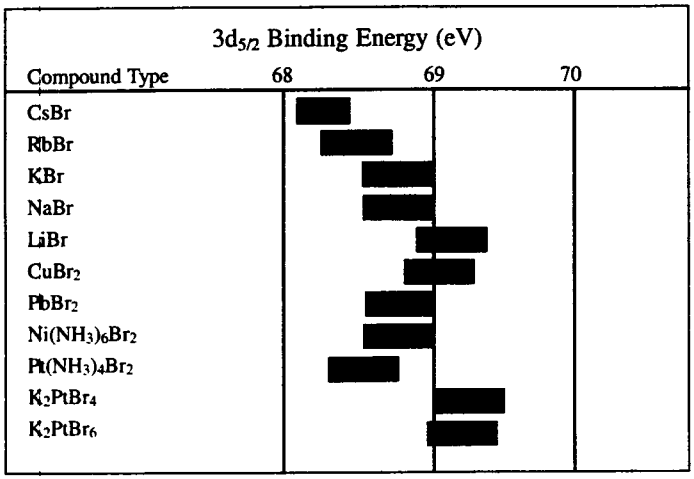
Auger Lines

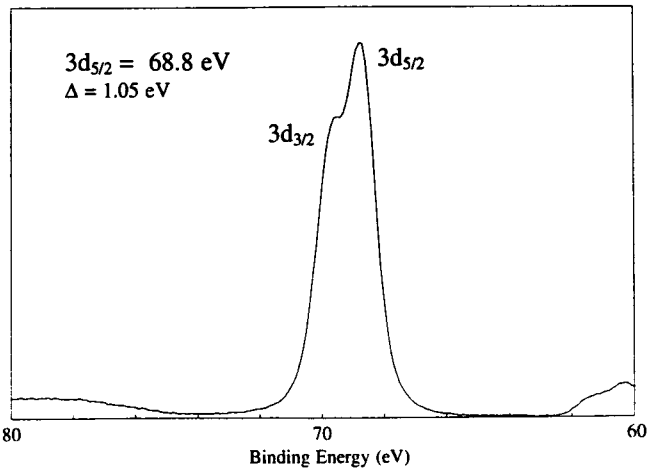
$M_{23}M_{45}N_{23}$
1386 (Al)
1153 (Mg)

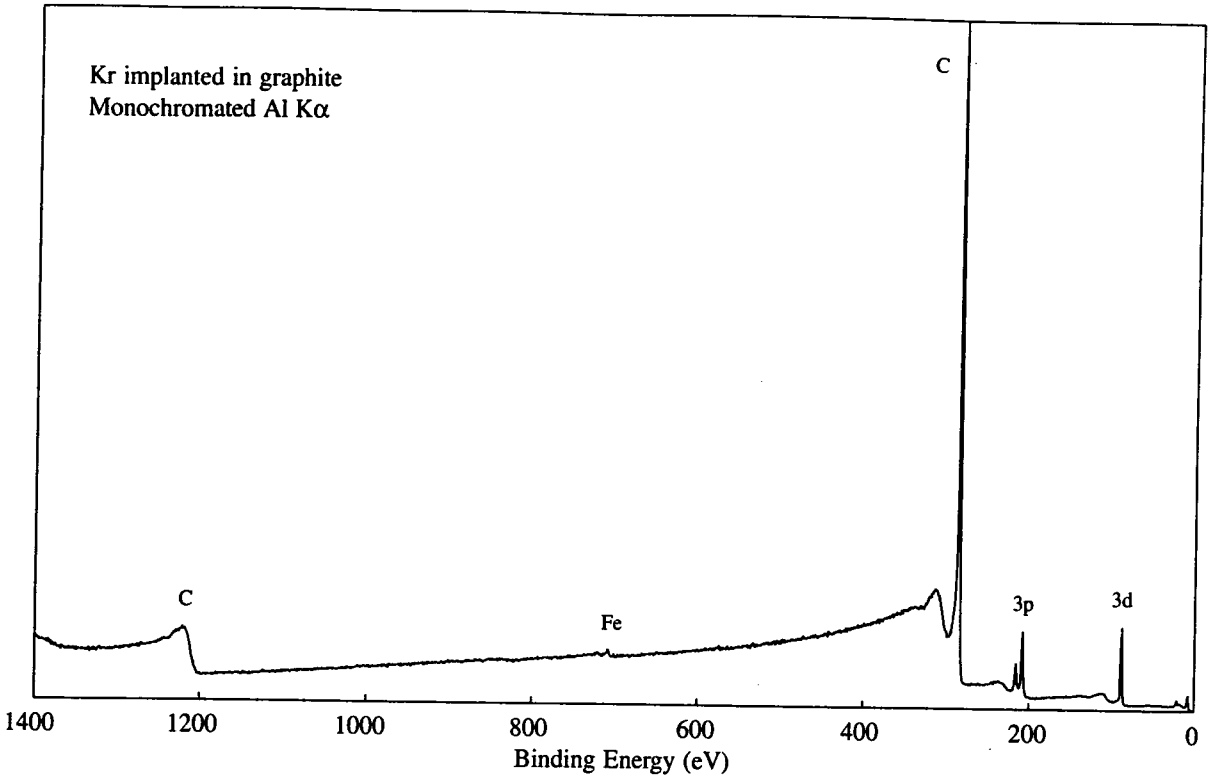
Bromine Br

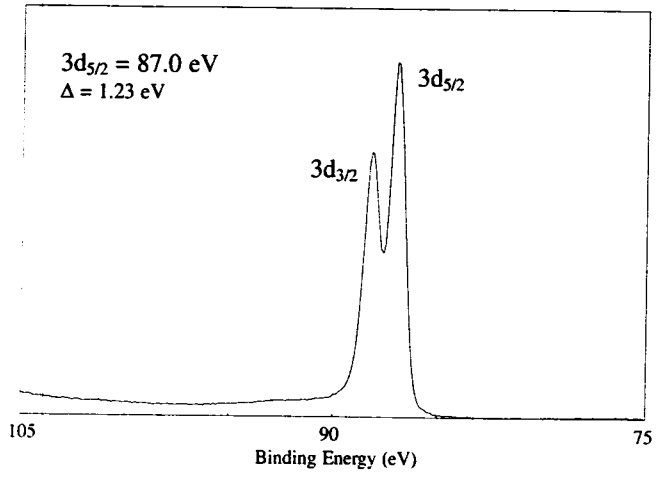
Atomic Number 35











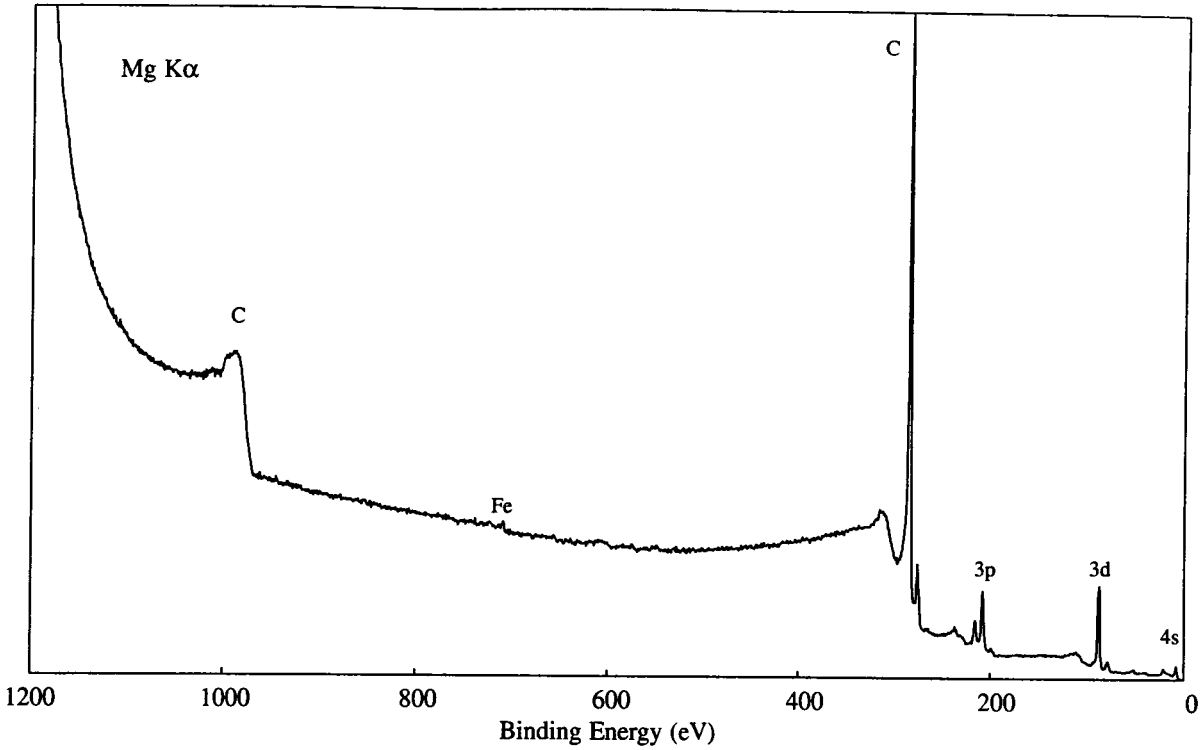
Line Positions (eV)

Photoelectron Lines

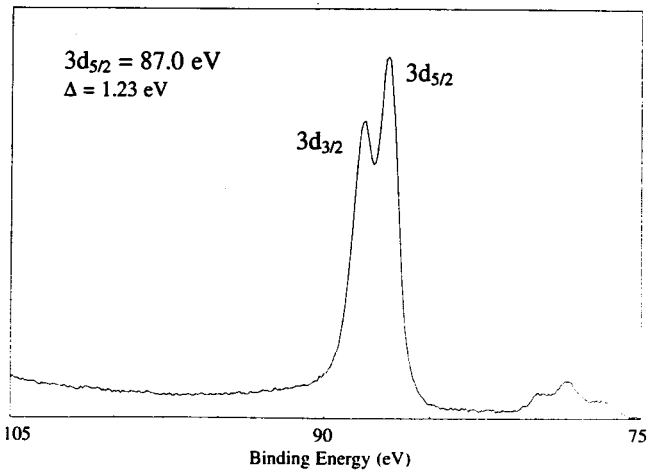
3s*	3p1/2	3p3/2	3d3/2	3d5/2	4s	4p
287	216	208	88	87	21	8

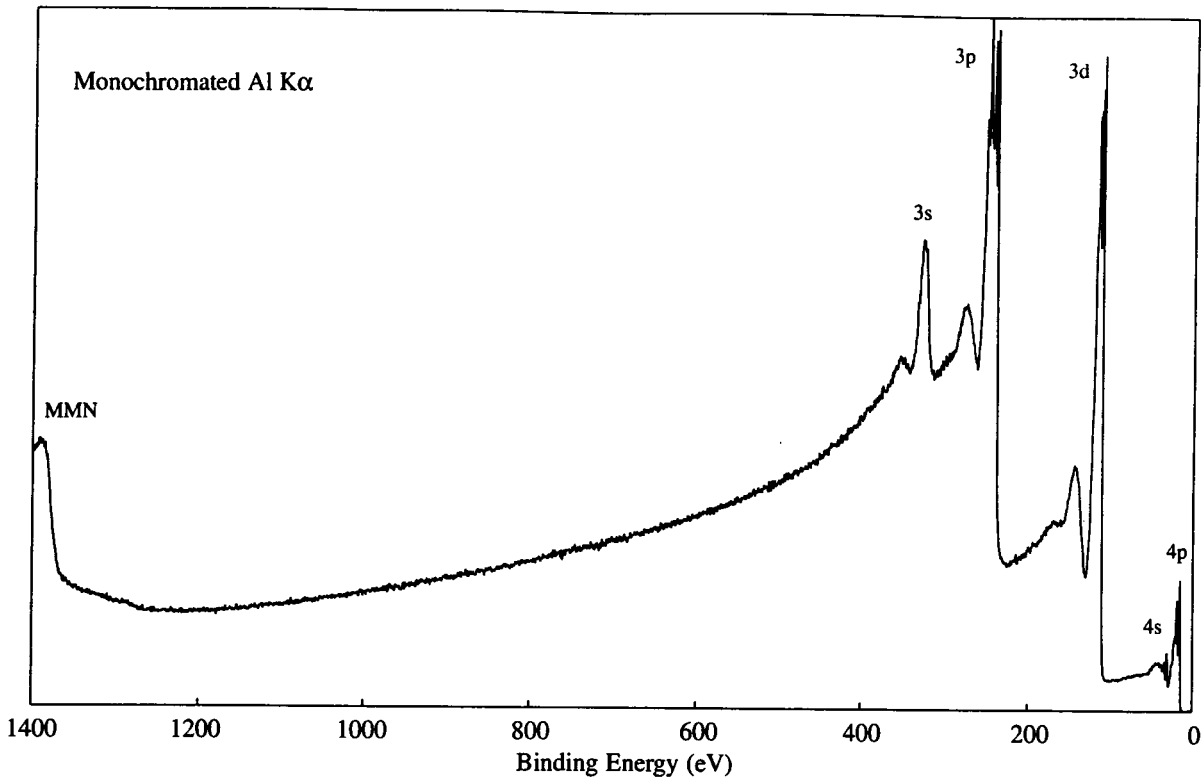
*Estimate

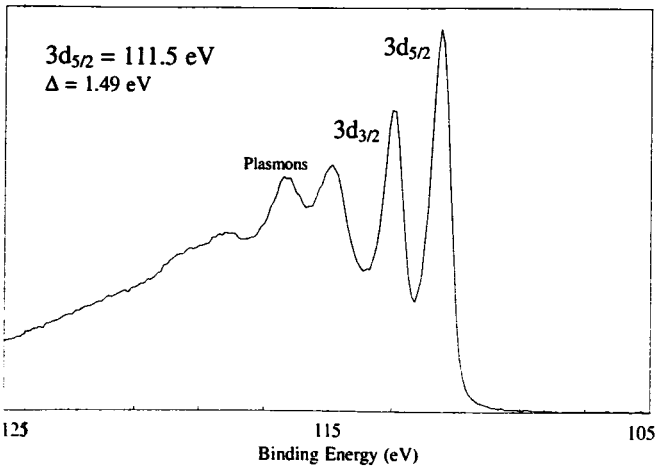
Krypton Kr
Atomic Number 36



Compound Type	$3d_{5/2}$ Binding Energy (eV) 84	86	88
Kr in graphite		■	







Line Positions (eV)

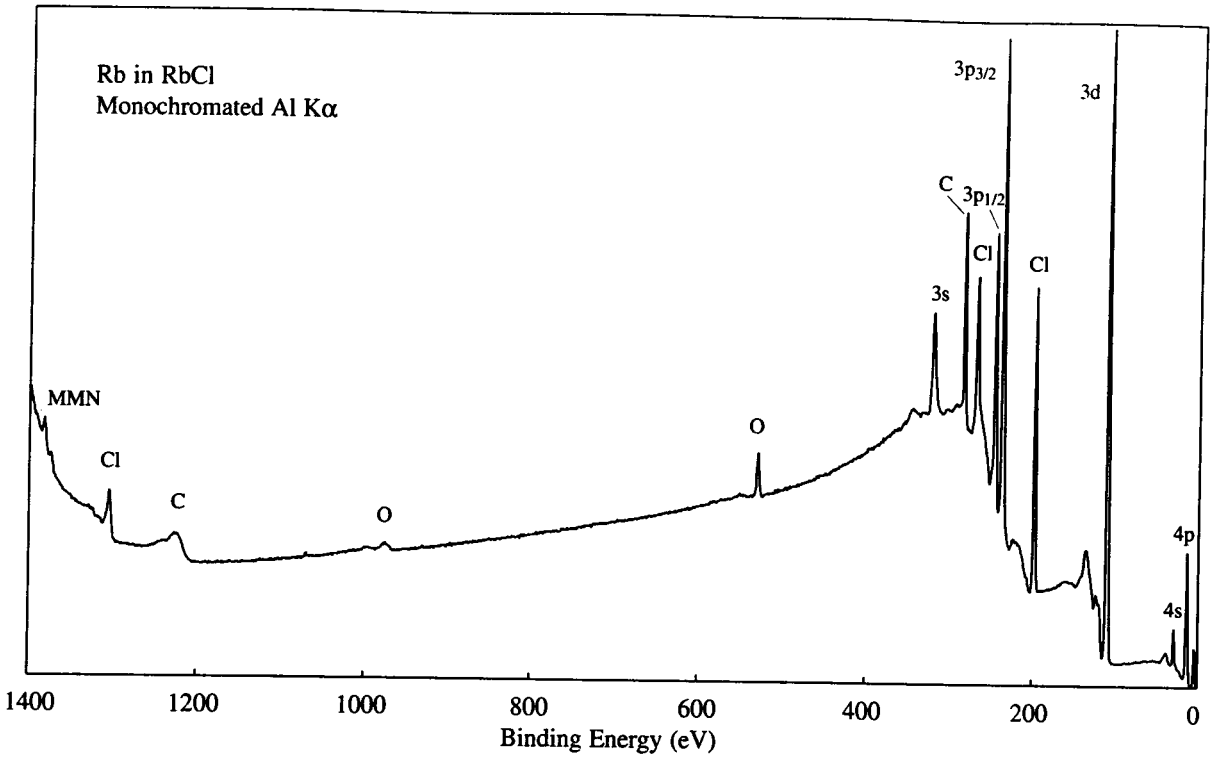
Photoelectron Lines

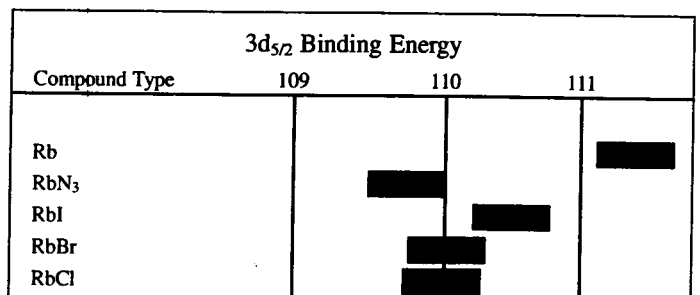
3s	$3p_{1/2}$	$3p_{3/2}$	$3d_{3/2}$	$3d_{5/2}$	4s	4p
325	249	240	113	111	31	16

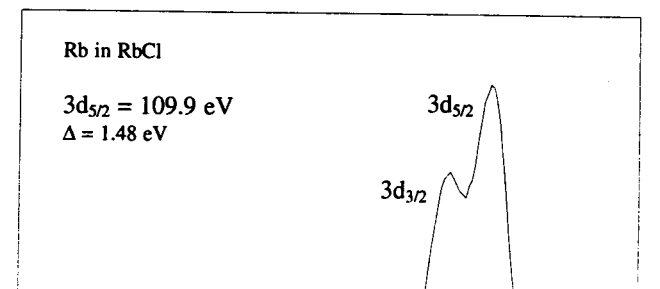
Auger Lines

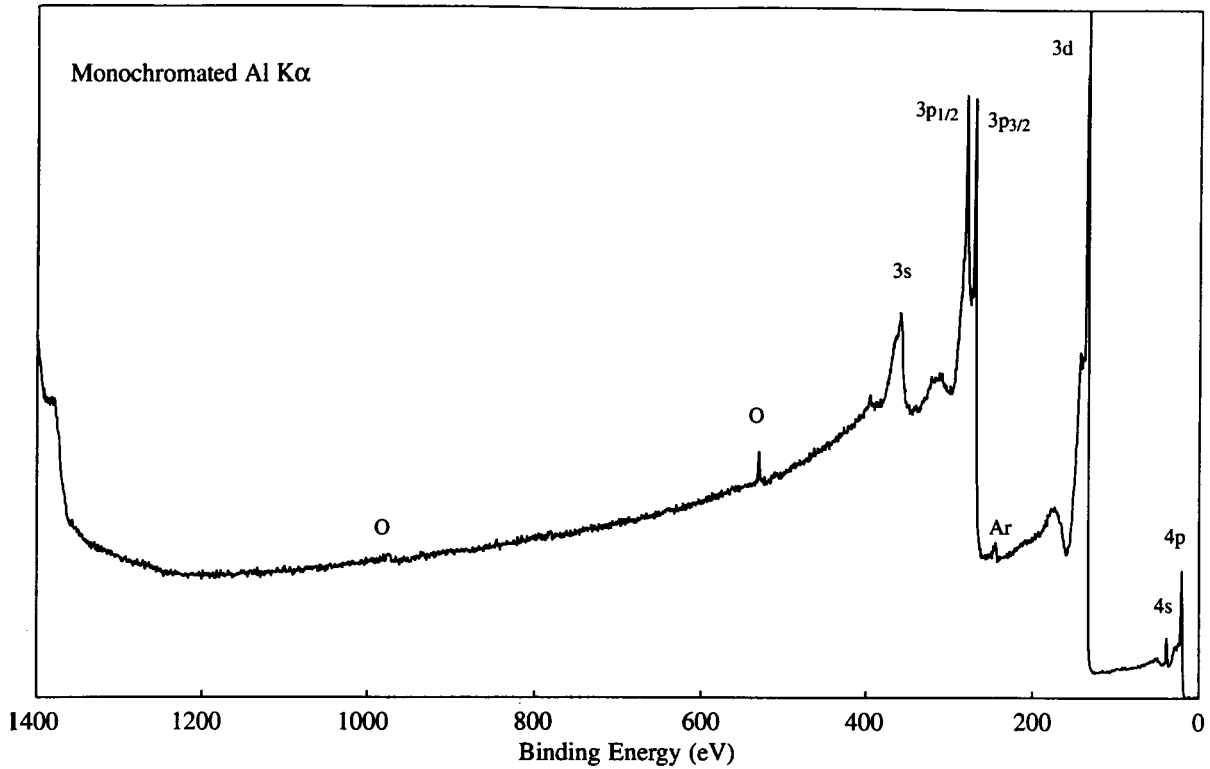
$M_{23}M_{45}N_{23}$
1385
1152

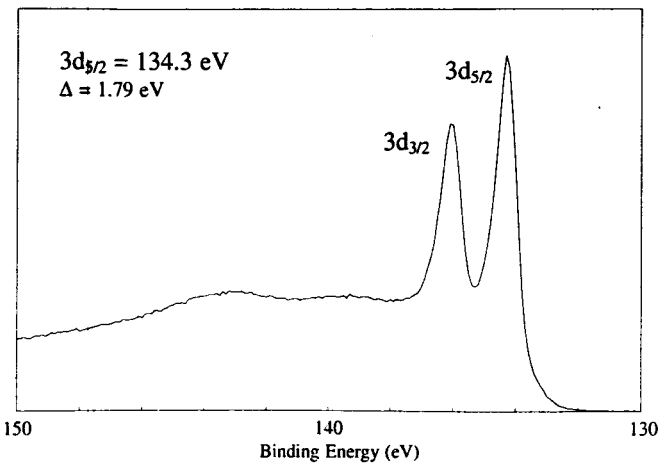
Rubidium Rb
Atomic Number 37







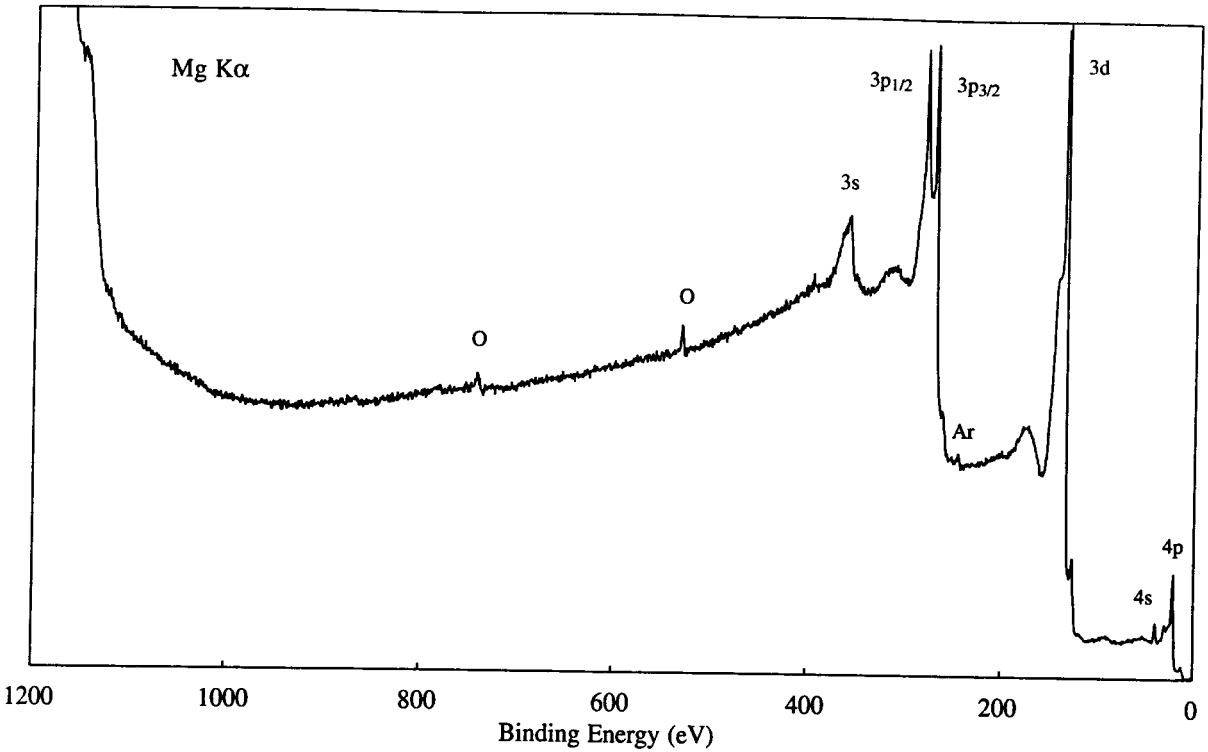


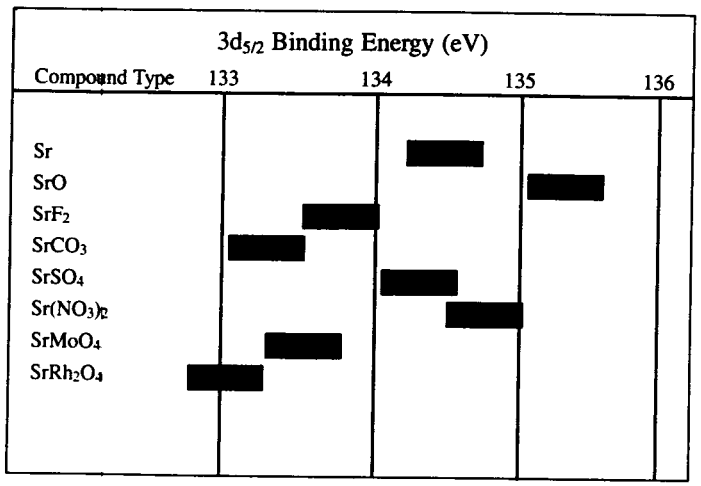


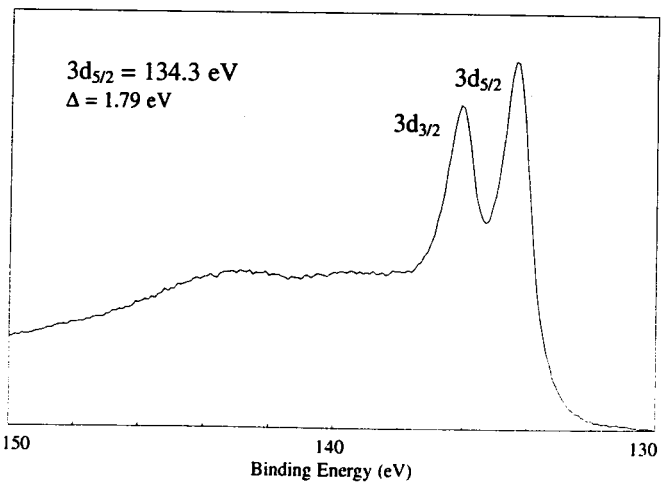
Line Positions (eV)

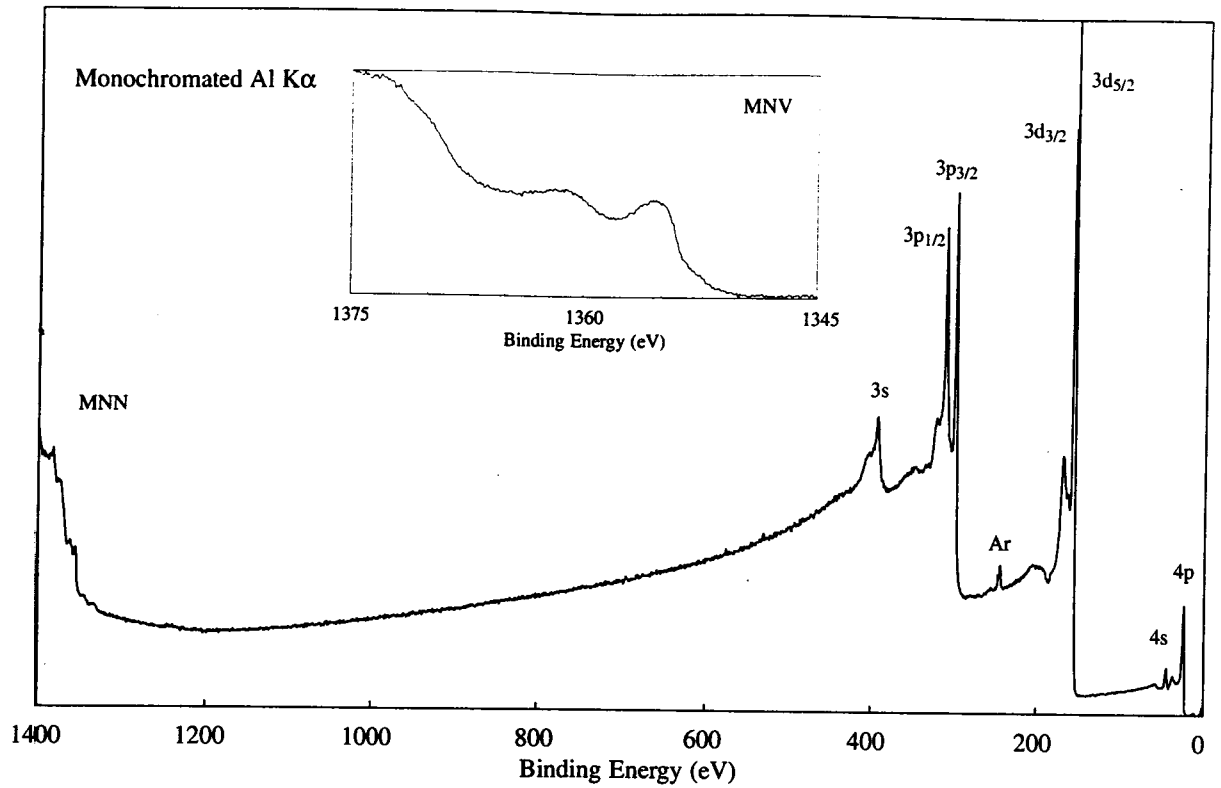
Photoelectron Lines						
3s	$3p_{1/2}$	$3p_{3/2}$	$3d_{3/2}$	$3d_{5/2}$	4s	4p
360	281	270	136	134	39	21

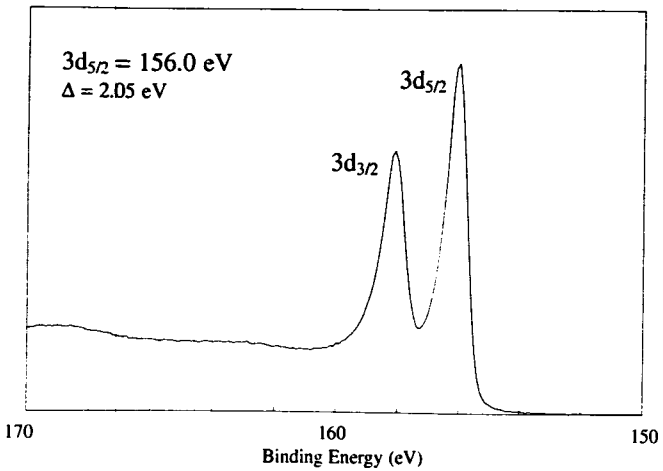
Strontium Sr
Atomic Number 38











Line Positions (eV)

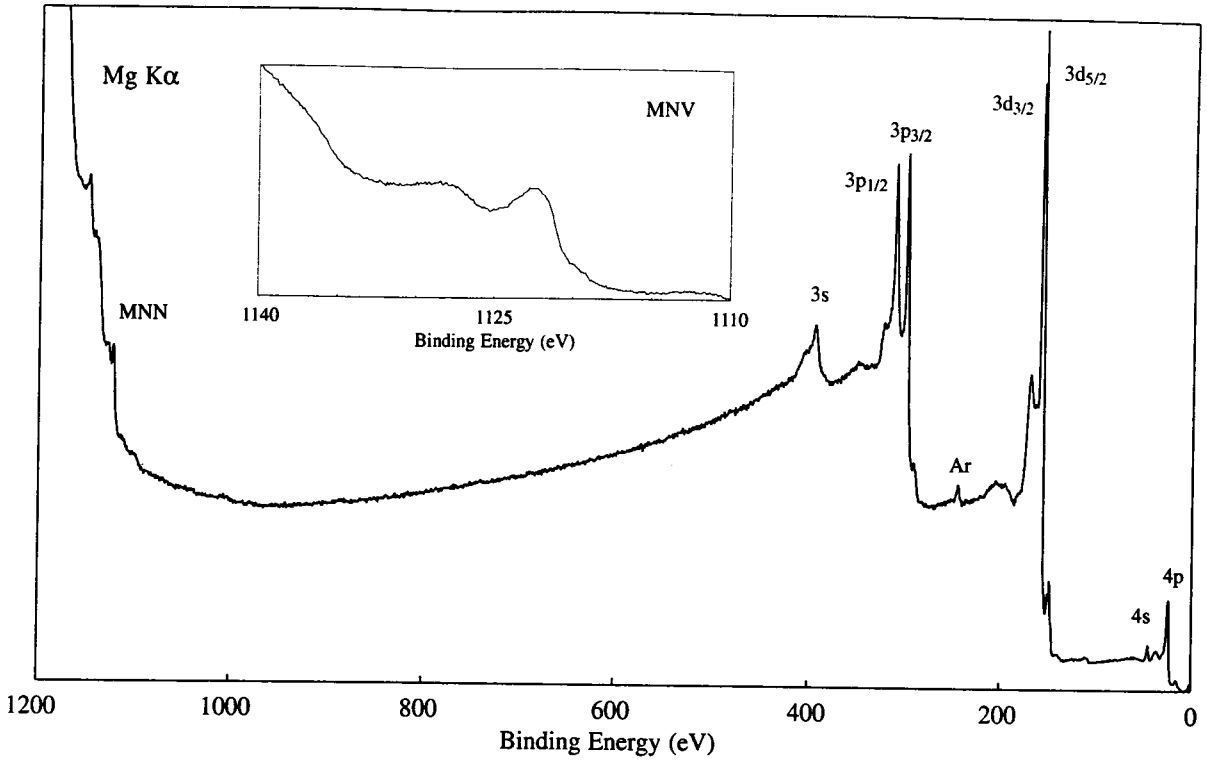
Photoelectron Lines

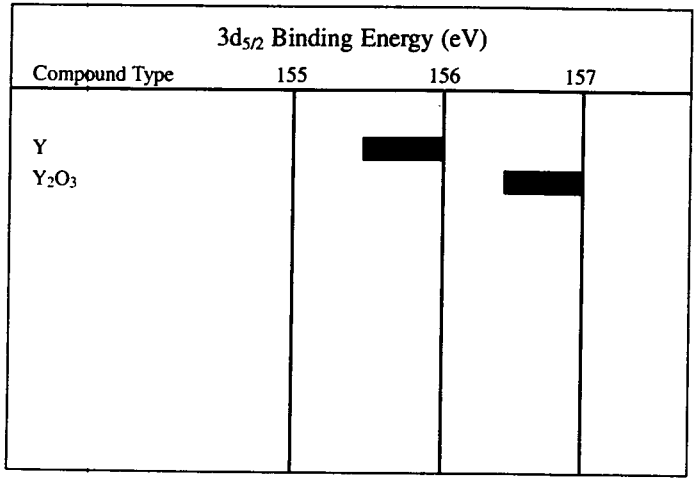
3s	3p1/2	3p3/2	3d3/2	3d5/2	4s	4p
394	311	299	158	156	45	24

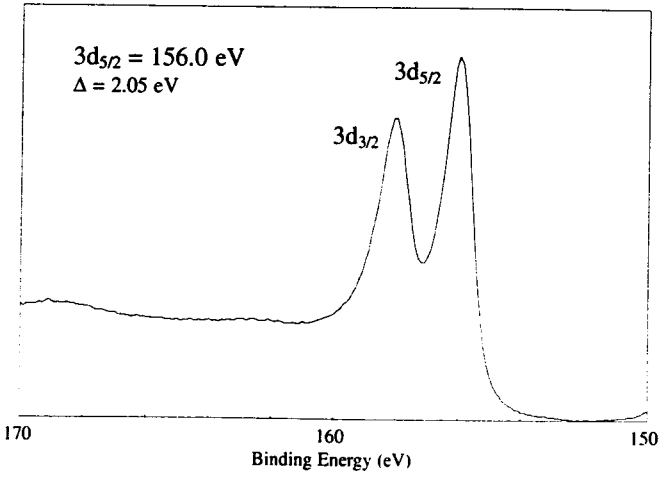
Auger Lines

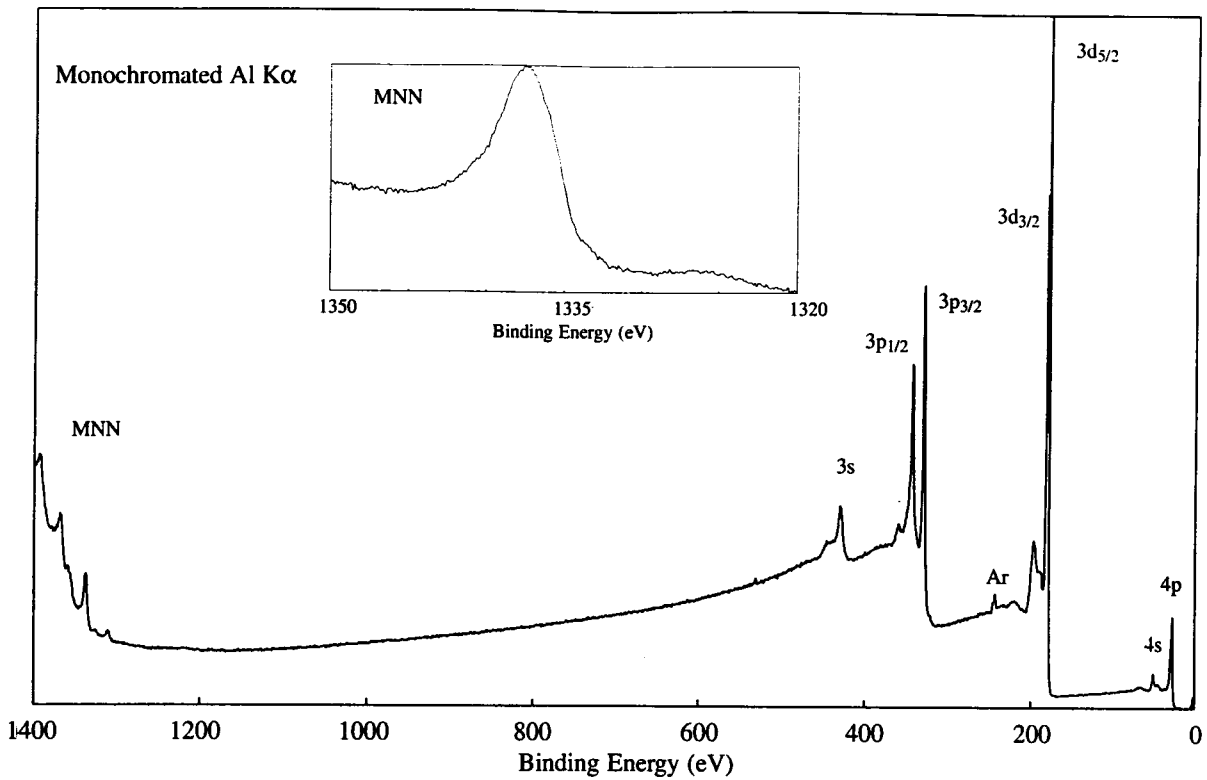
$M_{45}N_{23}V$
1356 (Al)
1123 (Mg)

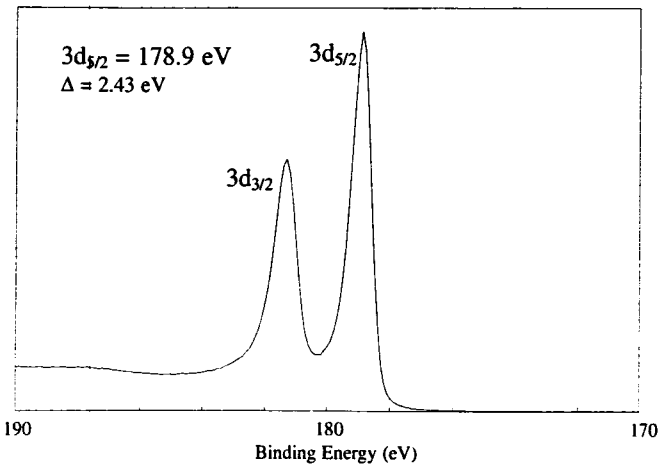
Yttrium Y
Atomic Number 39











Line Positions (eV)

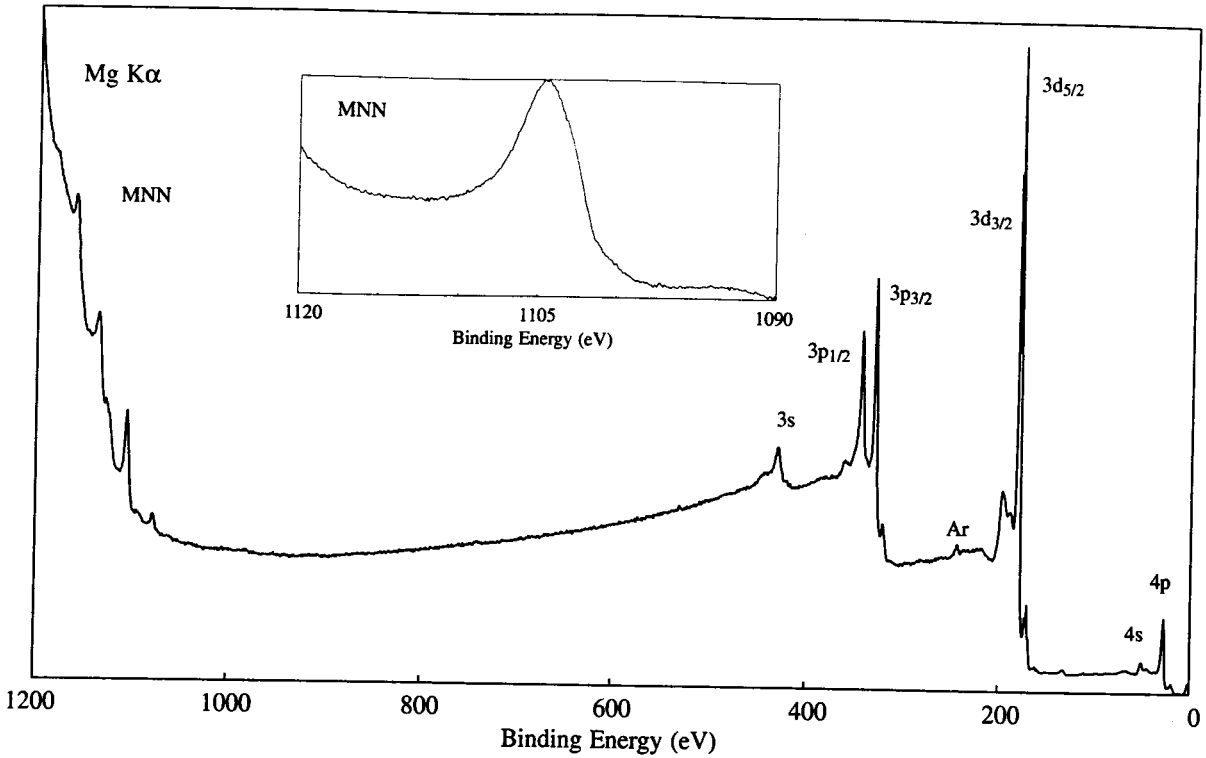
Photoelectron Lines

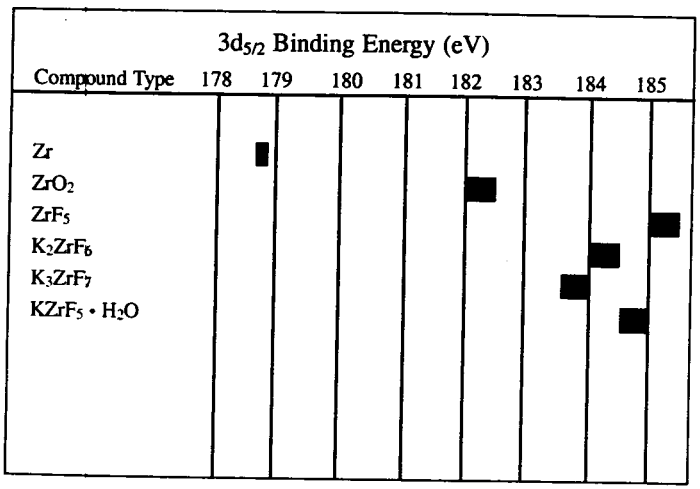
3s	3p1/2	3p3/2	3d3/2	3d5/2	4s	4p
430	343	330	181	179	51	28

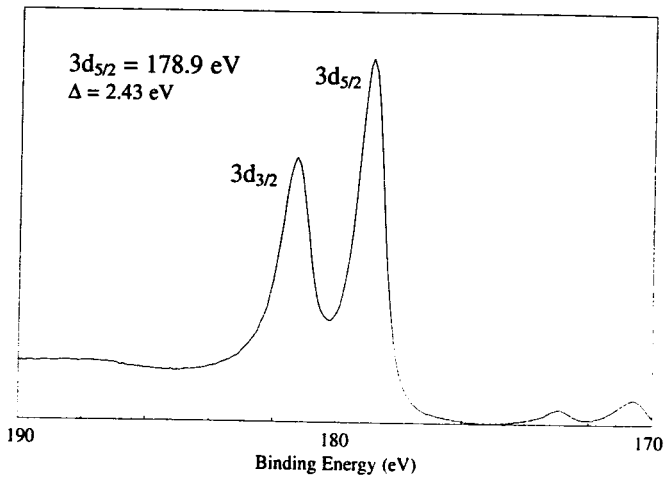
Auger Lines

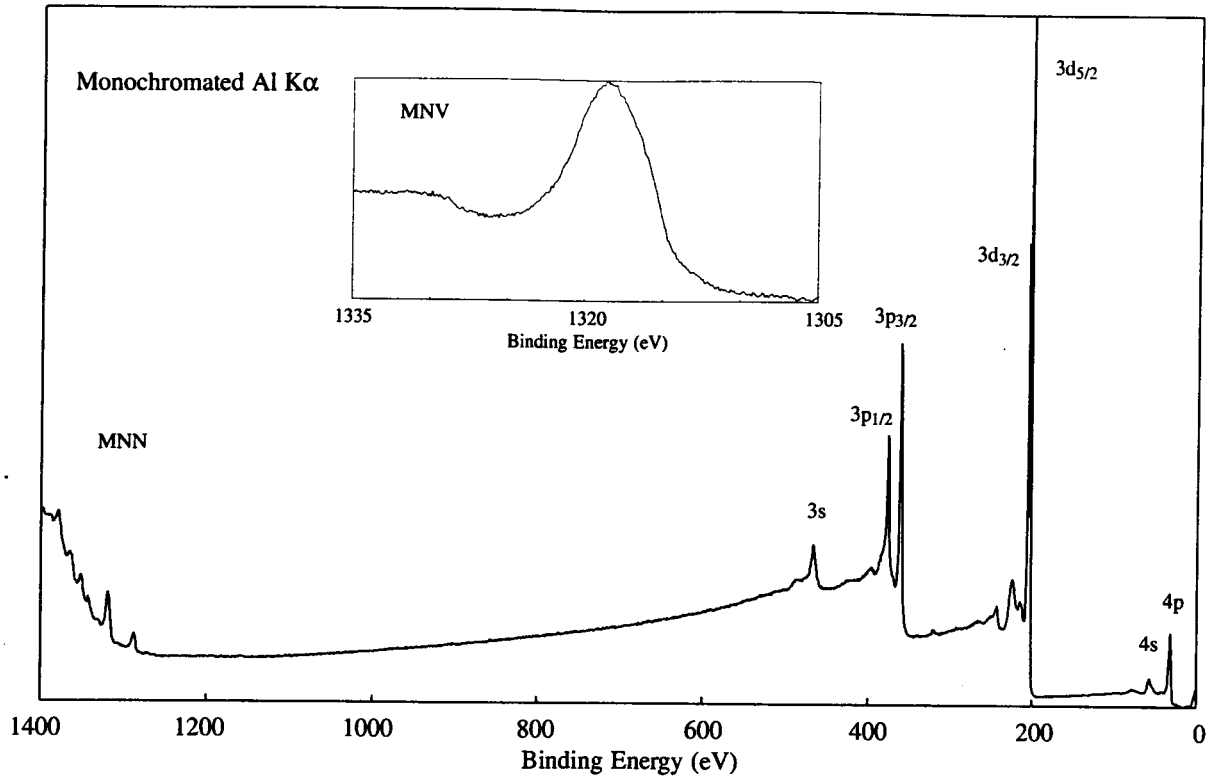
$M_{45}N_{23}N_{23}$	$M_{45}N_{23}V$	$M_{45}N_{45}N_{45}$	
1393	1368	1337	(Al)
1160	1135	1104	(Mg)

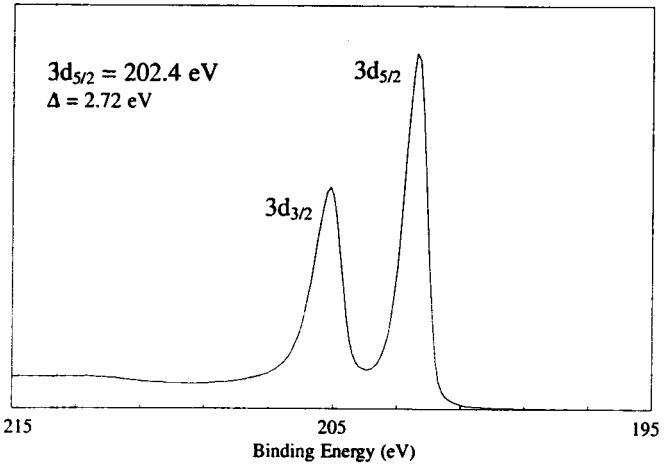
Zirconium Zr
Atomic Number 40











Line Positions (eV)

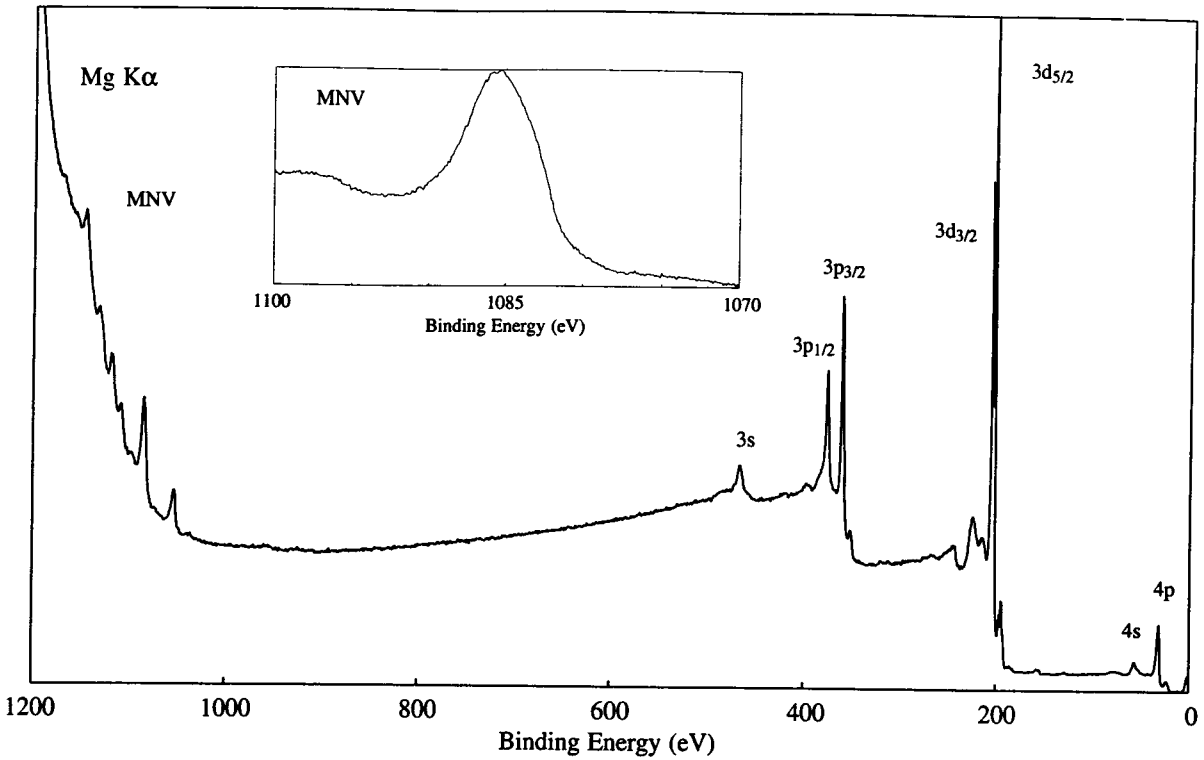
Photoelectron Lines

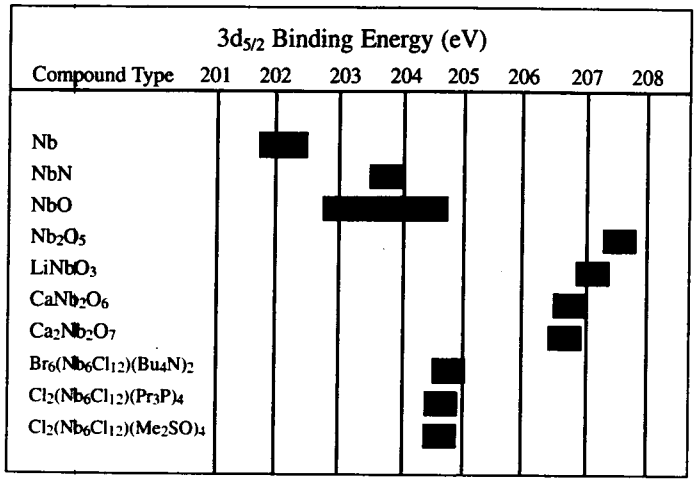
3s	3p1/2	3p3/2	3d3/2	3d5/2	4s	4p
467	376	361	205	202	56	31

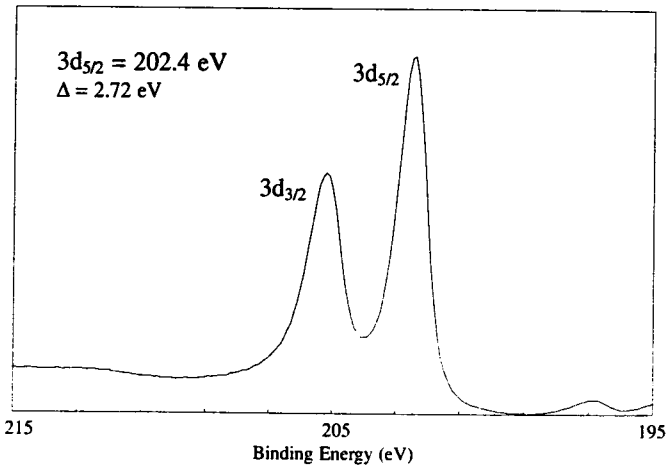
Auger Lines

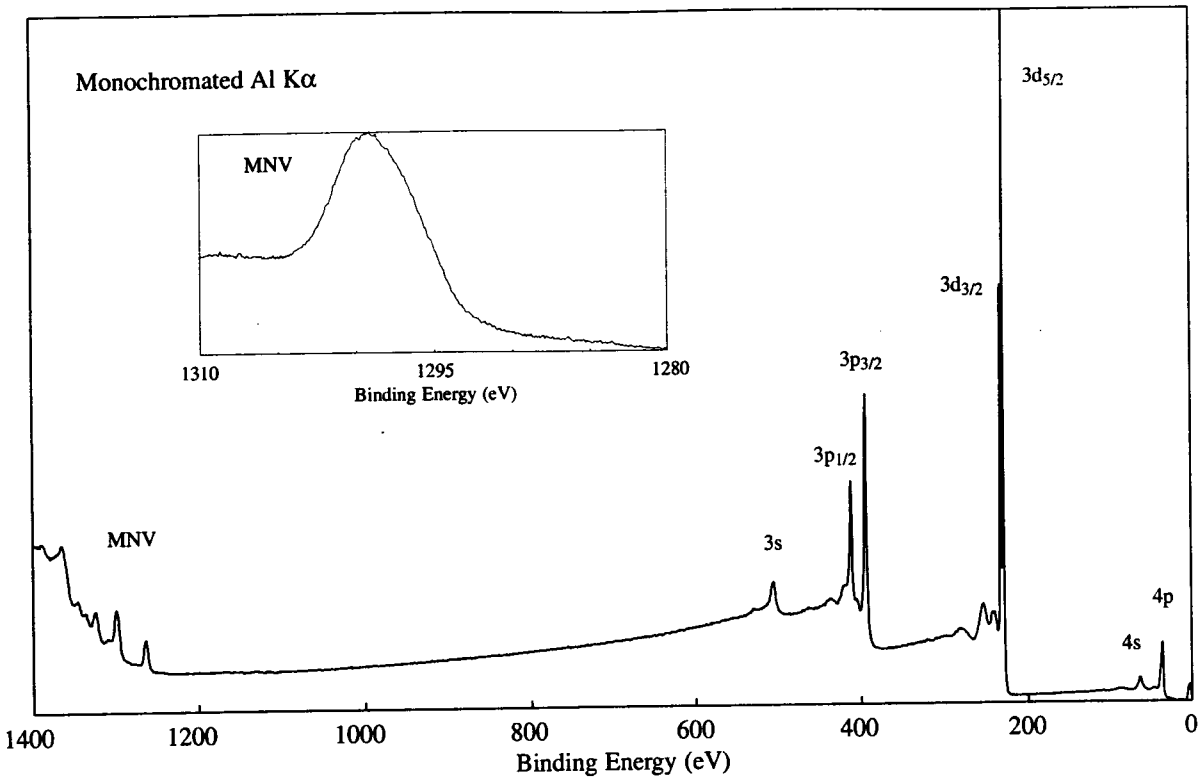
$M_{45}N_{23}V$	$M_{45}VV$	
1319	1287	(Al)
1086	1054	(Mg)

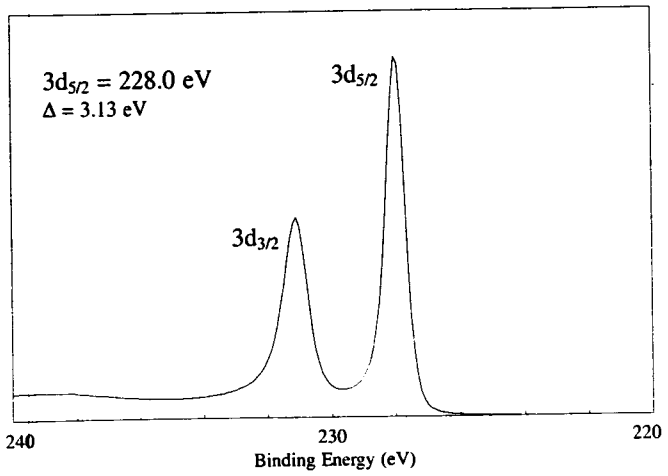
Niobium Nb
Atomic Number 41











Line Positions (eV)

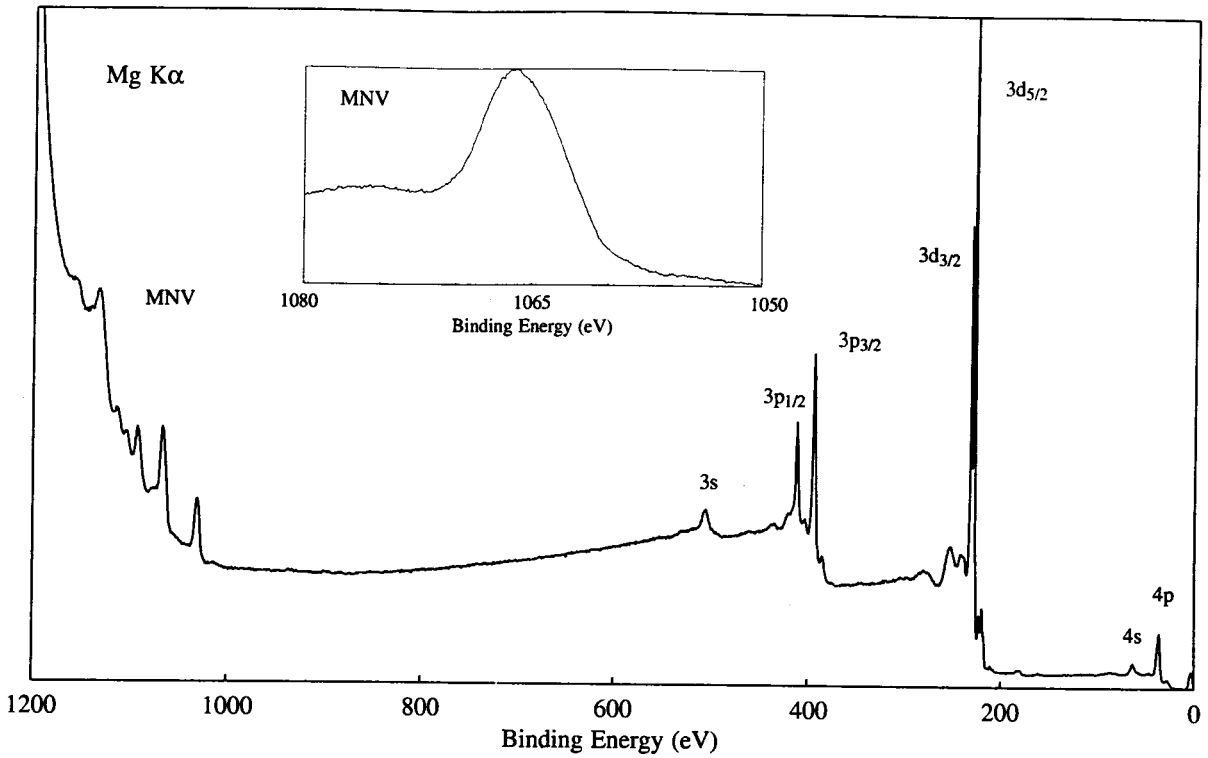
Photoelectron Lines

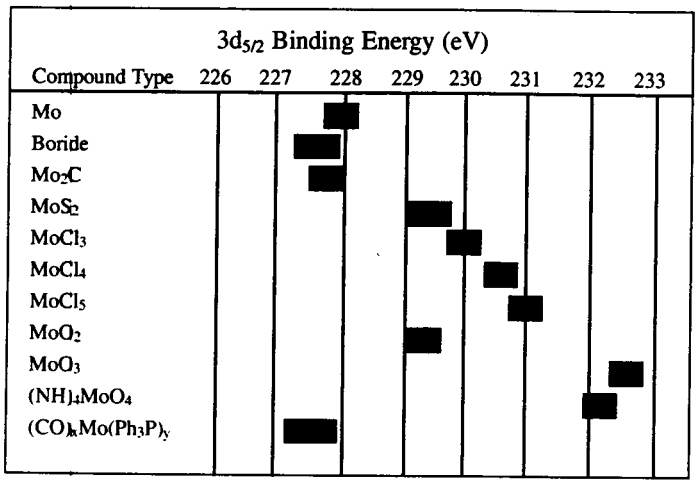
3s	3p1/2	3p3/2	3d3/2	3d5/2	4s	4p
506	412	394	231	228	63	36

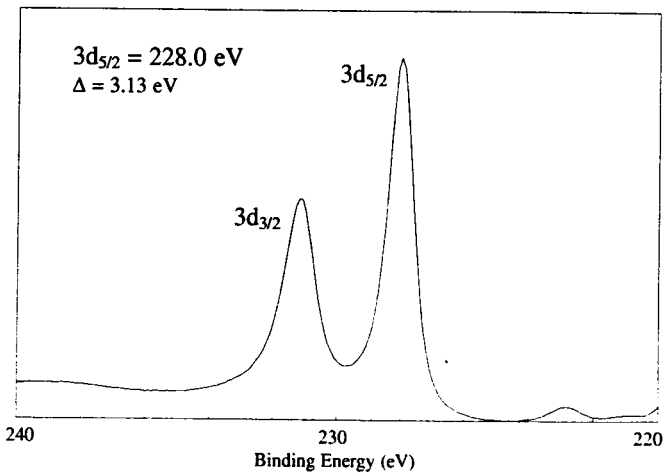
Auger Lines

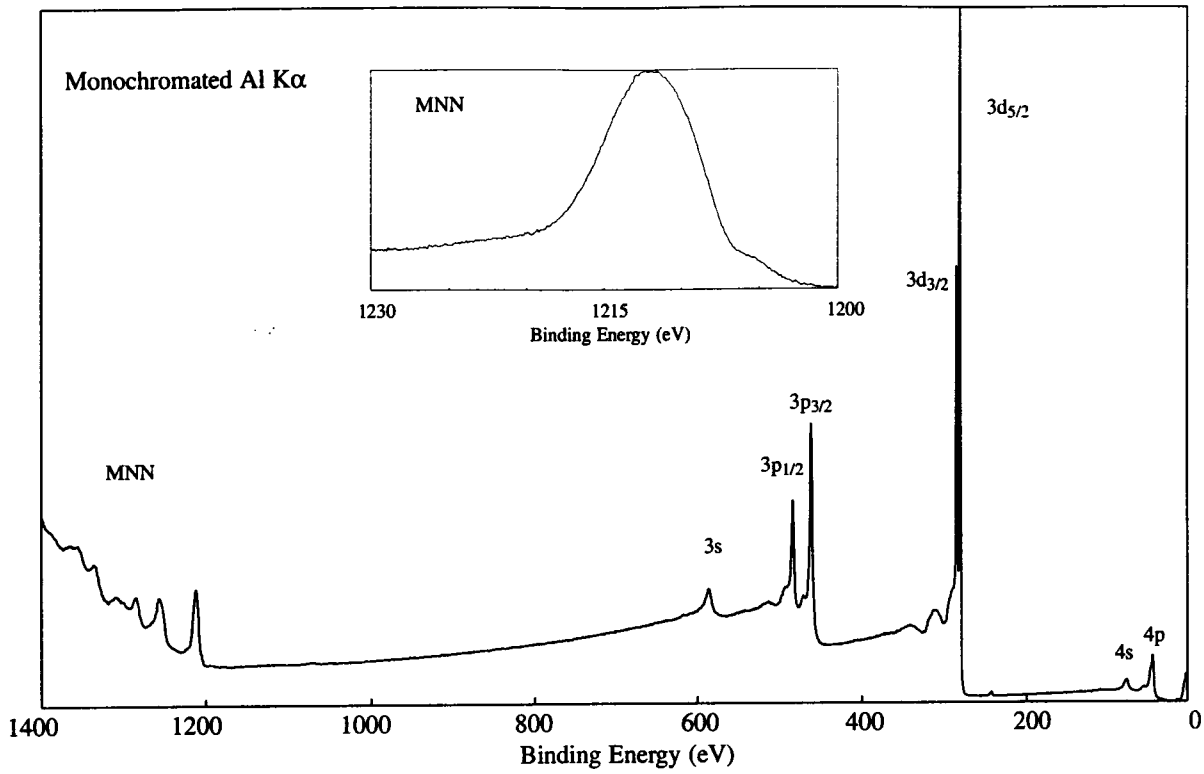
M45N23V	M45VV	
1299	1264	(Al)
1066	1031	(Mg)

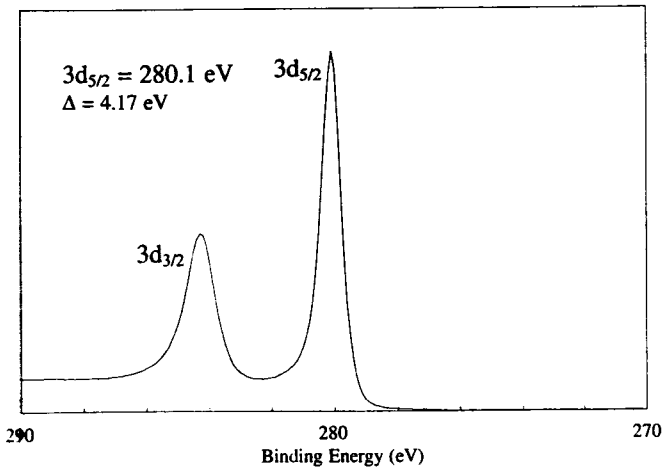
Molybdenum Mo
Atomic Number 42











Line Positions (eV)

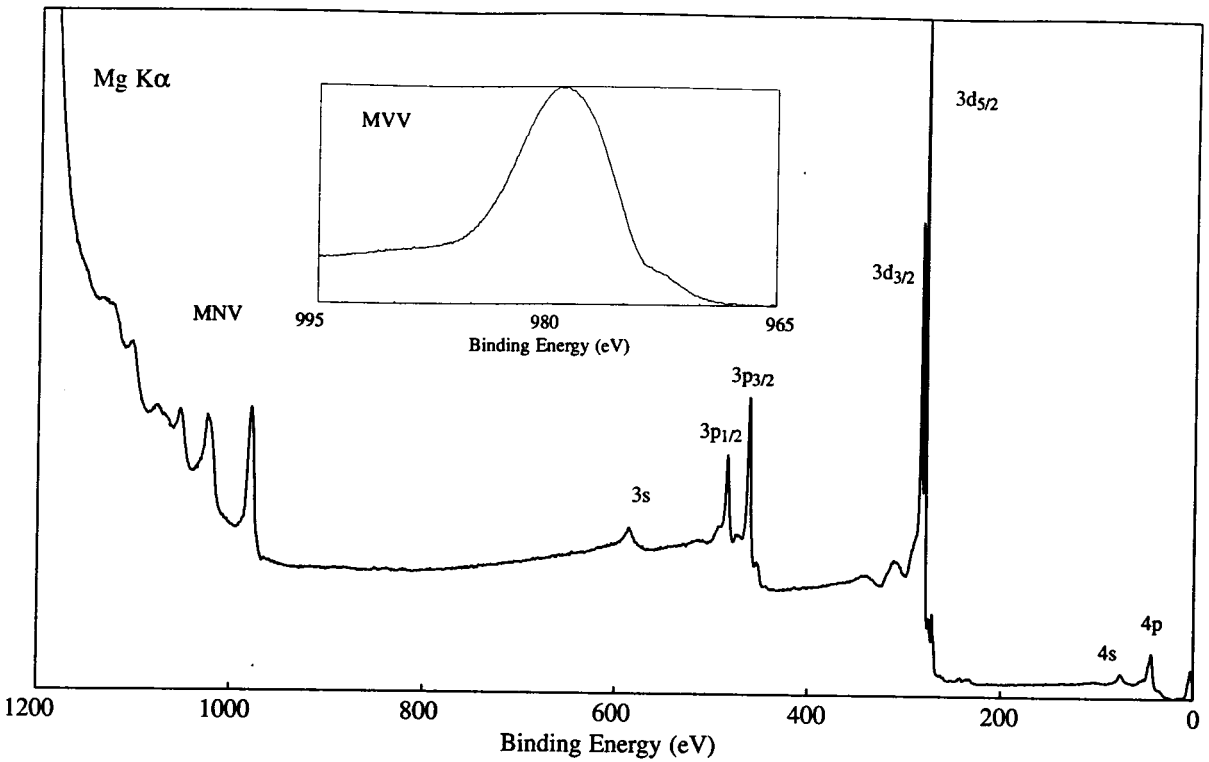
Photoelectron Lines

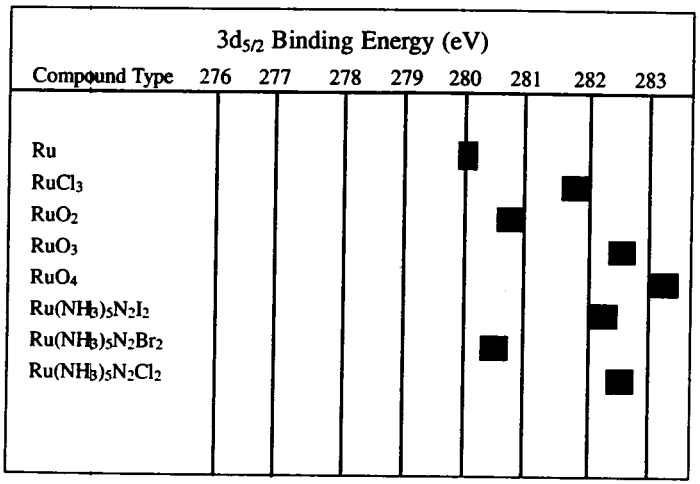
3s	3p1/2	3p3/2	3d3/2	3d5/2	4s	4p
586	484	462	284	280	75	43

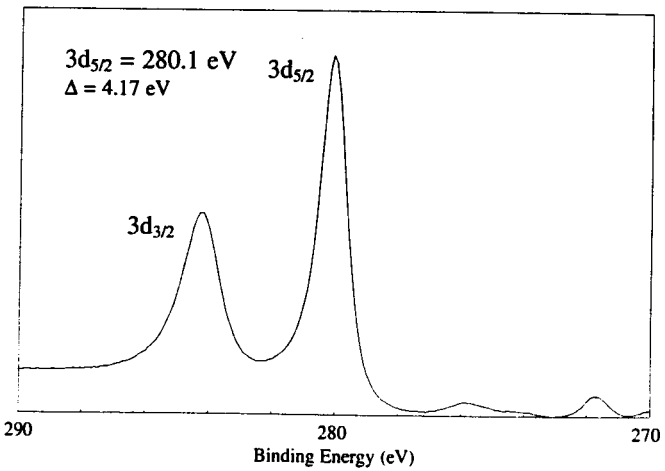
Auger Lines

$M_{45}N_{23}V$	$M_{45}VV$	
1256	1212	(Al)
1023	979	(Mg)

Ruthenium Ru
Atomic Number 44

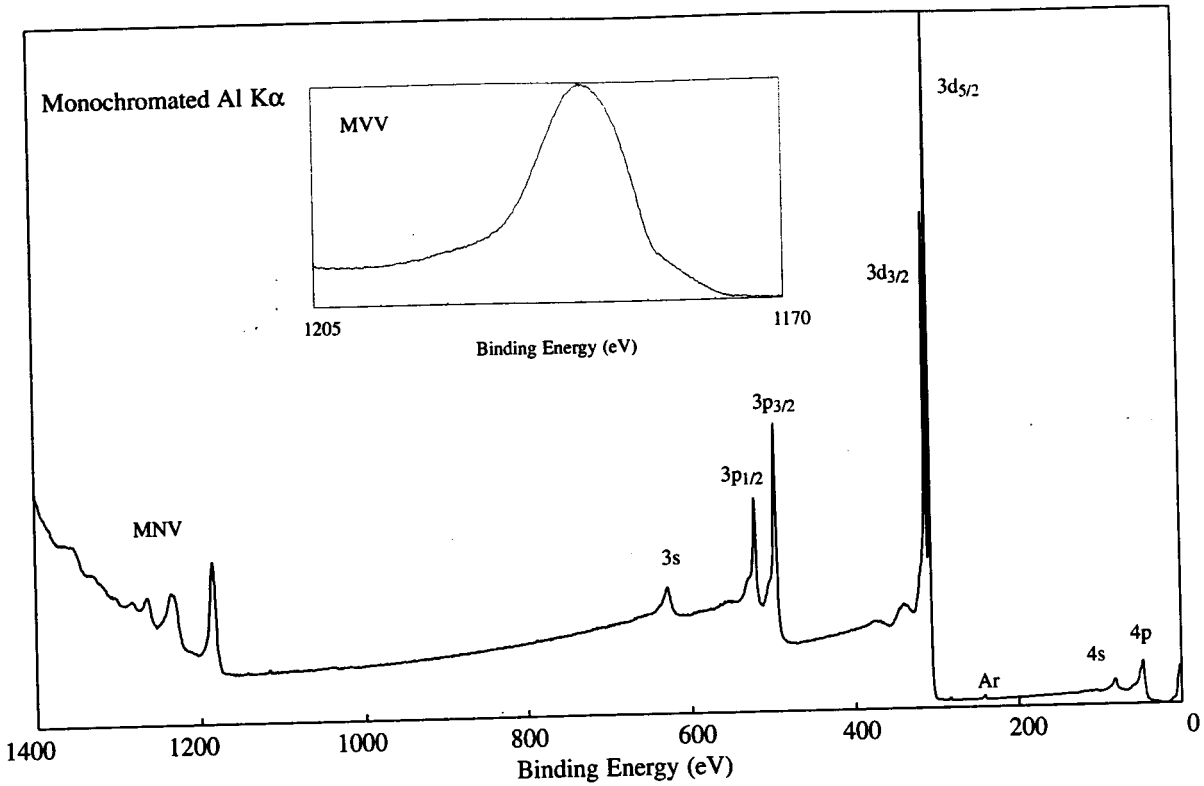


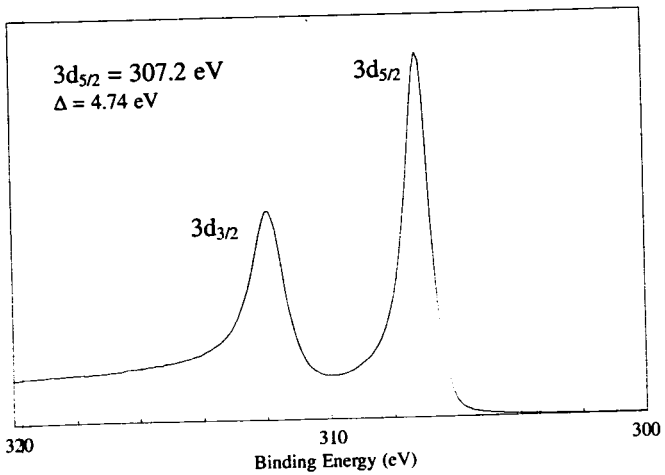




Rhodium Rh

Atomic Number 45





Line Positions (eV)

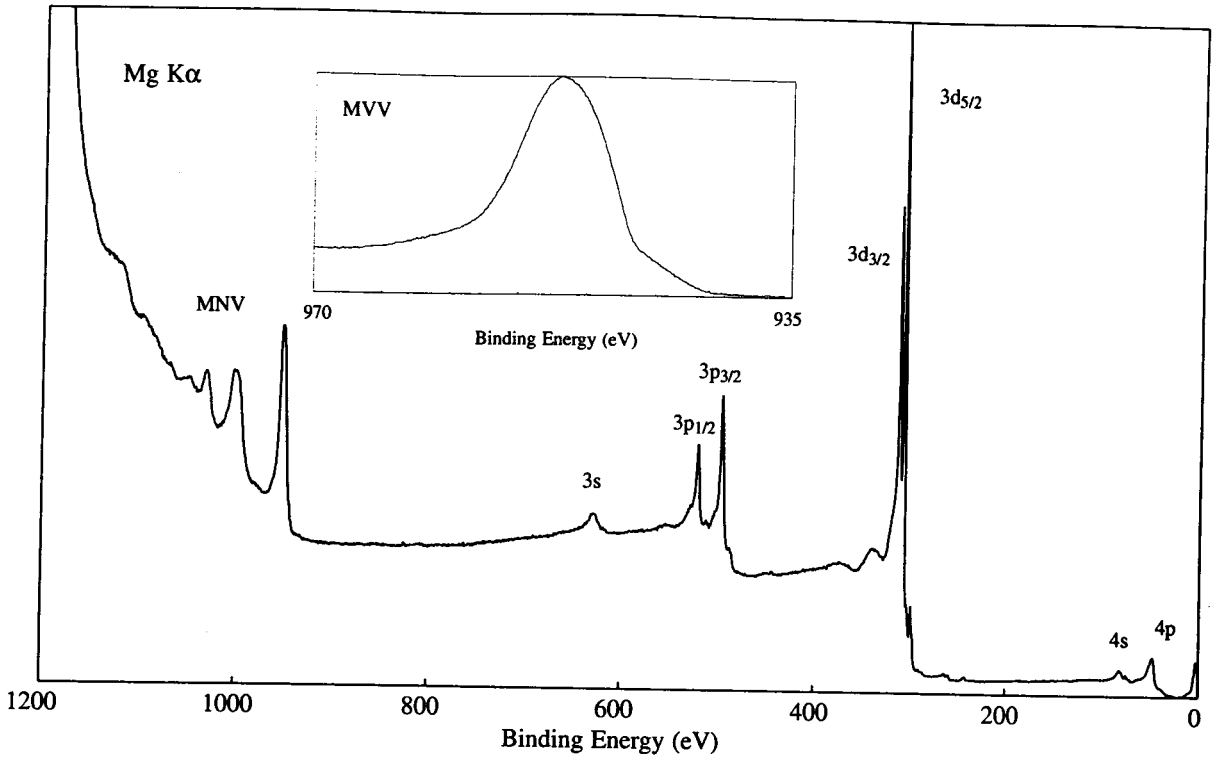
Photoelectron Lines

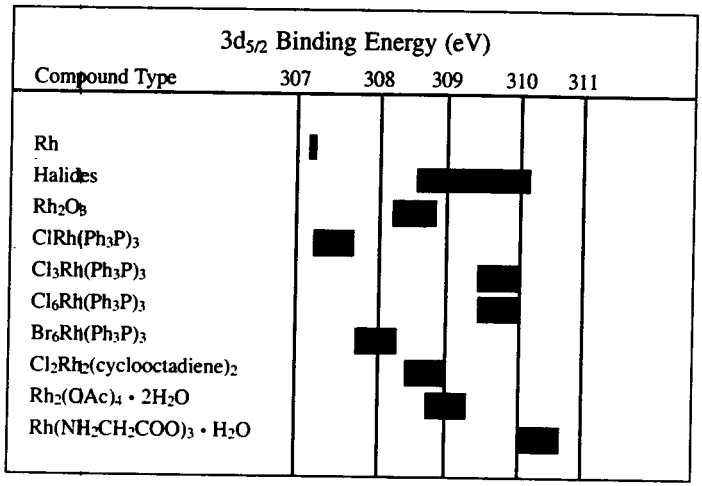
3s	3p1/2	3p3/2	3d3/2	3d5/2	4s	4p
629	521	497	312	307	81	48

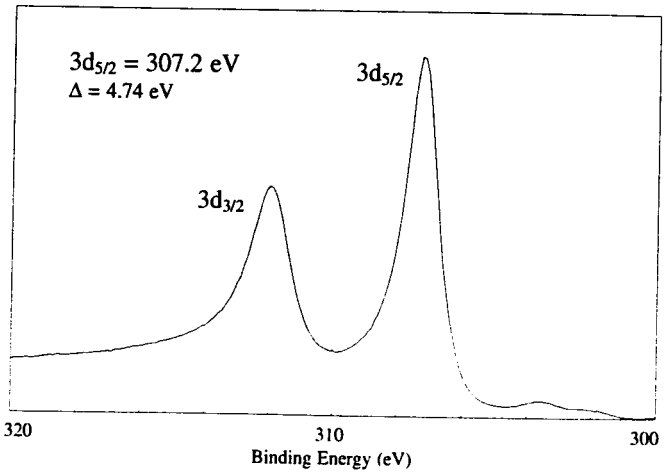
Auger Lines

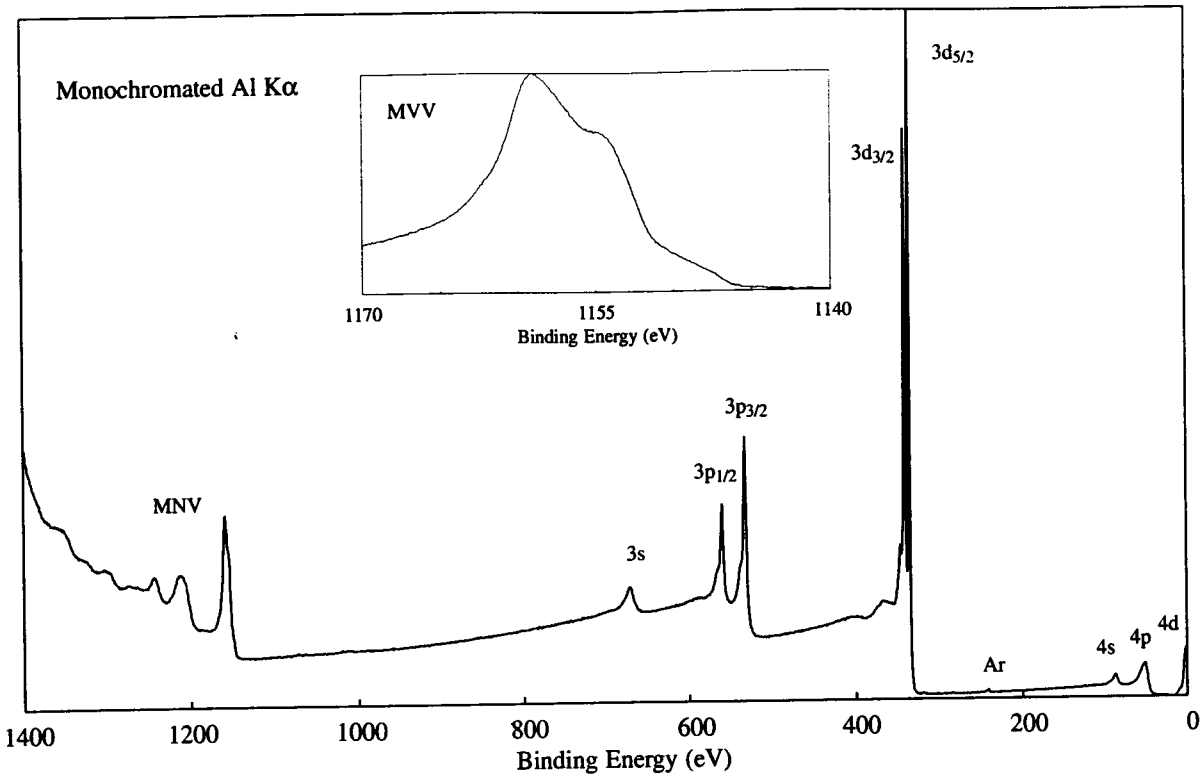
$M_{45}N_{23}V$	$M_{45}VV$	
1234	1185	(Al)
1001	952	(Mg)

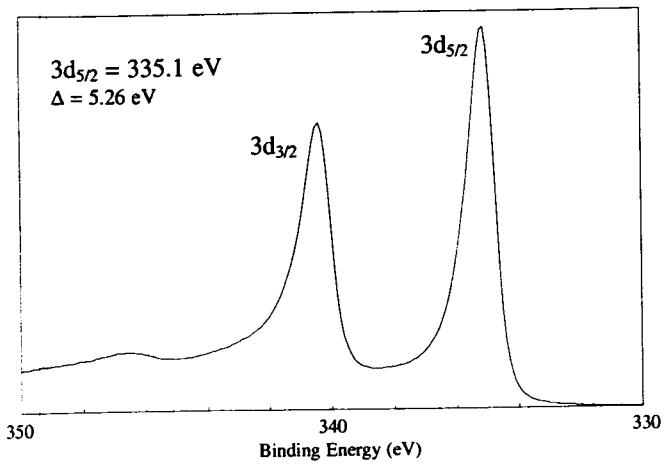
Rhodium Rh
Atomic Number 45











Line Positions (eV)

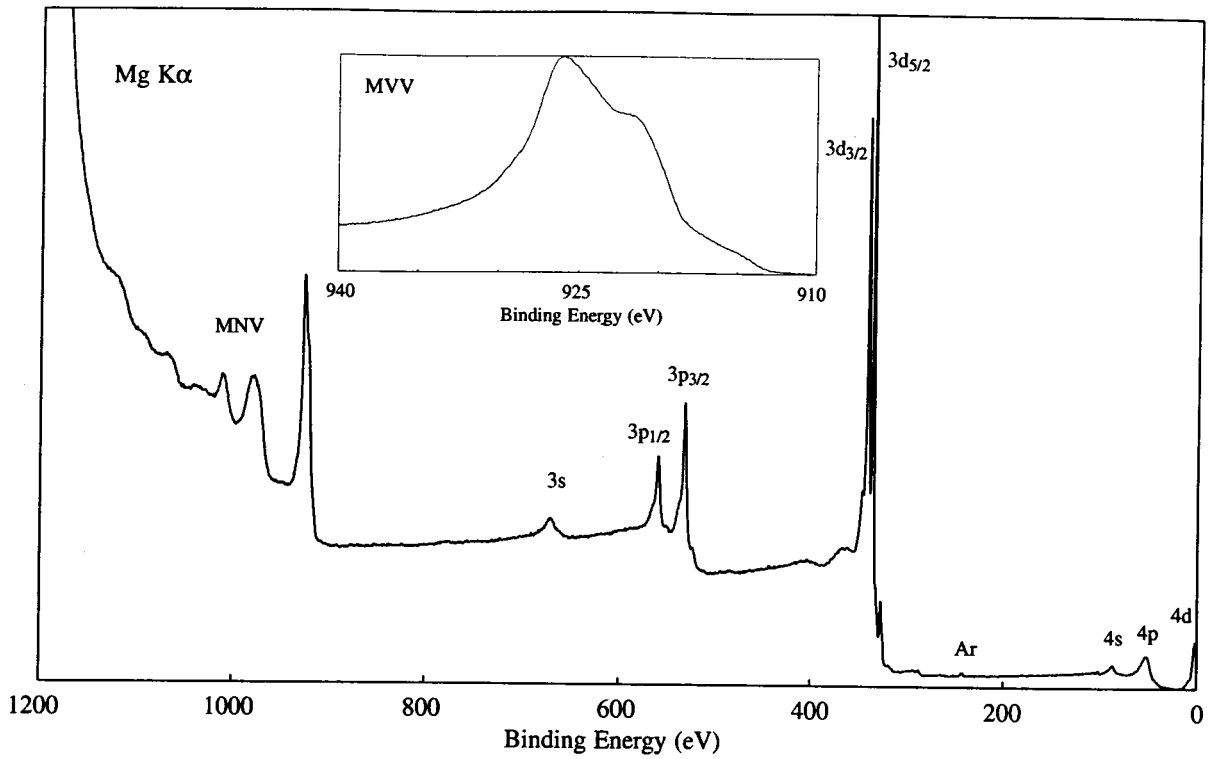
Photoelectron Lines

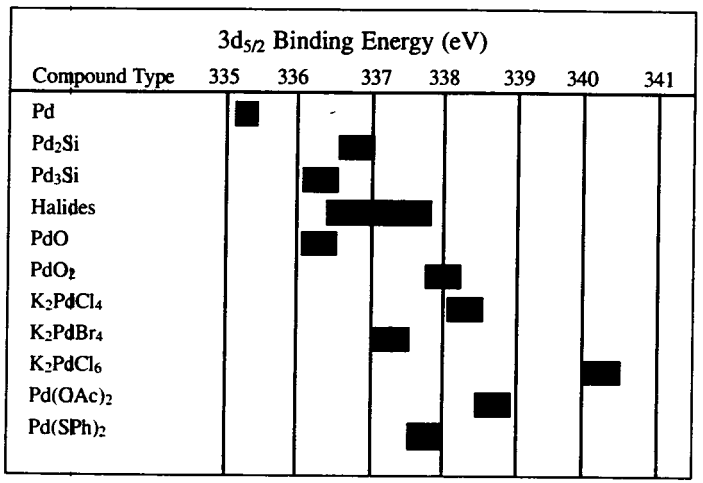
3s	3p1/2	3p3/2	3d3/2	3d5/2	4s	4p
671	560	533	340	335	88	52

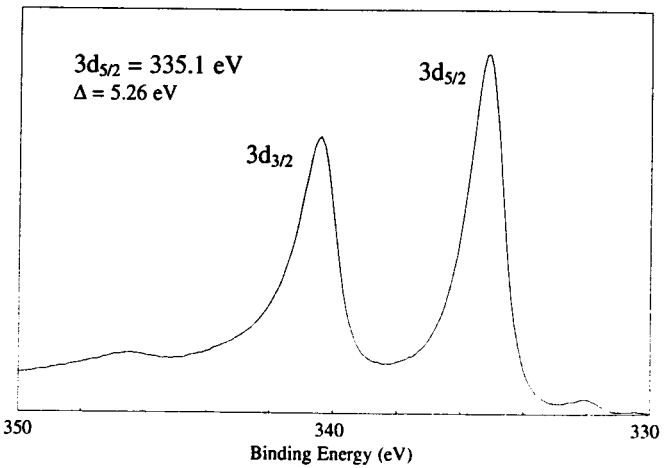
Auger Lines

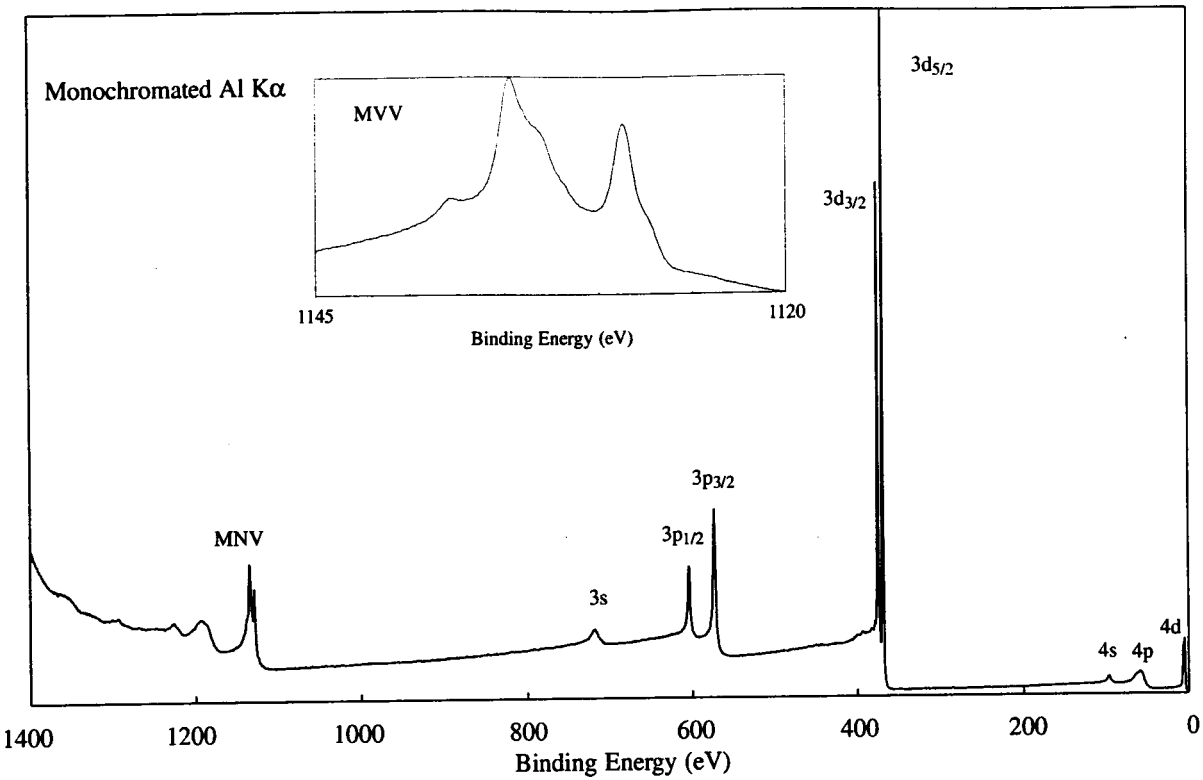
M45N23V	M45VV	
1211	1159	(Al)
978	926	(Mg)

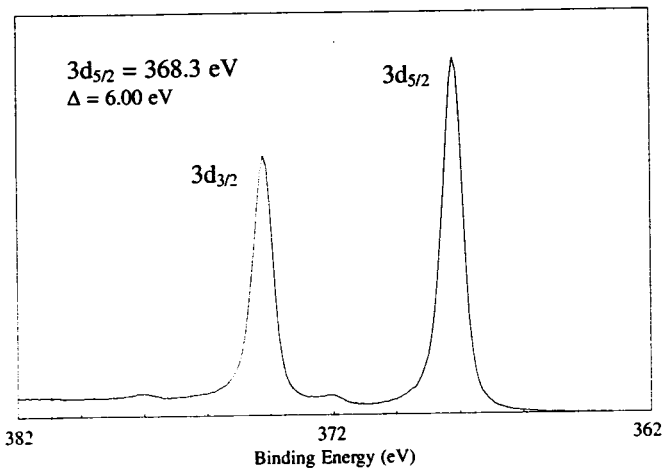
Palladium Pd
Atomic Number 46











Line Positions (eV)

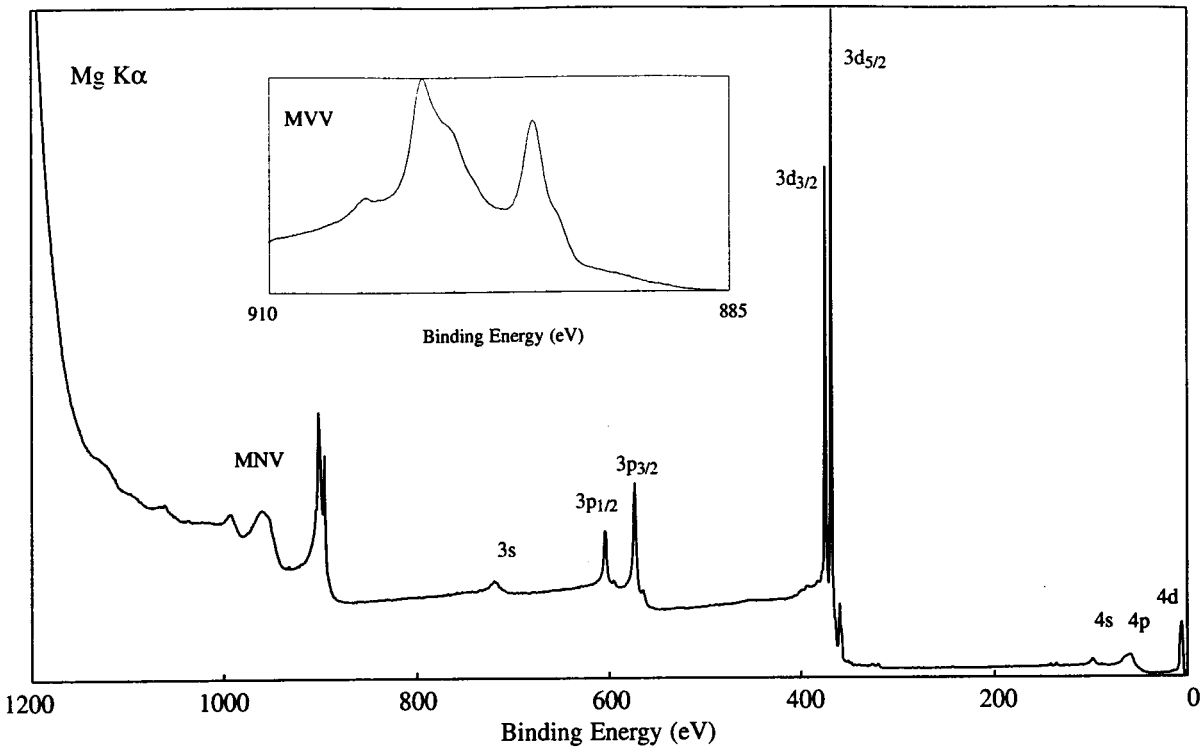
Photoelectron Lines

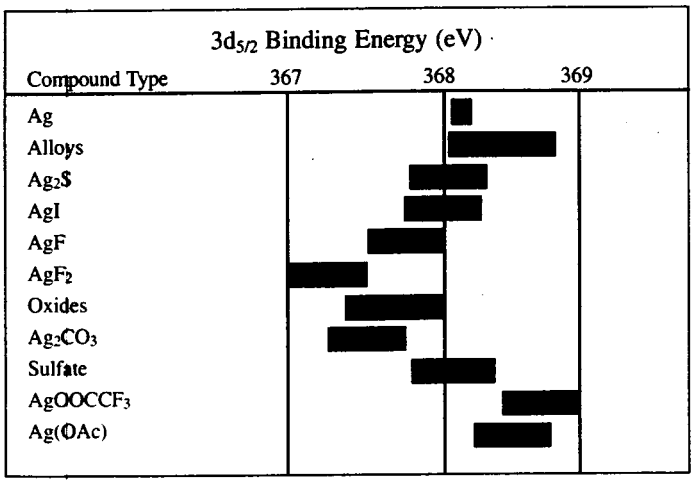
3s	3p1/2	3p3/2	3d3/2	3d5/2	4s	4p
719	604	573	374	368	98	60

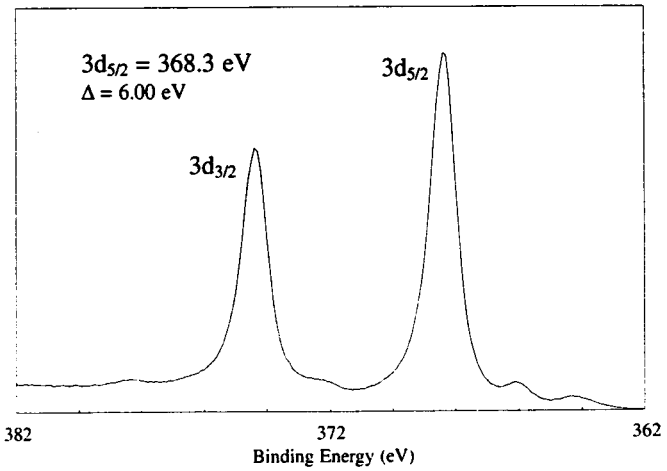
Auger Lines

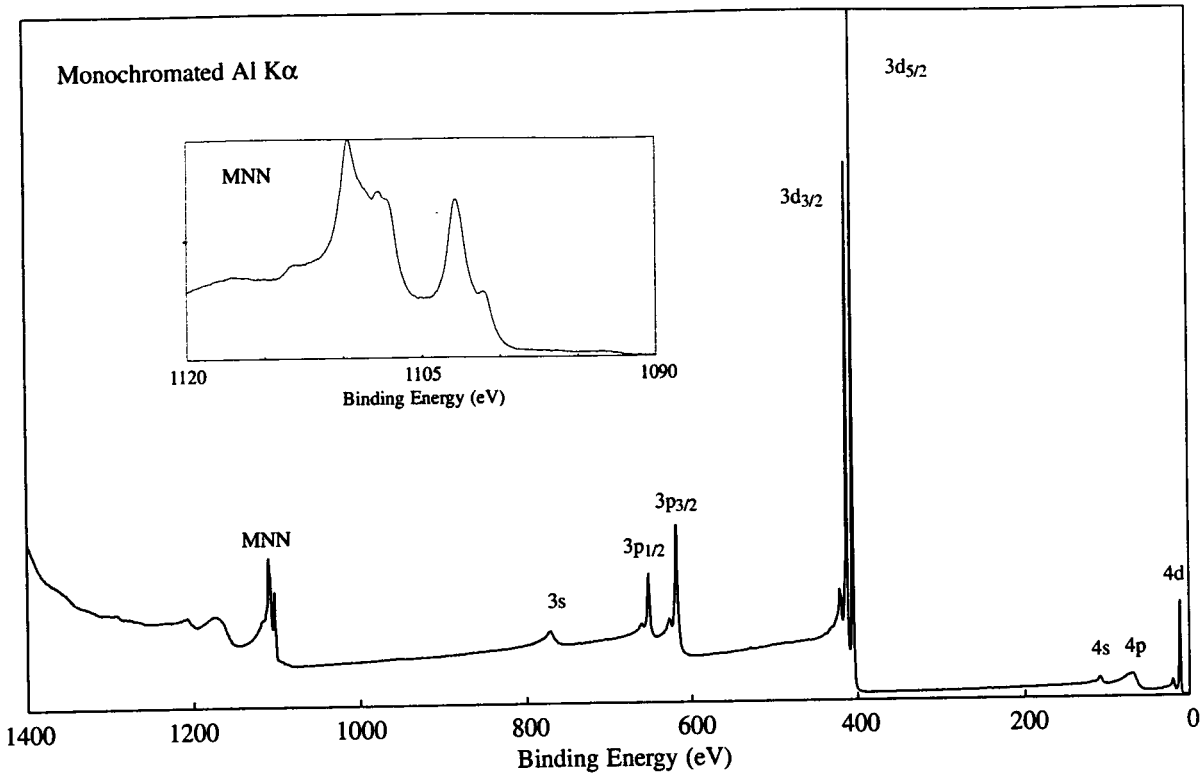
$M_{45}N_{23}V$	M_5VV	M_4VV	
1191	1135	1129	(Al)
958	902	896	(Mg)

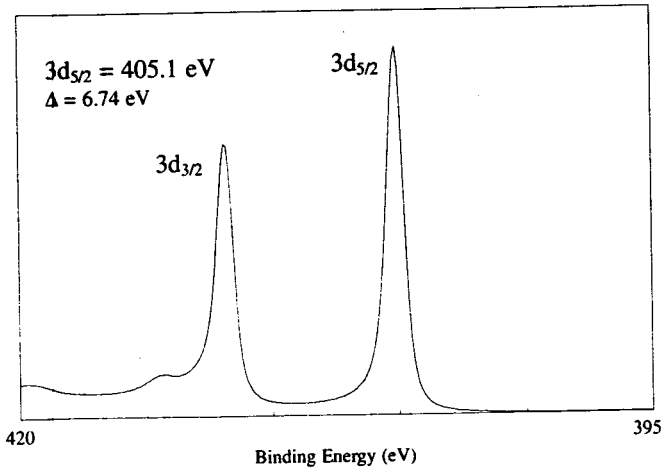
Silver Ag
Atomic Number 47











Line Positions (eV)

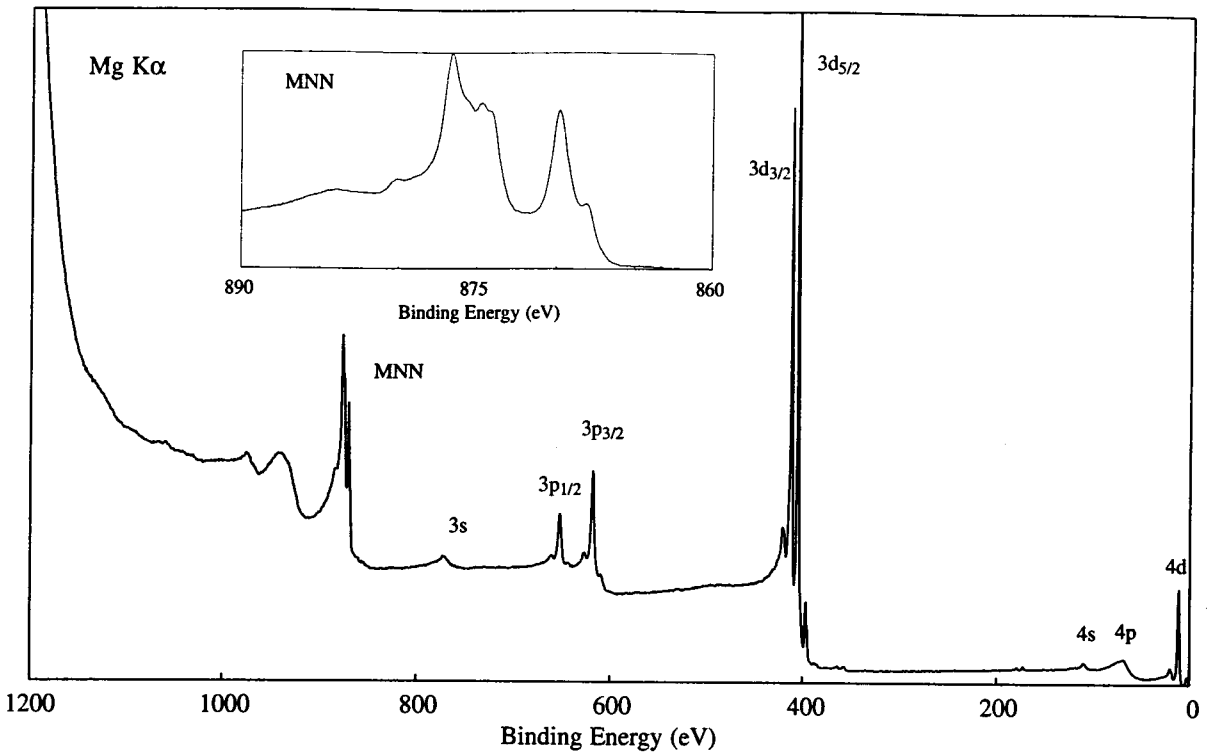
Photoelectron Lines

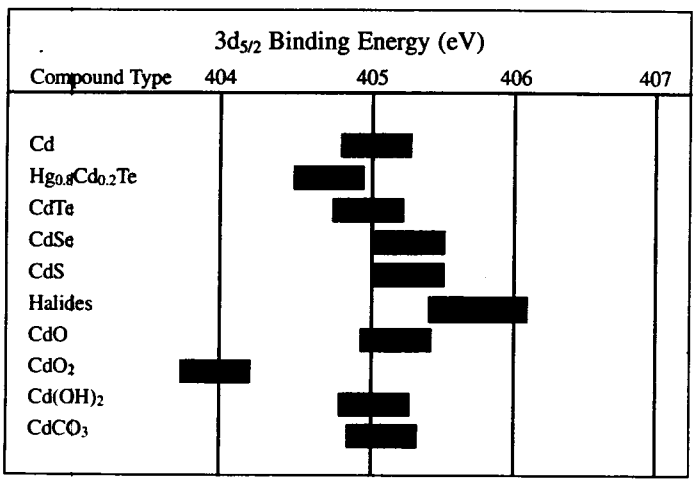
3s	3p1/2	3p3/2	3d3/2	3d5/2	4s	4p	4d
772	652	618	412	405	110	69	11

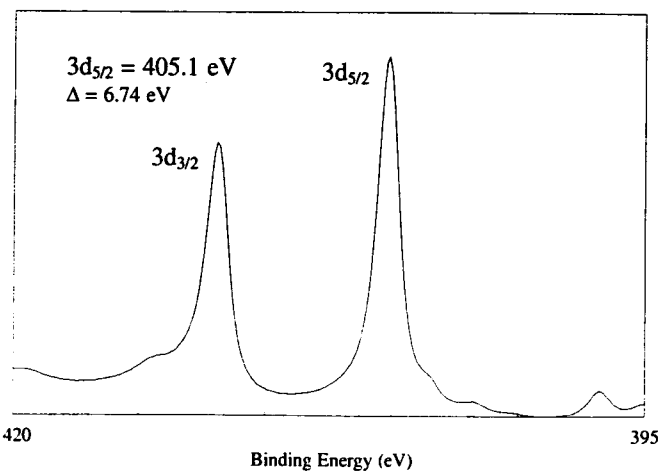
Auger Lines

M5N45N45	M4N45N45	
1110	1103	(Al)
877	870	(Mg)

Cadmium Cd
Atomic Number 48

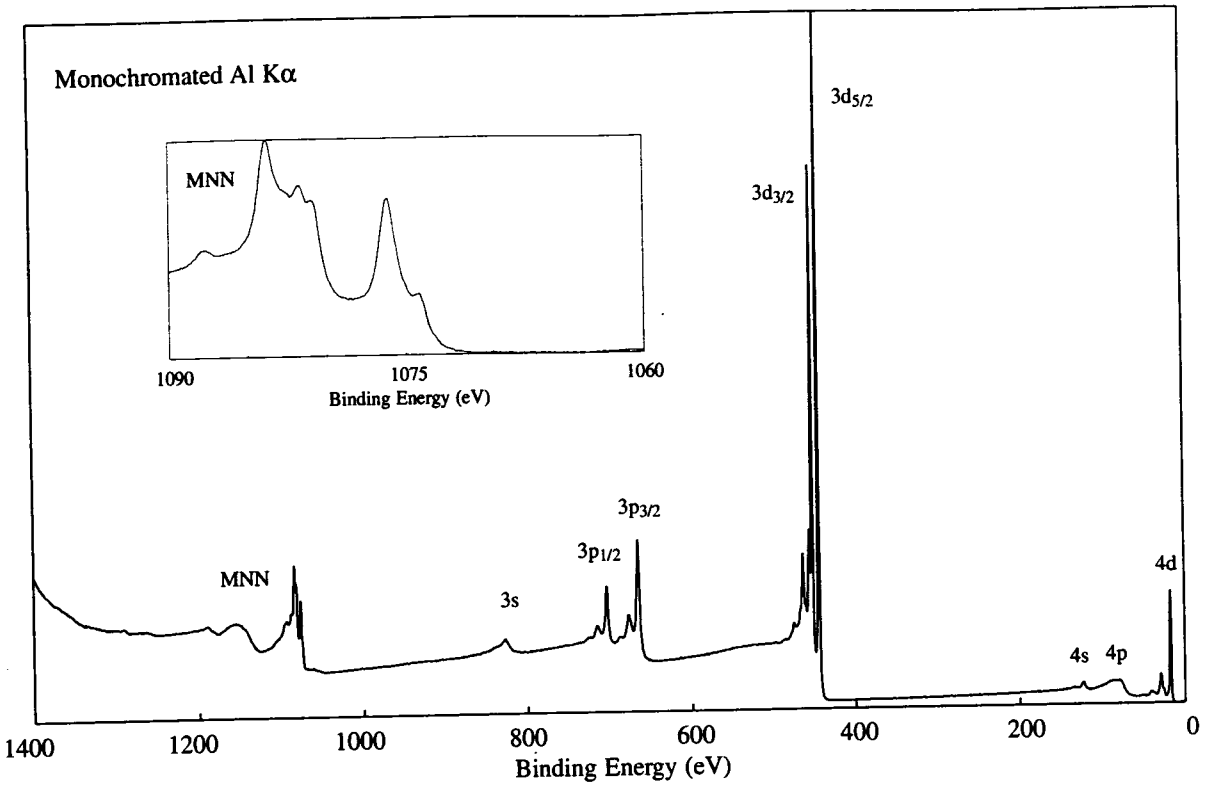


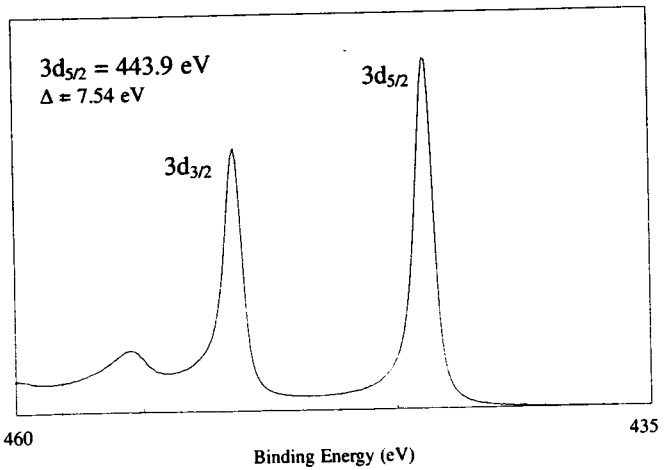




Indium In

Atomic Number 49





Line Positions (eV)

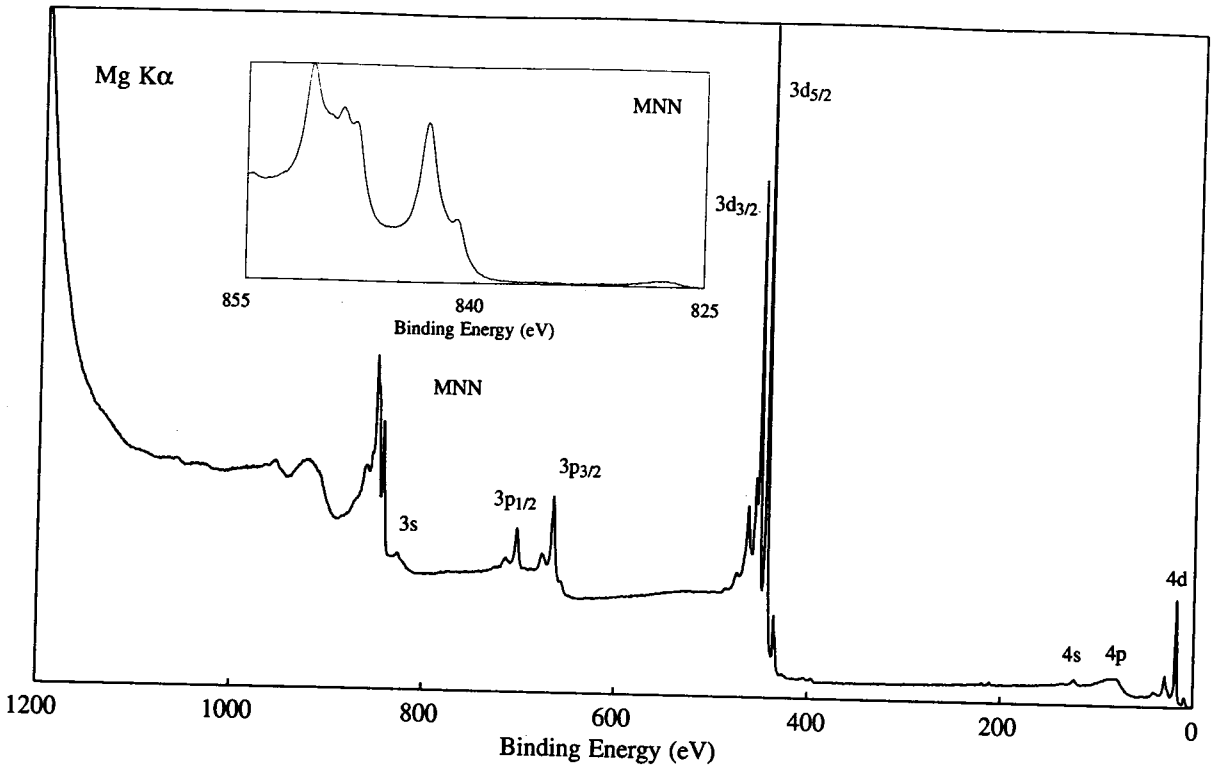
Photoelectron Lines

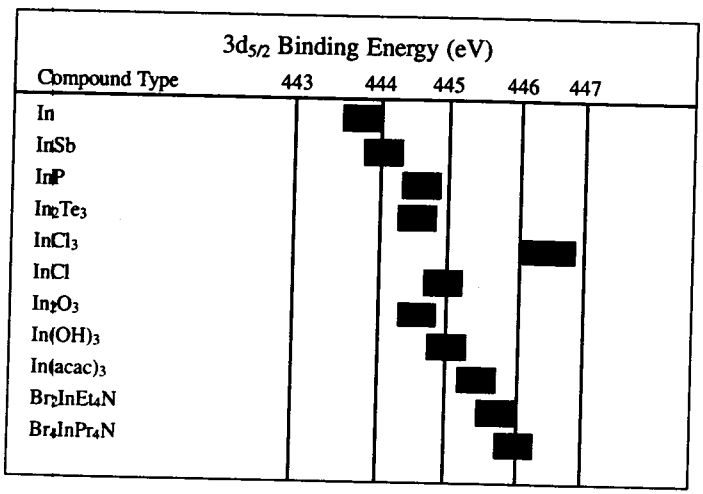
3s	3p1/2	3p3/2	3d3/2	3d5/2	4s	4p	4d
828	703	665	452	444	123	78	17

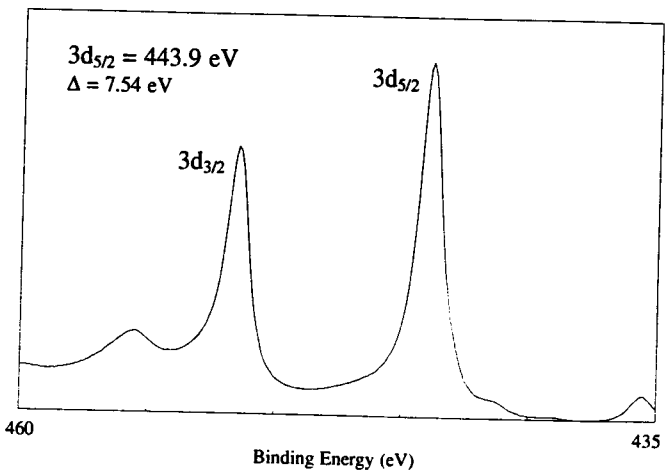
Auger Lines

$M_5N_{45}N_{45}$	$M_4N_{45}N_{45}$	
1084	1076	(Al)
851	843	(Mg)

Indium In
Atomic Number 49

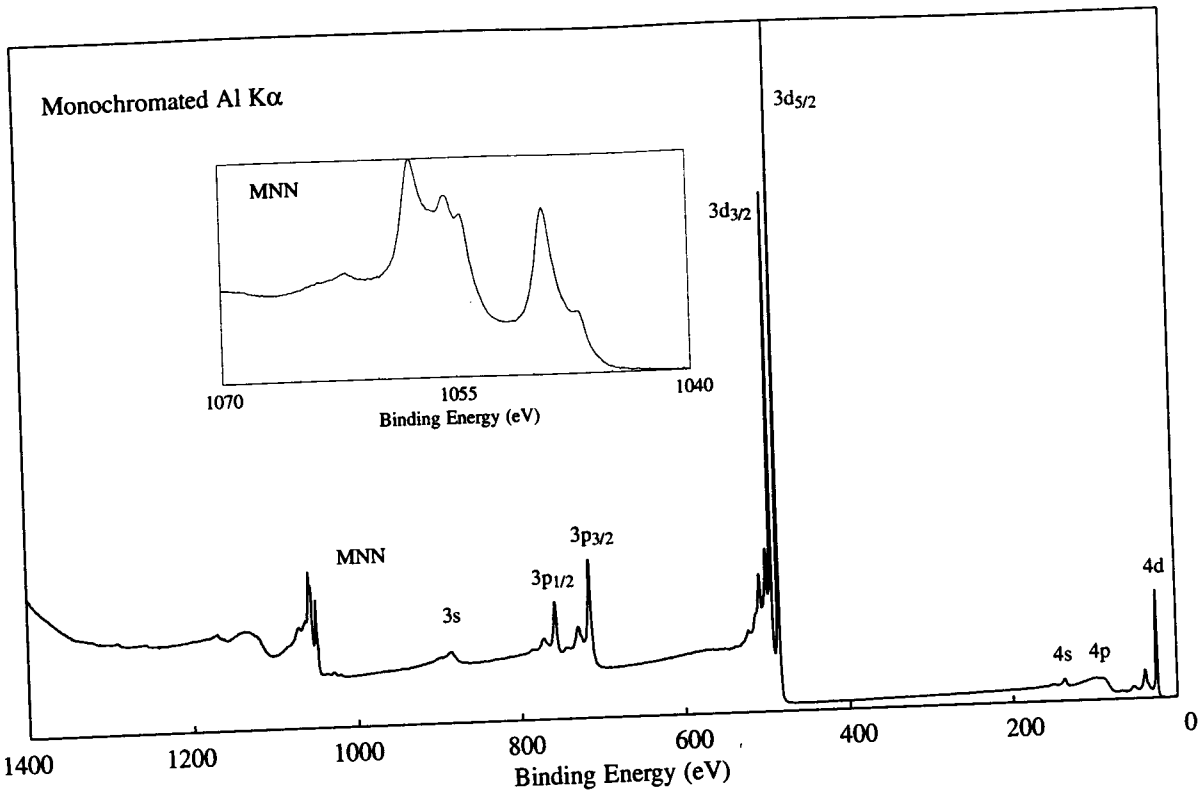


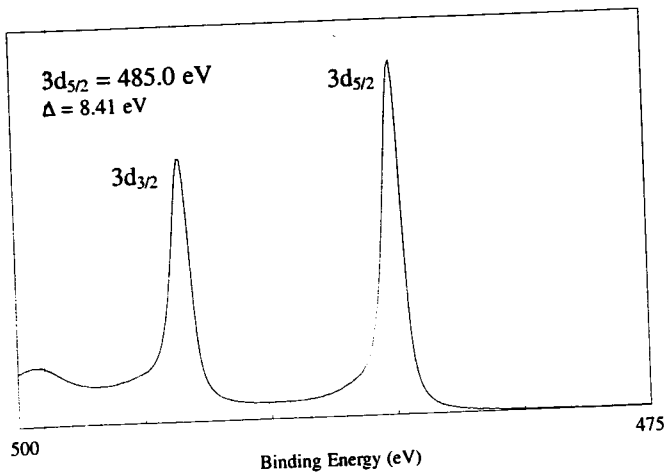




Tin Sn

Atomic Number 50





Line Positions (eV)

Photoelectron Lines

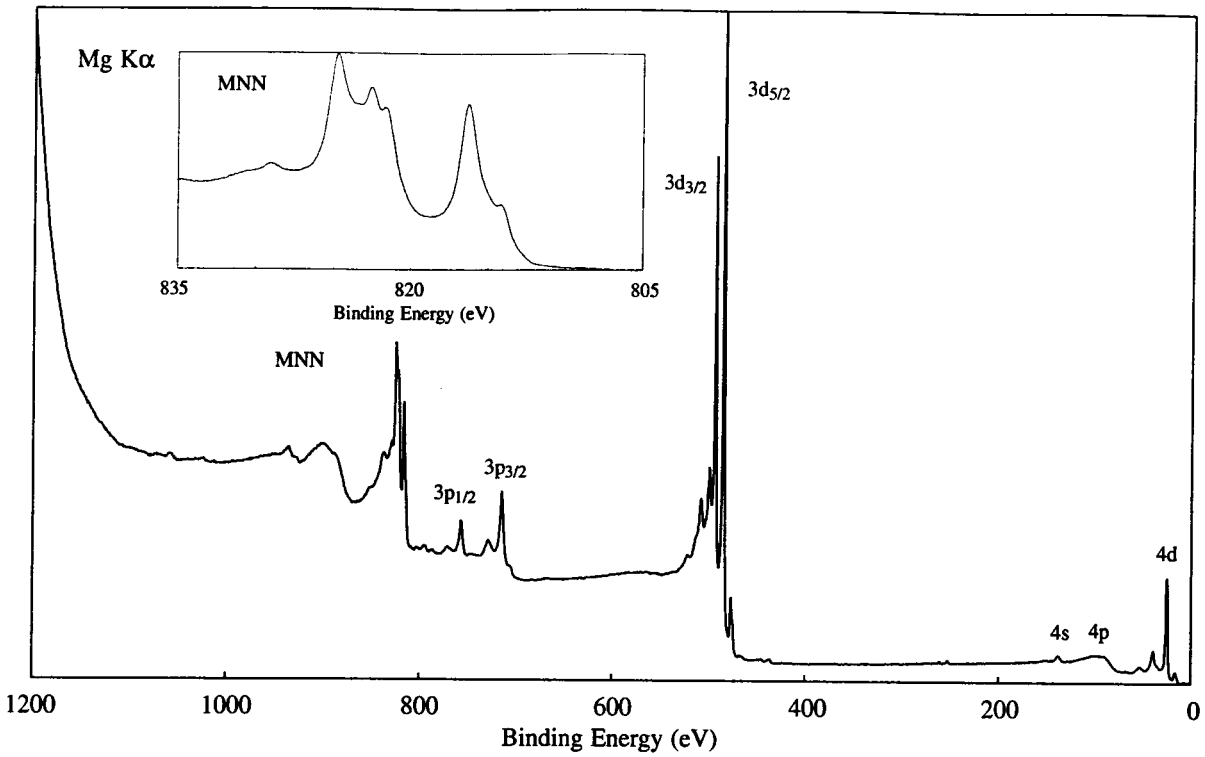
3s	3p1/2	3p3/2	3d3/2	3d5/2	4s	4p	4d
885	757	715	493	485	137	89	25

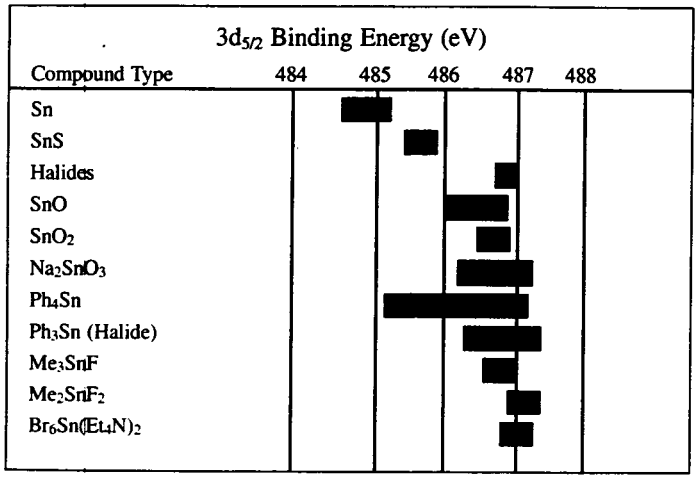
Auger Lines

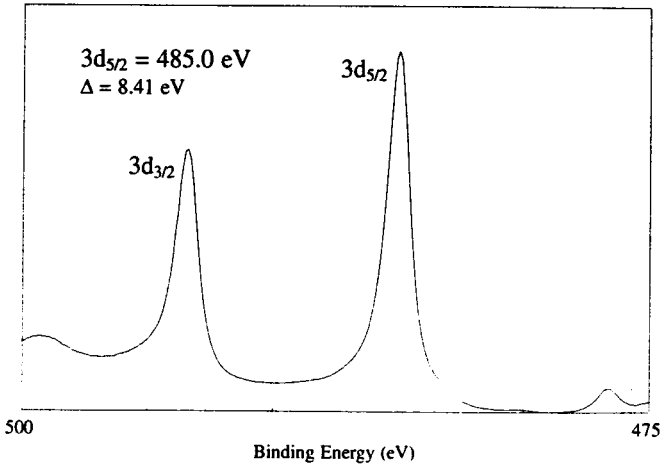
$M_5N_{45}N_{45}$	$M_4N_{45}N_{45}$	
1058	1049	(Al)
825	816	(Mg)

Tin Sn

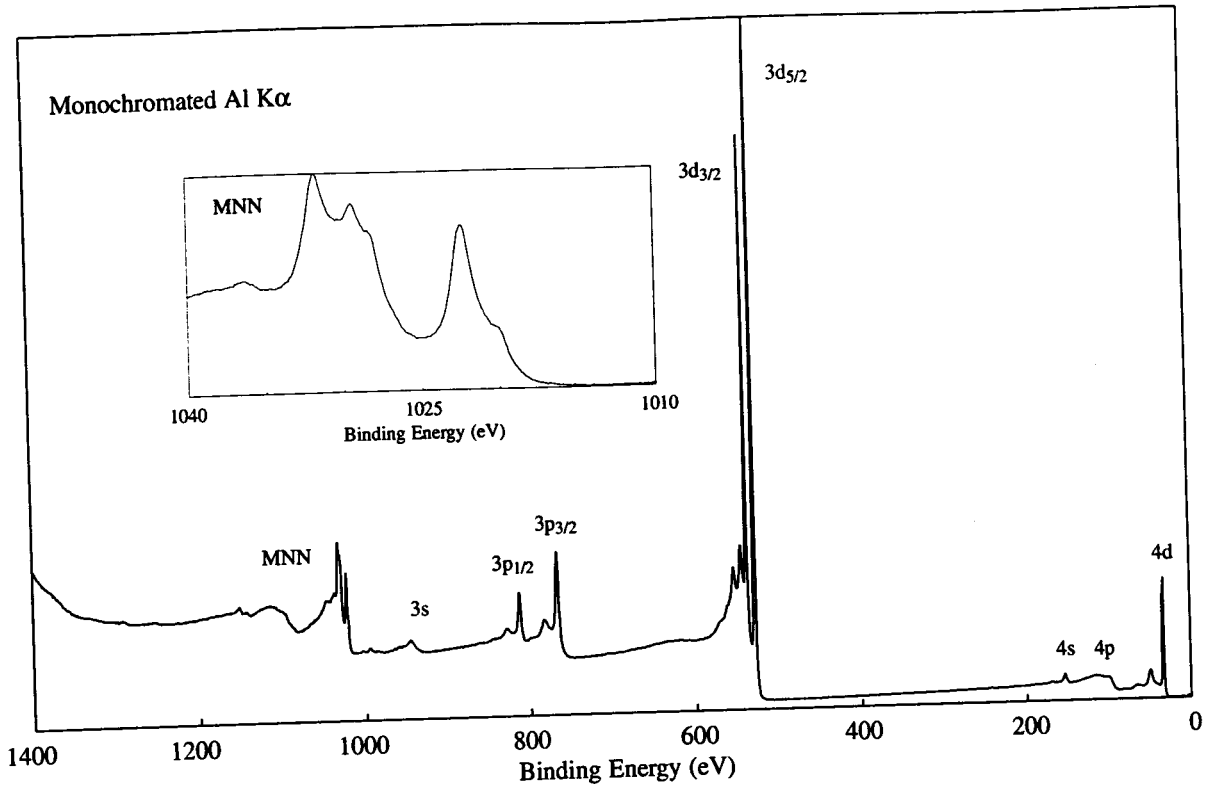
Atomic Number 50

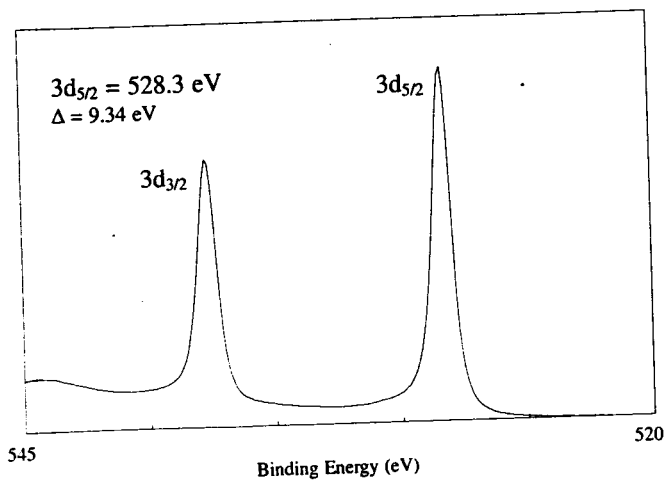






Antimony Sb
Atomic Number 51





Line Positions (eV)

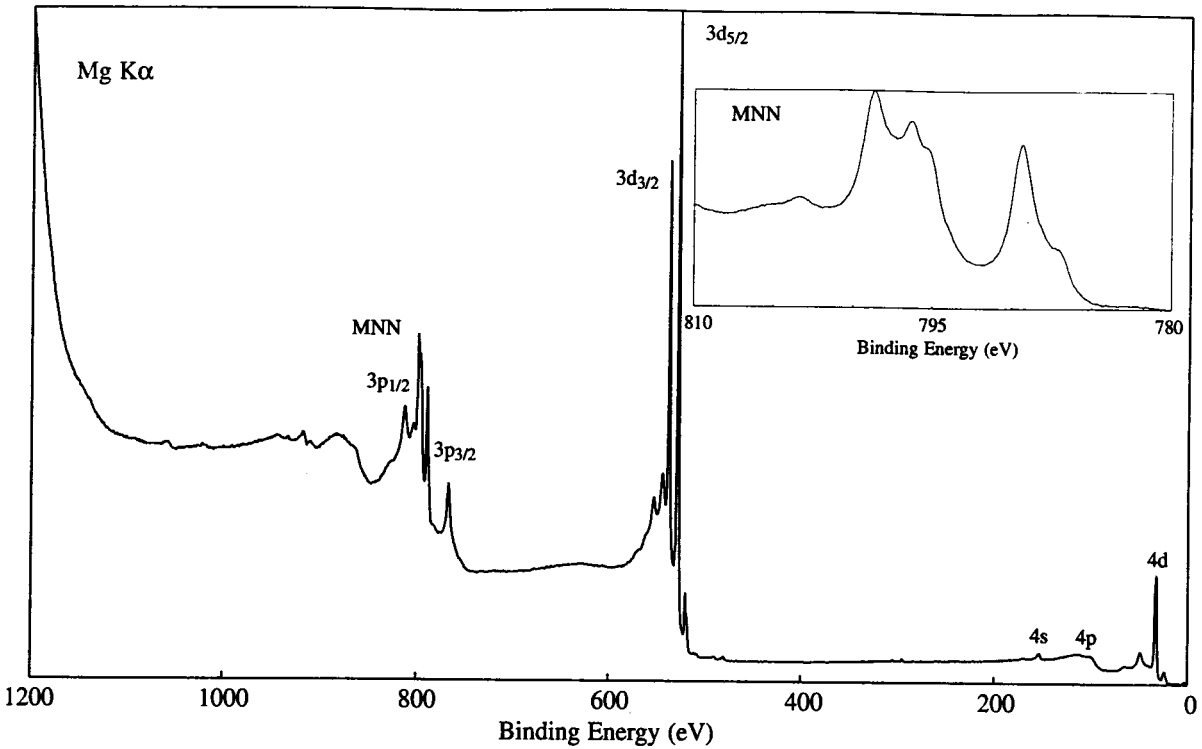
Photoelectron Lines

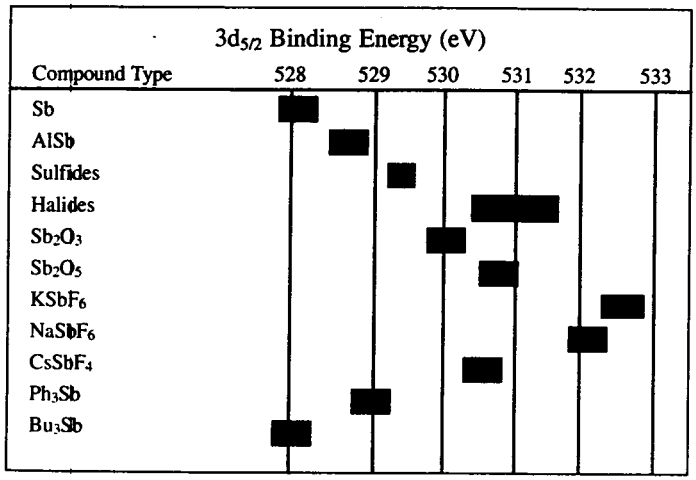
3s	3p1/2	3p3/2	3d3/2	3d5/2	4s	4p	4d
944	813	767	537	528	153	99	33

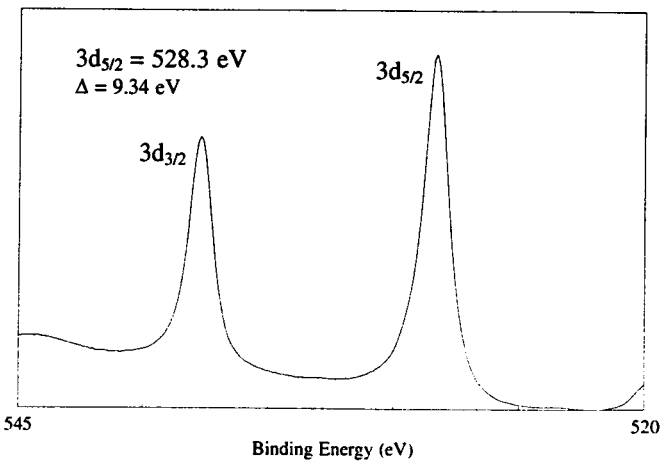
Auger Lines

$M_5N_{45}N_{45}$	$M_4N_{45}N_{45}$	
1032	1022	(Al)
799	789	(Mg)

Antimony Sb
Atomic Number 51

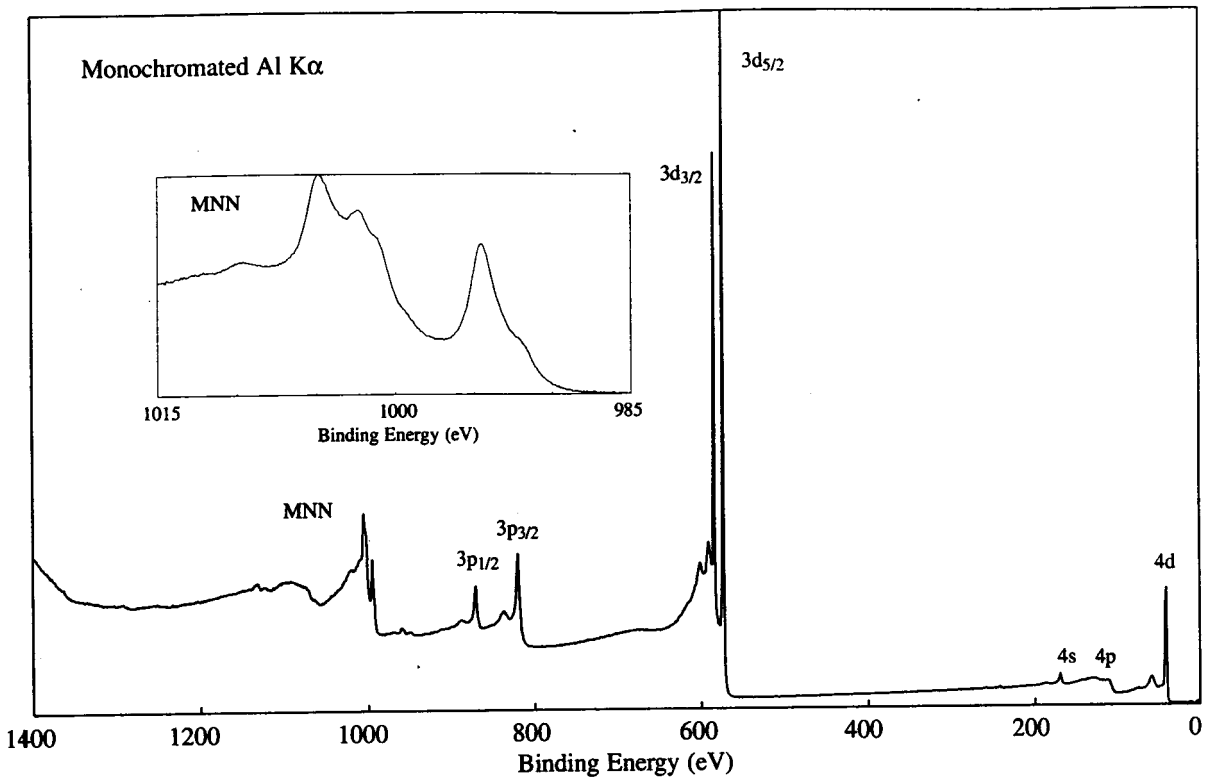


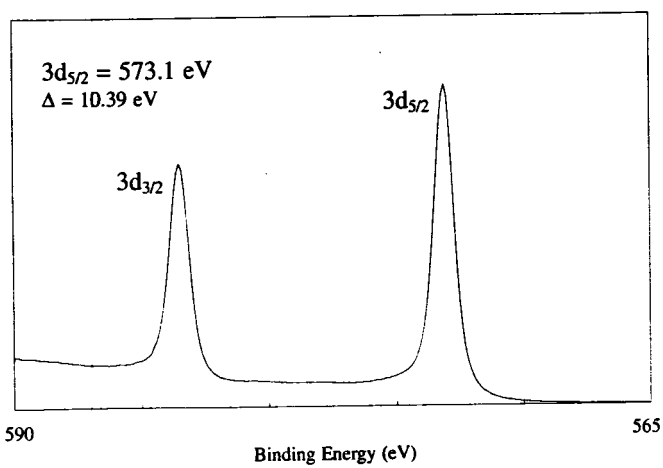




Tellurium Te

Atomic Number 52





Line Positions (eV)

Photoelectron Lines

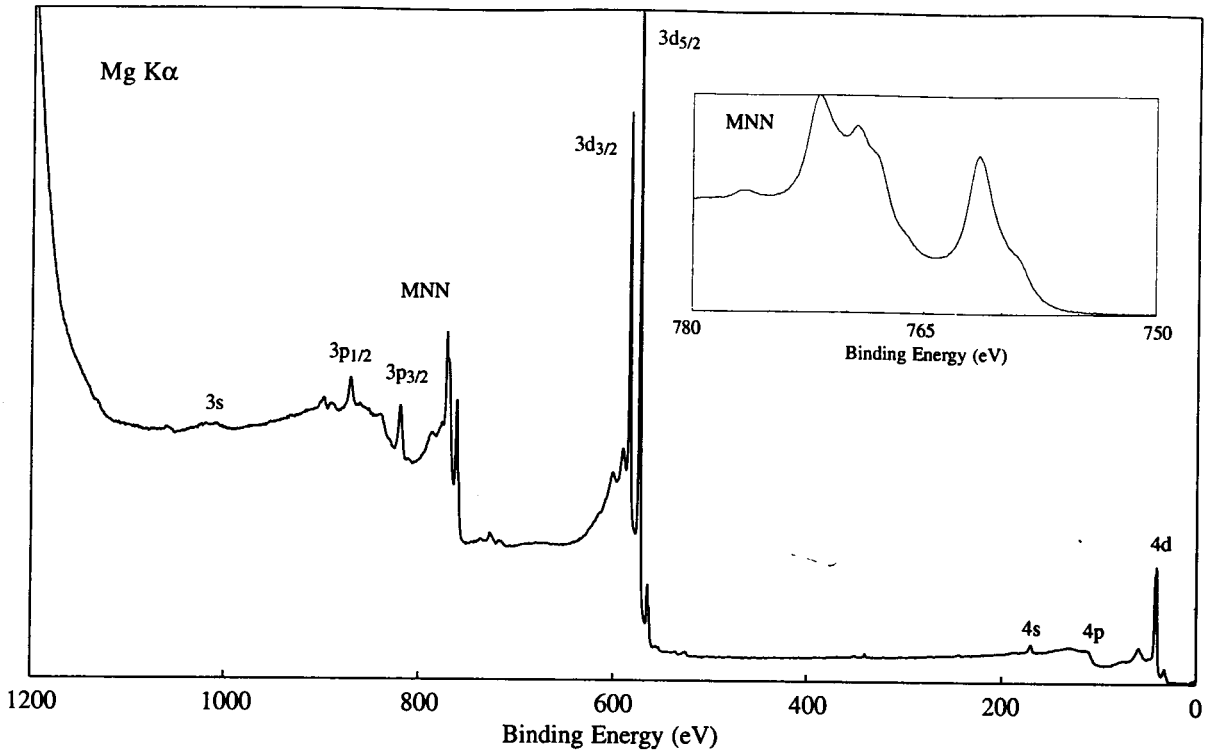
3s	3p1/2	3p3/2	3d3/2	3d5/2
1009	871	820	583	573

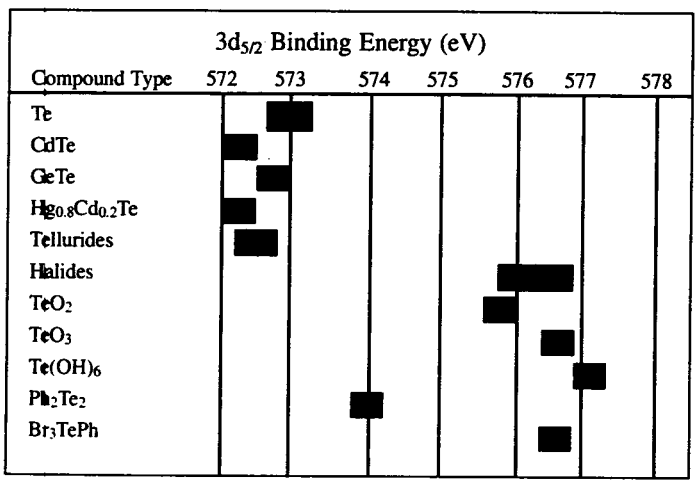
4s	4p	4d3/2	4d5/2	5s
170	111	42	41	12

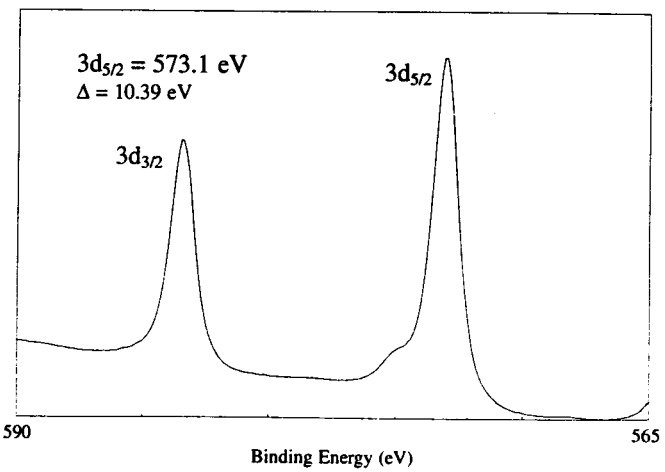
Auger Lines

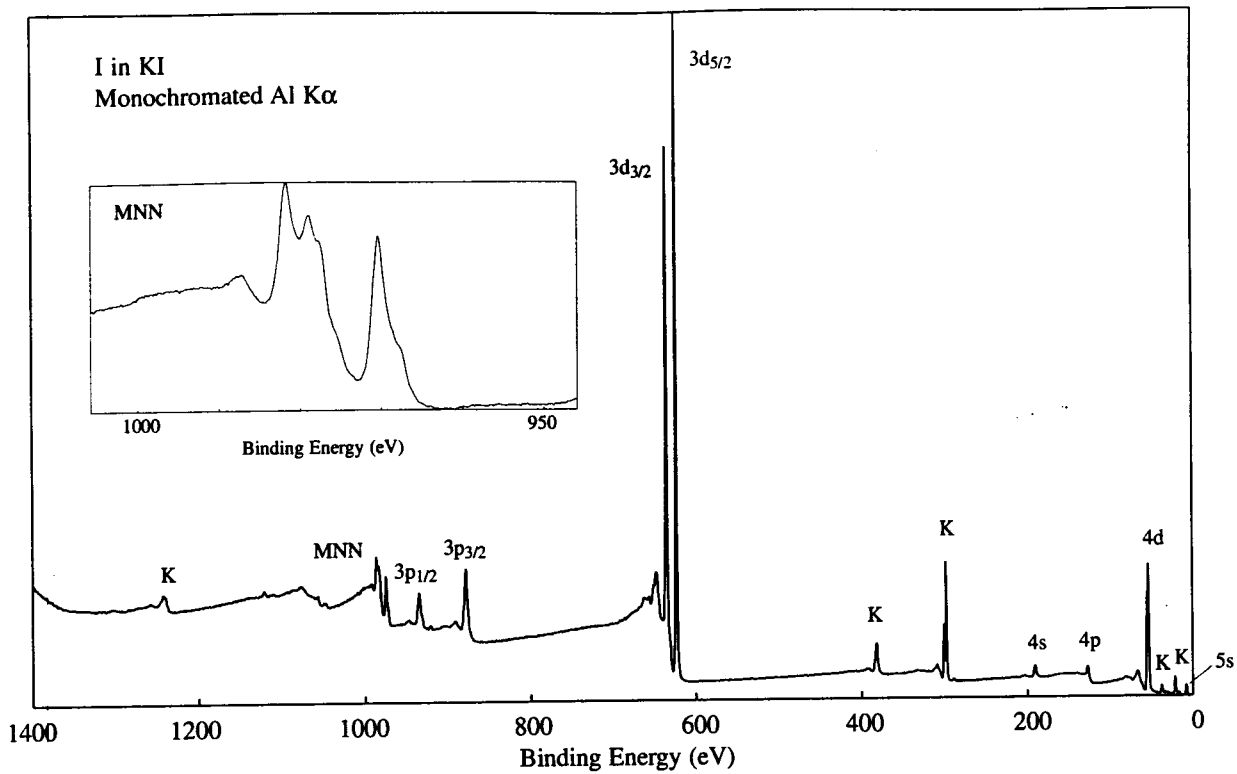
$M_5N_{45}N_{45}$	$M_4N_{45}N_{45}$	
1005	995	(Al)
772	762	(Mg)

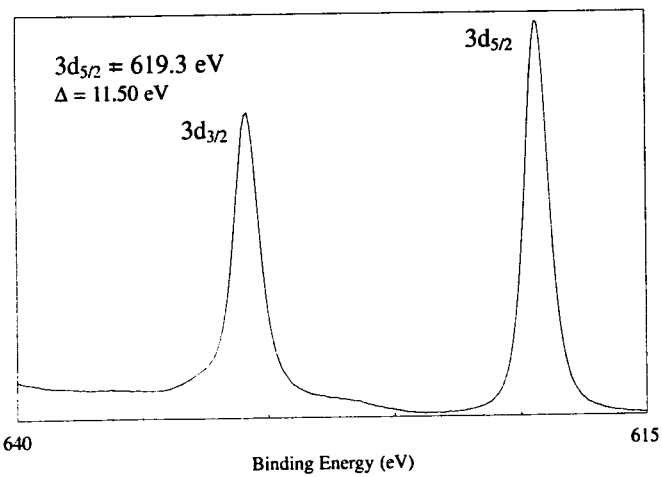
Tellurium Te
Atomic Number 52











Line Positions (eV)

Photoelectron Lines

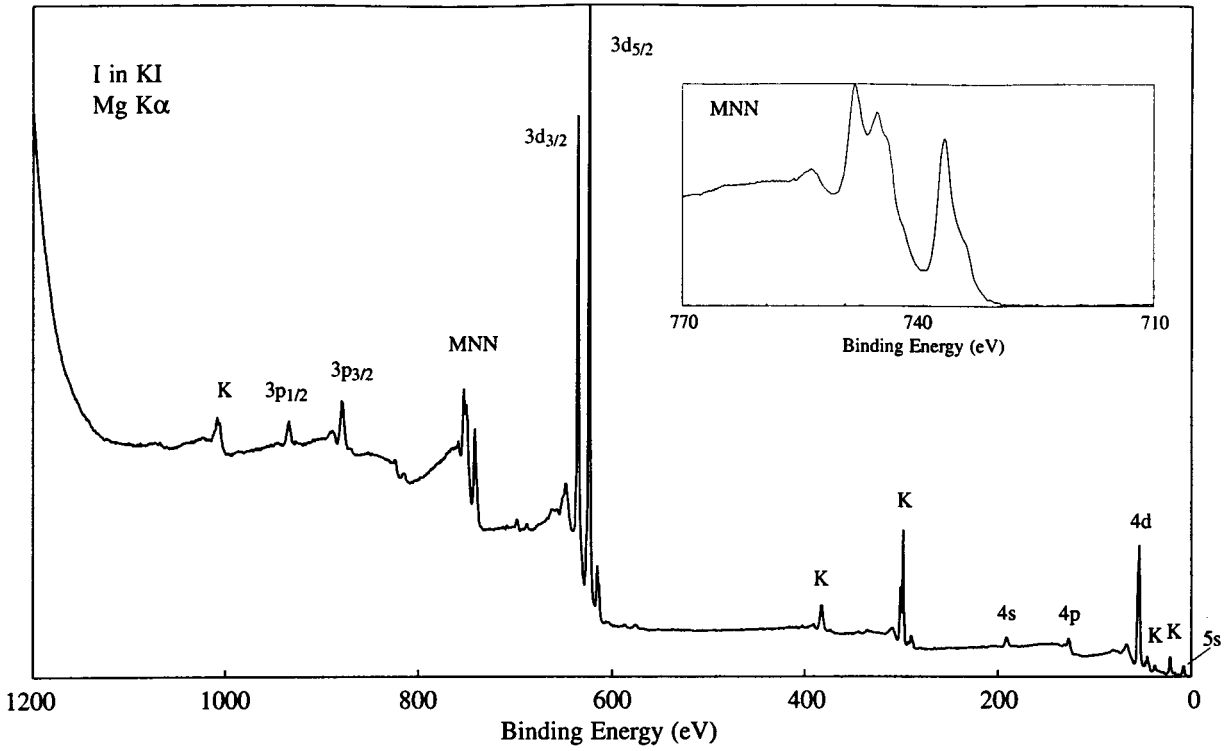
3s	3p1/2	3p3/2	3d3/2	3d5/2
1071	930	875	630	619

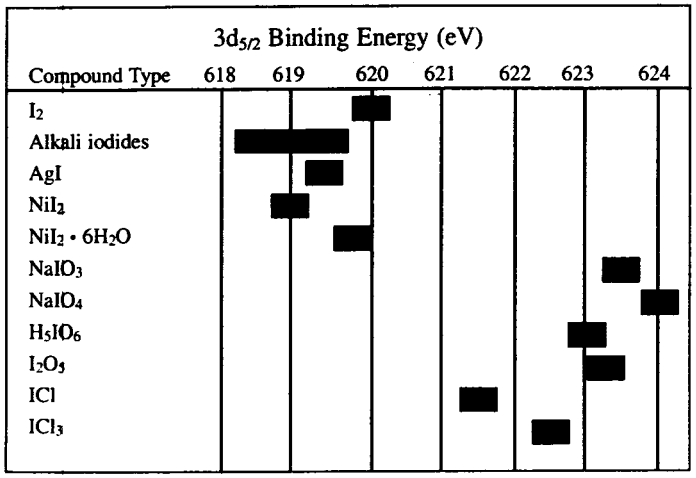
4s	4p	4d3/2	4d5/2	5s
187	123	51	49	18

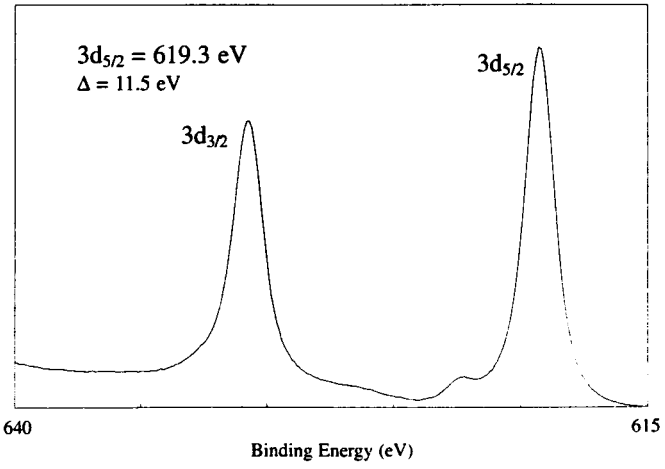
Auger Lines

$M_5N_{45}N_{45}$	$M_4N_{45}N_{45}$	
982	971	(Al)
749	738	(Mg)

Iodine I
Atomic Number 53

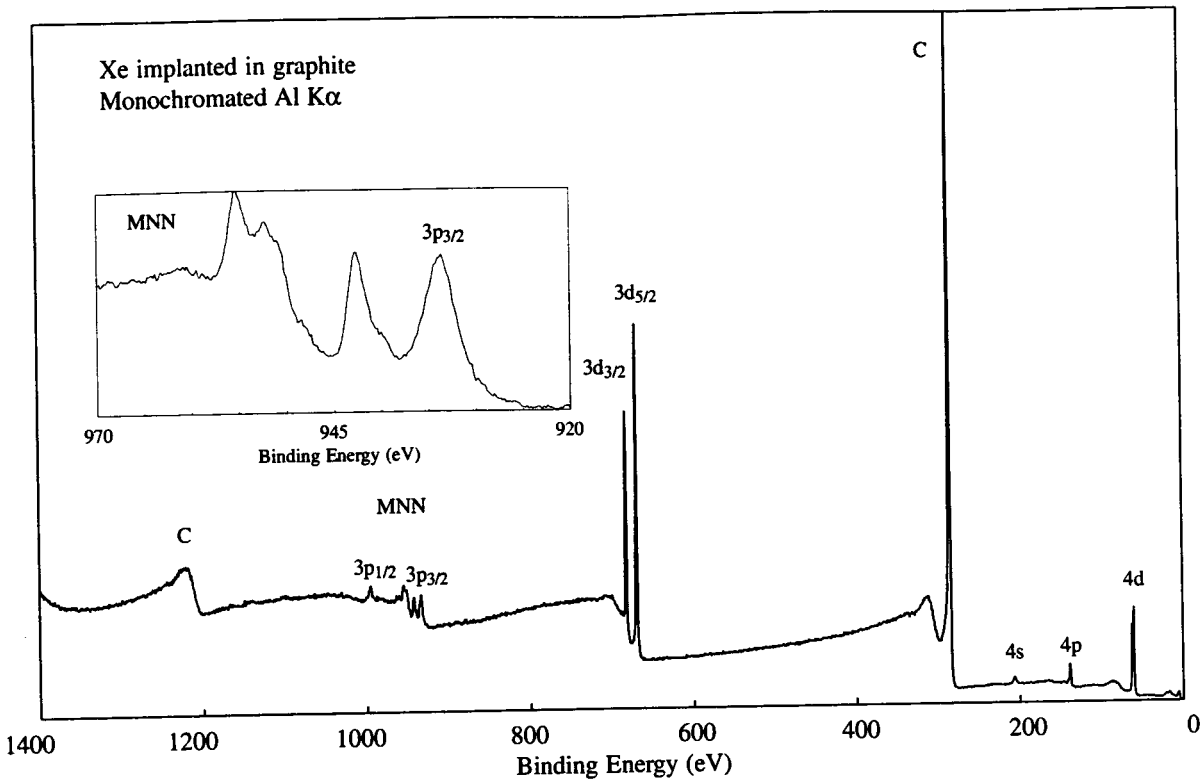


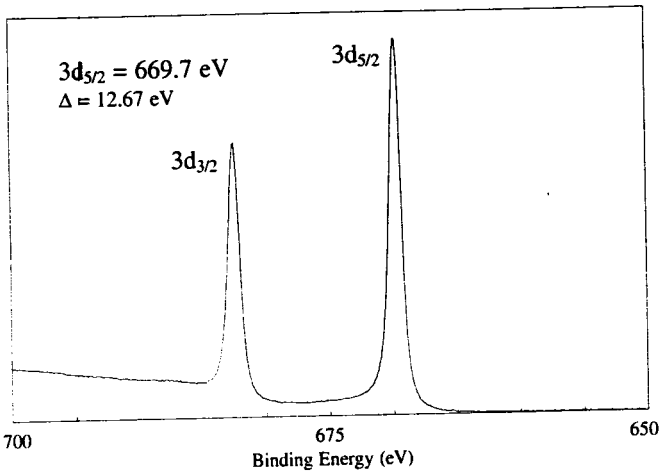




Xenon Xe

Atomic Number 54





Line Positions (eV)

Photoelectron Lines

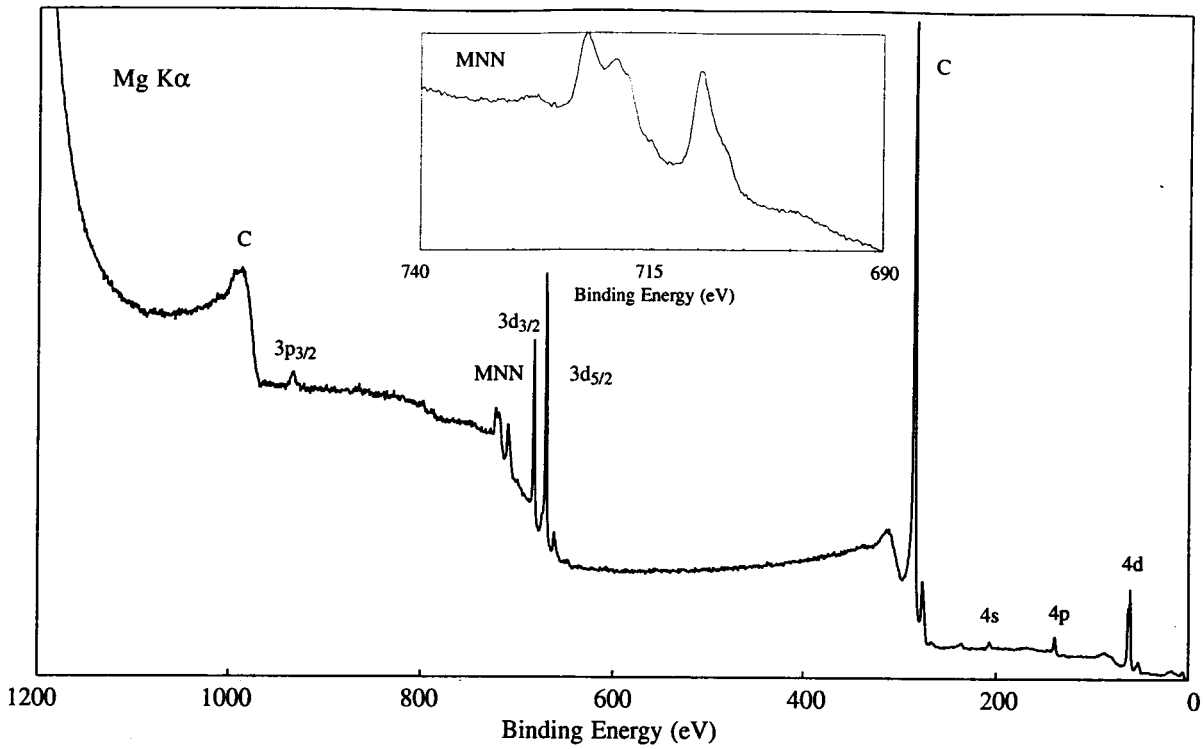
3s	3p1/2	3p3/2	3d3/2	3d5/2
1141	996	934	683	670

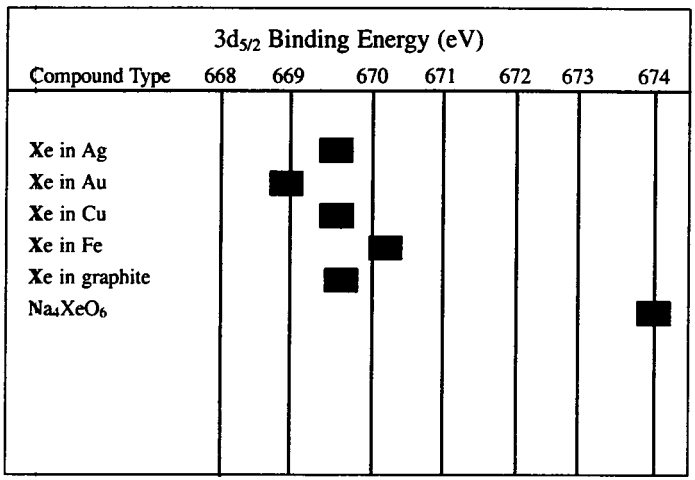
4s	4p	4d3/2	4d5/2	5s
207	139	63	61	17

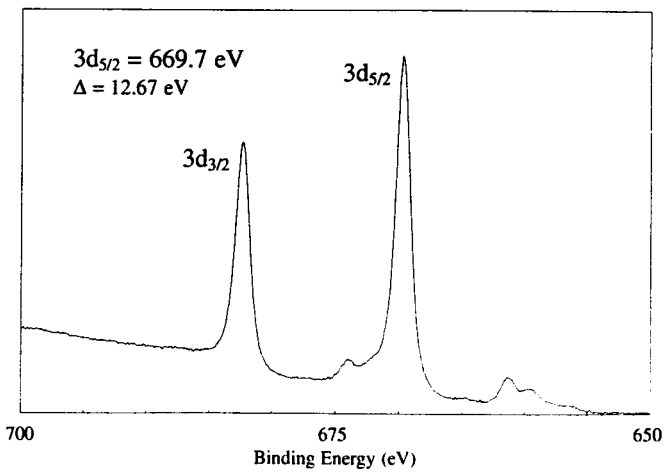
Auger Lines

$M_5N_{45}N_{45}$	$M_4N_{45}N_{45}$	
955	942	(Al)
722	709	(Mg)

Xenon Xe
Atomic Number 54

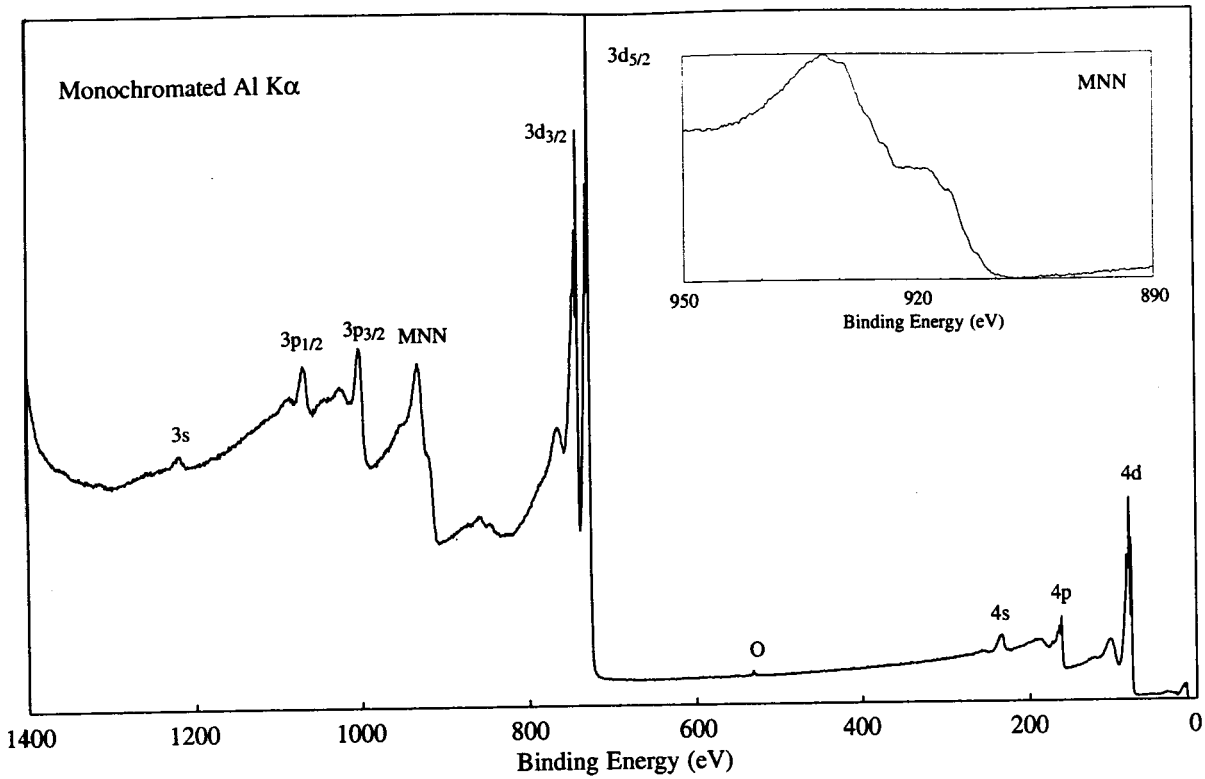


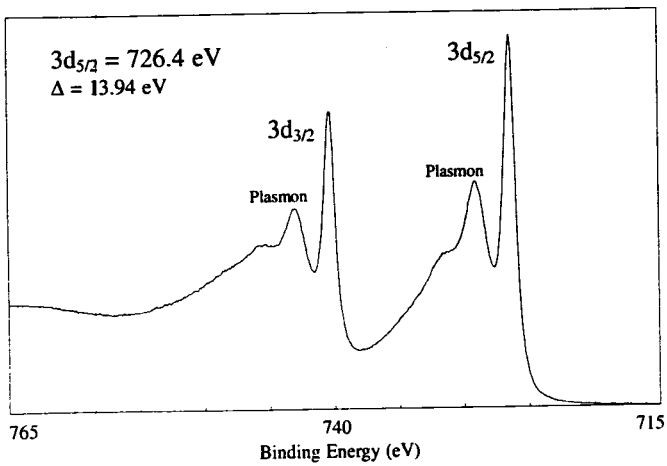




Cesium Cs

Atomic Number 55





Line Positions (eV)

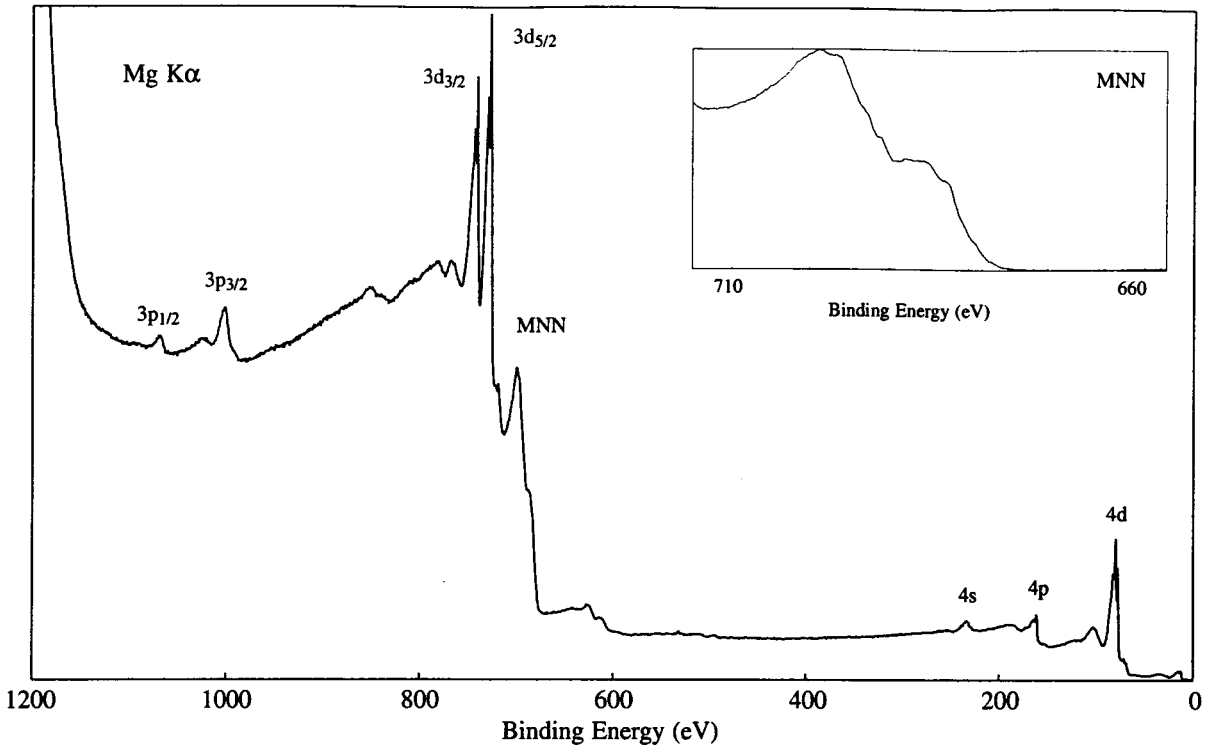
Photoelectron Lines

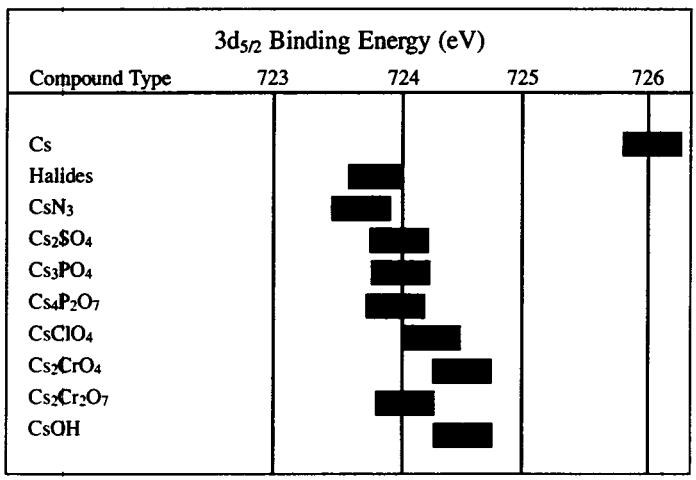
3s	3p1/2	3p3/2	3d3/2	3d5/2	
1219	1069	1002	740	726	
4s	4p1/2	4p3/2	4d3/2	4d5/2	5s
234	173	161	80	77	25

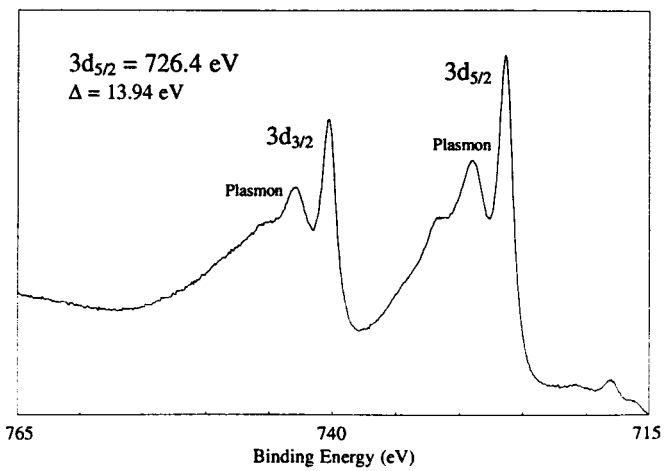
Auger Lines

$M_5N_{45}N_{45}$	$M_4N_{45}N_{45}$	
931	918	(Al)
698	685	(Mg)

Cesium Cs
Atomic Number 55

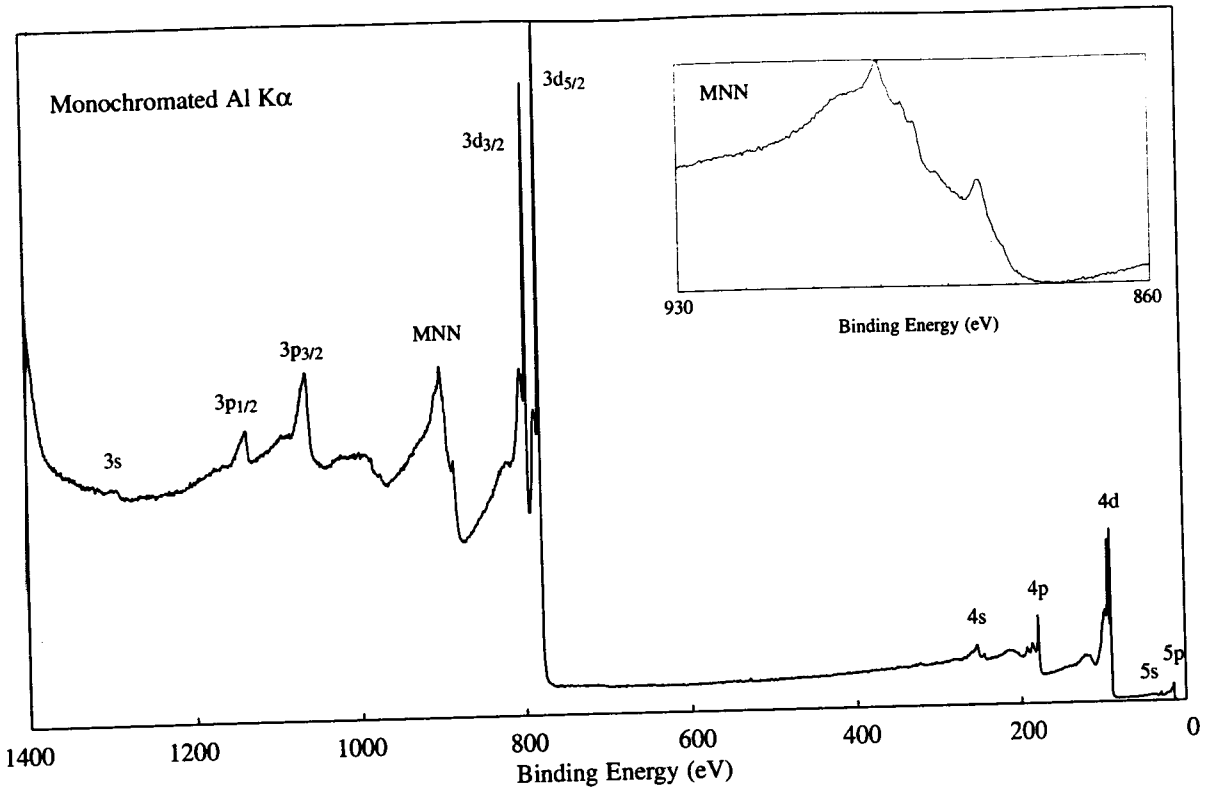


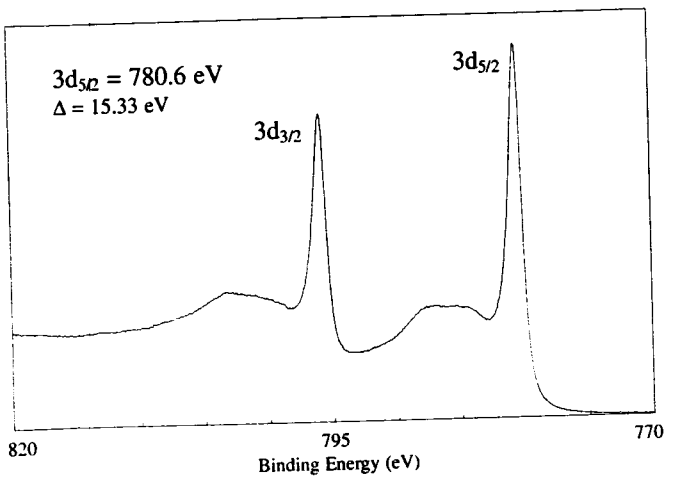




Barium Ba

Atomic Number 56





Line Positions (eV)

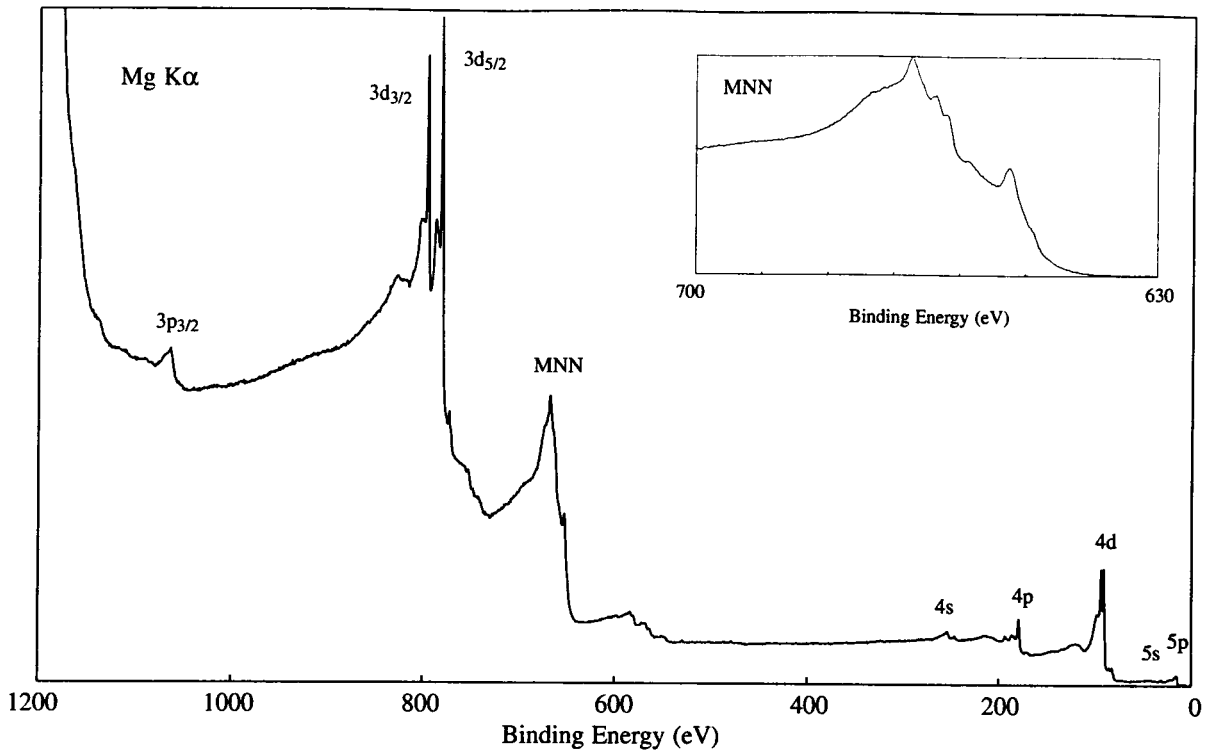
Photoelectron Lines

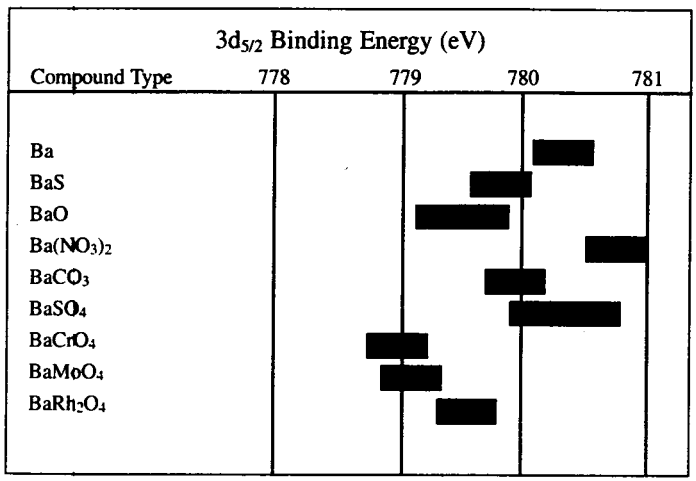
3s	3p1/2	3p3/2	3d3/2	3d5/2		
1292	1138	1064	796	781		
4s	4p1/2	4p3/2	4d3/2	4d5/2	5s	5p
254	193	179	93	90	31	15

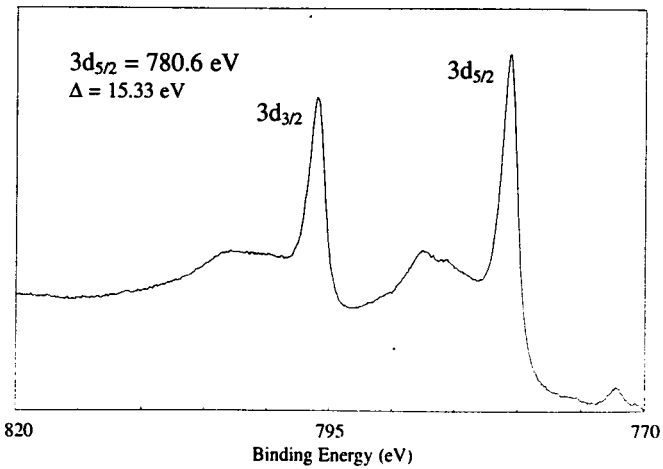
Auger Lines

$M_5N_{45}N_{45}$	$M_4N_{45}N_{45}$	
900	886	(Al)
667	653	(Mg)

Barium Ba
Atomic Number 56

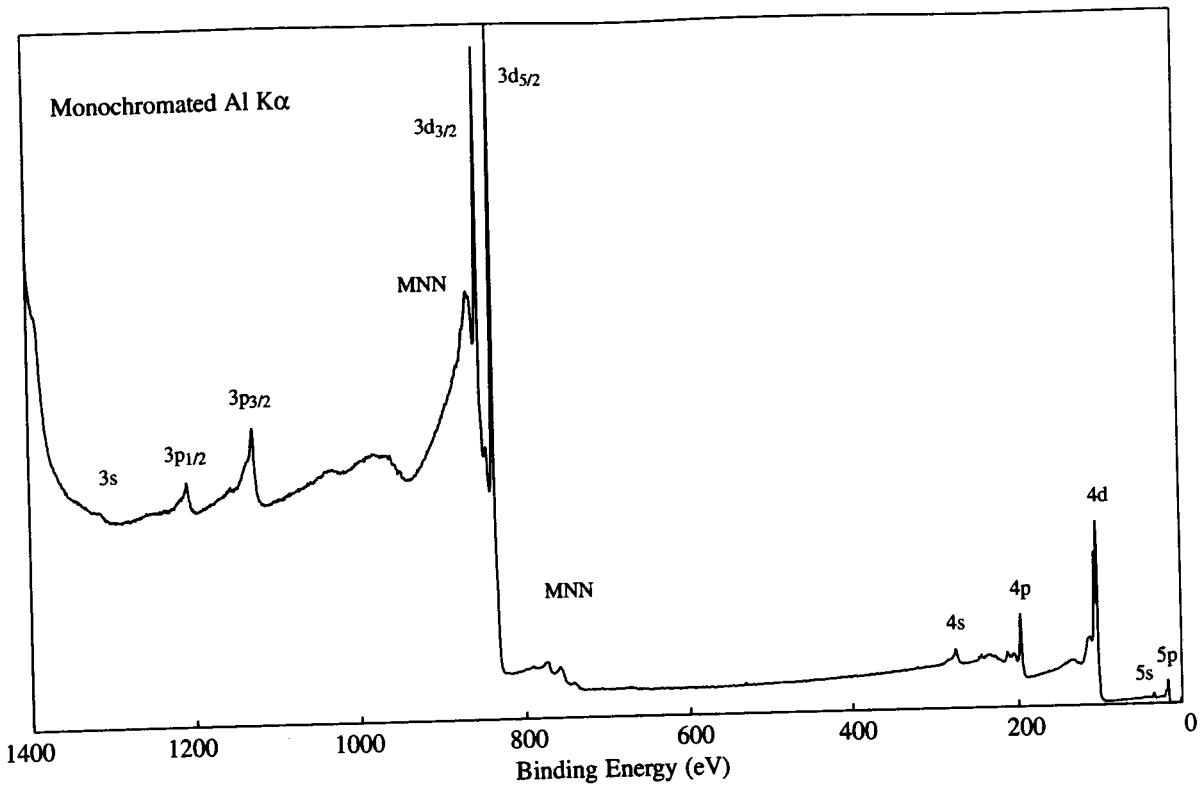


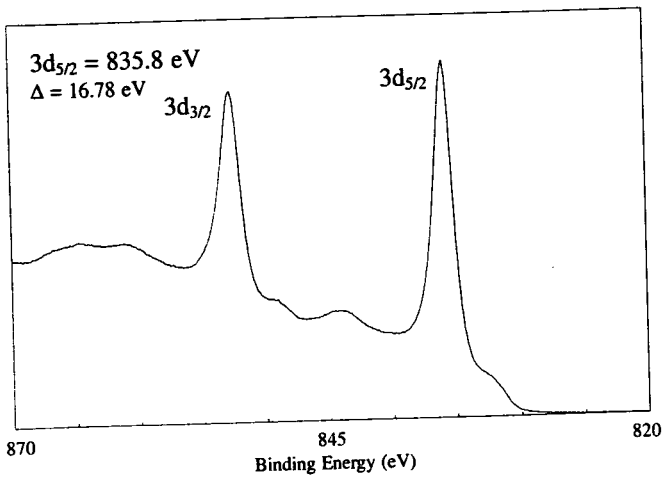




Lanthanum La

Atomic Number 57





Line Positions (eV)

Photoelectron Lines

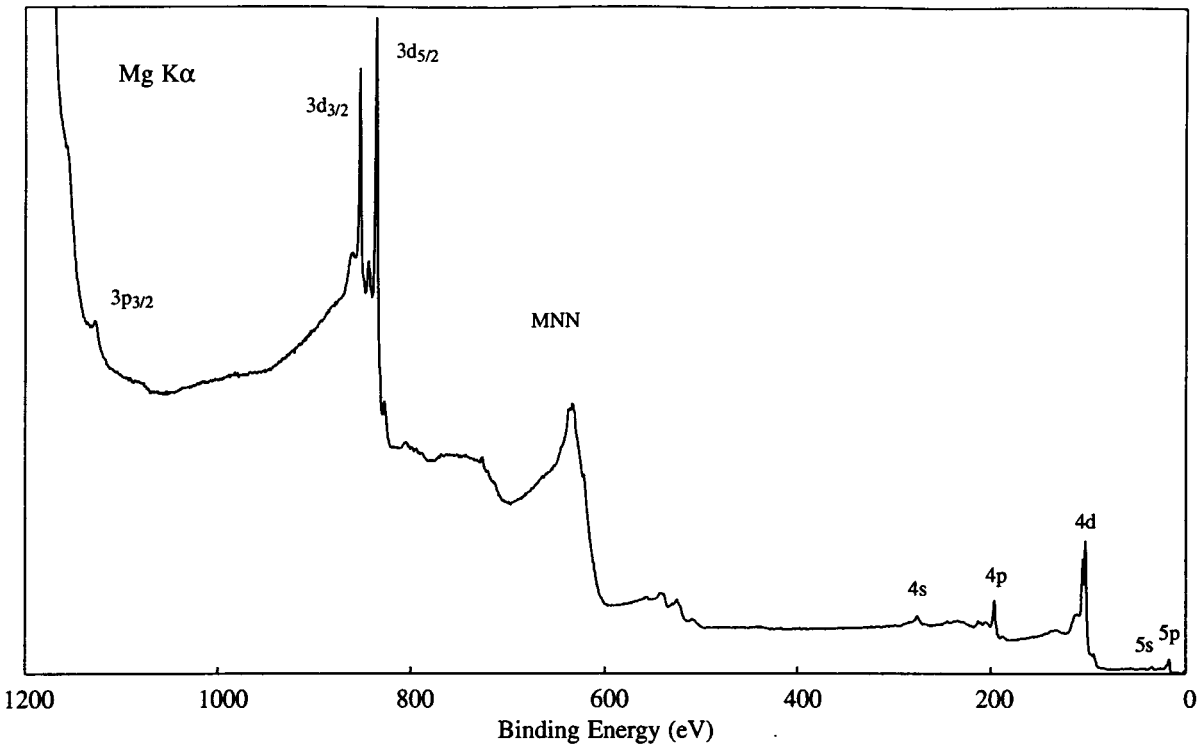
$3p_{1/2}$	$3p_{3/2}$	$3d_{3/2}$	$3d_{5/2}$			
1208	1128	853	836			
4s	$4p_{1/2}$	$4p_{3/2}$	$4d_{3/2}$	$4d_{5/2}$	5s	5p
275	213	197	106	103	34	17

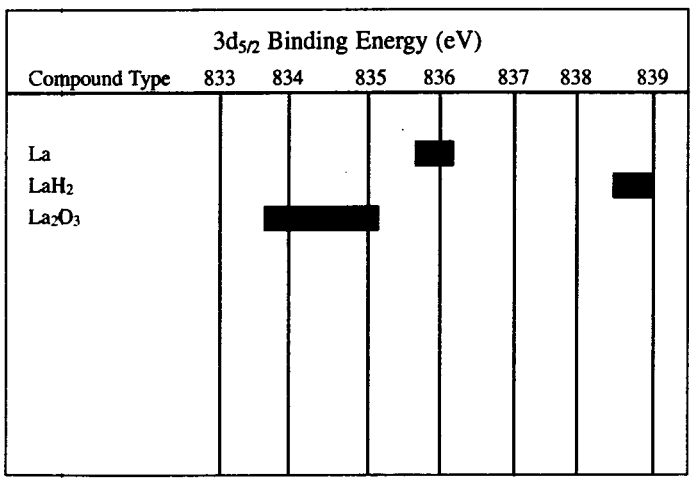
Auger Lines

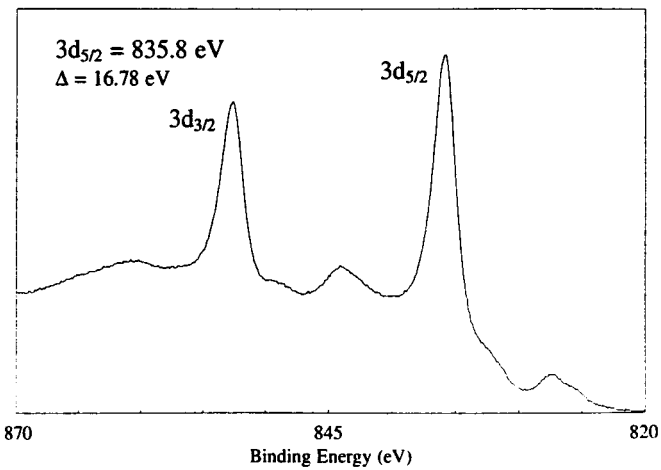
$M_5N_{45}N_{45}$	$M_4N_{45}N_{45}$	
867	854	(Al)
634	621	(Mg)

Lanthanum La

Atomic Number 57

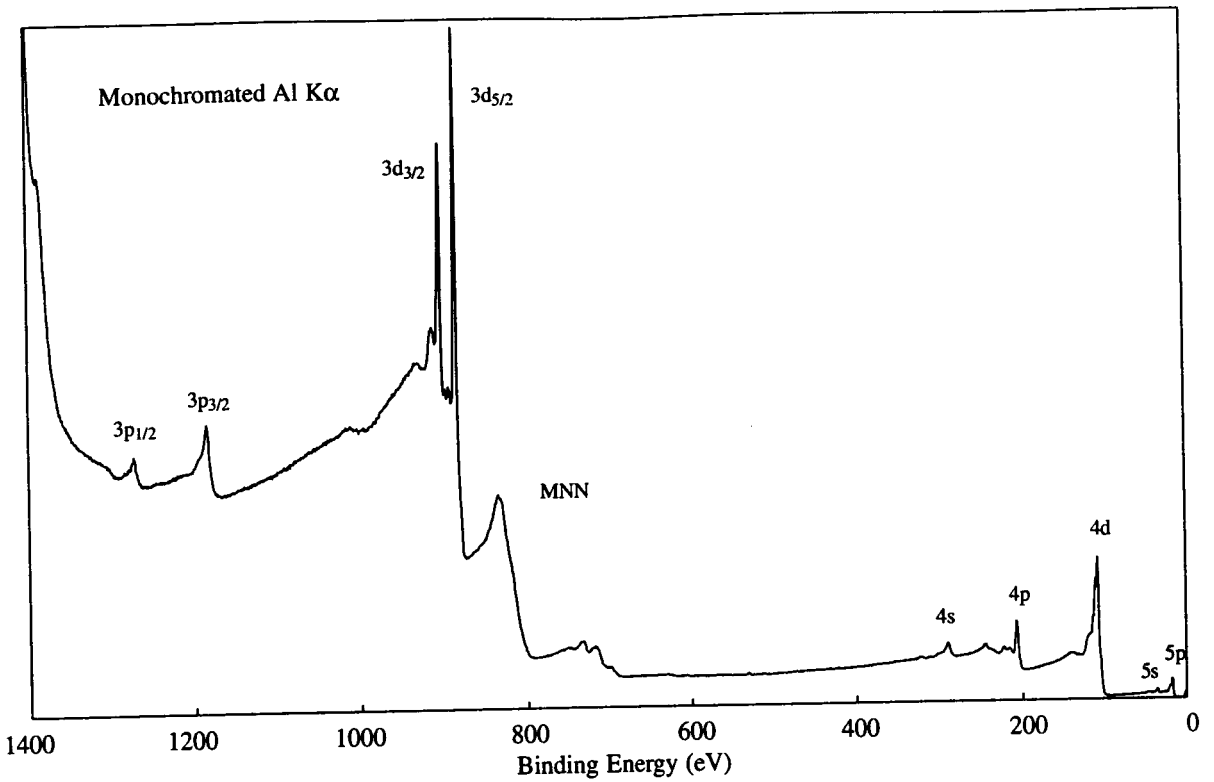


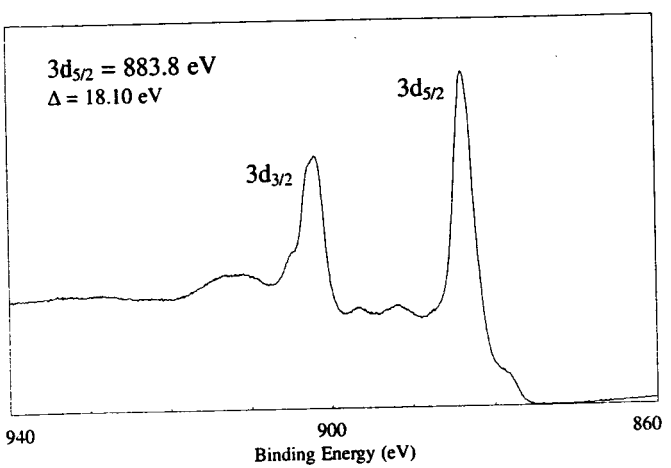




Cerium Ce

Atomic Number 58





Line Positions (eV)

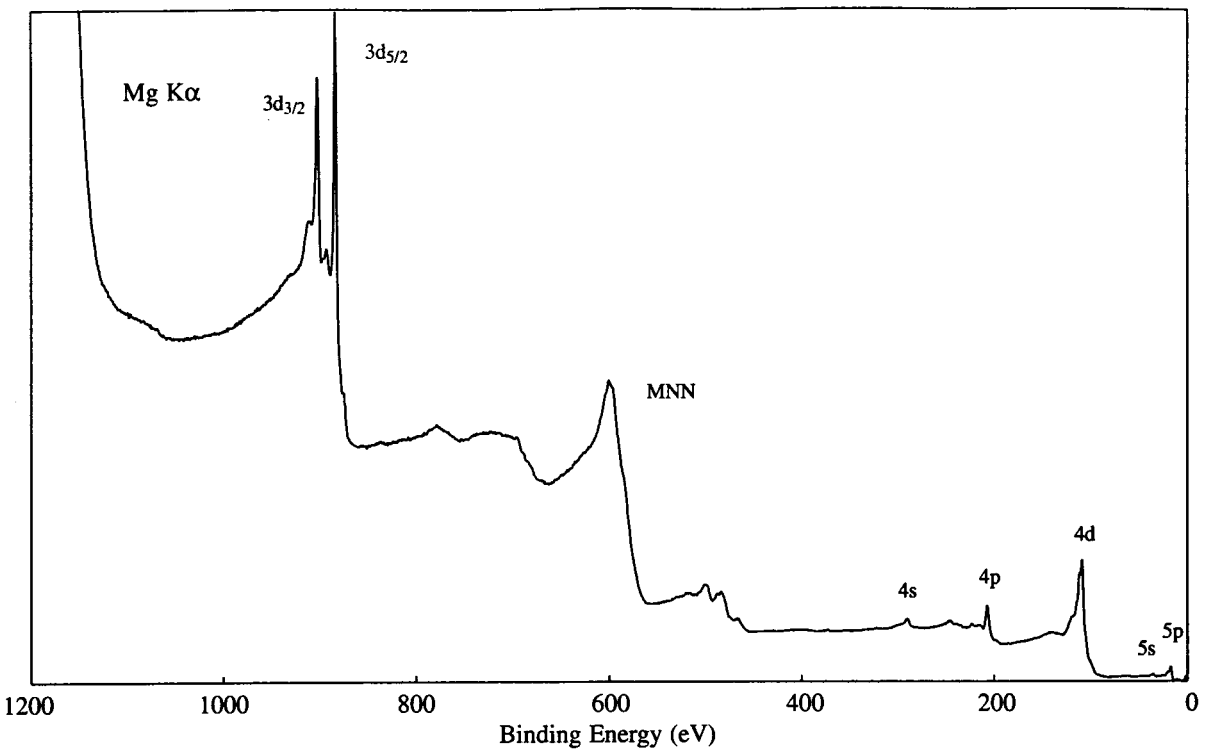
Photoelectron Lines

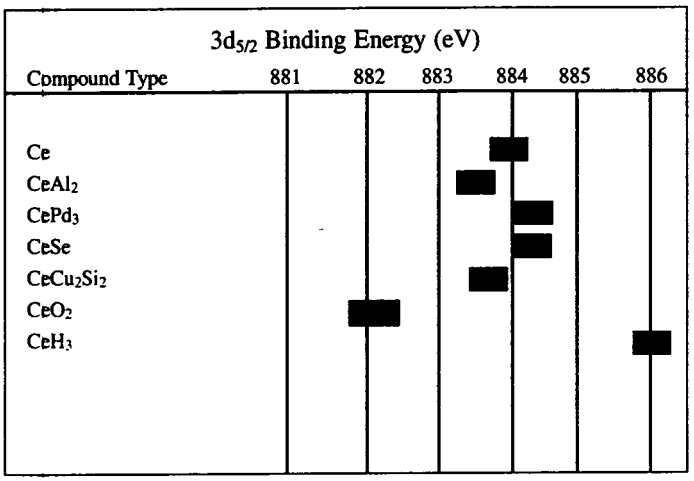
$3p_{1/2}$	$3p_{3/2}$	$3d_{3/2}$	$3d_{5/2}$			
1272	1184	902	884			
4s	**$4p_{1/2}$**	**$4p_{3/2}$**	**$4d_{3/2}$**	**$4d_{5/2}$**	**5s**	**5p**
290	223	207	112	109	36	18

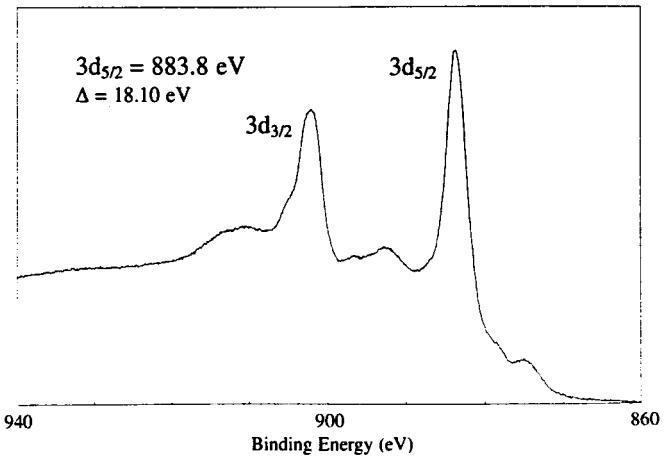
Auger Lines

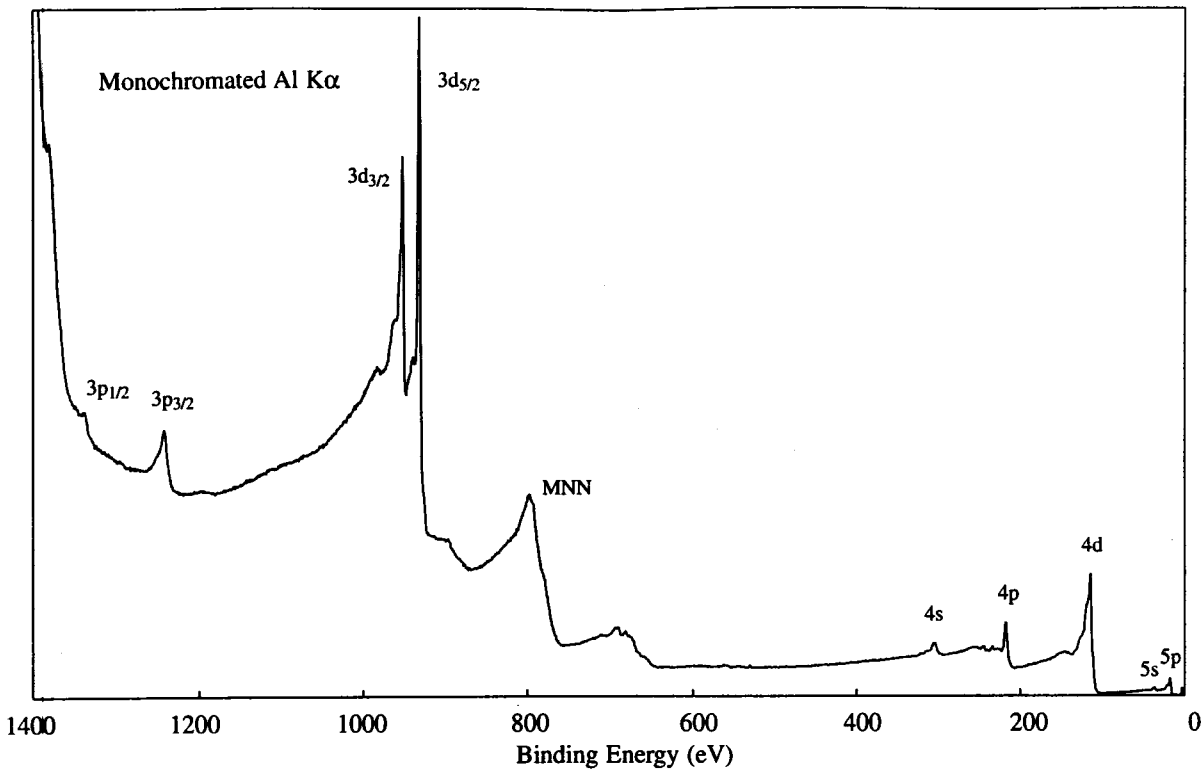
$M_{45}N_{45}N_{45}$	
833	(Al)
600	(Mg)

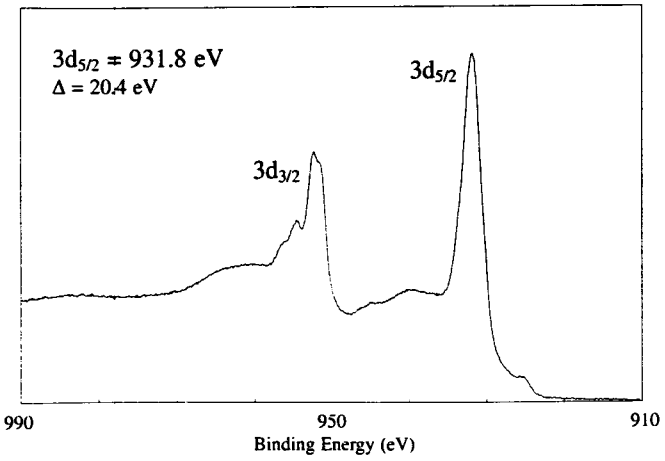
Cerium Ce
Atomic Number 58











Line Positions (eV)

Photoelectron Lines

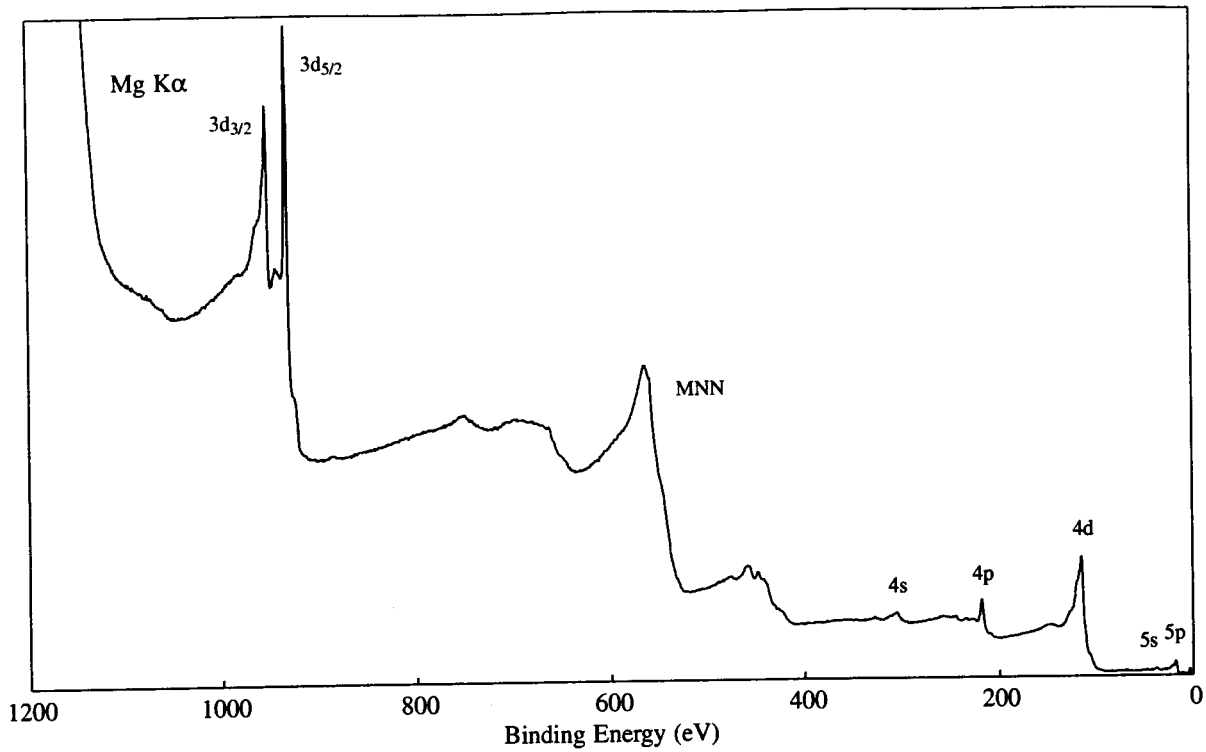
$3p_{1/2}$	$3p_{3/2}$	$3d_{3/2}$	$3d_{5/2}$		
1339	1242	952	932		
4s	$4p_{1/2}$	$4p_{3/2}$	4d	5s	5p
305	234	218	115	38	18

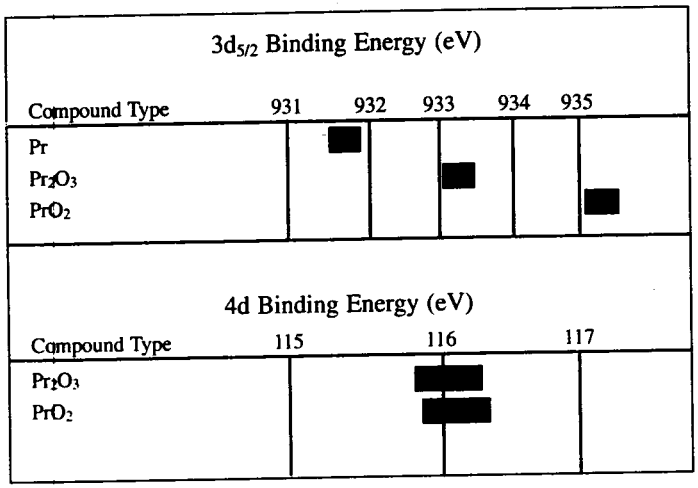
Auger Lines

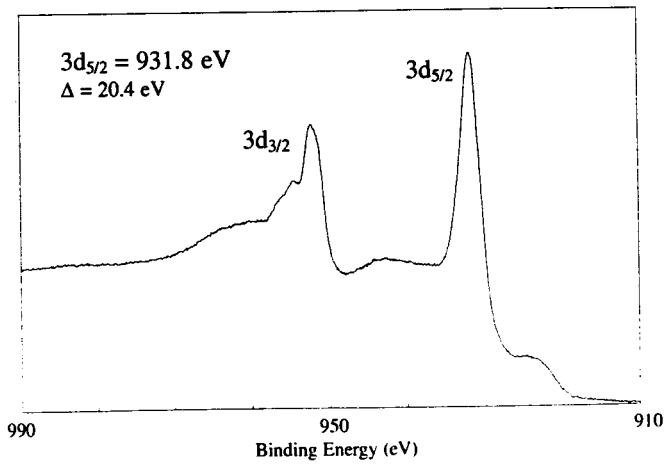
$M_{45}N_{45}N_{45}$	
797	(Al)
564	(Mg)

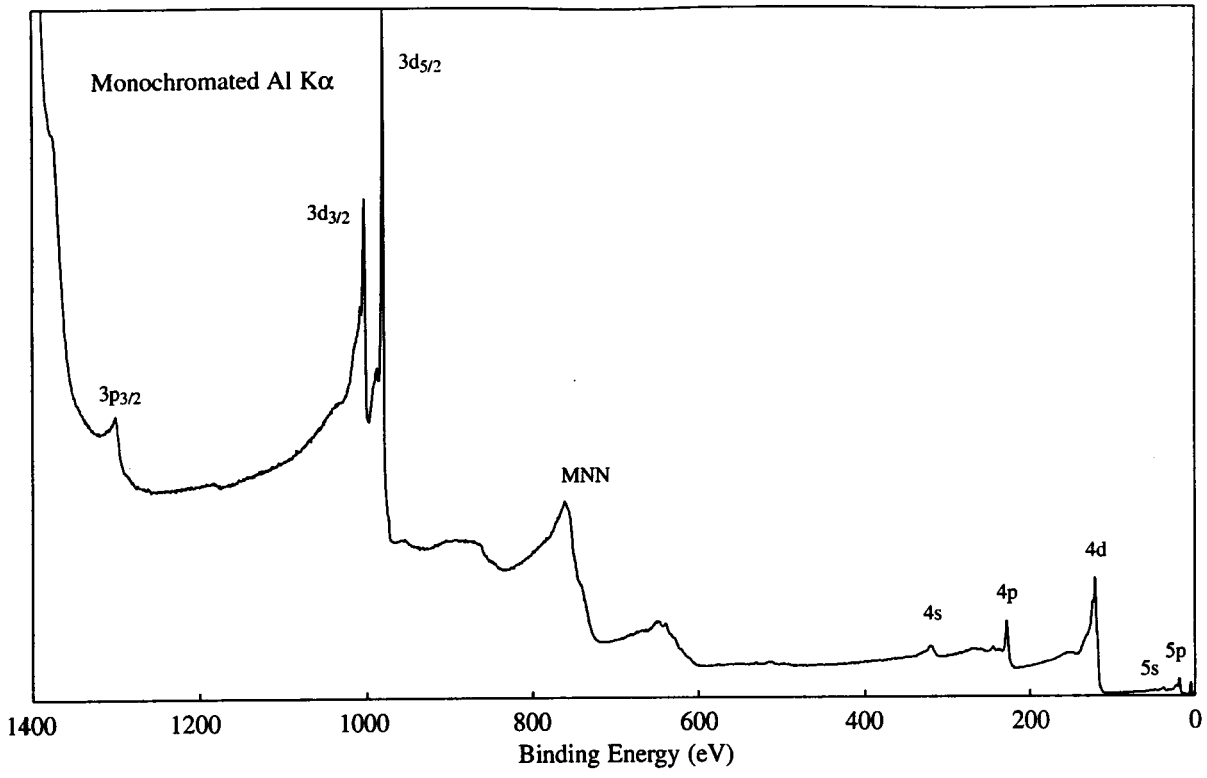
Praseodymium Pr

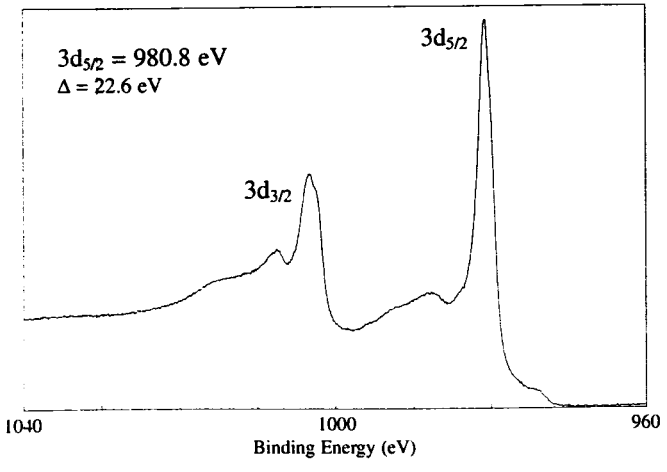
Atomic Number 59











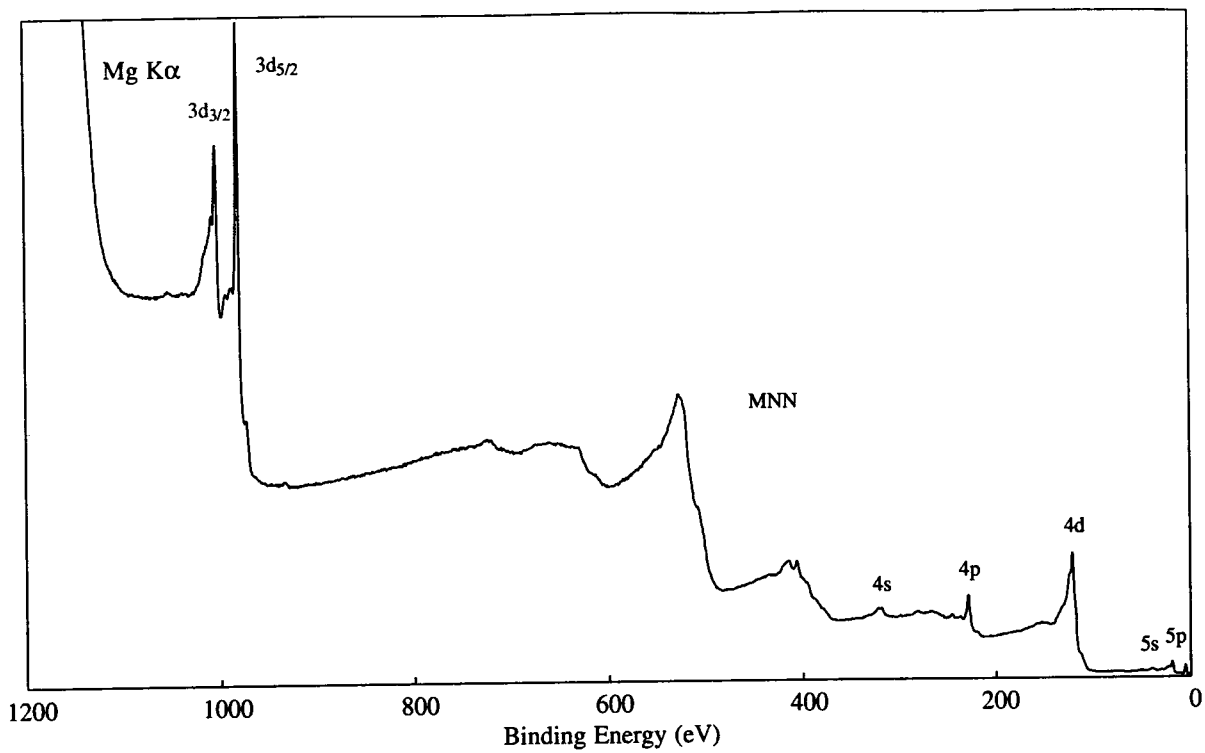
Line Positions (eV)

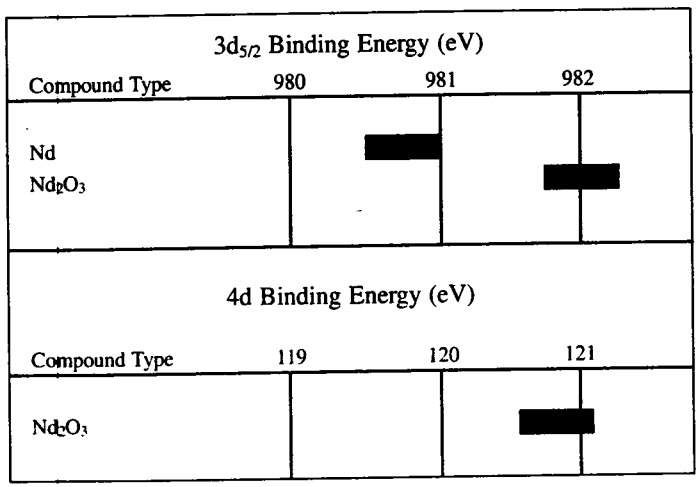
Photoelectron Lines

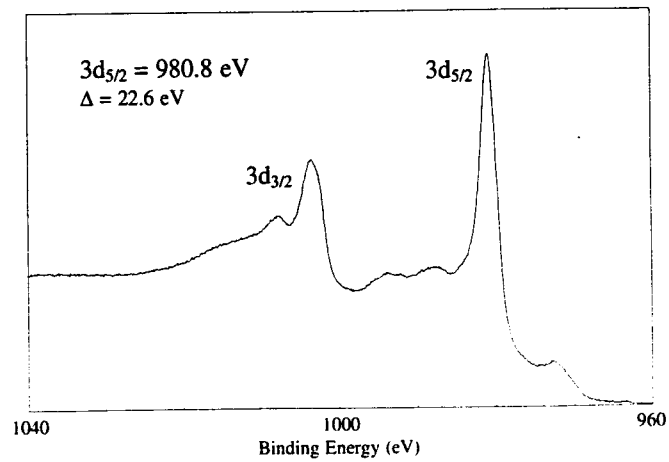
$3p_{3/2}$	$3d_{3/2}$	$3d_{5/2}$			
1301	1003	981			
4s	$4p_{1/2}$	$4p_{3/2}$	4d	5s	5p
320	245	228	121	39	19

Auger Lines

$M_{45}N_{45}N_{45}$	
758	(Al)
525	(Mg)

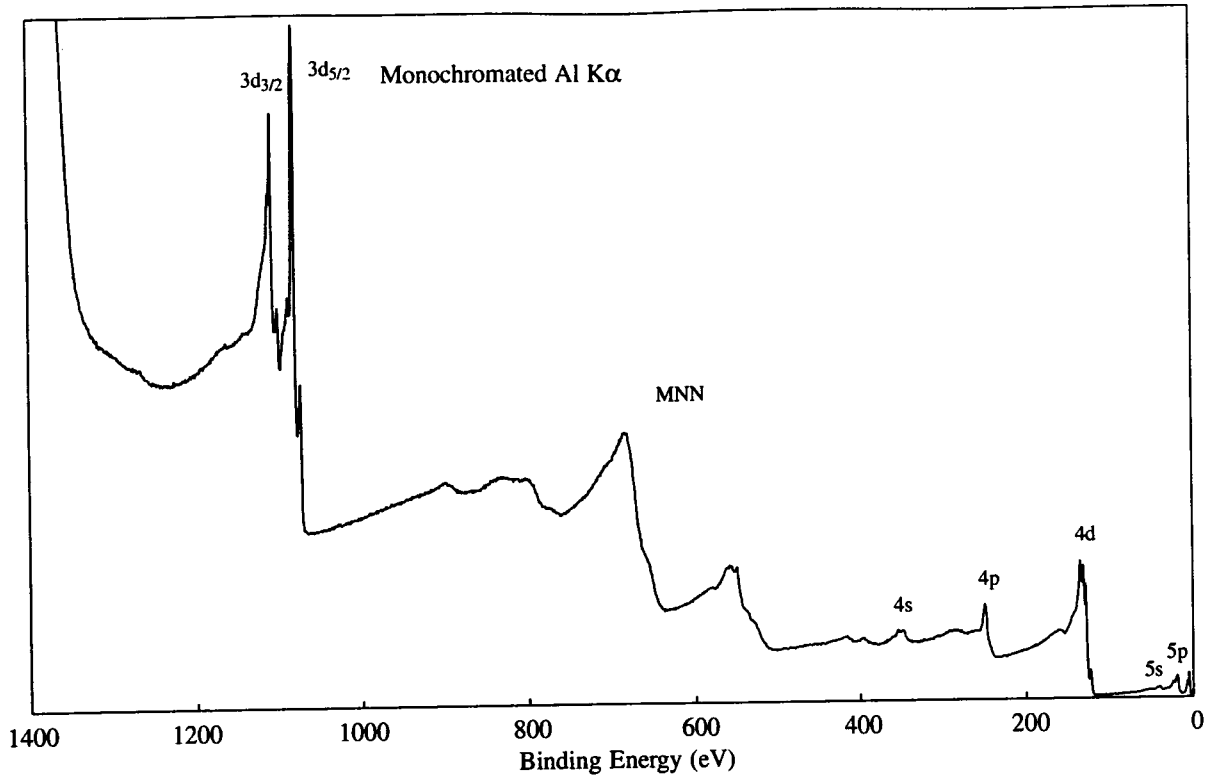

Mg Kα
3d5/2
3d3/2
MNN
4d
4s
4p
5s
5p
1200
1000
800
600
400
200
0
Binding Energy (eV)

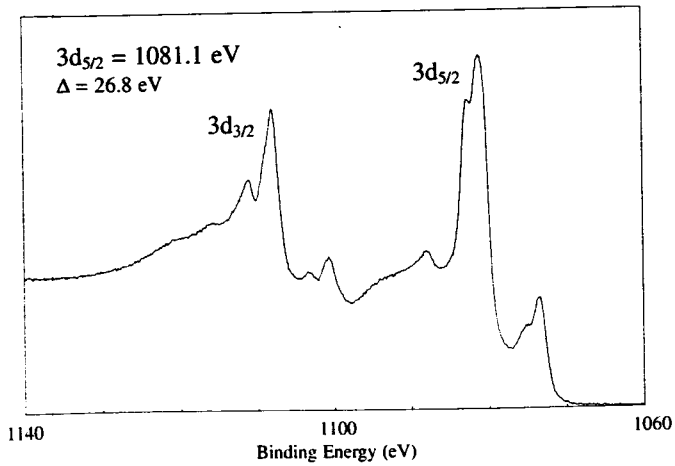

3d5/2 Binding Energy (eV)
Compound Type
980
981
982
Nd
Nd2O3
4d Binding Energy (eV)
Compound Type
119
120
121
Nd2O3


3d5/2 = 980.8 eV
Δ = 22.6 eV
3d5/2
3d3/2
1040
1000
960
Binding Energy (eV)

Samarium Sm

Atomic Number 62





Line Positions (eV)

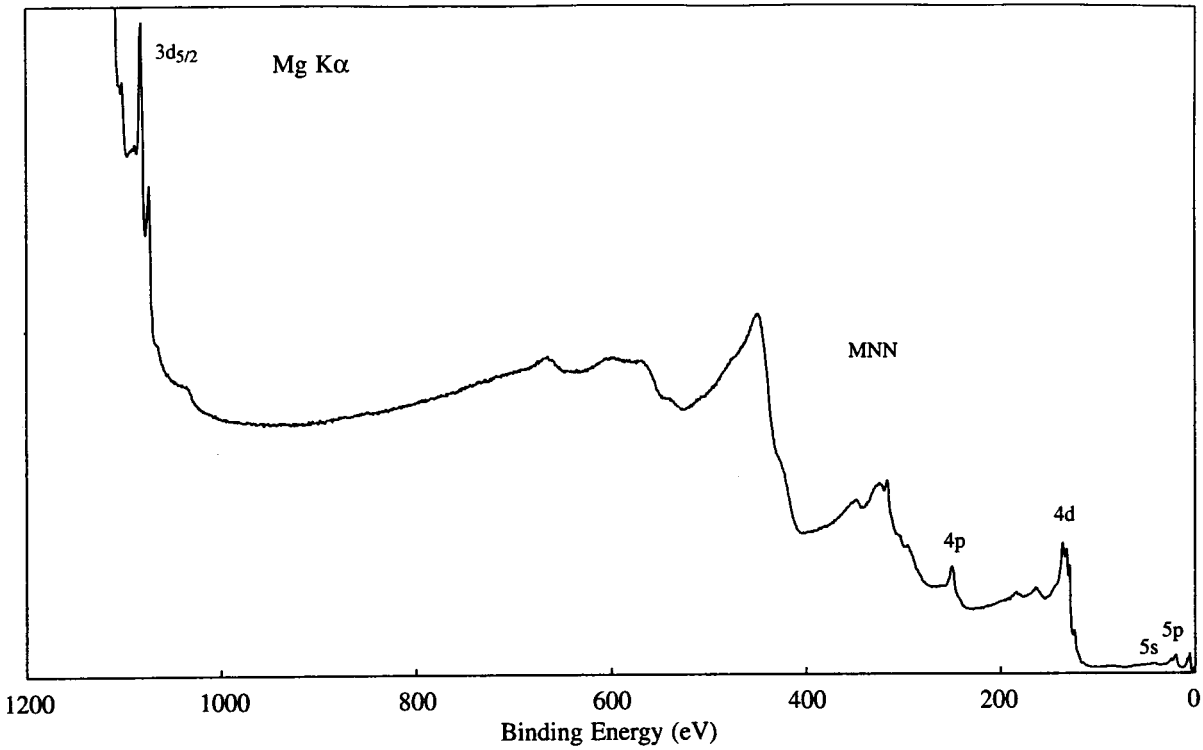
Photoelectron Lines

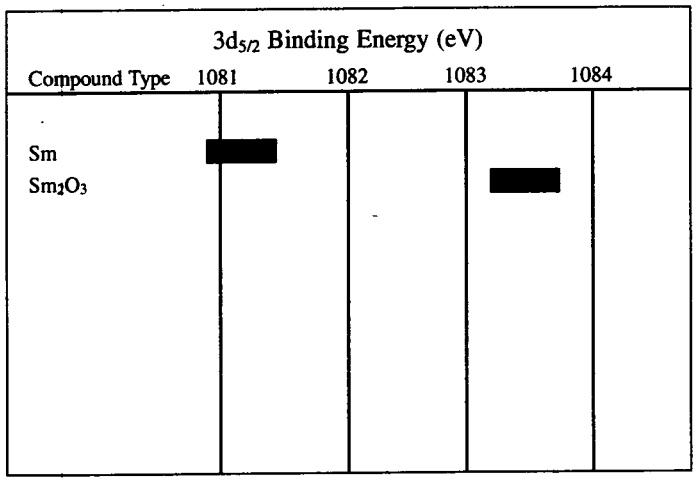
3d3/2	3d5/2	4s	4p1/2	4p3/2	4d	5s	5p
1108	1081	349	283	250	129	41	19

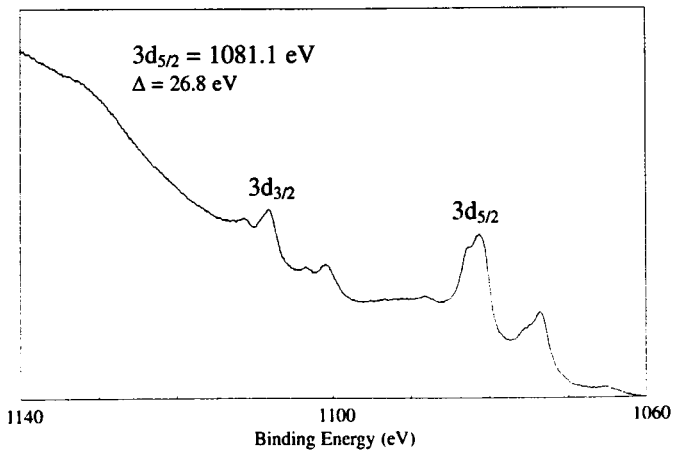
Auger Lines

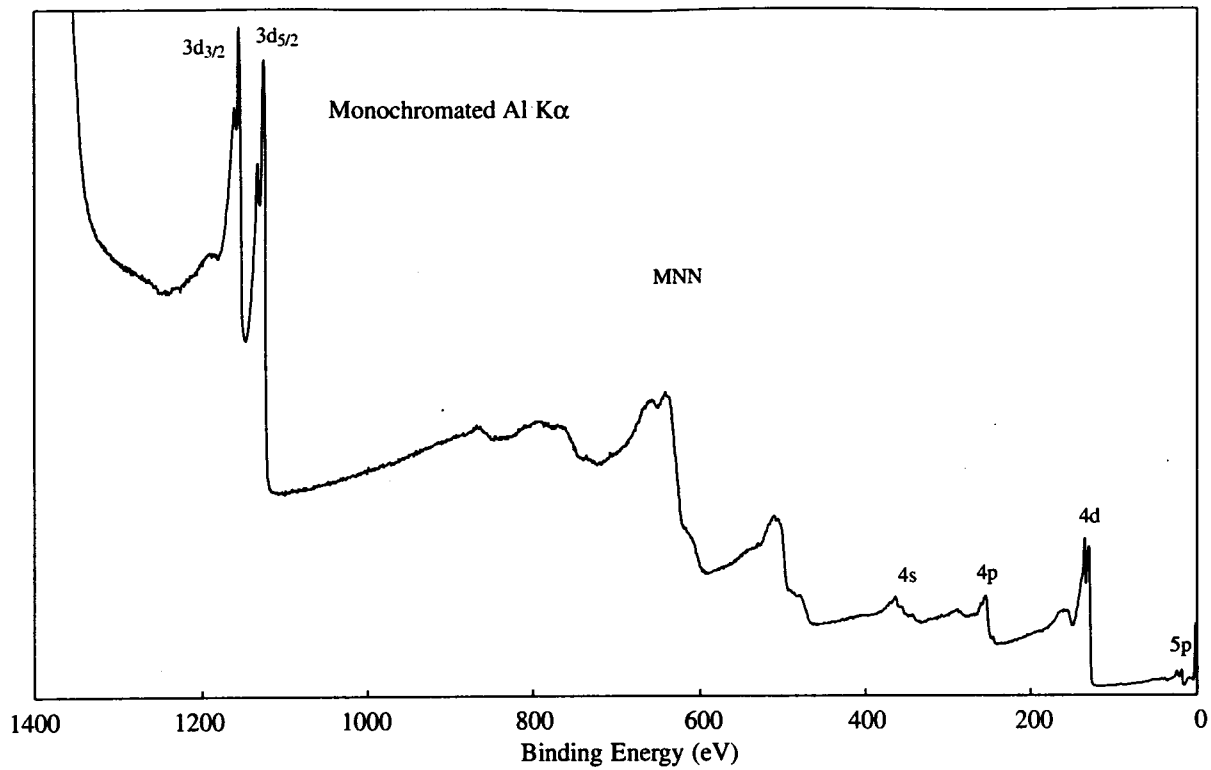
M45N45N45
682 (Al)
449 (Mg)

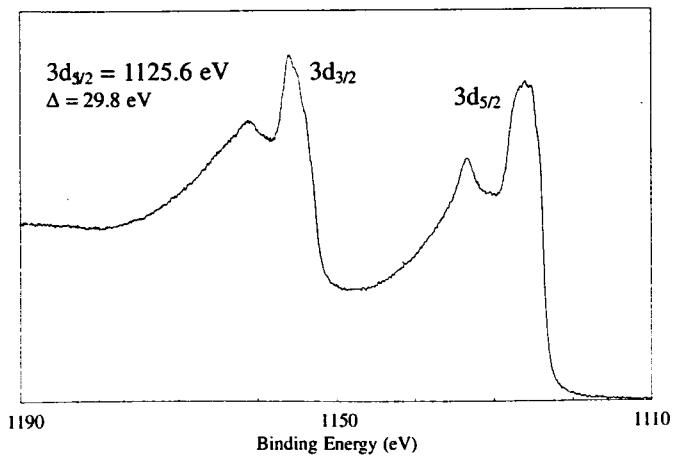
Samarium Sm
Atomic Number 62











Line Positions (eV)

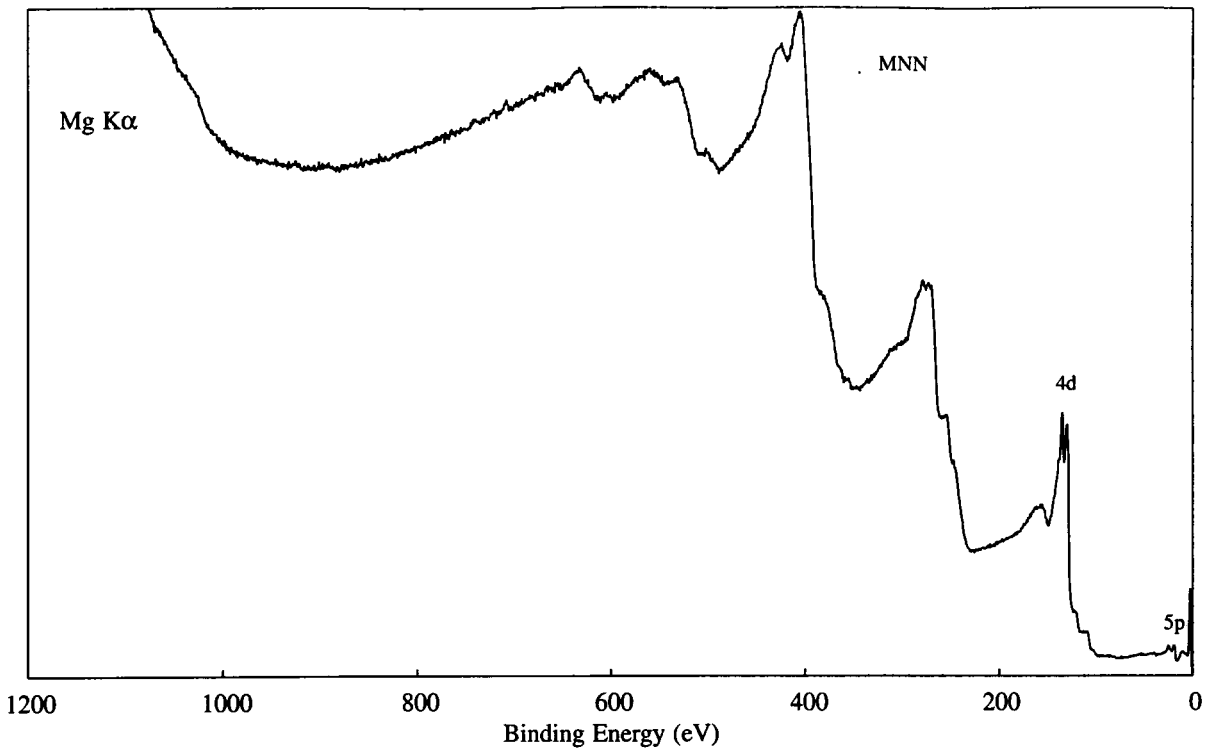
Photoelectron Lines

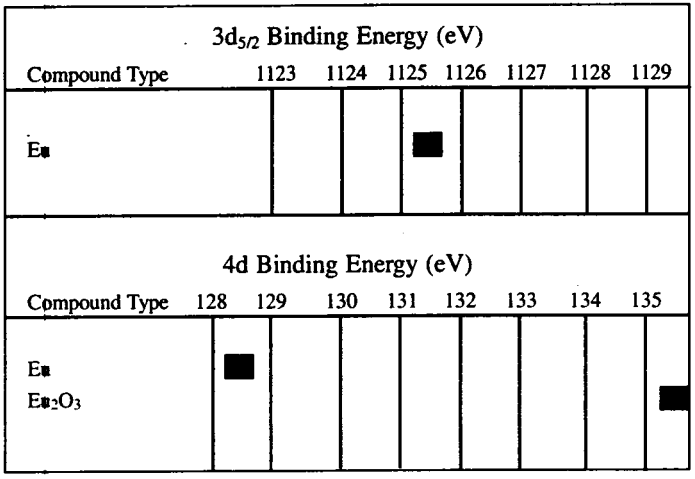
$3d_{3/2}$	$3d_{5/2}$	4s	$4p_{1/2}$	$4p_{3/2}$	4d	5s	5p
1155	1126	363	289	255	128	39	19

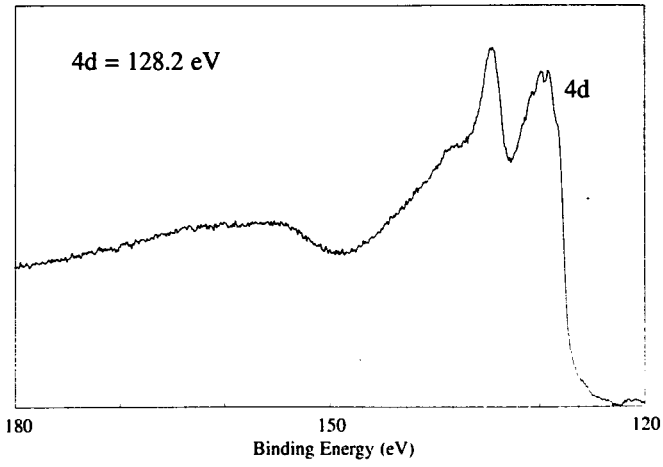
Auger Lines

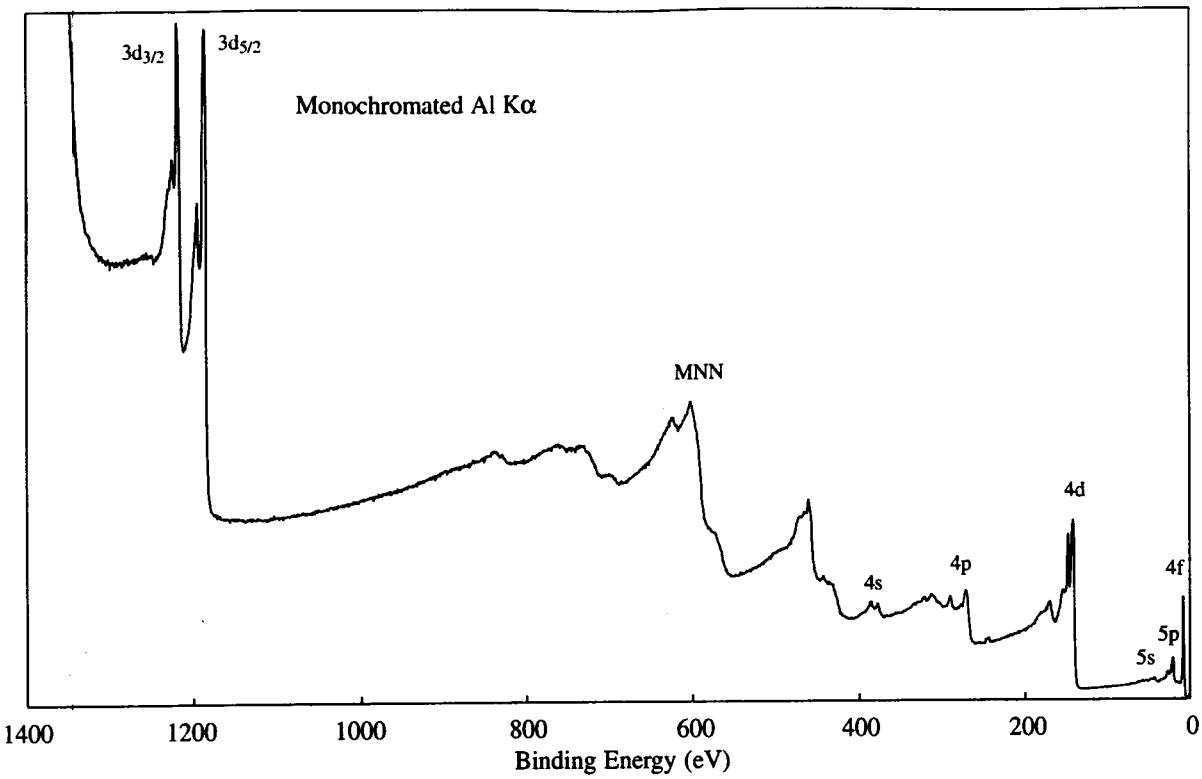
$M_{45}N_{45}N_{45}$
637 (Al)
404 (Mg)

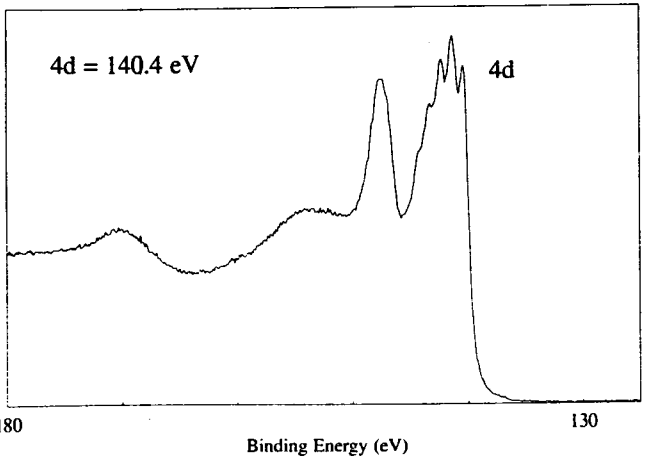
Europium Eu
Atomic Number 63











Line Positions (eV)

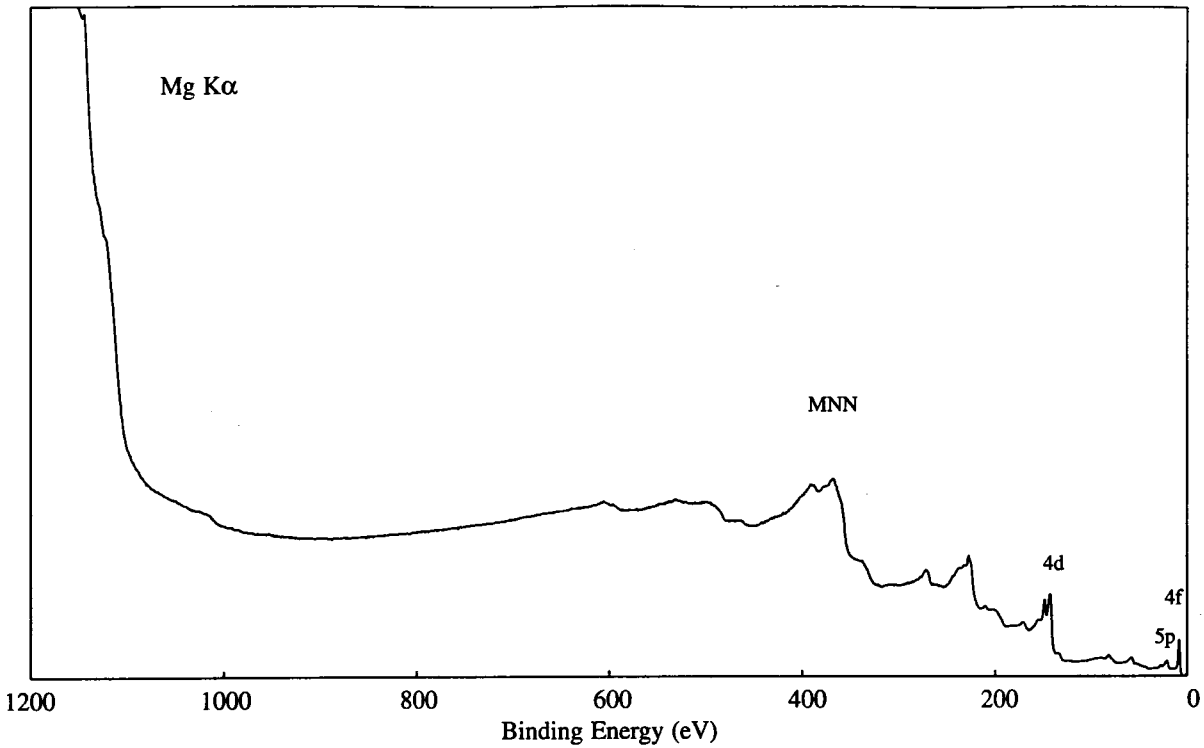
Photoelectron Lines

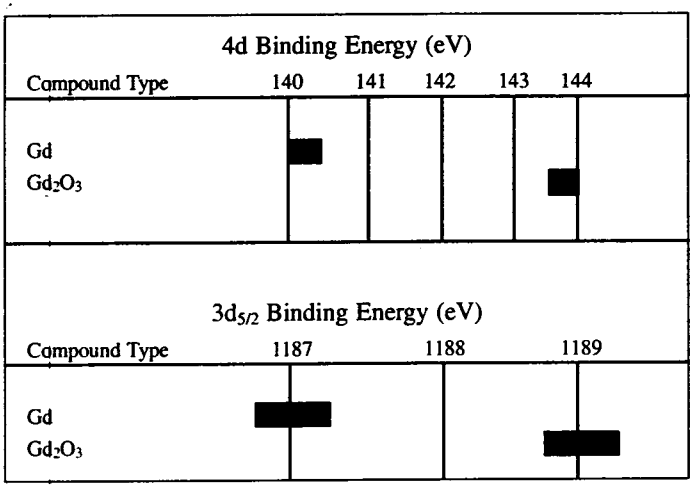
$3d_{3/2}$	$3d_{5/2}$					
1218	1186					
4s	$4p_{1/2}$	$4p_{3/2}$	4d	5s	5p	4f
378	291	272	140	43	21	8

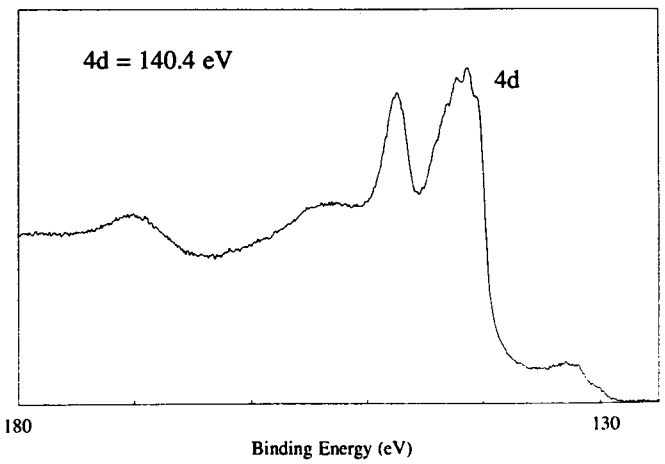
Auger Lines

$M_{45}N_{45}N_{45}$	
602	(Al)
369	(Mg)

Gadolinium Gd
Atomic Number 64

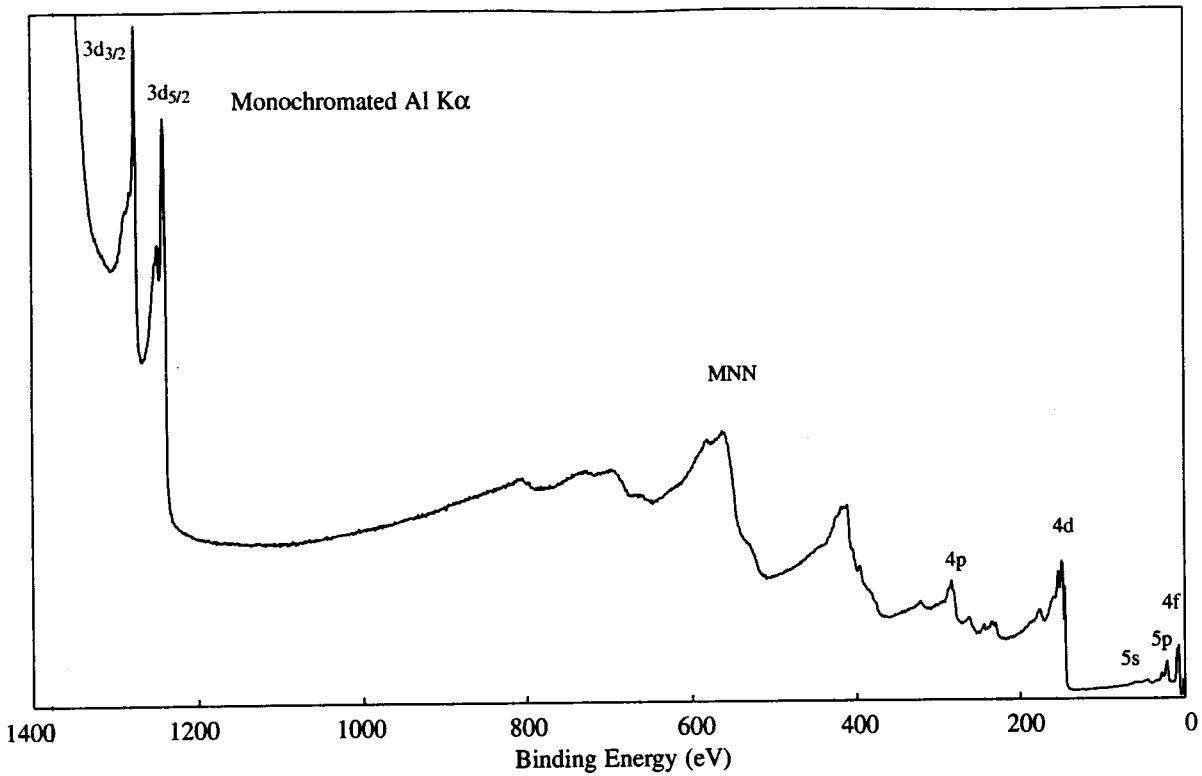


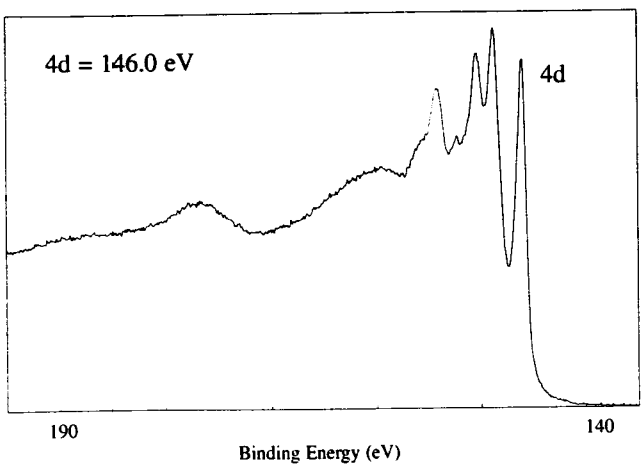




Terbium Tb

Atomic Number 65





Line Positions (eV)

Photoelectron Lines

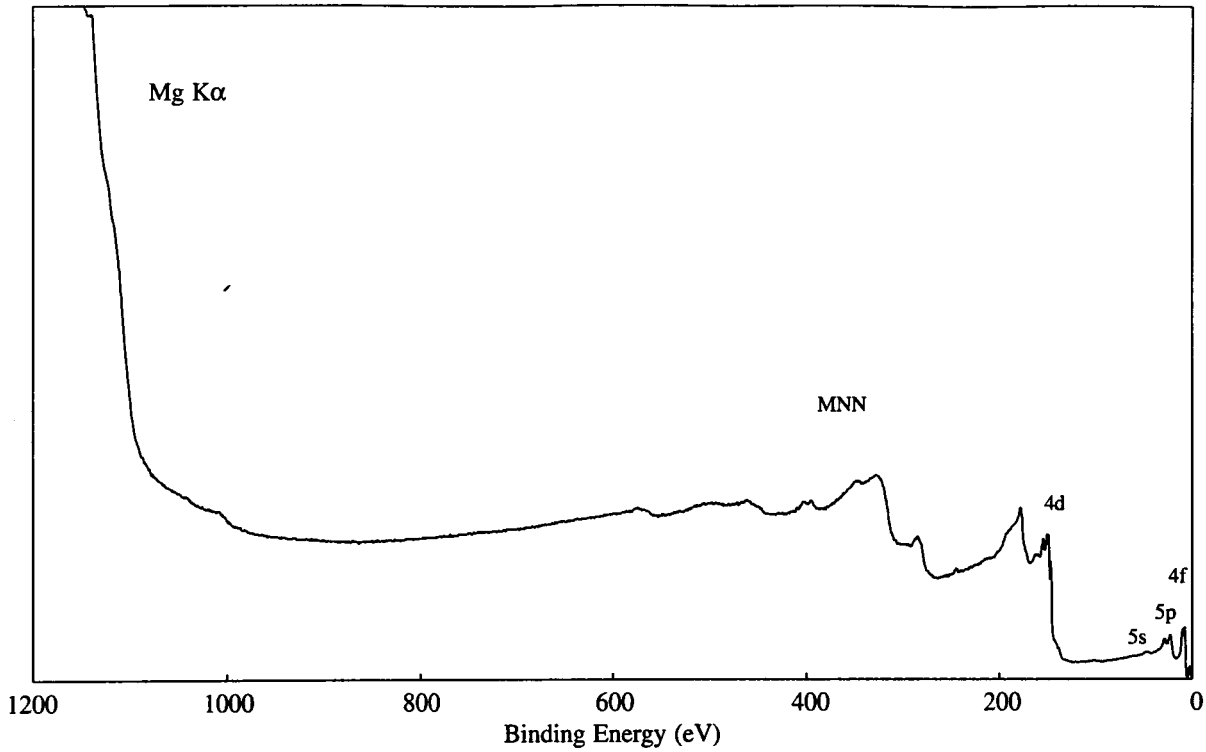
$3d_{3/2}$	$3d_{5/2}$					
1276	1241					
4s	$4p_{1/2}$	$4p_{3/2}$	4d	5s	5p	4f
396	322	285	146	45	22	8

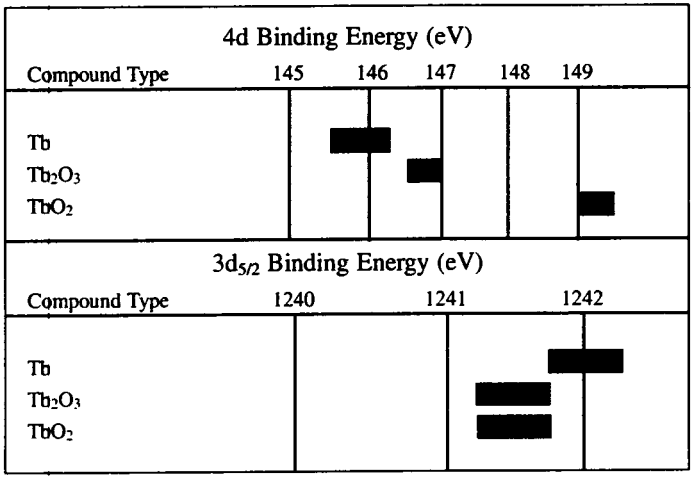
Auger Lines

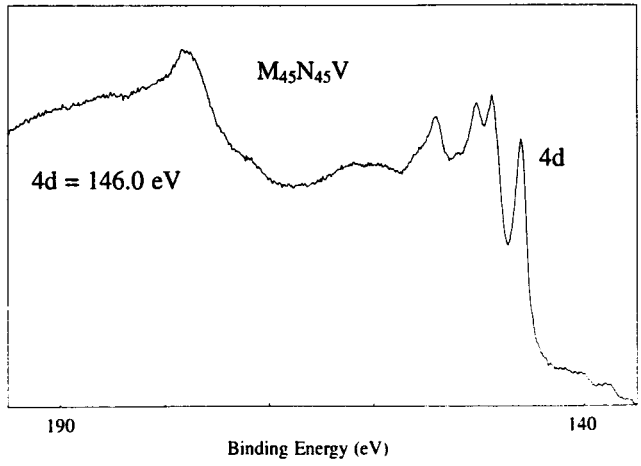
$M_{45}N_{45}N_{45}$	$M_{45}N_{45}V$	M_5VV	M_4VV	
559	411	260	230	(Al)
326	178			(Mg)

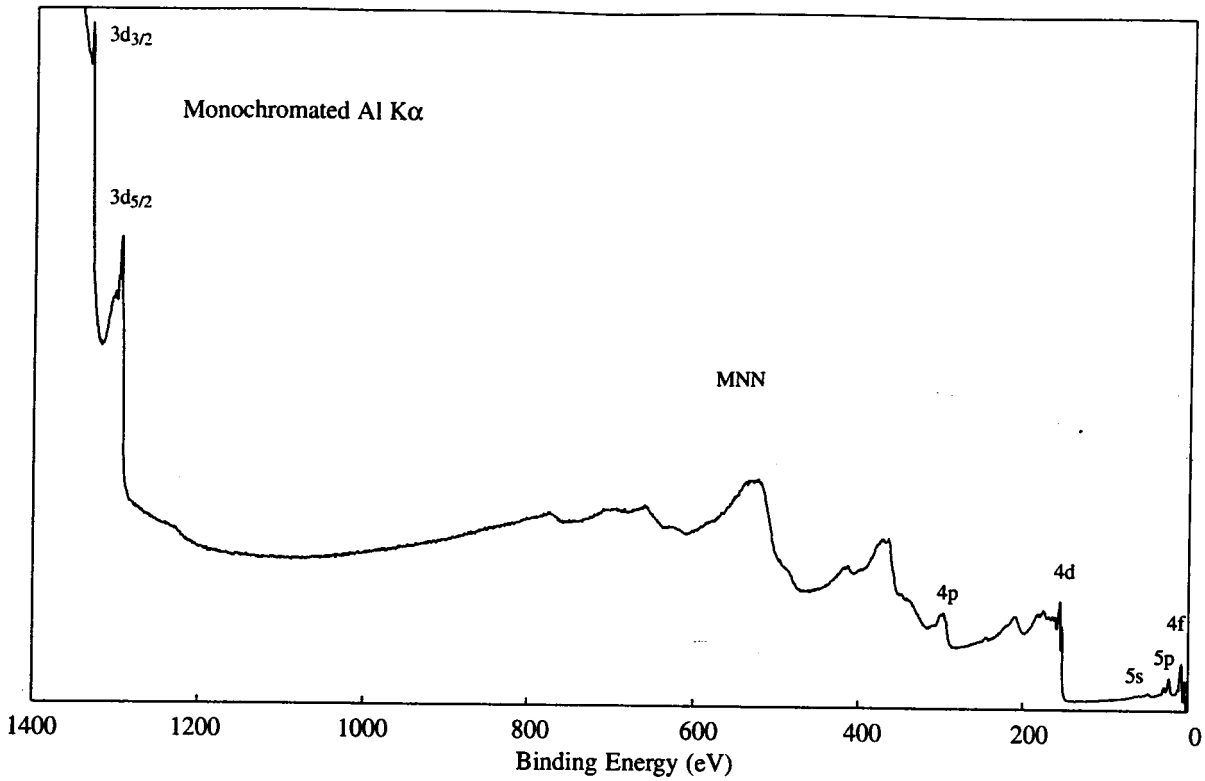
Terbium Tb

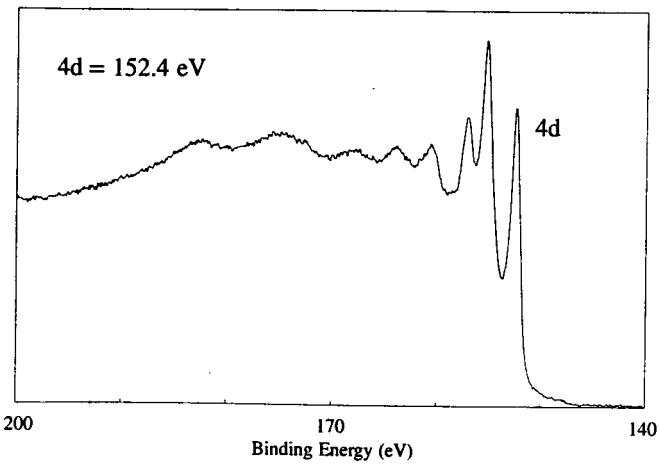
Atomic Number 65











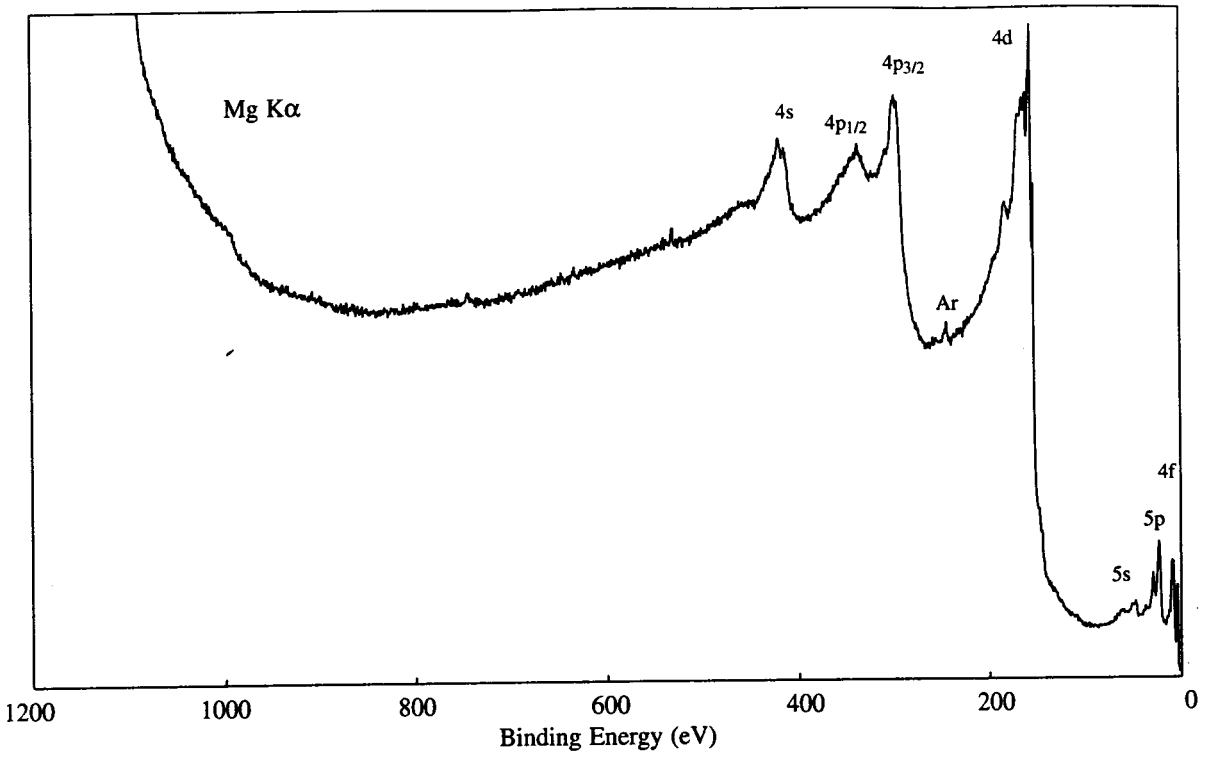
Line Positions (eV)

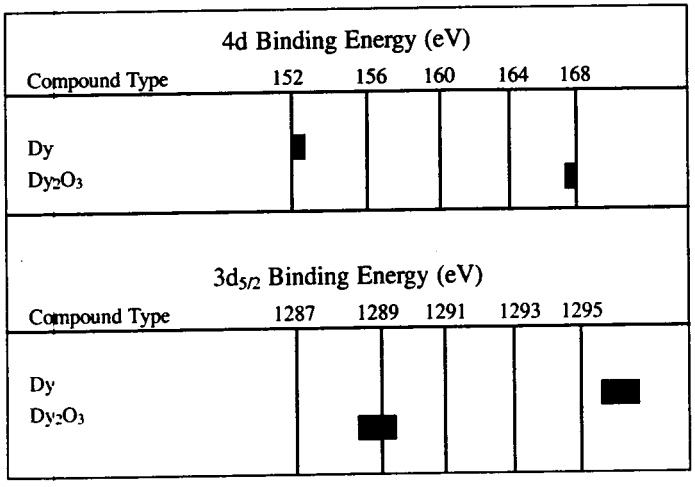
Photoelectron Lines

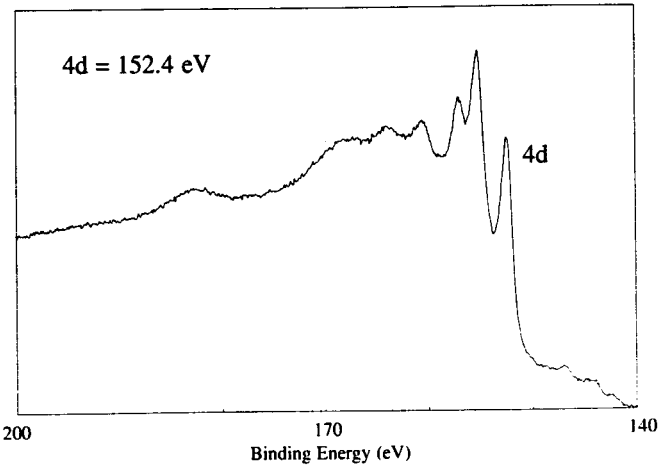
$3d_{3/2}$	$3d_{5/2}$					
1333	1296					
4s	$4p_{1/2}$	$4p_{3/2}$	4d	5s	5p	4f
417	337	297	152	48	23	8

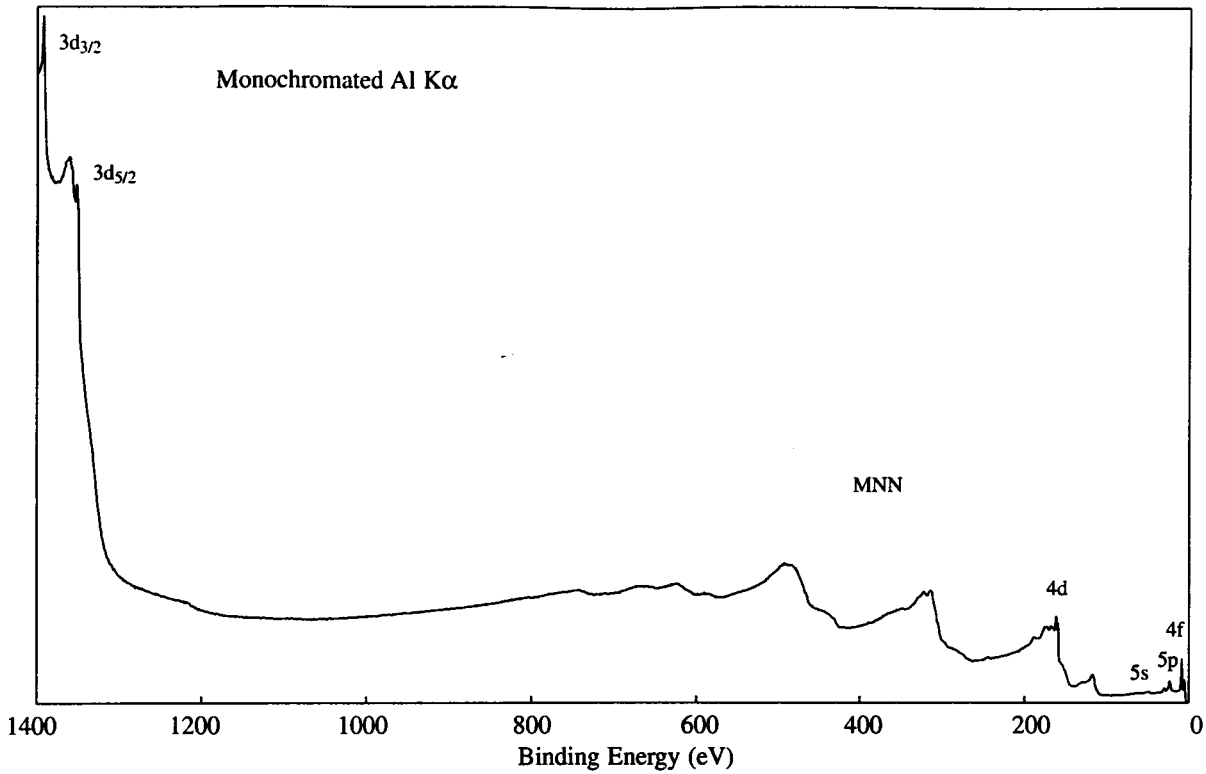
Auger Lines

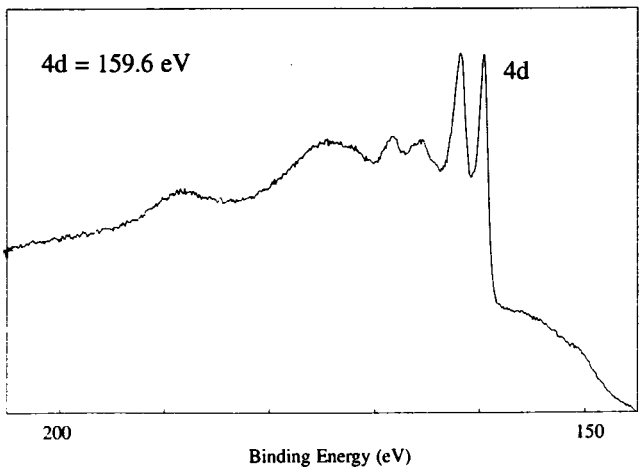
$M_{45}N_{45}N_{45}$	$M_{45}N_{45}V$	
526	368	(Al)


Mg Kα
4s
4p1/2
4p3/2
4d
Ar
4f
5p
5s
1200
1000
800
600
400
200
0
Binding Energy (eV)


4d Binding Energy (eV)
Compound Type
152
156
160
164
168
Dy
Dy2O3
3d5/2 Binding Energy (eV)
Compound Type
1287
1289
1291
1293
1295
Dy
Dy2O3


4d = 152.4 eV
4d
200
170
140
Binding Energy (eV)





Line Positions (eV)

Photoelectron Lines

$3d_{3/2}$	$3d_{5/2}$	4s	$4p_{1/2}$	$4p_{3/2}$	4d
1393	1352	435	353	309	160

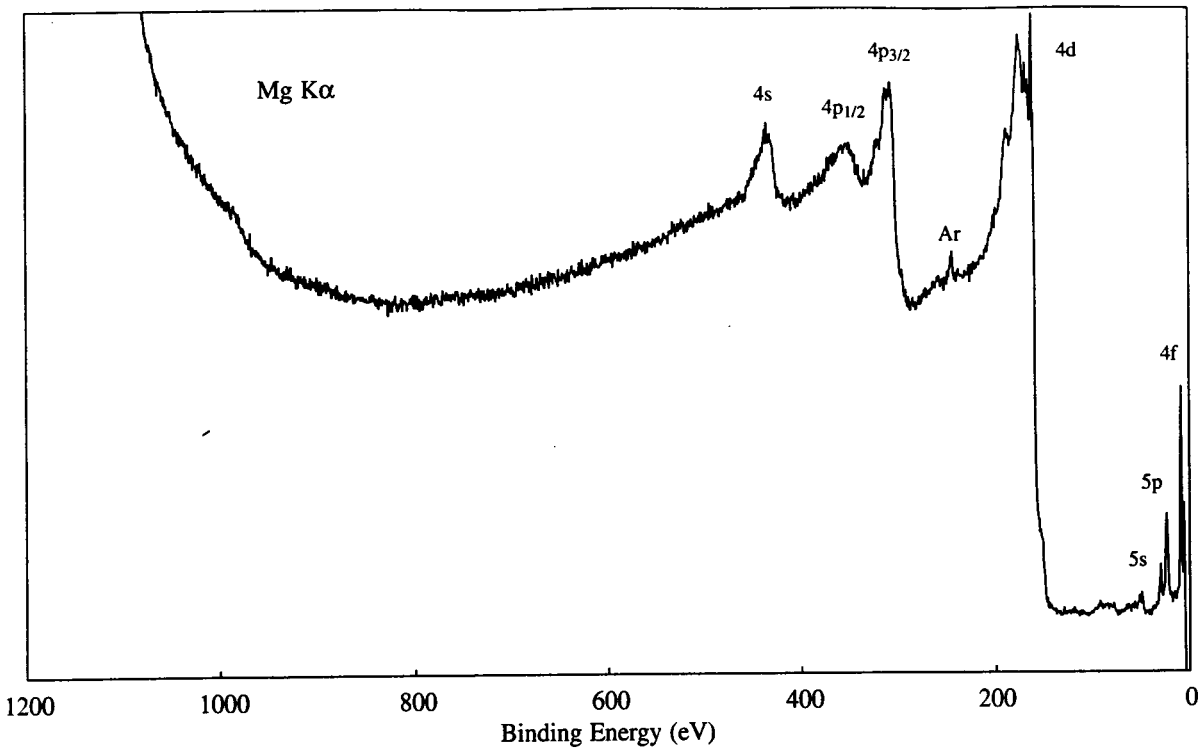
5s	$5p_{1/2}$	$5p_{3/2}$	4f
49	30	24	9

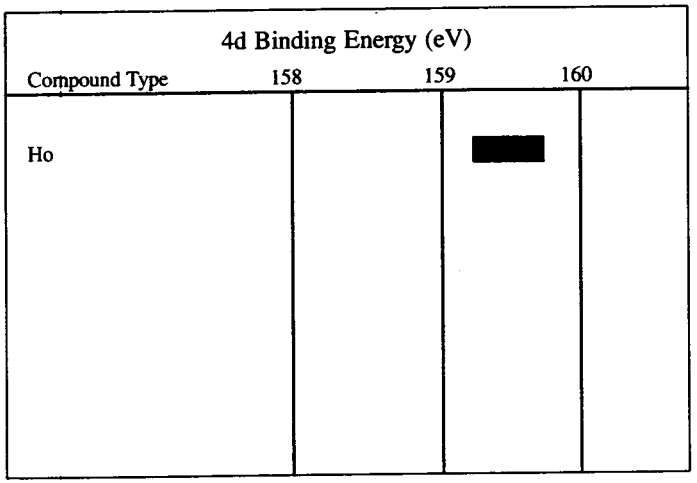
Auger Lines

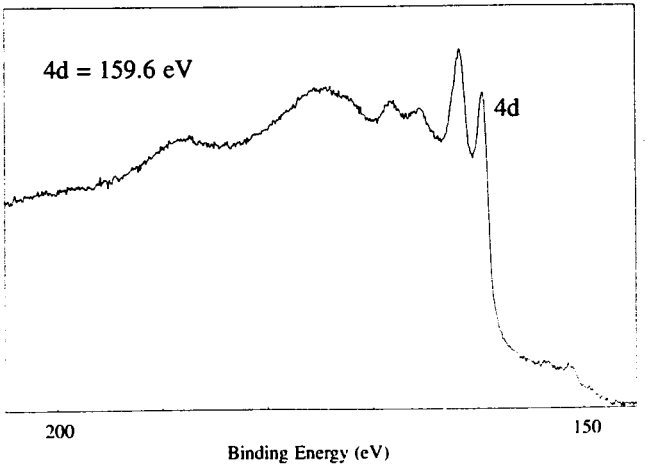
$M_{45}N_{45}N_{45}$	$M_{45}N_{45}V$	M_4VV	
488	314	117	(Al)

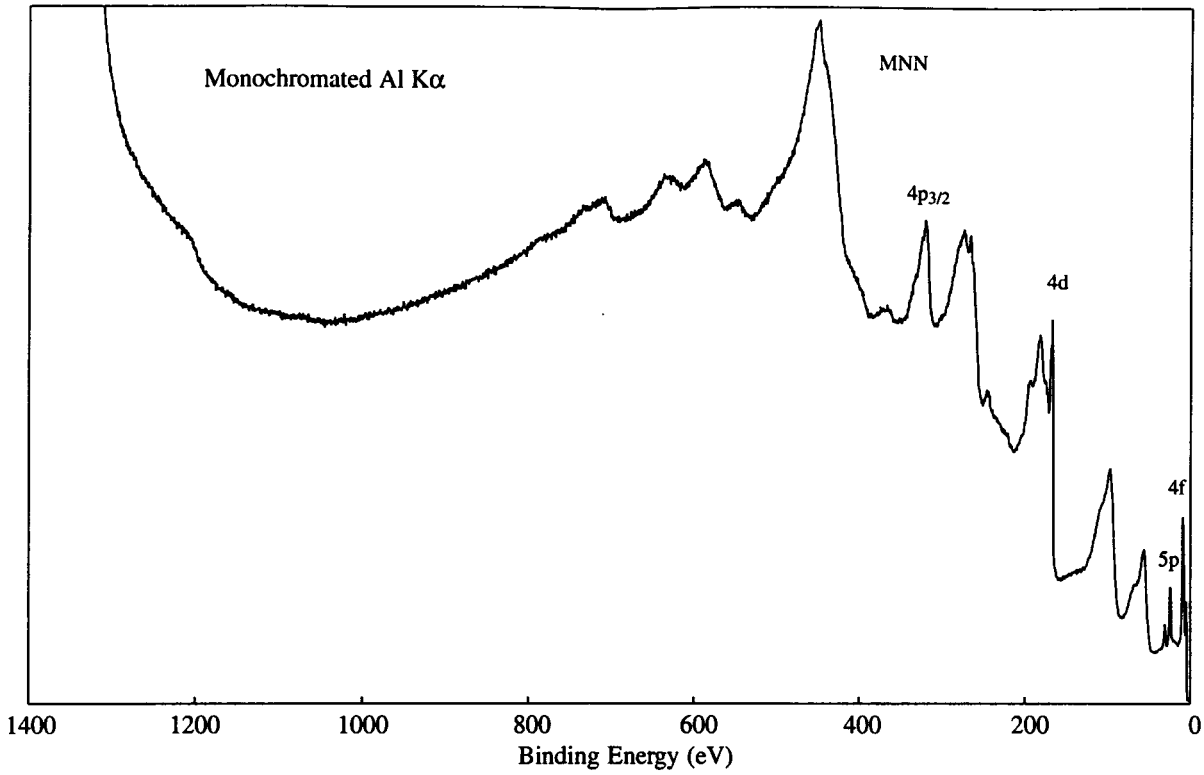
Holmium Ho

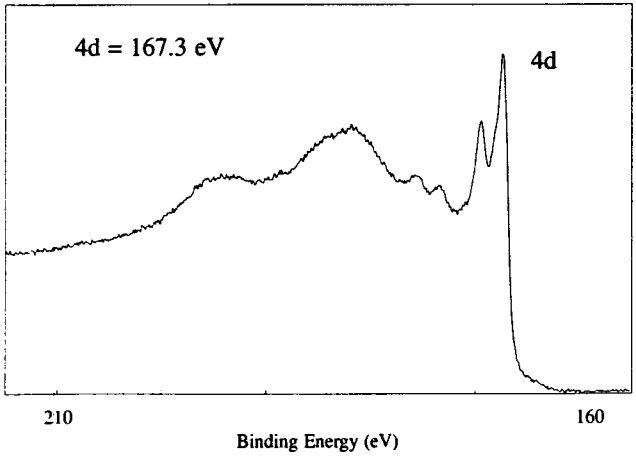
Atomic Number 67











Line Positions (eV)

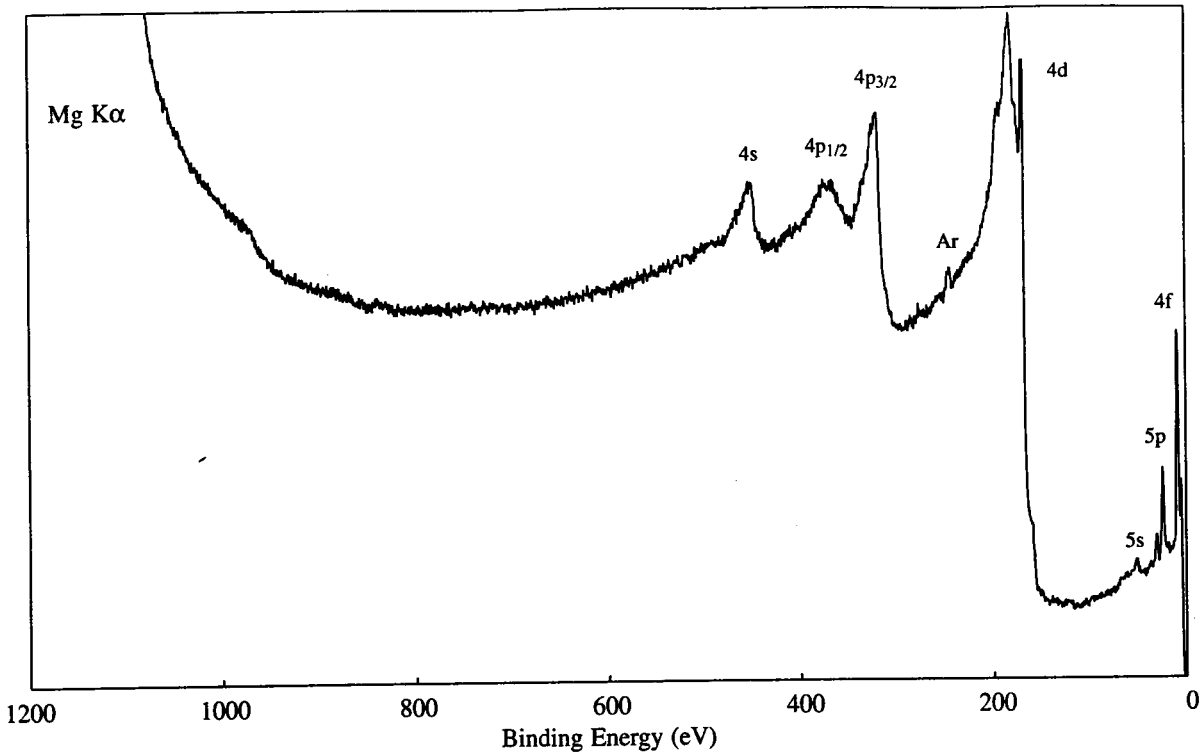
Photoelectron Lines

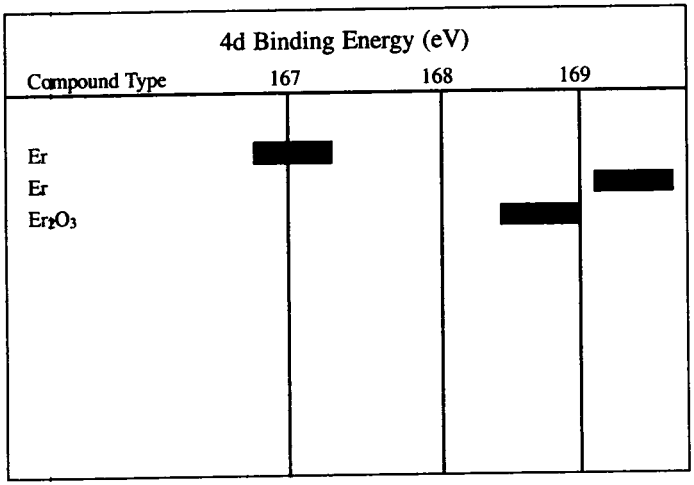
4s	$4p_{1/2}$	$4p_{3/2}$	4d	5s	$5p_{1/2}$	$5p_{3/2}$	4f
451	368	321	167	52	31	24	9

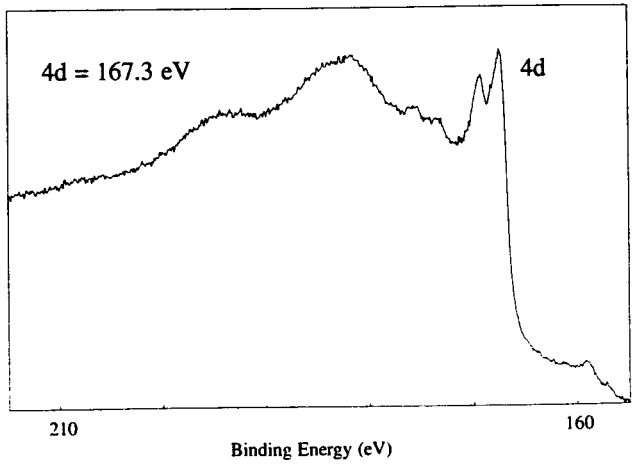
Auger Lines

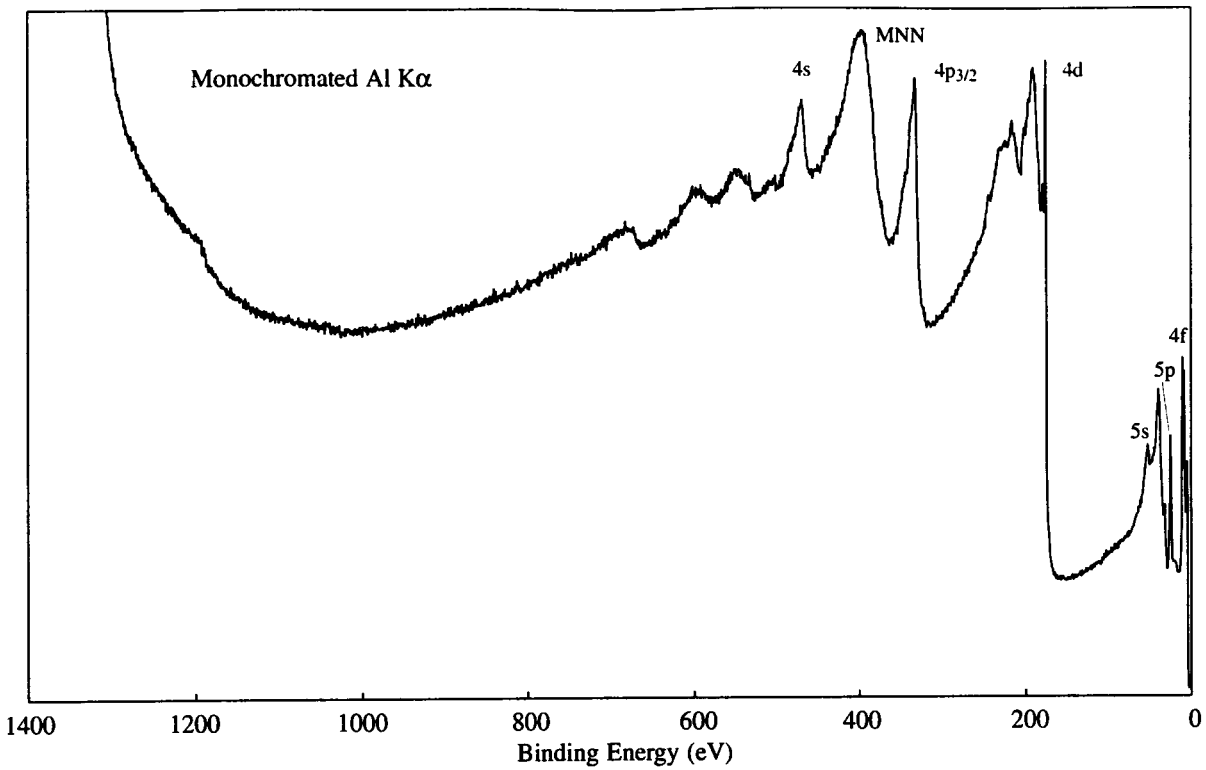
$M_{45}N_{45}N_{45}$	$M_{45}N_{45}V$	M_5VV	M_4VV	
440	273	98	56	(Al)

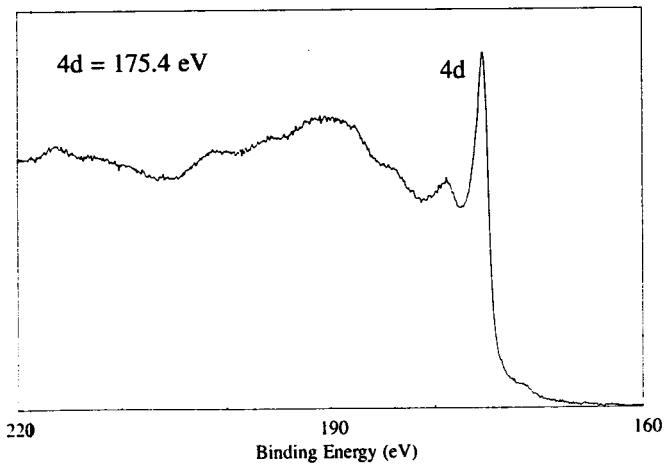
Erbium Er
Atomic Number 68











Line Positions (eV)

Photoelectron Lines

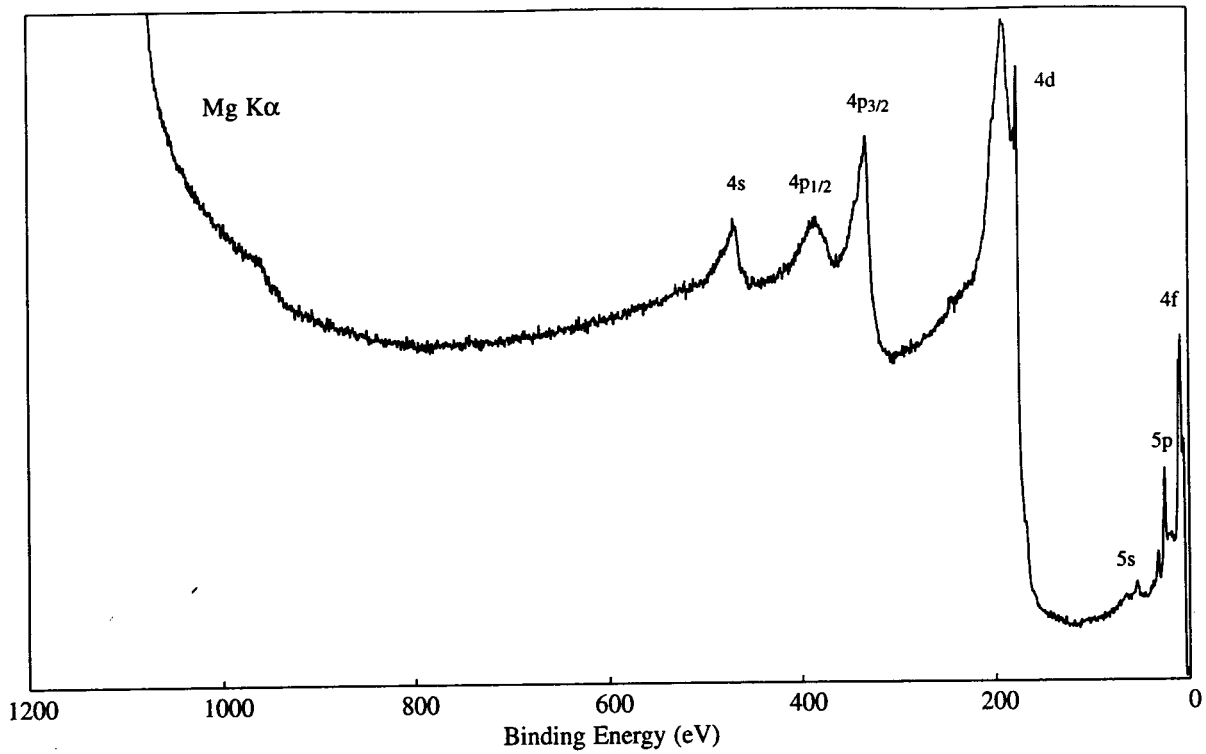
4s	4p1/2	4p3/2	4d	5s	5p1/2	5p3/2	4f
470	384	333	175	53	32	25	8

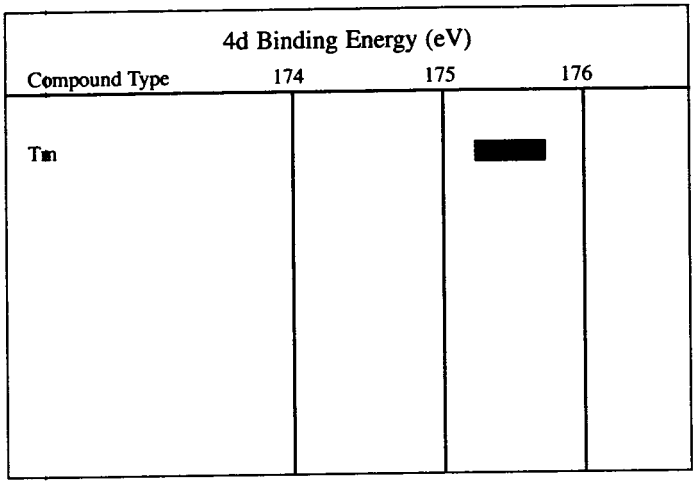
Auger Lines

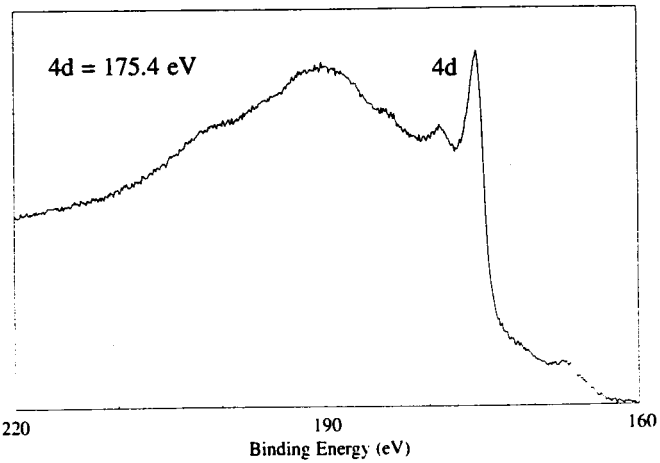
$M_{45}N_{45}N_{45}$	
398	(Al)

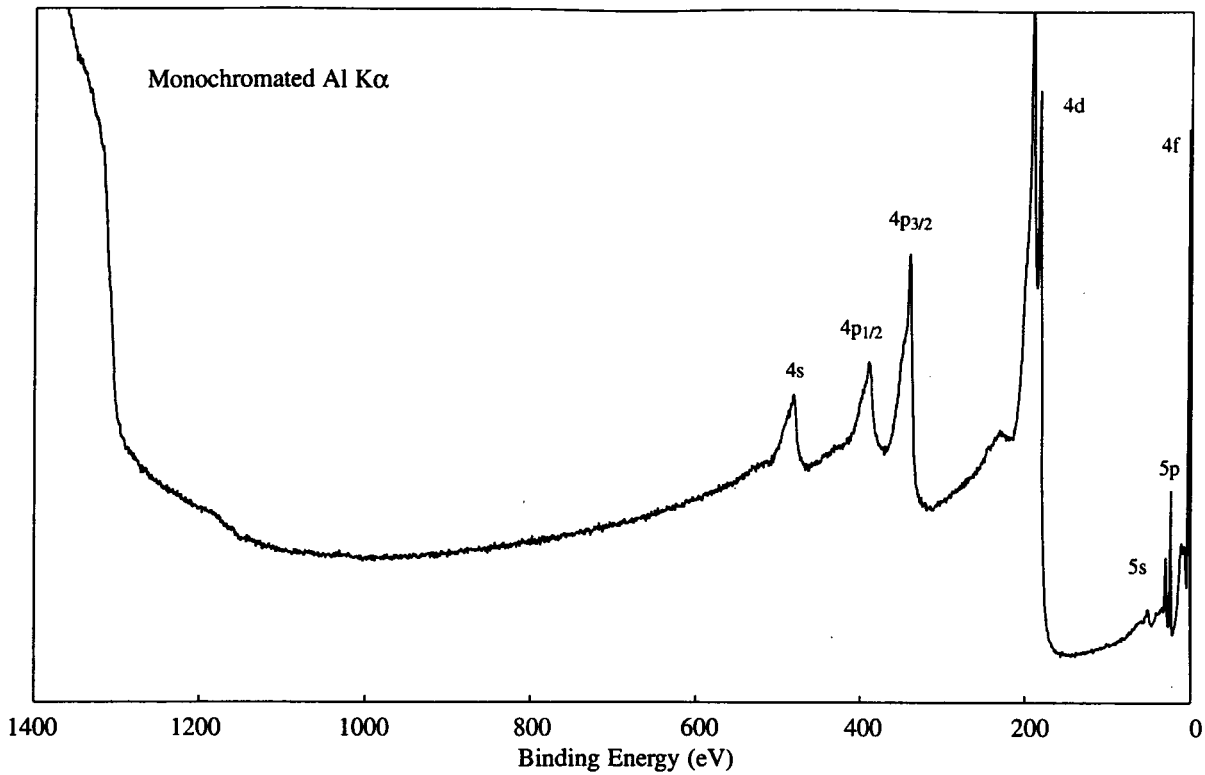
Thulium Tm

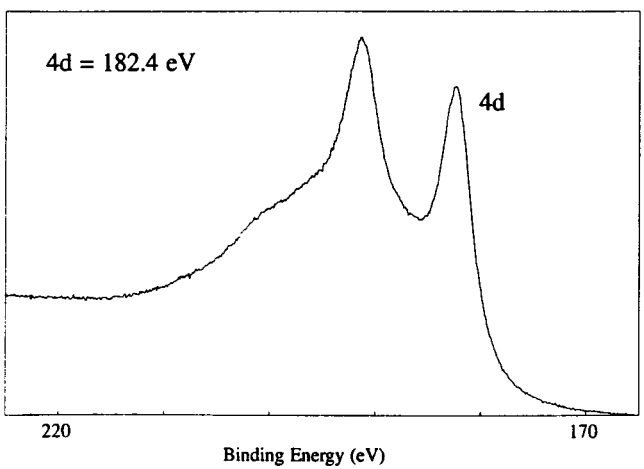
Atomic Number 69









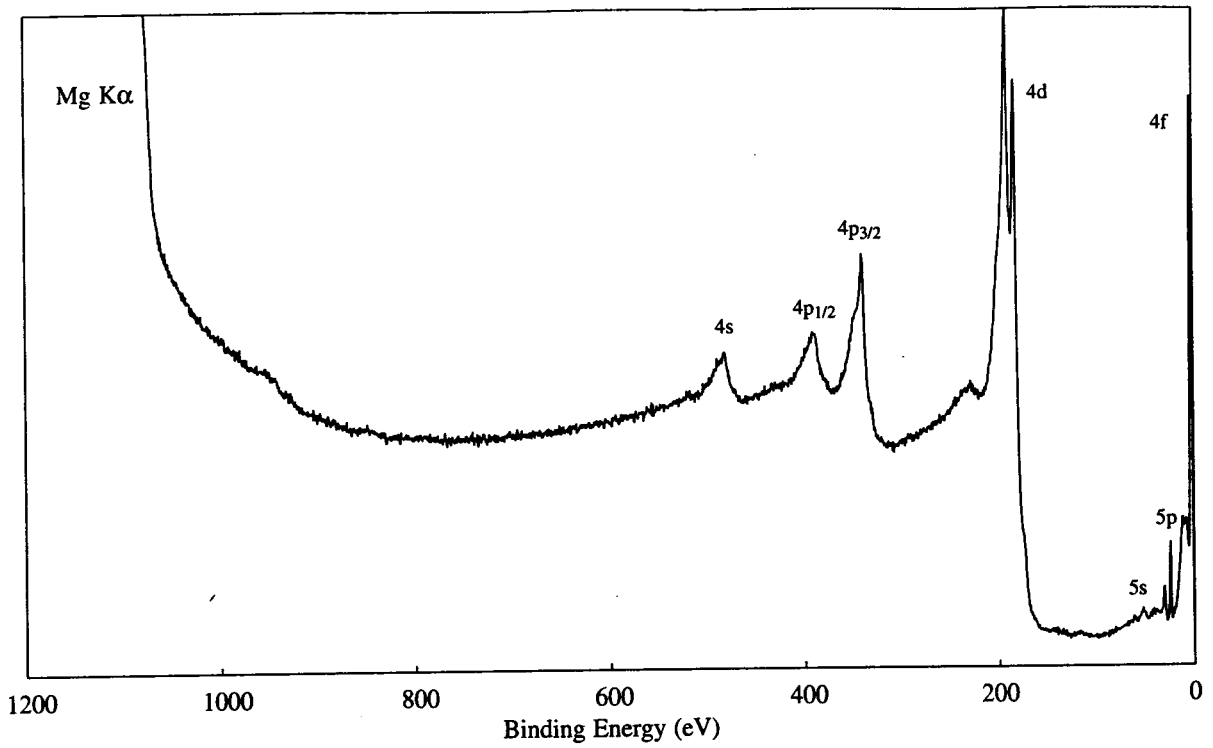


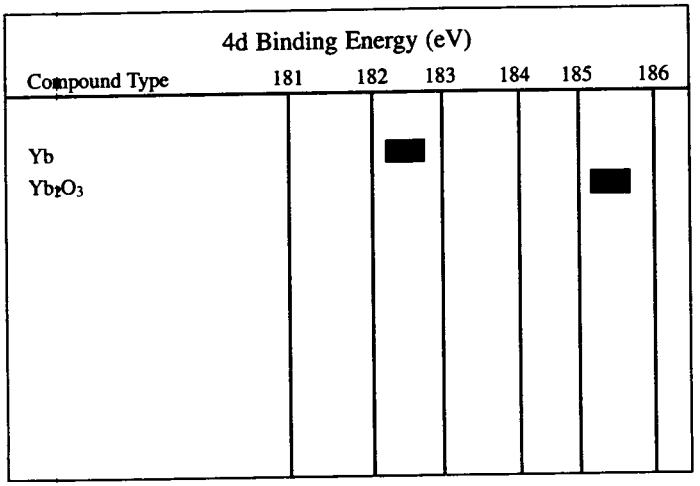
Line Positions (eV)

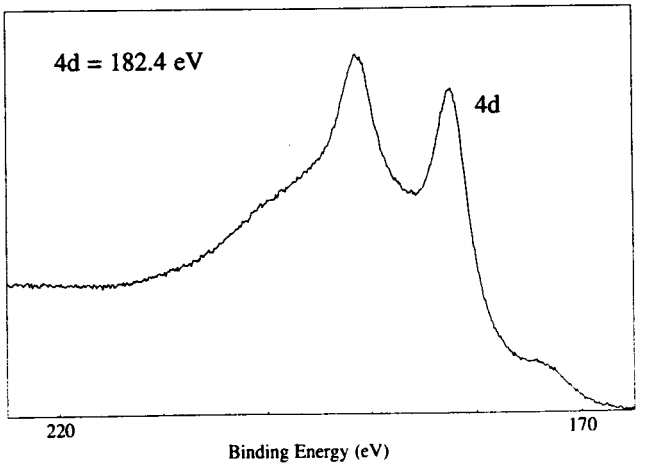
Photoelectron Lines

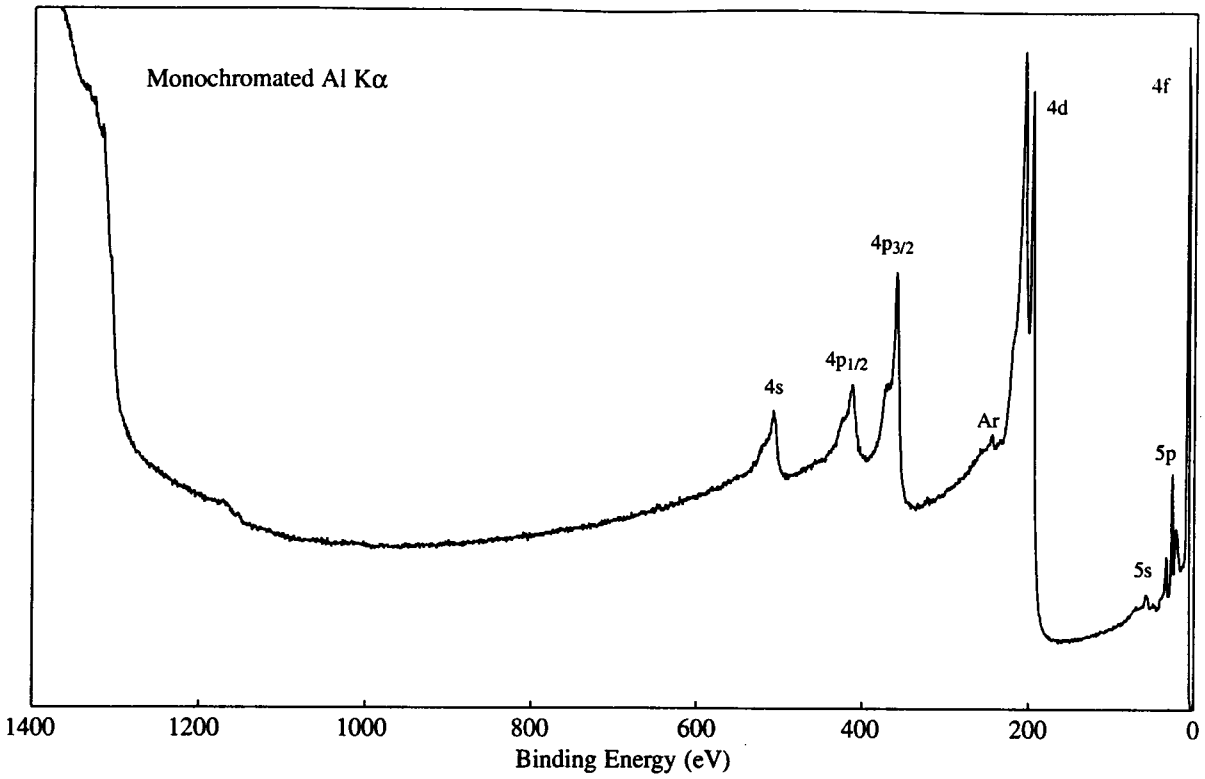
4s	4p1/2	4p3/2	4d	5s	5p1/2	5p3/2	4f
482	389	341	182	51	30	24	3

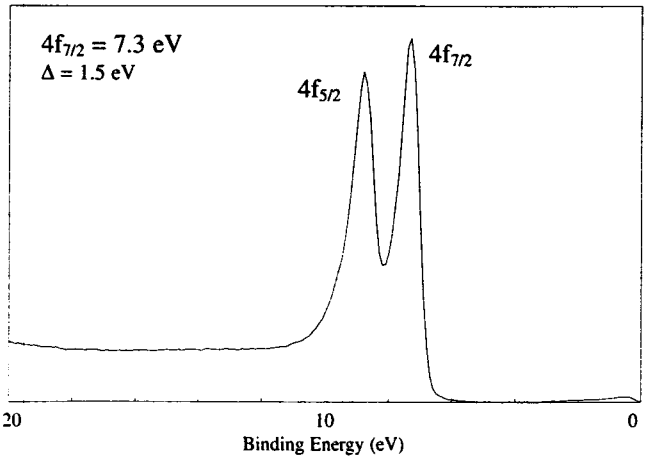
Ytterbium Yb
Atomic Number 70











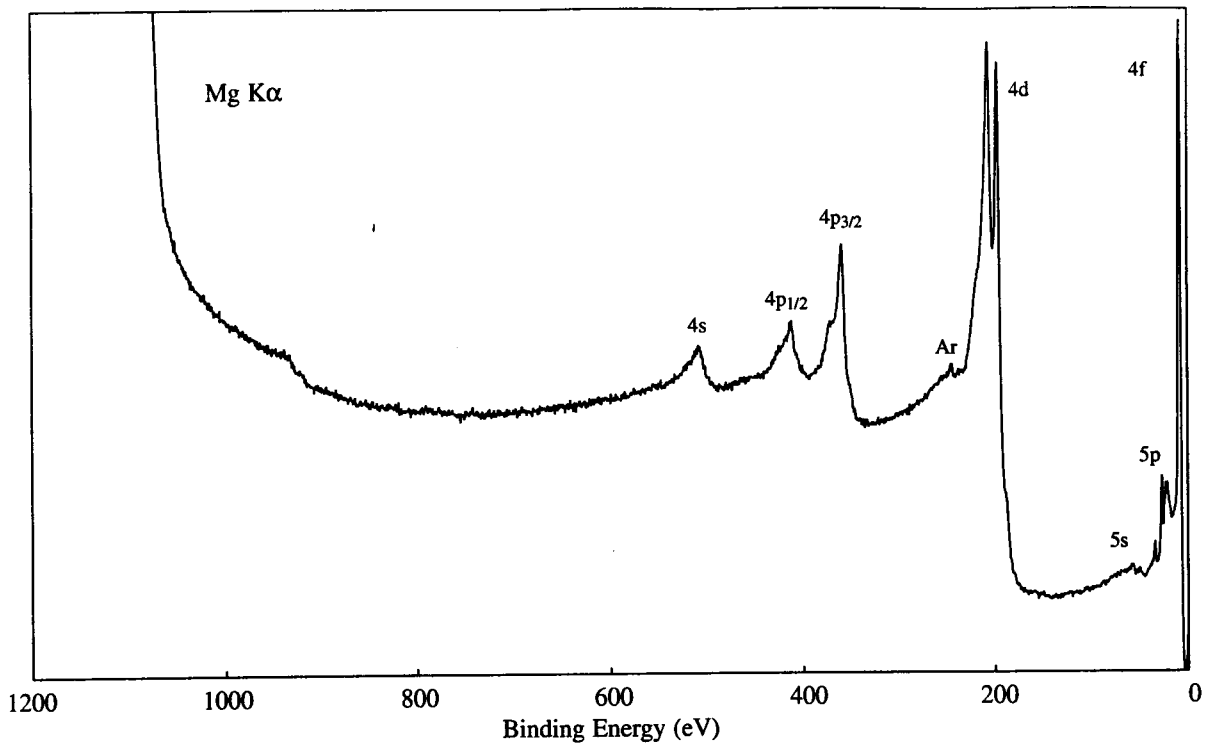
Line Positions (eV)

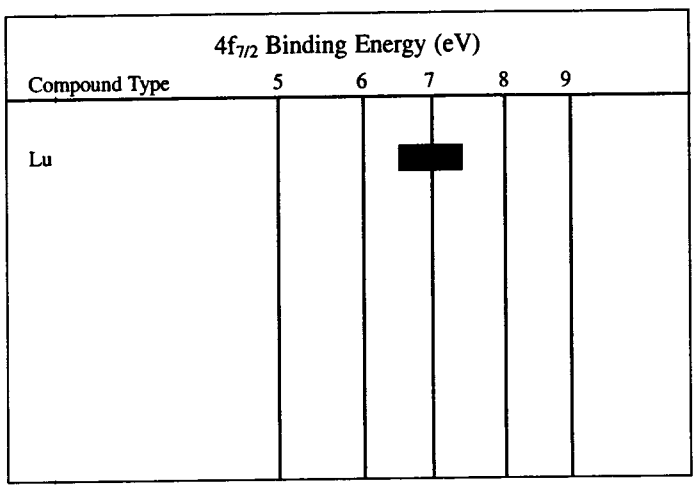
Photoelectron Lines

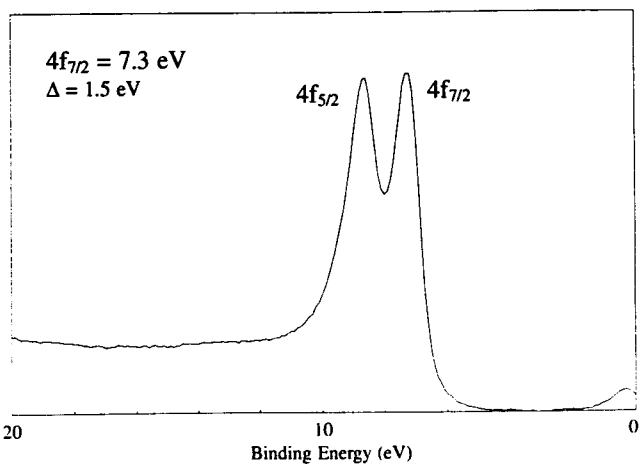
4s	4p1/2	4p3/2	4d3/2	4d5/2
509	413	360	206	196

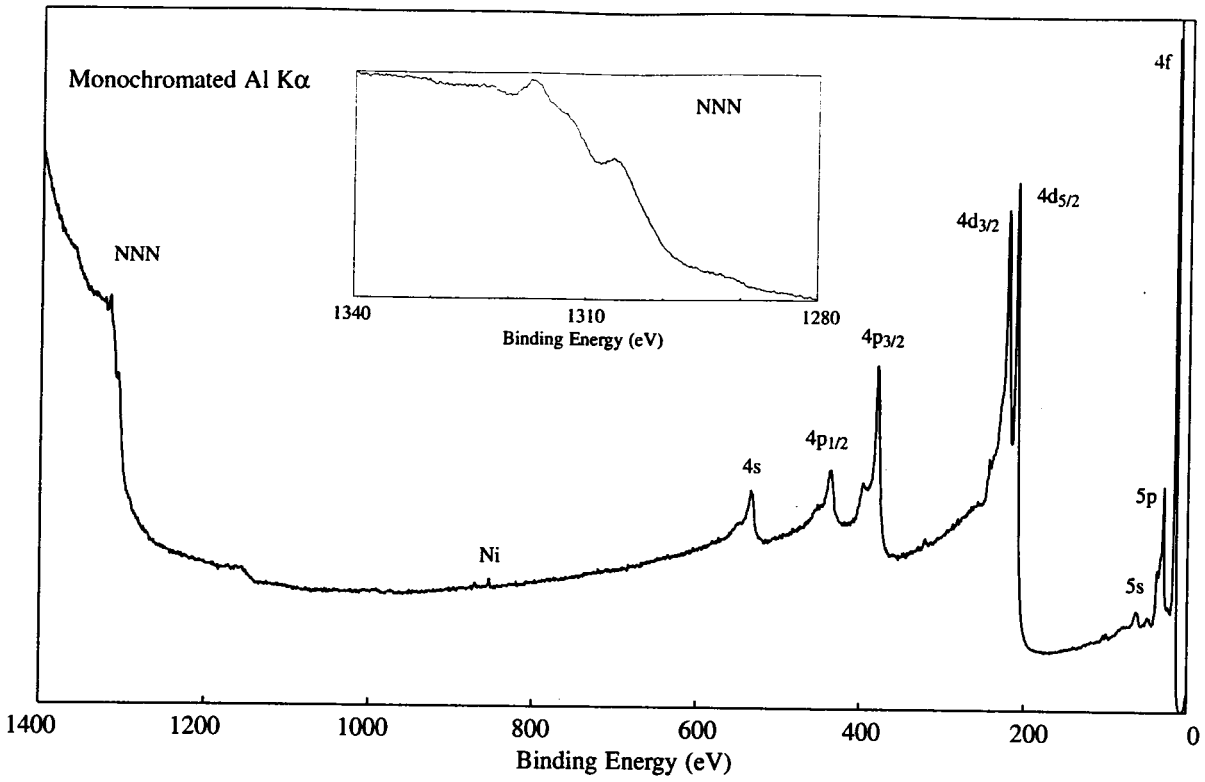
5s	5p1/2	5p3/2	4f5/2	4f7/2
57	34	27	9	7

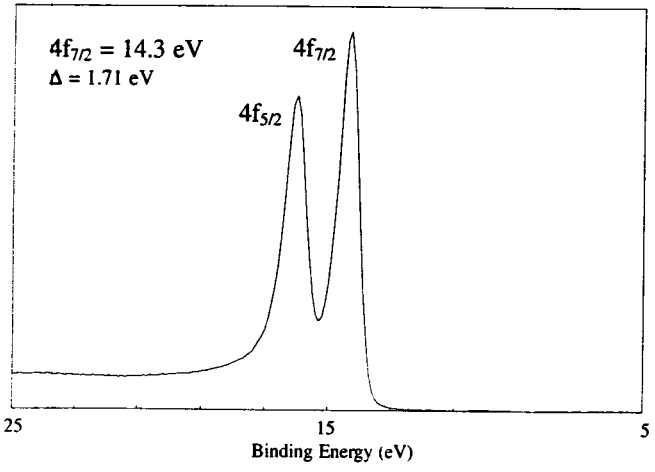
Lutetium Lu
Atomic Number 71











Line Positions (eV)

Photoelectron Lines

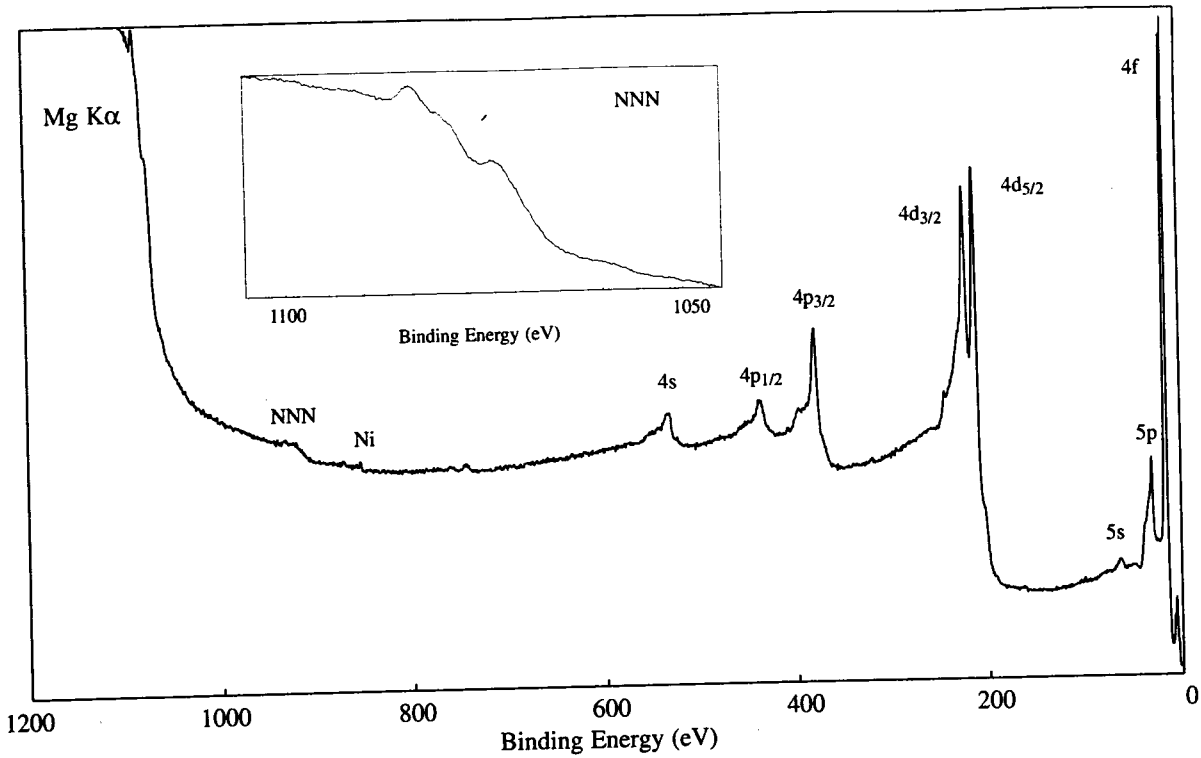
4s	4p1/2	4p3/2	4d3/2	4d5/2
534	437	380	222	211

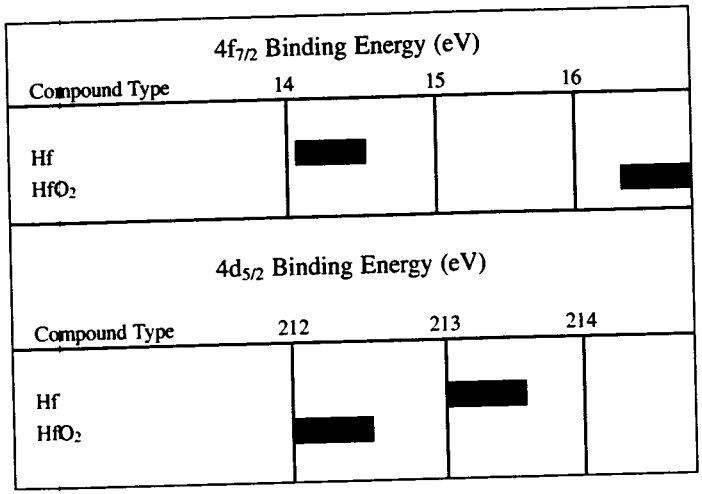
5s	5p1/2	5p3/2	4f5/2	4f7/2
63	38	30	16	14

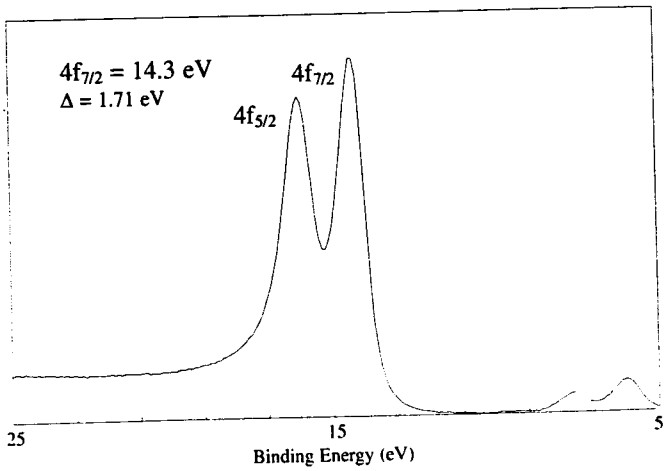
Auger Lines

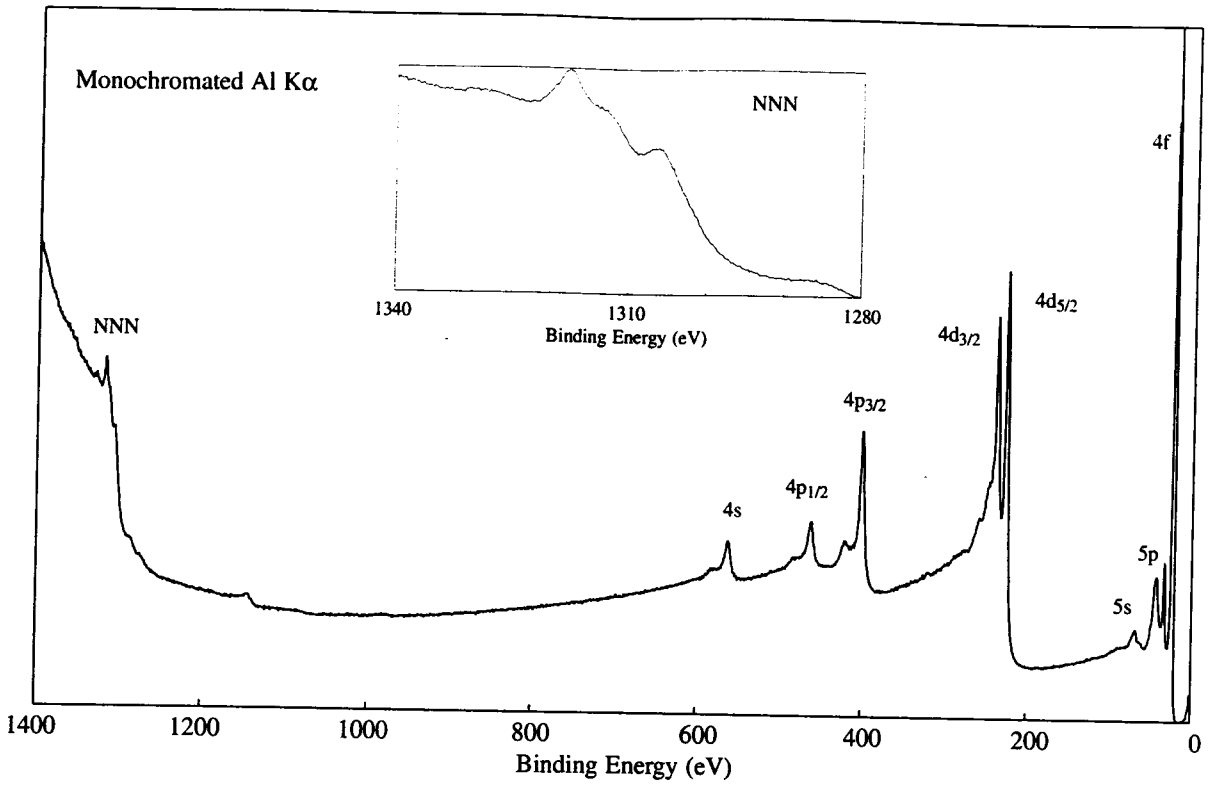
$N_5N_{67}N_7$	$N_4N_{67}N_7$	
1317	1306	(Al)
1084	1073	(Mg)

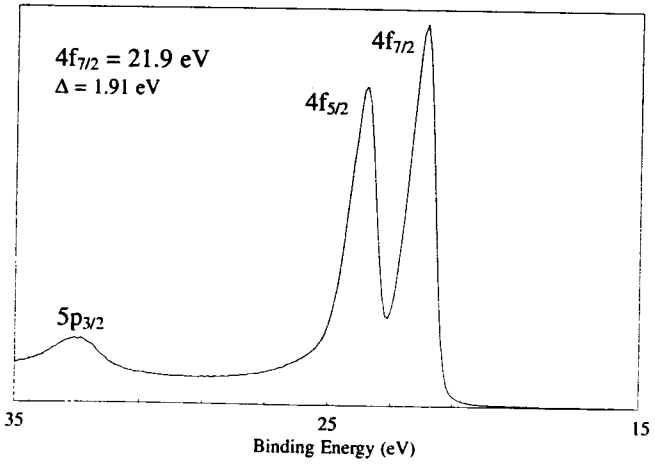
Hafnium Hf
Atomic Number 72











Line Positions (eV)

Photoelectron Lines

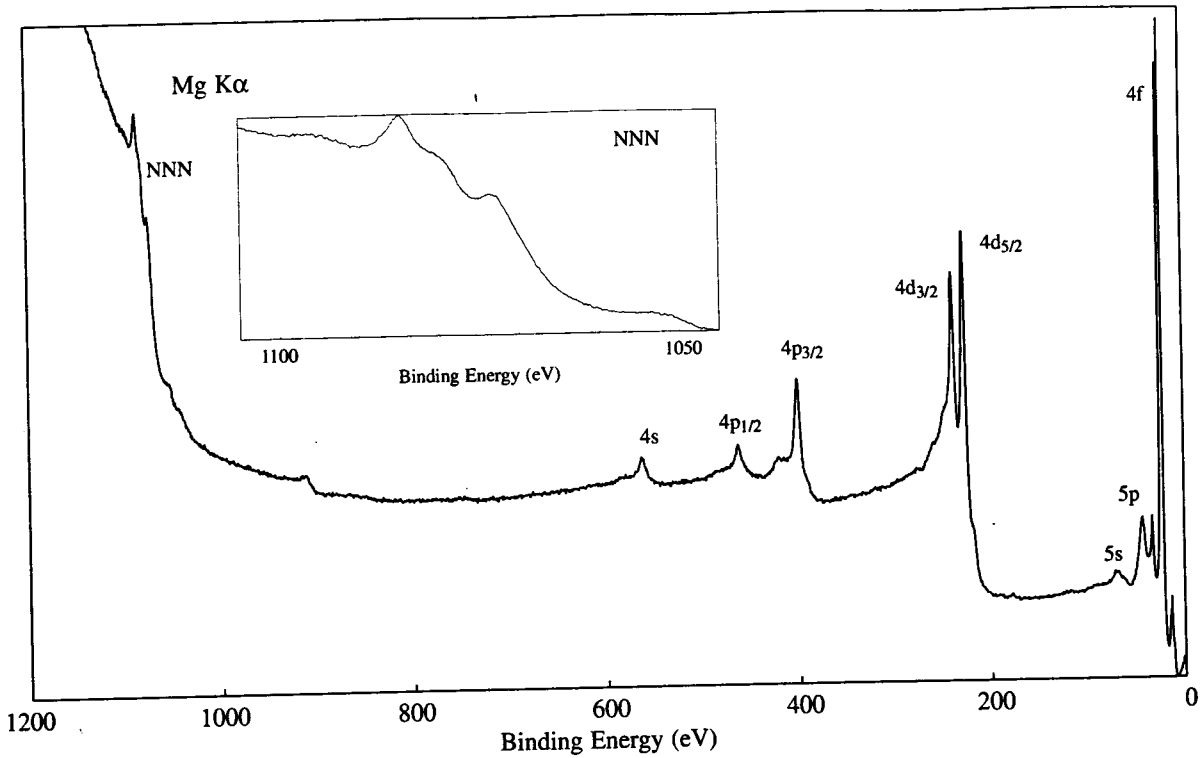
4s	4p1/2	4p3/2	4d3/2	4d5/2
563	463	401	238	226

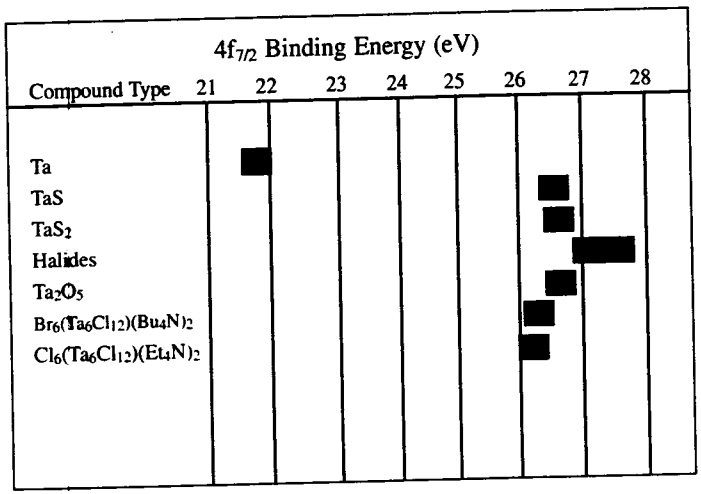
5s	5p1/2	5p3/2	4f5/2	4f7/2
69	43	33	24	22

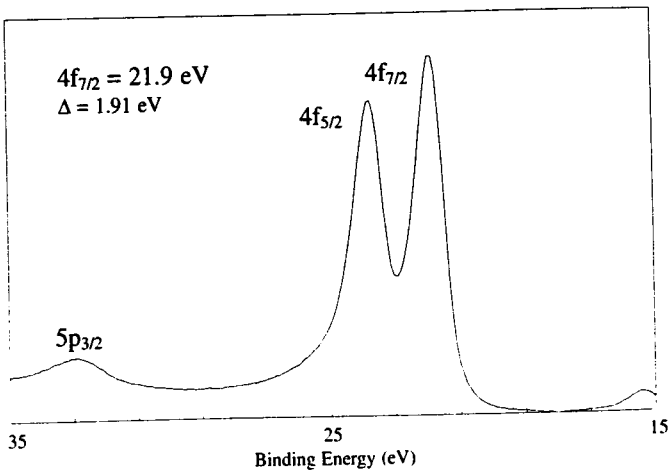
Auger Lines

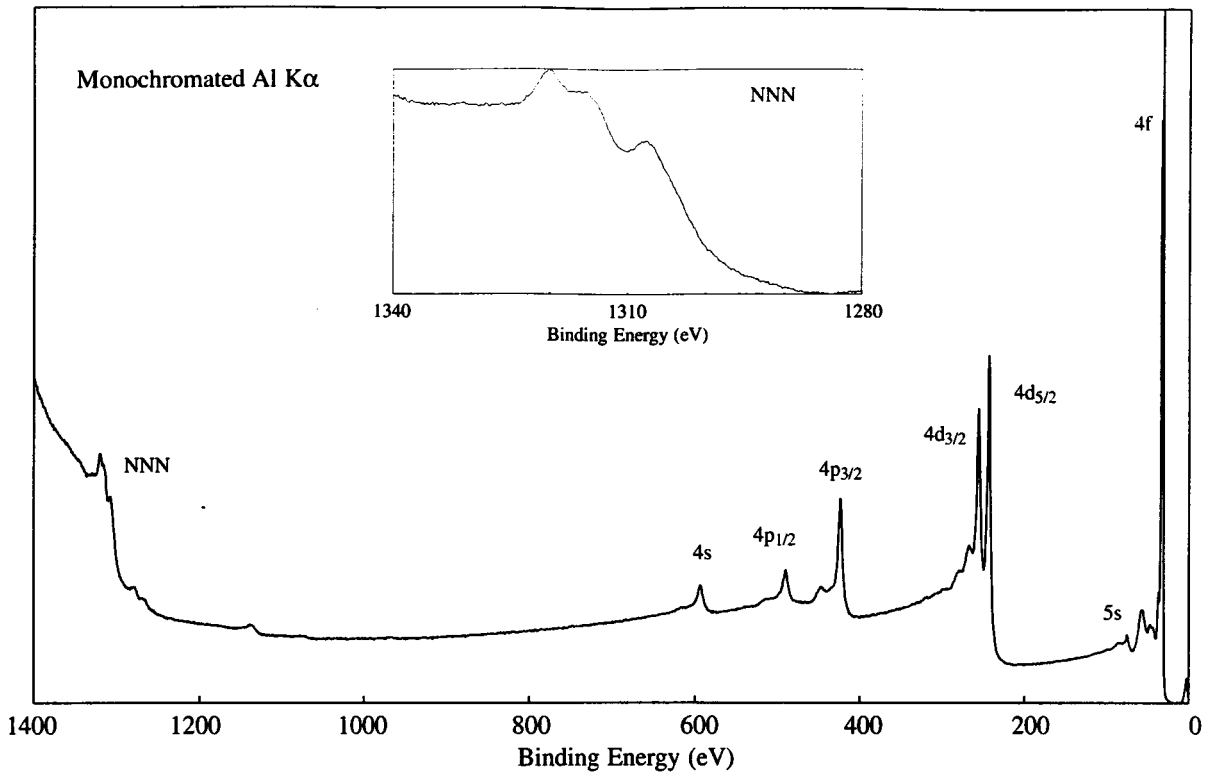
$N_5N_{67}N_7$	$N_4N_{67}N_7$	
1318	1306	(Al)
1085	1073	(Mg)

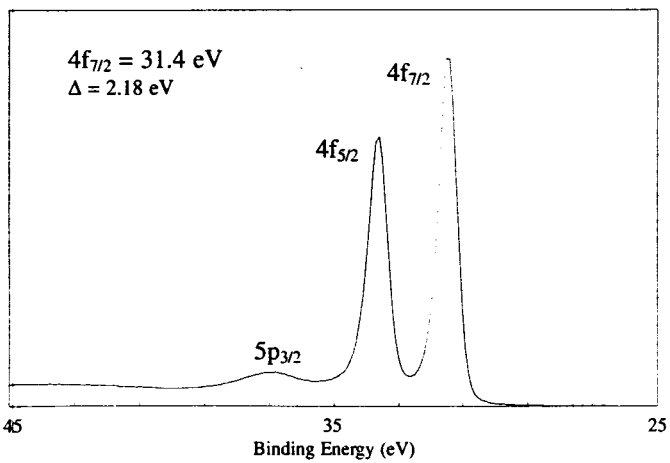
Tantalum Ta
Atomic Number 73











Line Positions (eV)

Photoelectron Lines

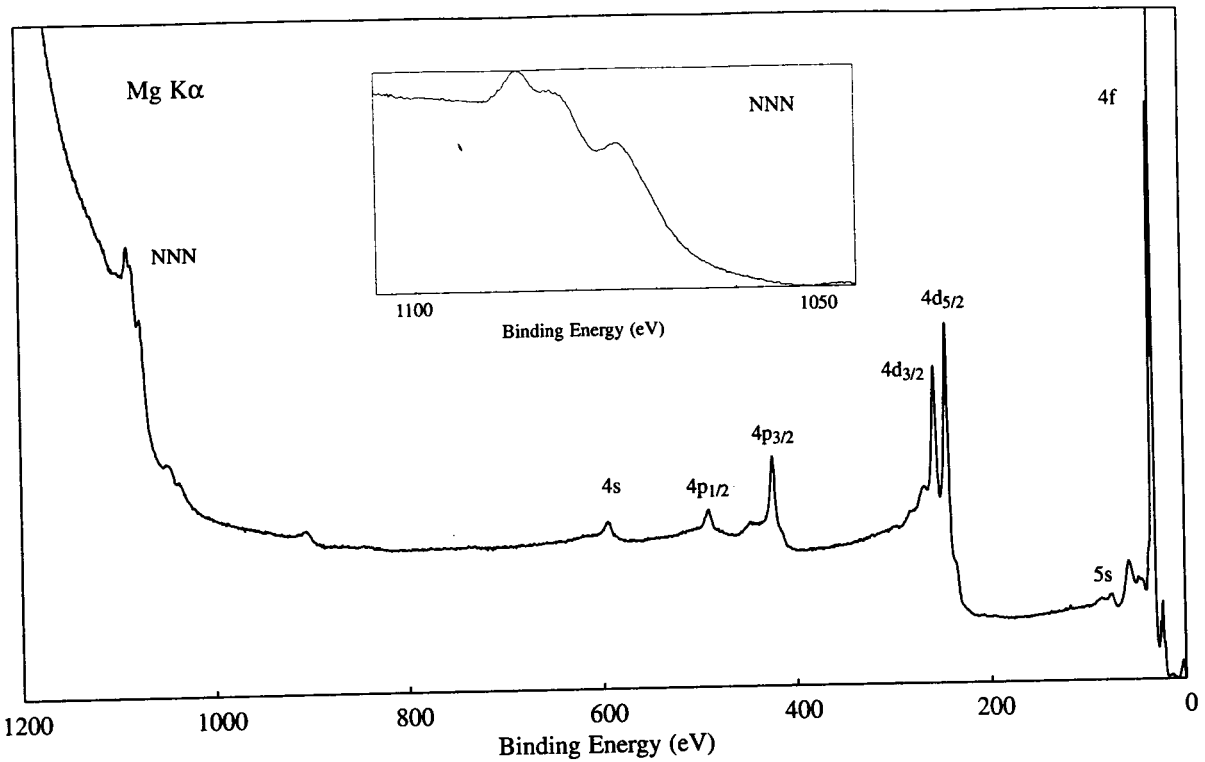
4s	4p1/2	4p3/2	4d3/2	4d5/2
594	491	424	256	243

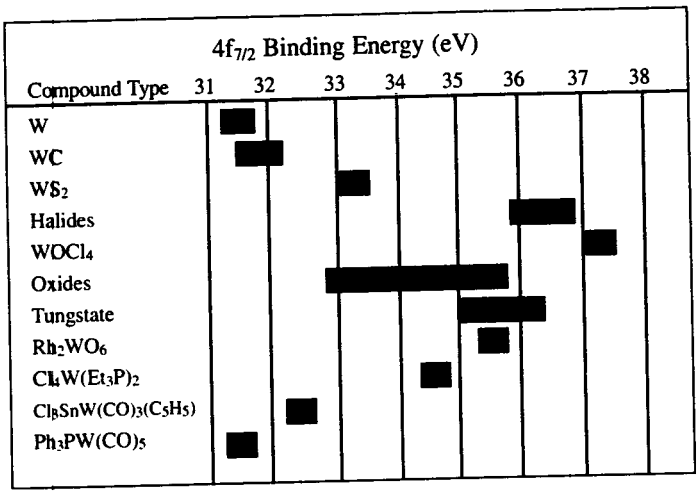
5s	5p1/2	5p3/2	4f5/2	4f7/2
75	47	37	33	31

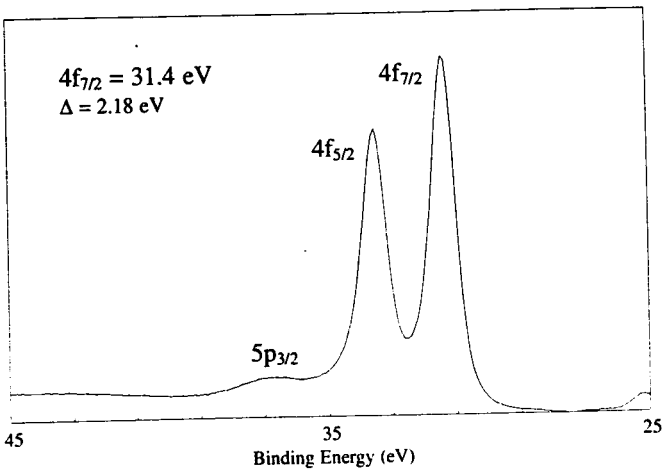
Auger Lines

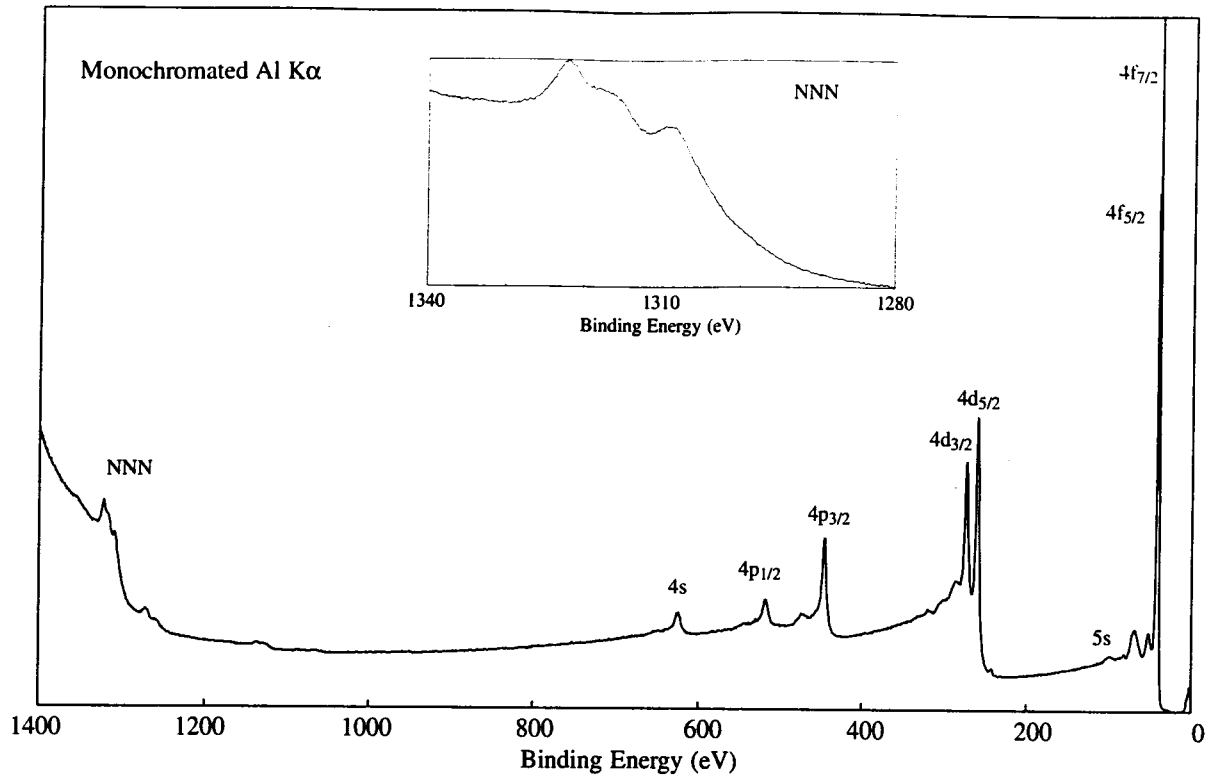
$N_5N_{67}N_7$	$N_4N_{67}N_7$	
1320	1307	(Al)
1087	1074	(Mg)

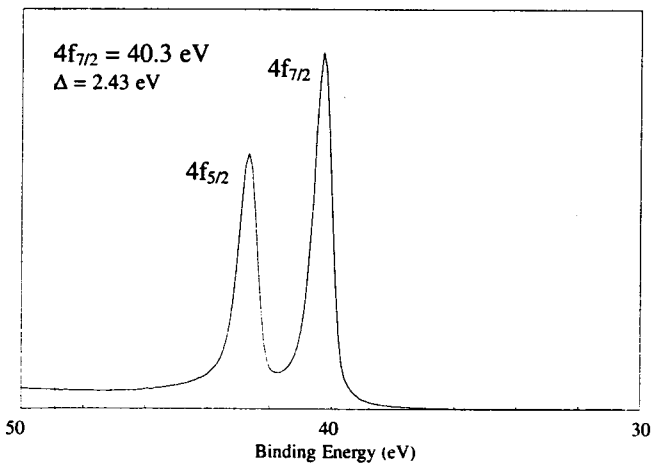
Tungsten W
Atomic Number 74











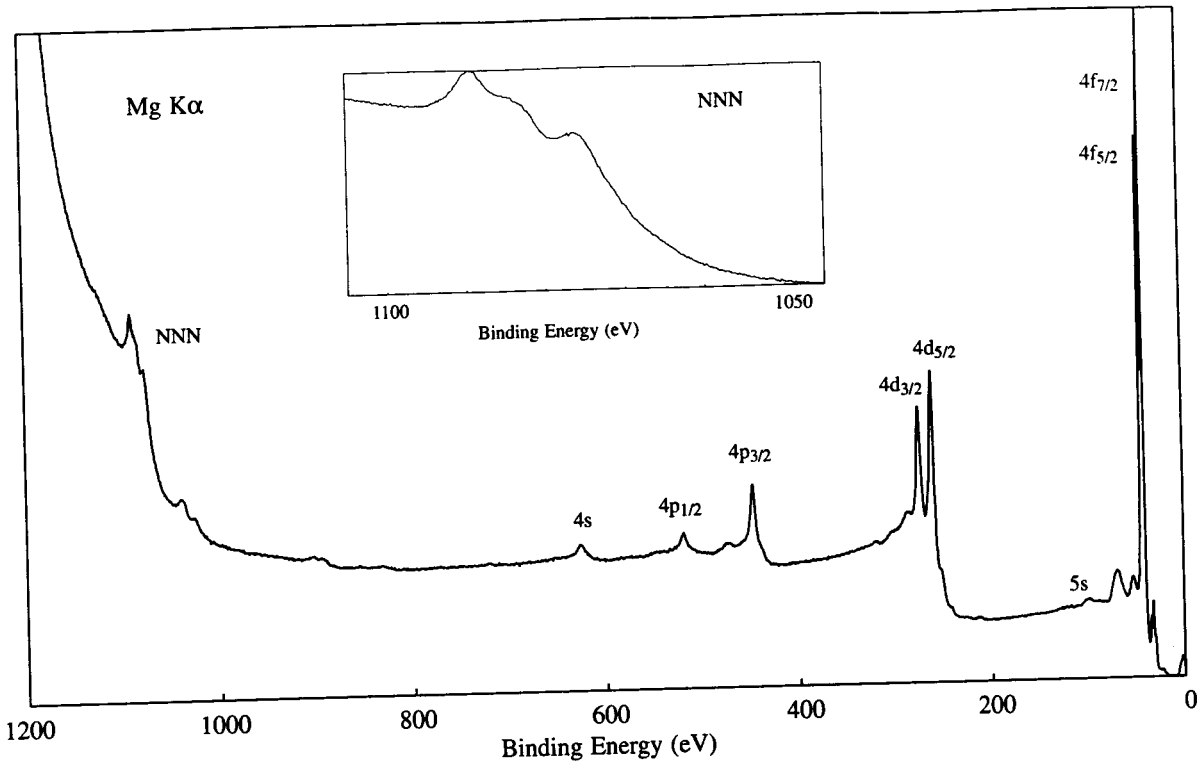
Line Positions (eV)

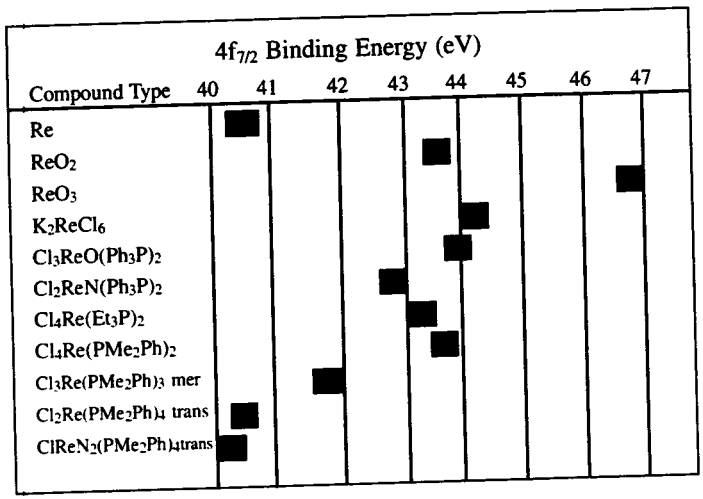
Photoelectron Lines

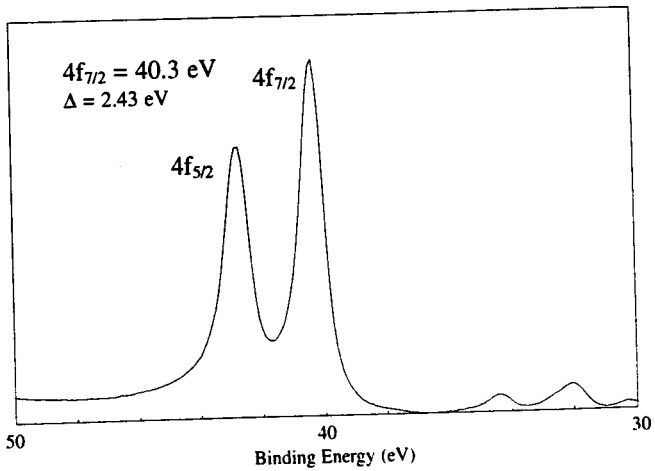
4s	4p1/2	4p3/2	4d3/2	4d5/2	5s	4f5/2	4f7/2
625	518	446	274	260	99	42	40

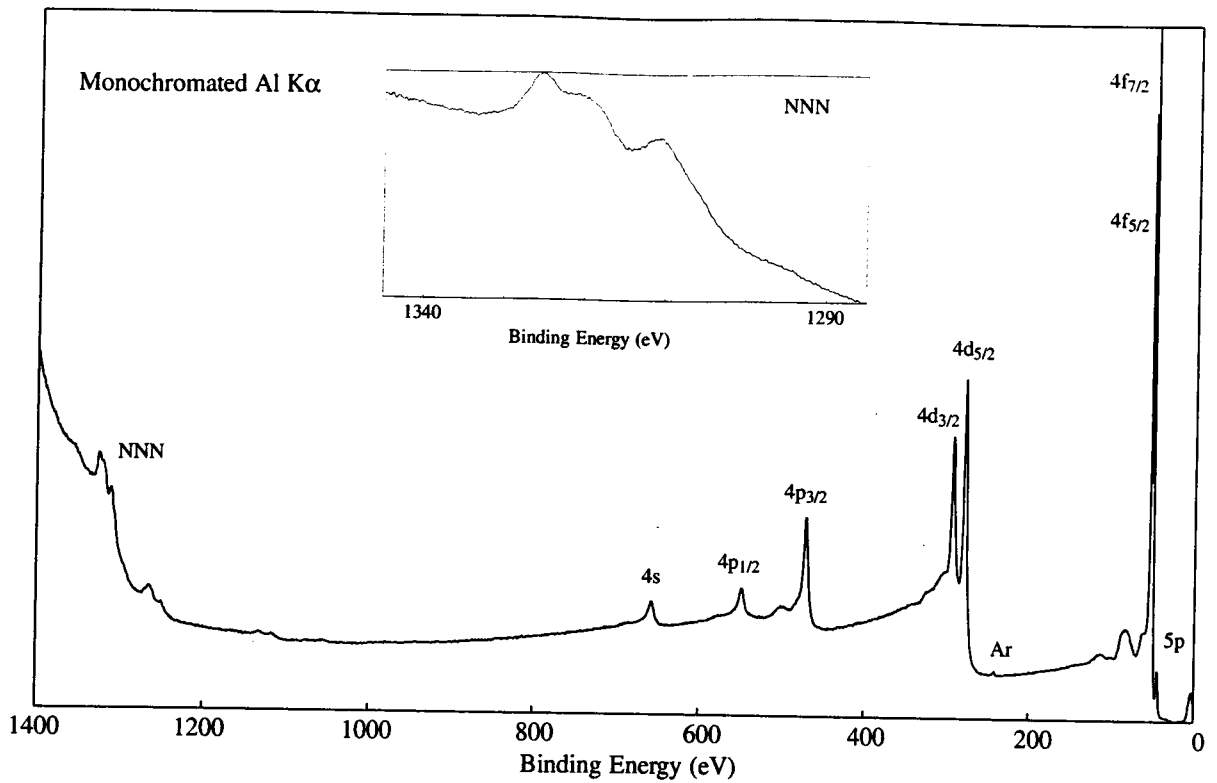
Auger Lines

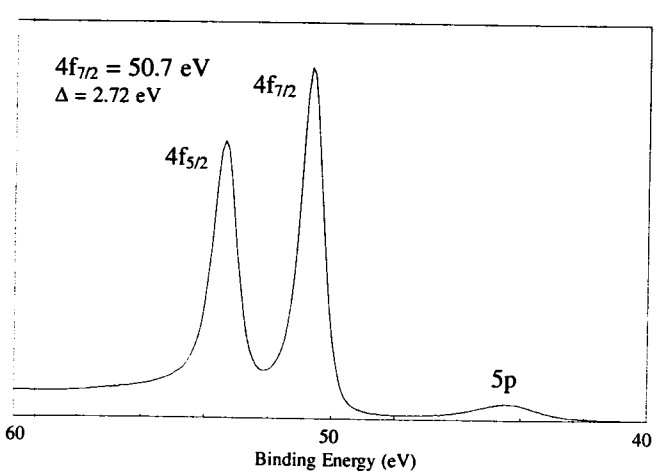
$N_5N_{67}N_7$	$N_4N_{67}N_7$	
1322	1309	(Al)
1089	1076	(Mg)


Mg Kα
NNN
1100
1050
Binding Energy (eV)
4f7/2
4f5/2
NNN
4d5/2
4d3/2
4p3/2
4p1/2
4s
5s
1200
1000
800
600
400
200
0
Binding Energy (eV)


4f7/2 Binding Energy (eV)
Compound Type
40
41
42
43
44
45
46
47
Re
ReO2
ReO3
K2ReCl6
Cl3ReO(Ph3P)2
Cl2ReN(Ph3P)2
Cl4Re(Et3P)2
Cl4Re(PMe2Ph)2
Cl3Re(PMe2Ph)3 mer
Cl2Re(PMe2Ph)4 trans
ClReN2(PMe2Ph)4trans


4f7/2 = 40.3 eV
Δ = 2.43 eV
4f7/2
4f5/2
50
40
30
Binding Energy (eV)





Line Positions (eV)

Photoelectron Lines

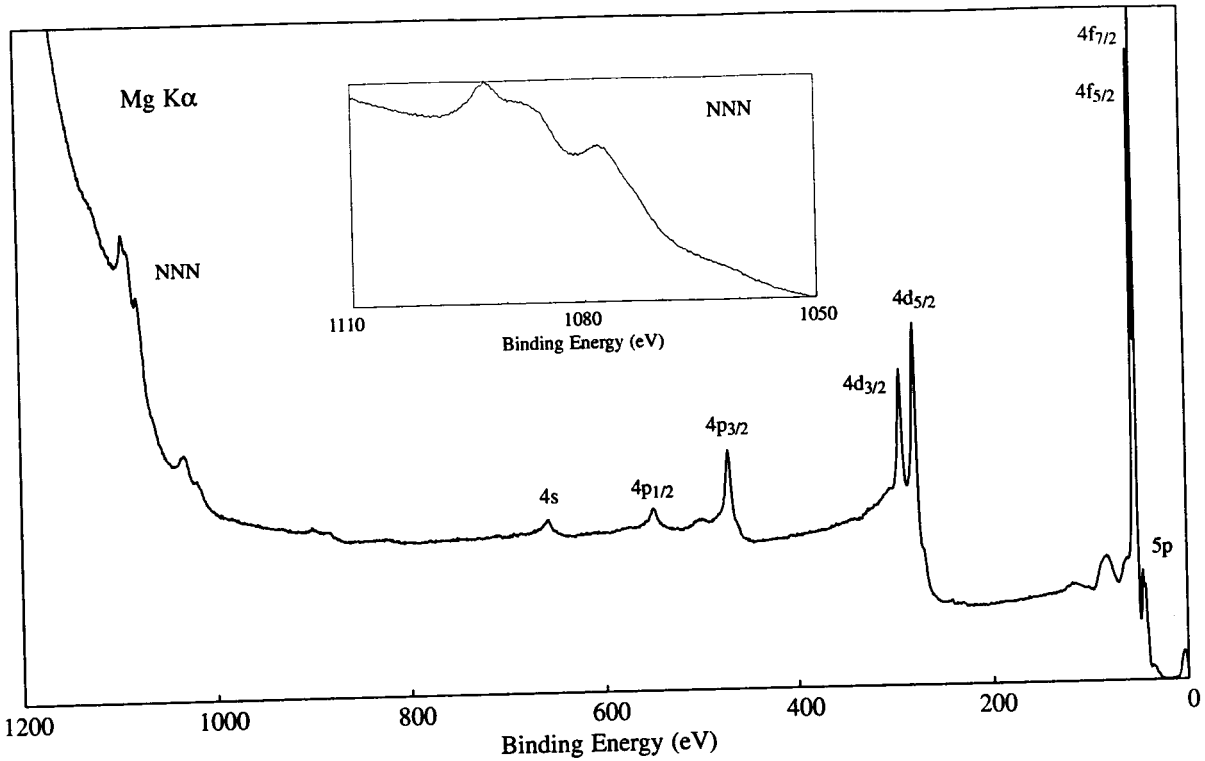
4s	4p1/2	4p3/2	4d3/2	4d5/2
658	548	471	293	279

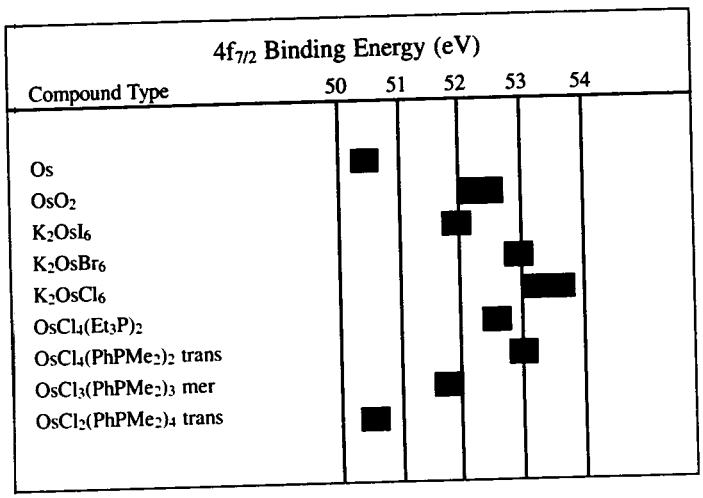
5s*	4f5/2	4f7/2	5p
89	54	51	44

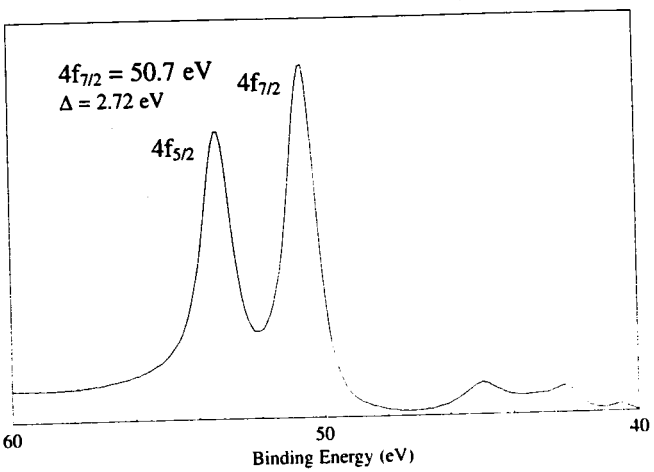
Auger Lines

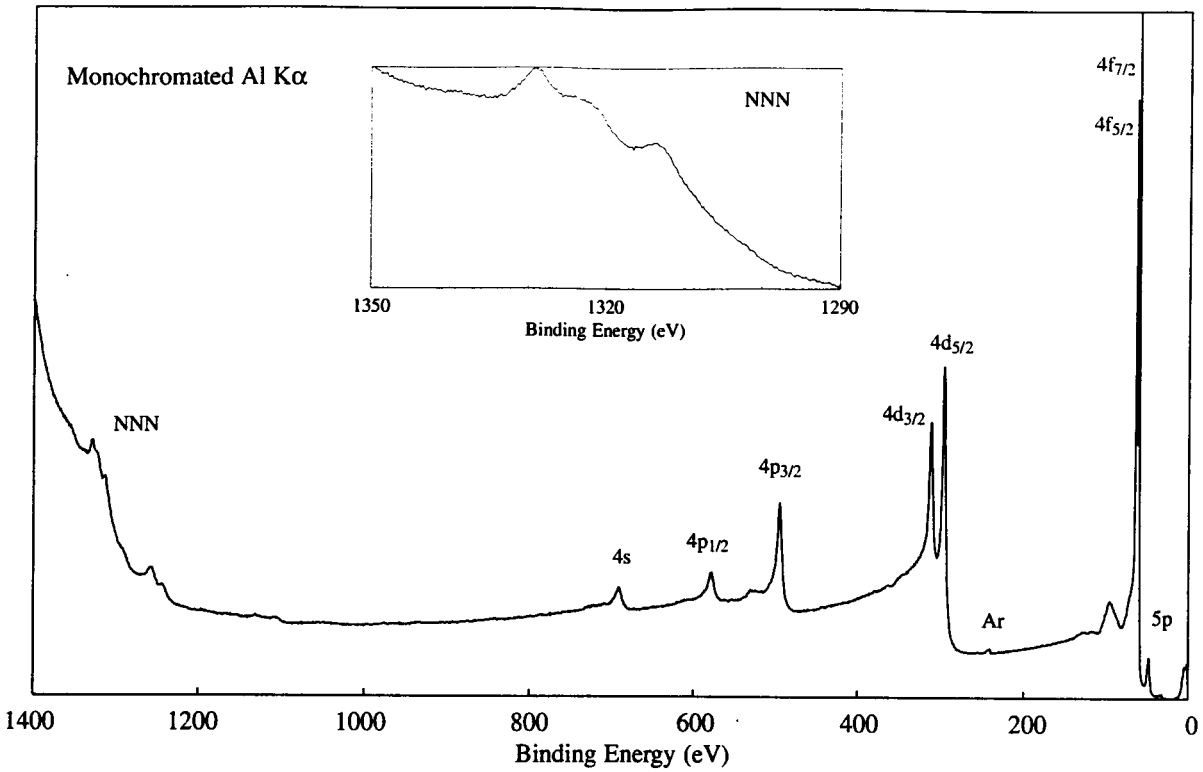
$N_5N_{67}N_7$	$N_4N_{67}N_7$	
1326	1311	(Al)
1093	1078	(Mg)

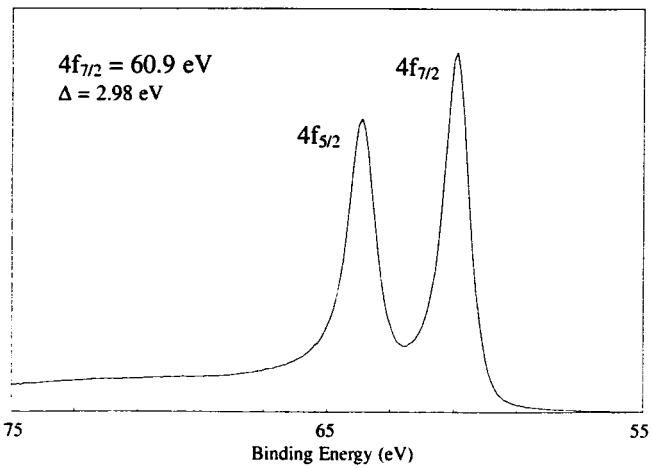
*Estimate


Mg Kα
NNN
NNN
1110
1080
1050
Binding Energy (eV)
4f7/2
4f5/2
4d5/2
4d3/2
4p3/2
4p1/2
4s
5p
1200
1000
800
600
400
200
0
Binding Energy (eV)


4f7/2 Binding Energy (eV)
Compound Type
50
51
52
53
54
Os
OsO2
K2OsI6
K2OsBr6
K2OsCl6
OsCl4(Et3P)2
OsCl4(PhPMe2)2 trans
OsCl3(PhPMe2)3 mer
OsCl2(PhPMe2)4 trans


4f7/2 = 50.7 eV
Δ = 2.72 eV
4f7/2
4f5/2
60
50
40
Binding Energy (eV)





Line Positions (eV)

Photoelectron Lines

4s	4p1/2	4p3/2	4d3/2	4d5/2
692	578	495	312	297

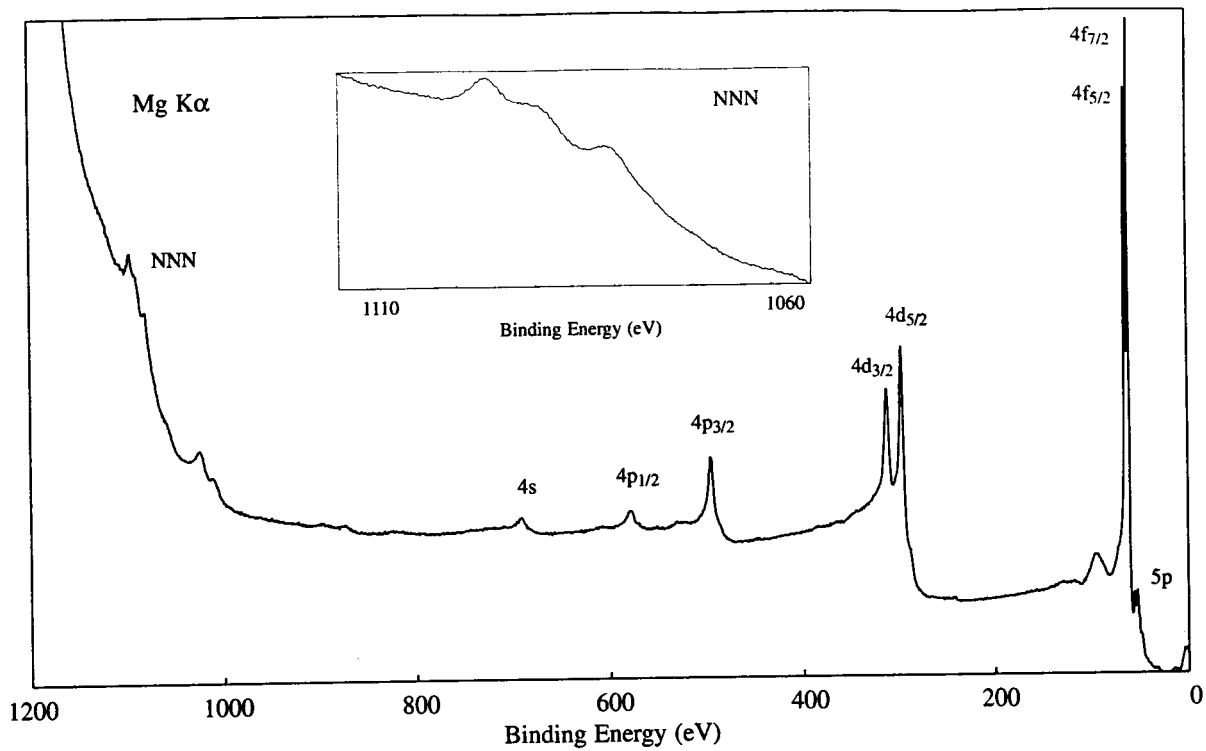
5s*	4f5/2	4f7/2	5p
96	64	61	48

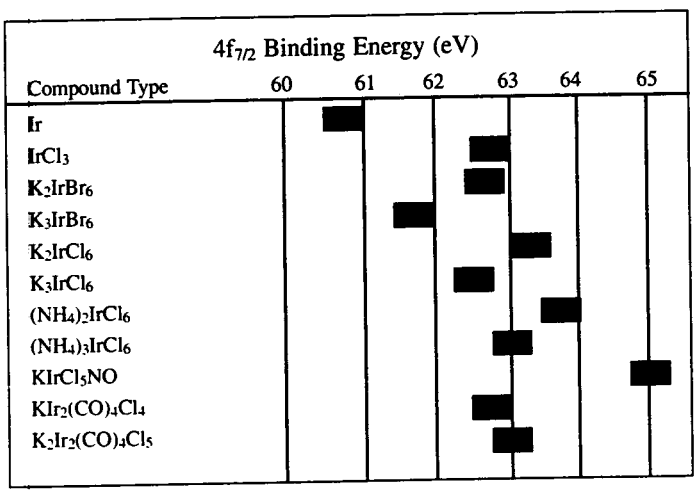
Auger Lines

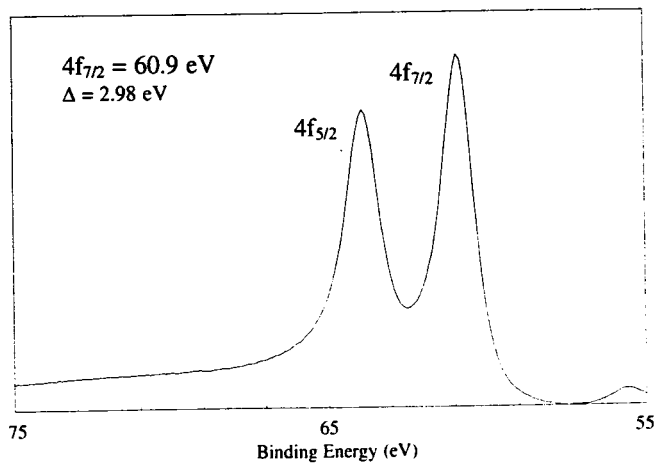
$N_5N_{67}N_7$	$N_4N_{67}N_7$	
1329	1314	(Al)
1096	1081	(Mg)

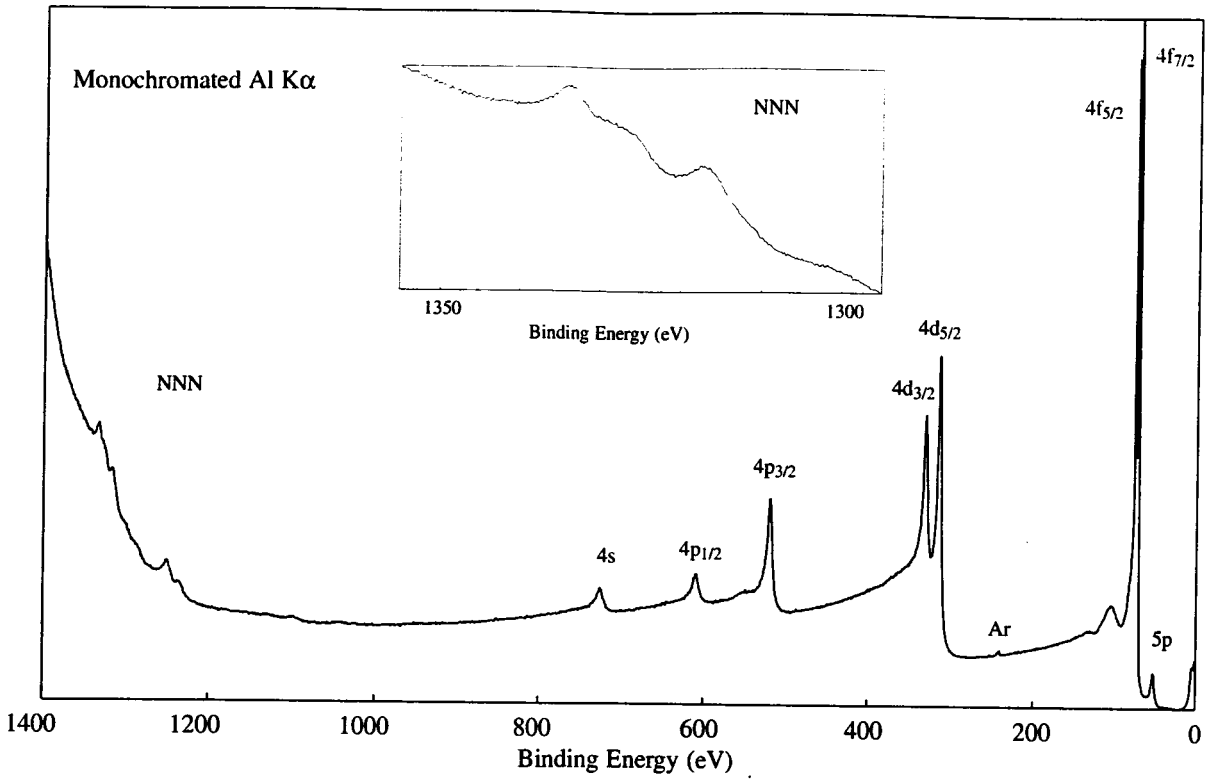
*Estimate

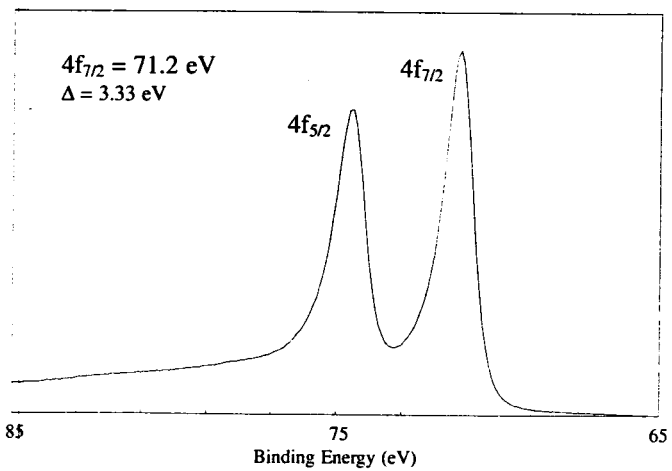
Iridium Ir
Atomic Number 77











Line Positions (eV)

Photoelectron Lines

4s	4p1/2	4p3/2	4d3/2	4d5/2
725	609	520	332	315

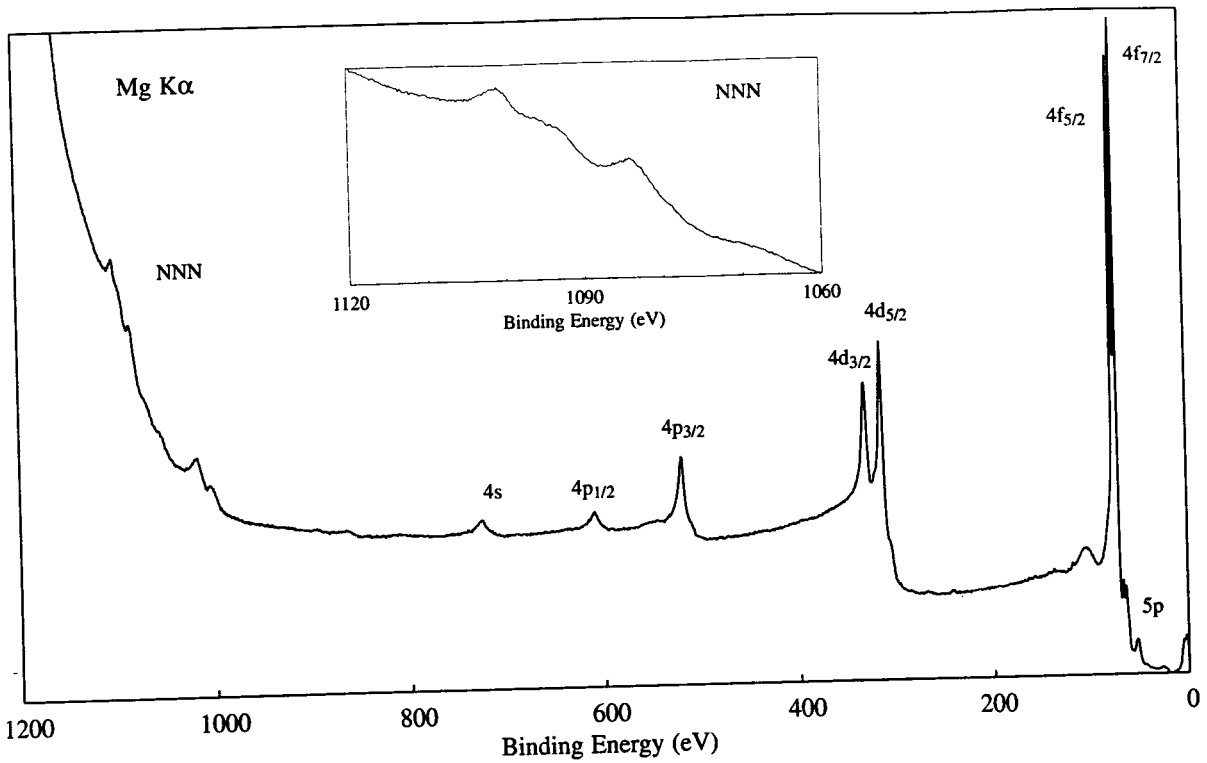
5s*	4f5/2	4f7/2	5p
103	74	71	52

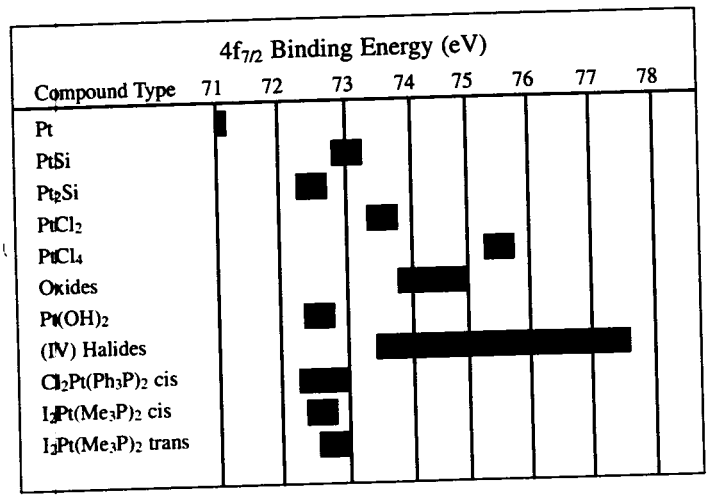
Auger Lines

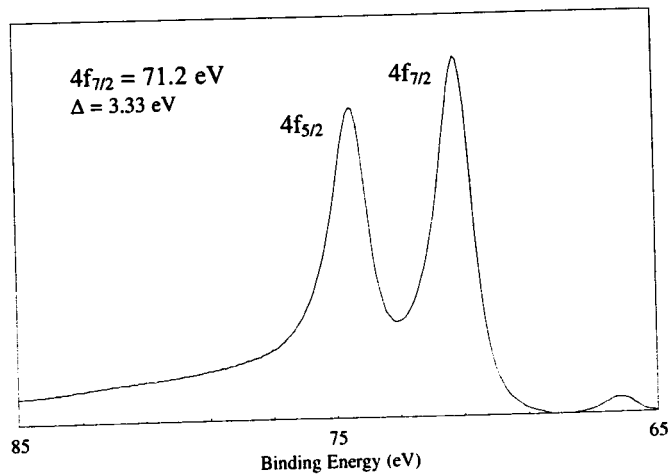
	$N_5N_{67}N_7$	$N_4N_{67}N_7$	
	1334	1317	(Al)
	1101	1084	(Mg)

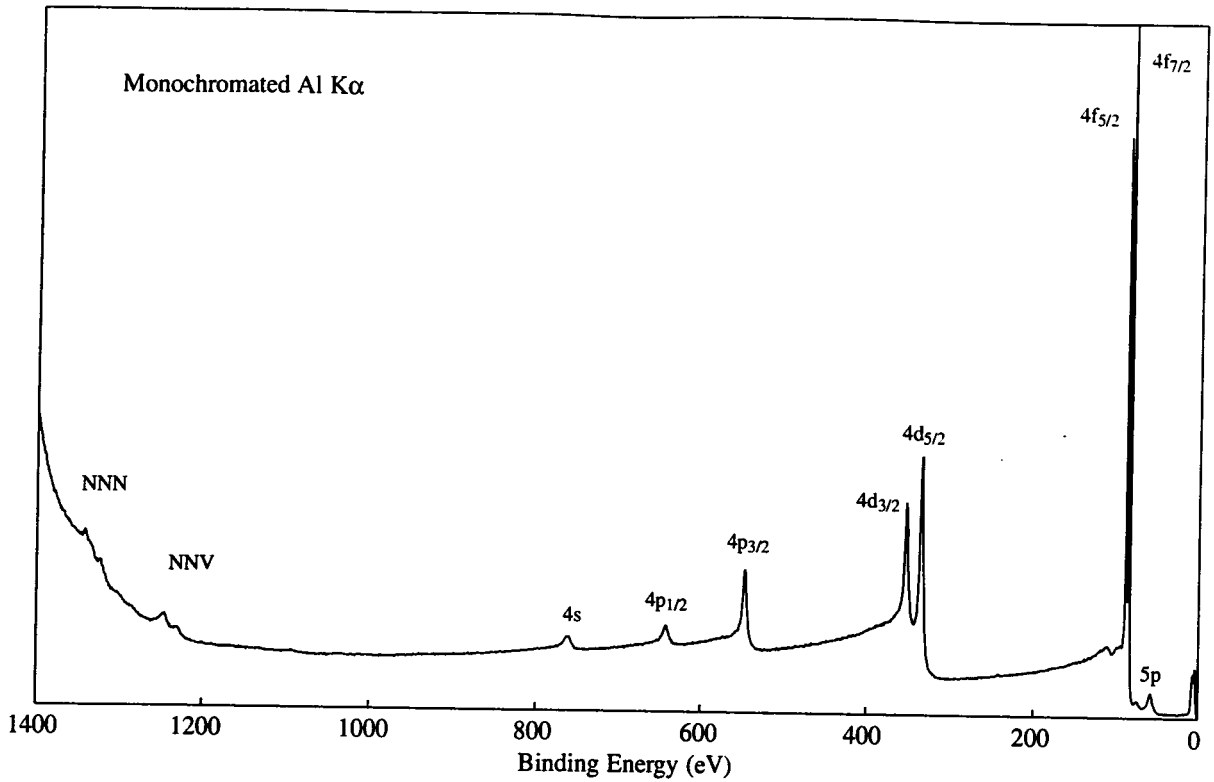
*Estimate

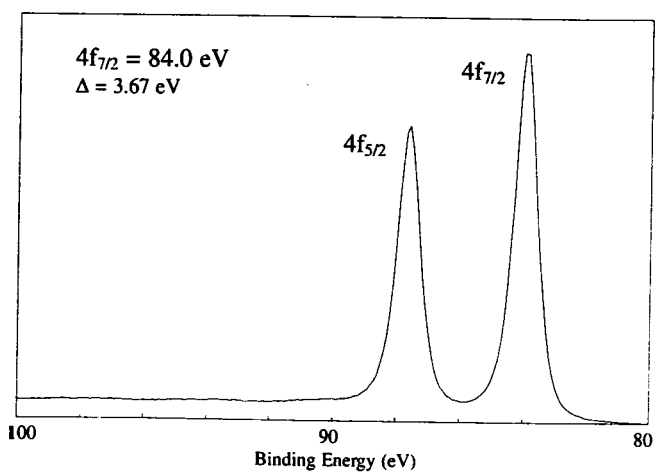
Platinum Pt
Atomic Number 78











Line Positions (eV)

Photoelectron Lines

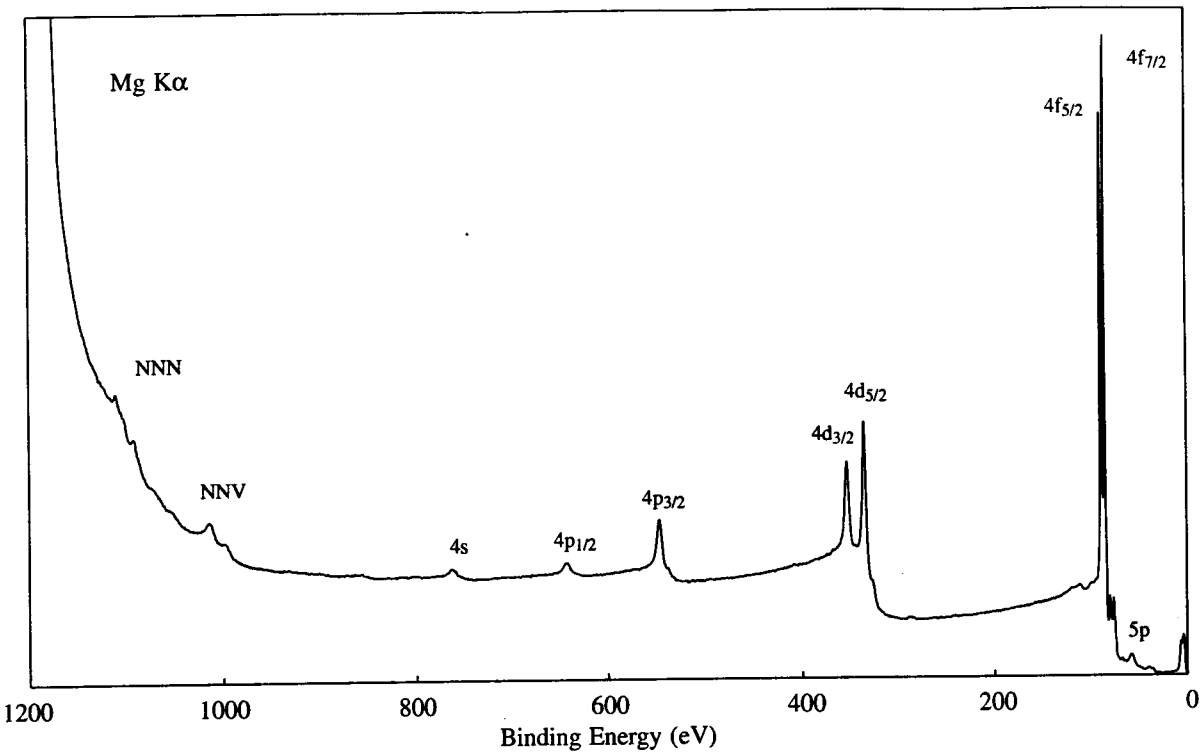
4s	4p1/2	4p3/2	4d3/2	4d5/2
763	643	547	353	335

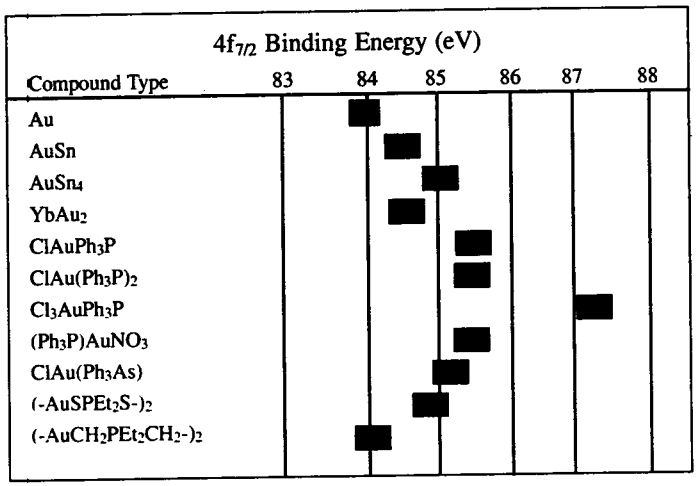
5s*	4f5/2	4f7/2	5p1/2	5p3/2
110	88	84	74	57

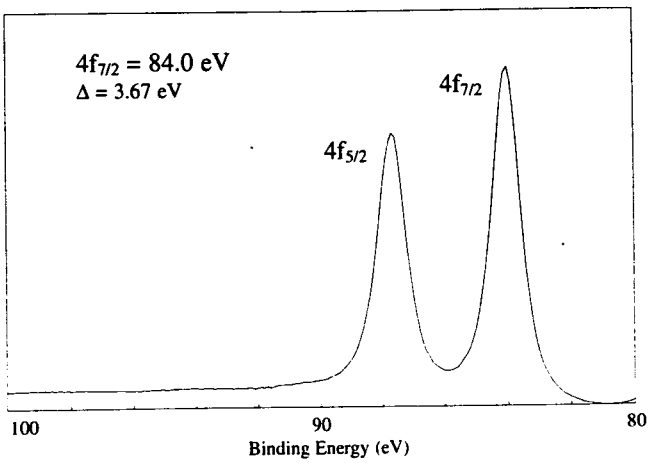
Auger Lines

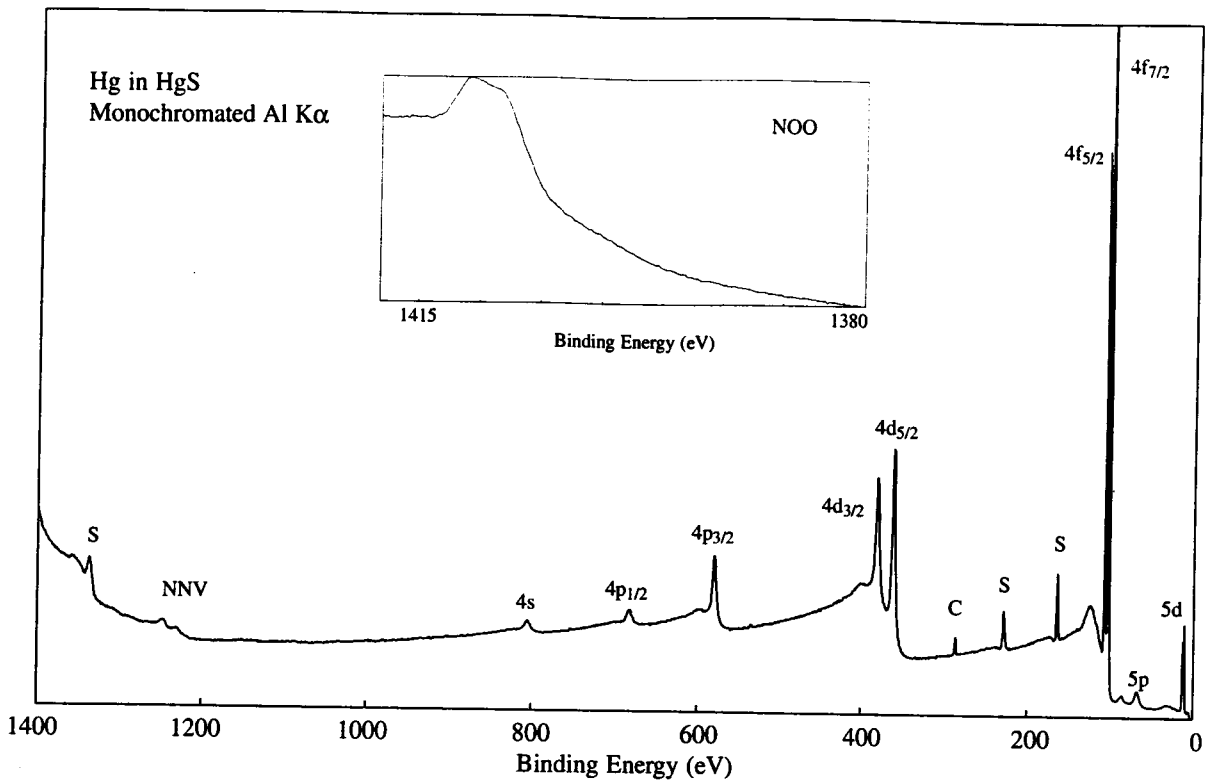
$N_{67}O_{45}O_{45}$	$N_5N_6N_{67}$	$N_4N_6N_{67}$	$N_5N_{67}V$	
1416	1342	1324	1247	(Al)
1183	1109	1091	1014	(Mg)

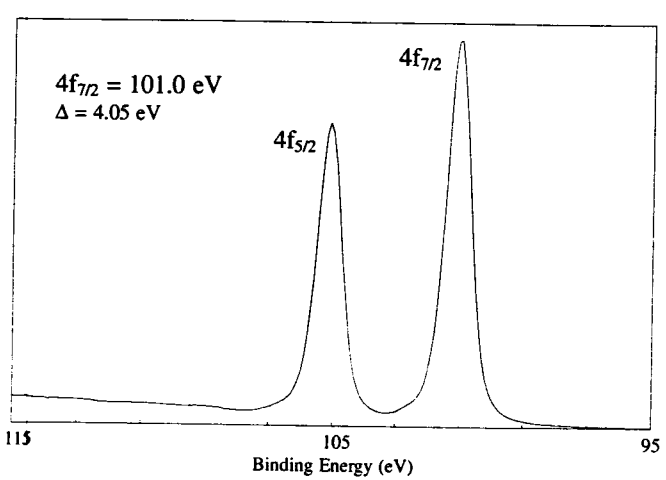
*Estimate


Mg Kα
4f7/2
4f5/2
NNN
4d5/2
4d3/2
NNV
4p3/2
4s
4p1/2
5p
1200
1000
800
600
400
200
0
Binding Energy (eV)


4f7/2 Binding Energy (eV)
Compound Type
83
84
85
86
87
88
Au
AuSn
AuSn4
YbAu2
ClAuPh3P
ClAu(Ph3P)2
Cl3AuPh3P
(Ph3P)AuNO3
ClAu(Ph3As)
(-AuSPEt2S-)2
(-AuCH2PEt2CH2-)2


4f7/2 = 84.0 eV
Δ = 3.67 eV
4f7/2
4f5/2
100
90
80
Binding Energy (eV)





Line Positions (eV)

Photoelectron Lines

4s	$4p_{1/2}$	$4p_{3/2}$	$4d_{3/2}$	$4d_{5/2}$	5s*
805	682	579	381	361	125

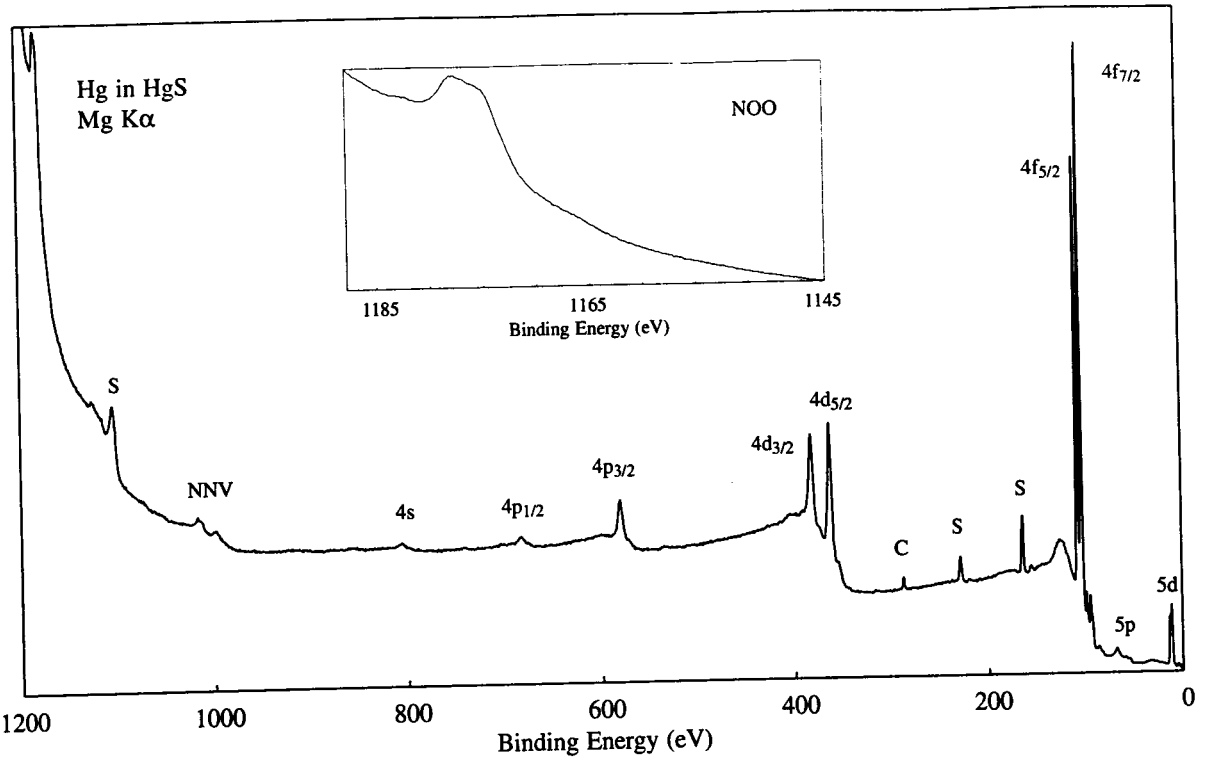
$4f_{5/2}$	$4f_{7/2}$	$5p_{1/2}$	$5p_{3/2}$	$5d_{3/2}$	$5d_{5/2}$
105	101	85	67	12	10

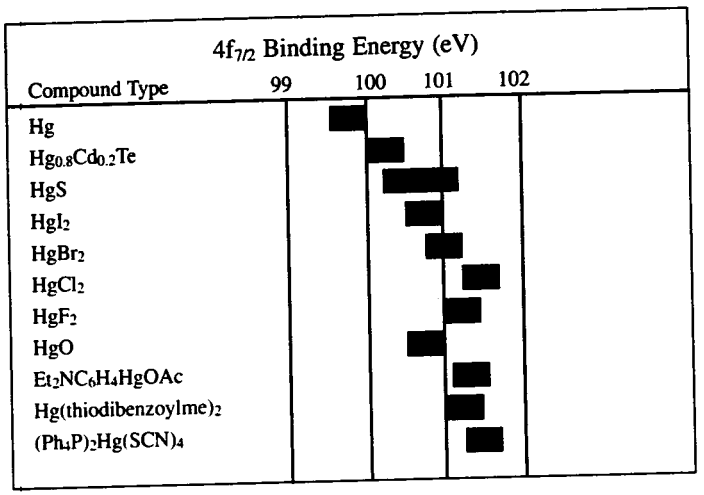
Auger Lines

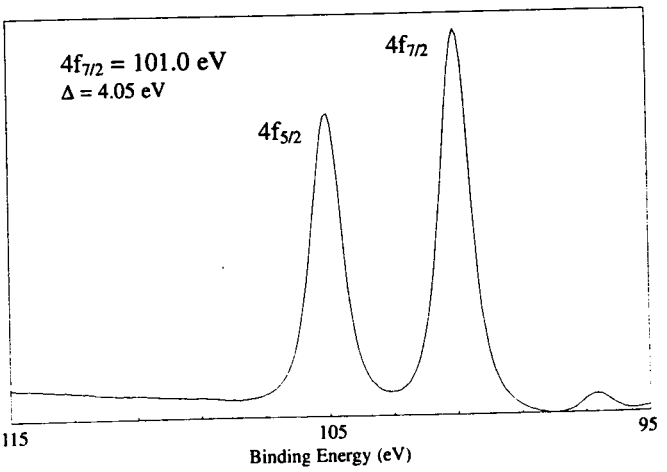
$N_7O_{45}O_{45}$	N_5N_7O	N_4N_6O	
1412	1246	1230	(Al)
1179	1013	997	(Mg)

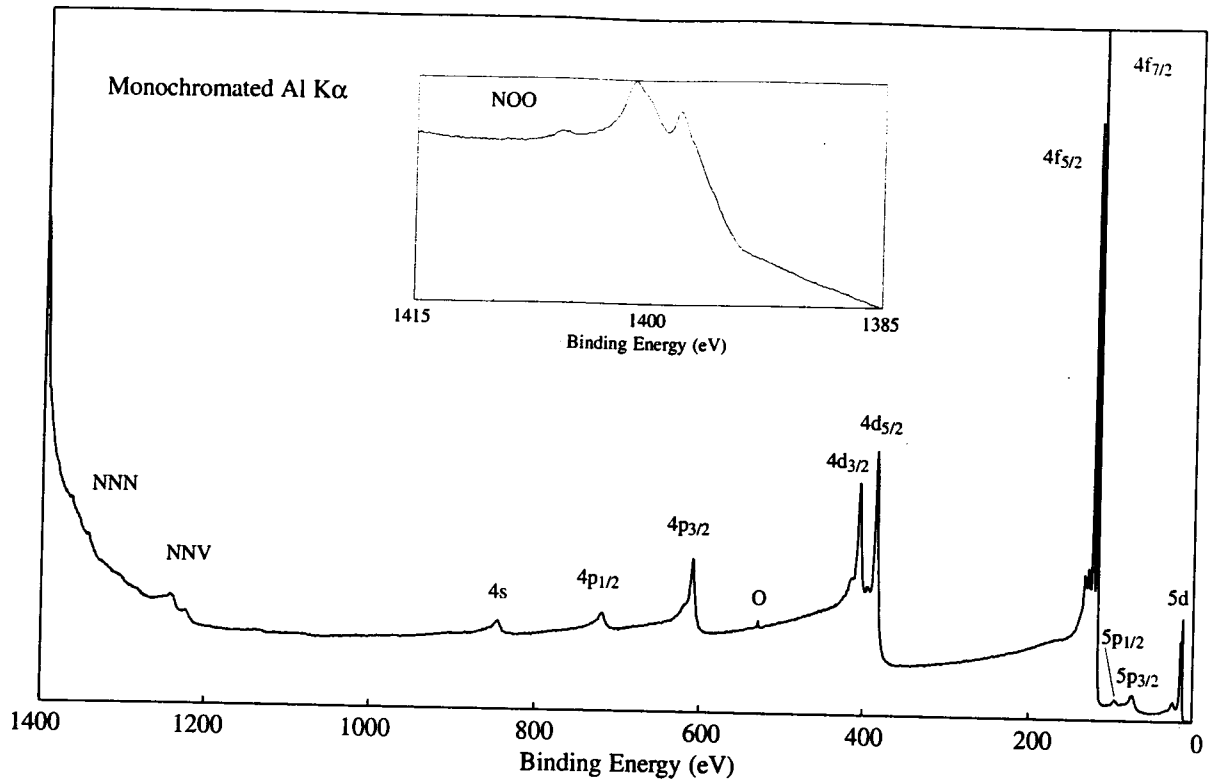
*Estimate

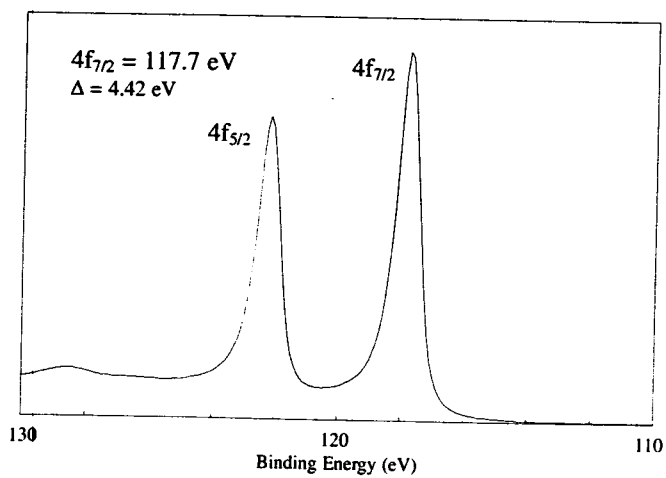
Mercury Hg
Atomic Number 80











Line Positions (eV)

Photoelectron Lines

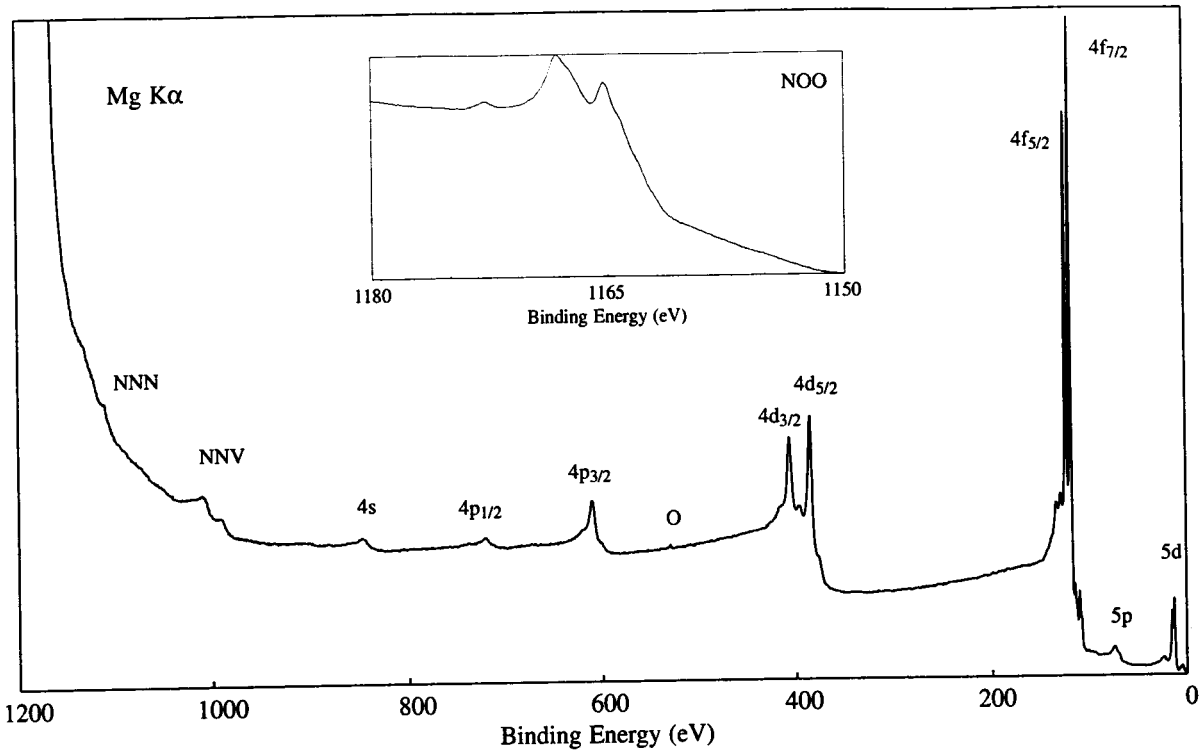
4s	4p1/2	4p3/2	4d3/2	4d5/2	5s*
847	720	610	406	385	133

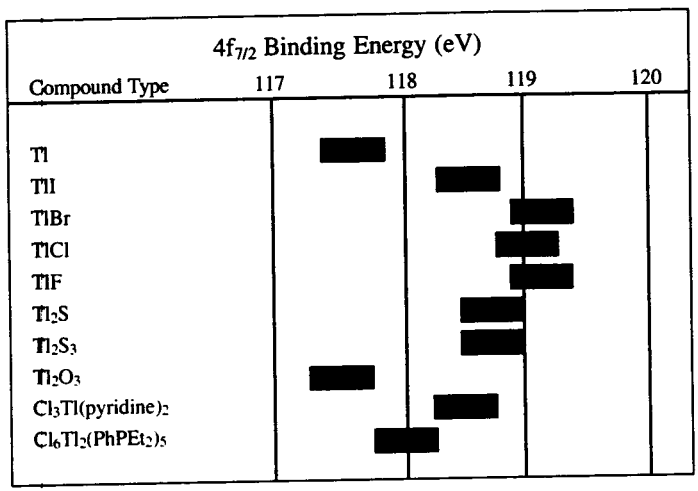
4f5/2	4f7/2	5p1/2	5p3/2	5d3/2	5d5/2
122	118	95	74	15	13

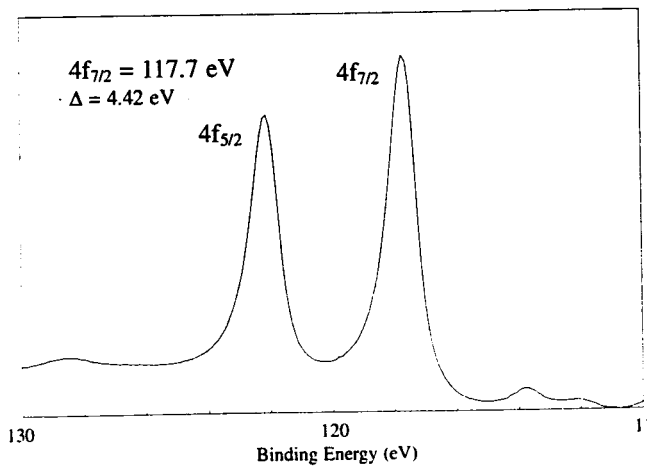
Auger Lines

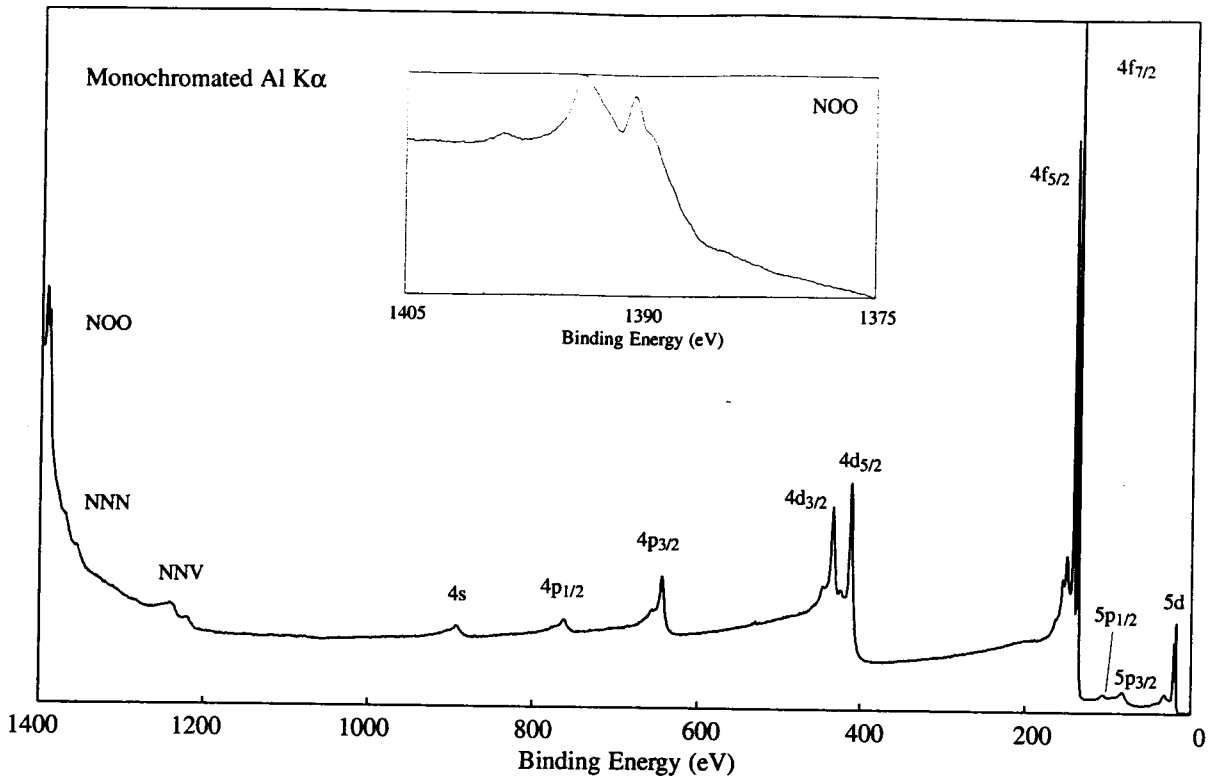
N7O45O45	N6O45O45	N5N7O5	N4N67O5	
1401	1399	1241	1222	(Al)
1168	1166	1008	989	(Mg)

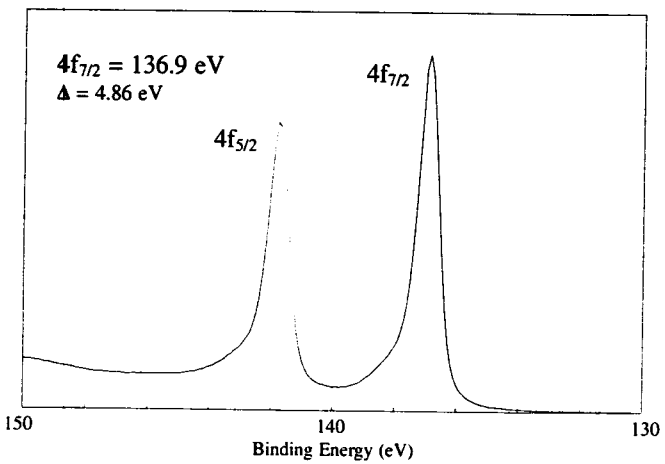
*Estimate


Mg Kα
NOO
1180
1165
1150
Binding Energy (eV)
4f7/2
4f5/2
NNN
NNV
4s
4p1/2
4p3/2
O
4d5/2
4d3/2
5d
5p
1200
1000
800
600
400
200
0
Binding Energy (eV)


4f7/2 Binding Energy (eV)
Compound Type
117
118
119
120
Tl
TlI
TlBr
TlCl
TlF
Tl2S
Tl2S3
Tl2O3
Cl3Tl(pyridine)2
Cl6Tl2(PhPEt2)5


4f7/2 = 117.7 eV
Δ = 4.42 eV
4f7/2
4f5/2
130
120
110
Binding Energy (eV)





Line Positions (eV)

Photoelectron Lines

4s	4p1/2	4p3/2	4d3/2	4d5/2	5s*
893	762	644	434	412	150

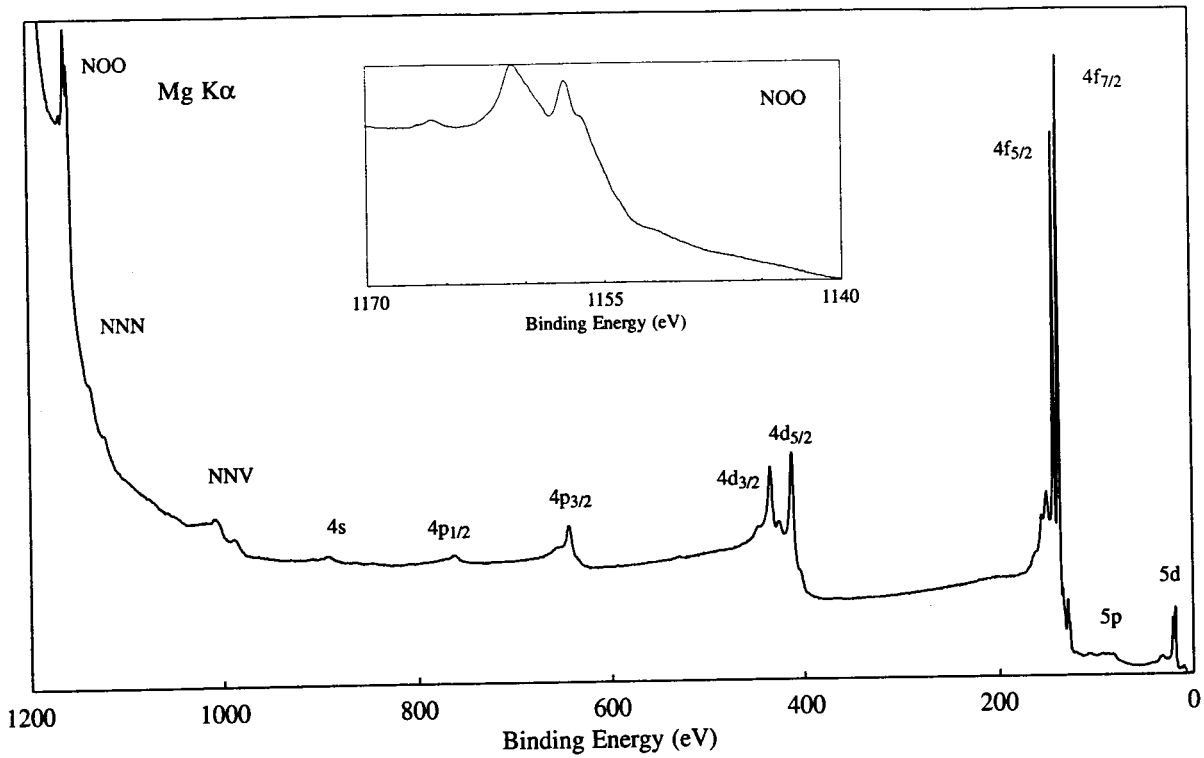
4f5/2	4f7/2	5p1/2	5p3/2	5d3/2	5d5/2
142	137	107	84	21	18

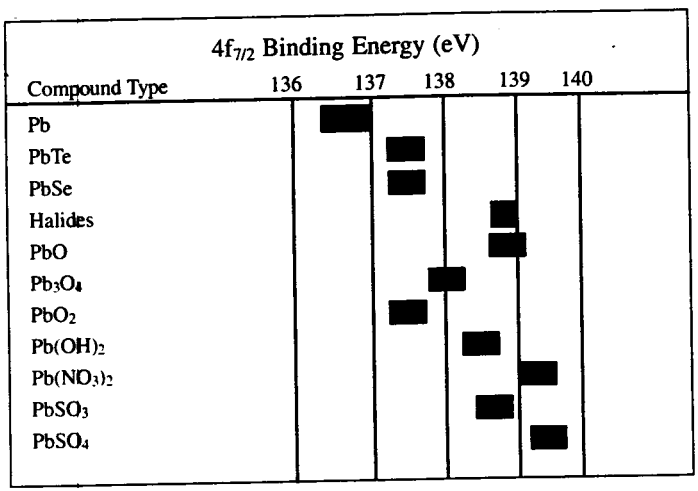
Auger Lines

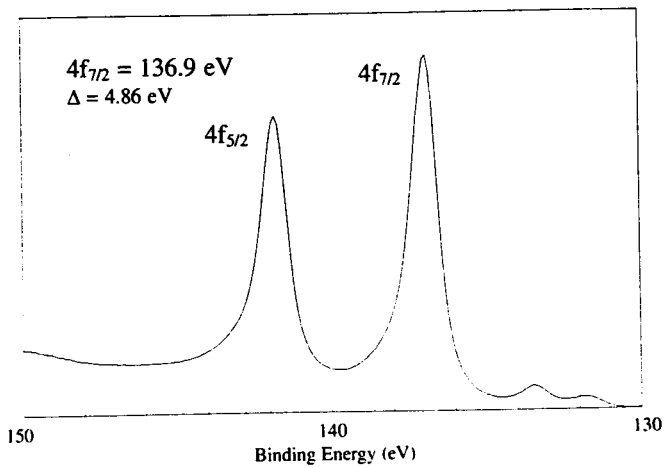
$N_7O_{45}O_{45}$	$N_6O_{45}O_{45}$	
1394	1391	(Al)
1161	1158	(Mg)

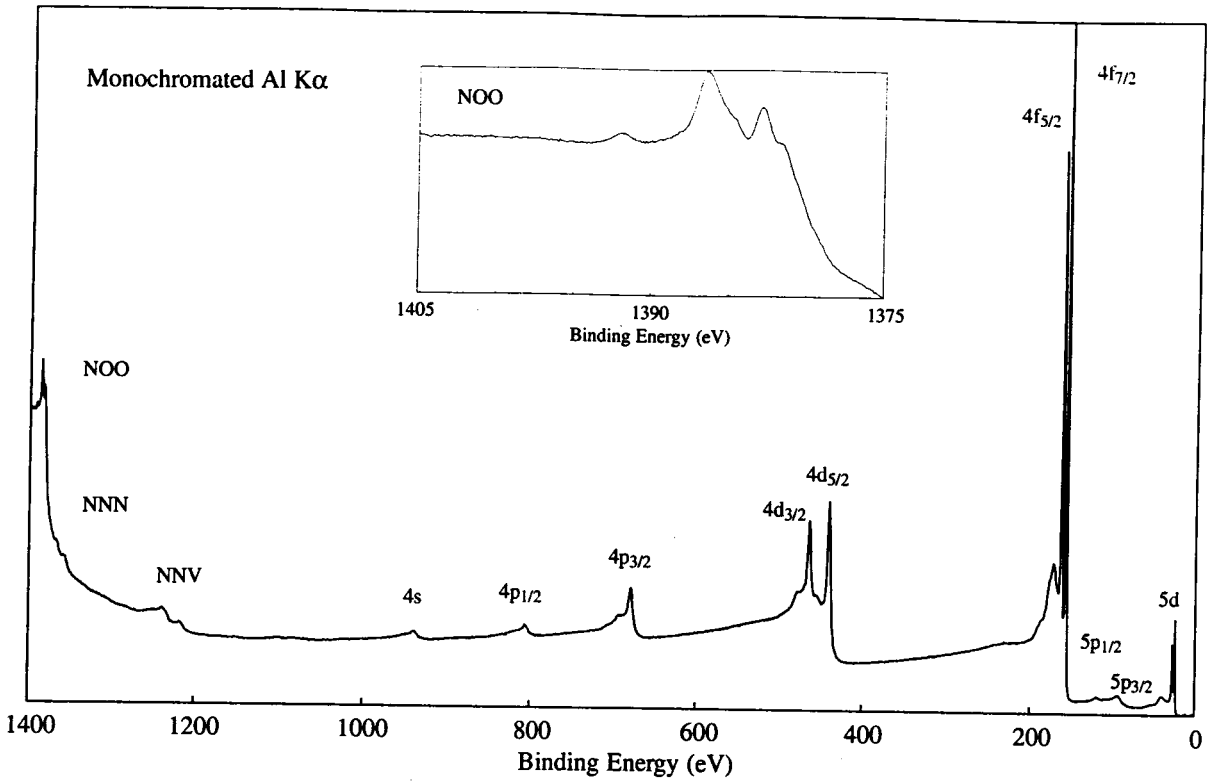
*Estimate

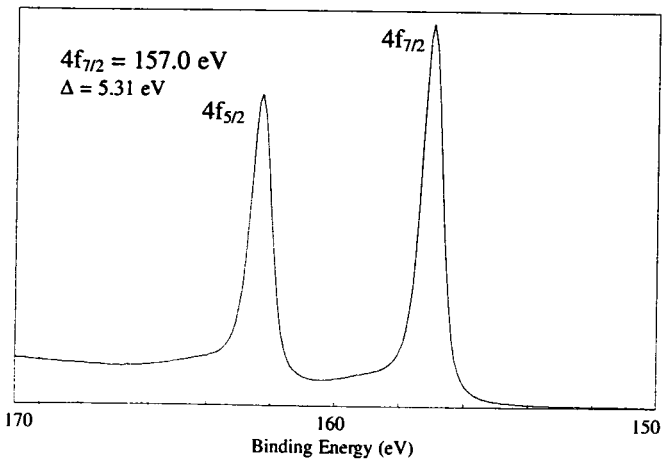
Lead Pb
Atomic Number 82











Line Positions (eV)

Photoelectron Lines

4s	4p1/2	4p3/2	4d3/2	4d5/2	5s*
940	806	679	464	440	161

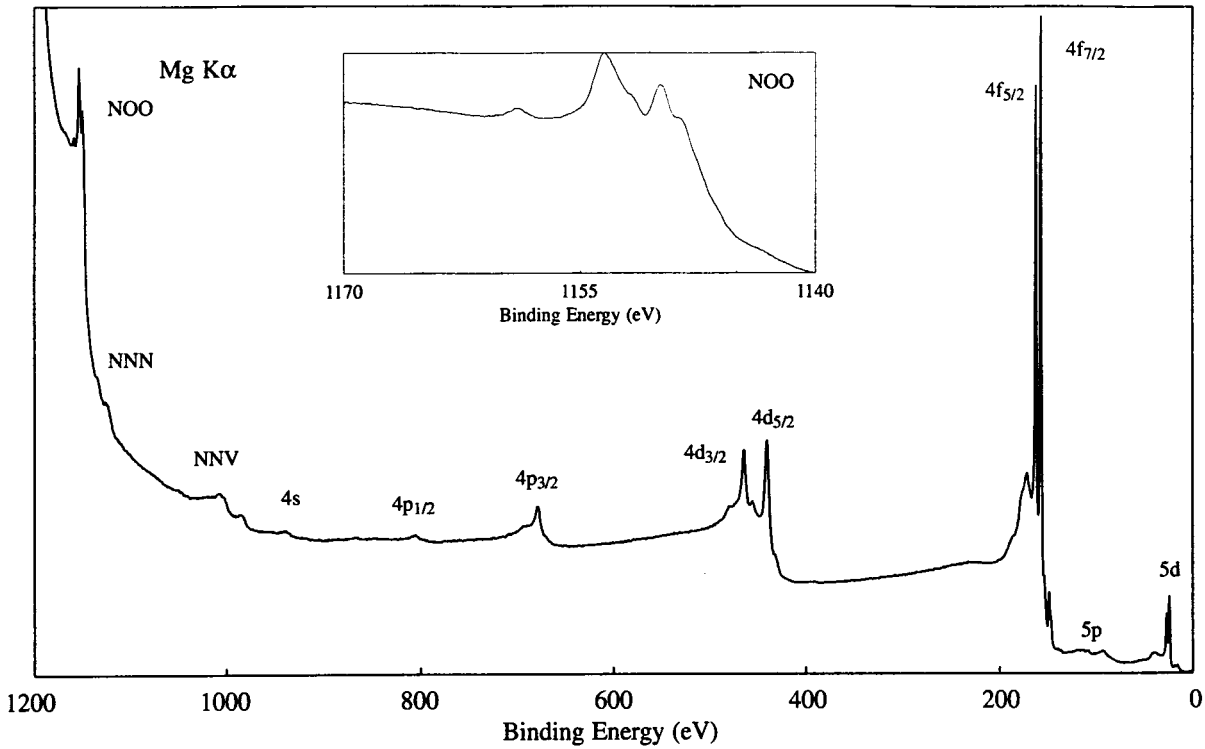
4f5/2	4f7/2	5p1/2	5p3/2	5d3/2	5d5/2
162	157	119	93	27	24

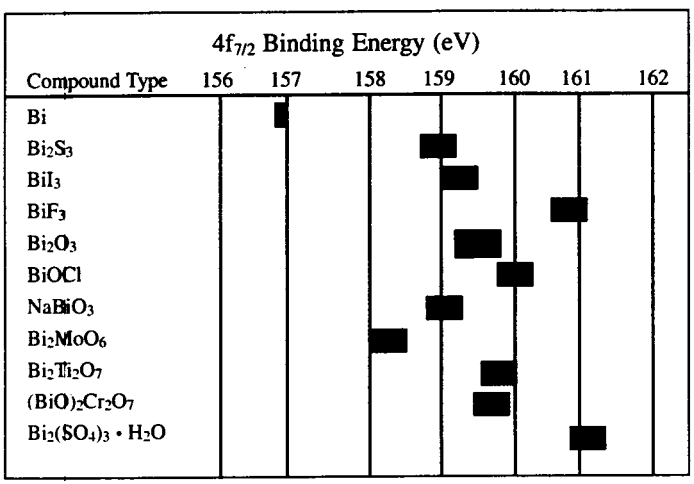
Auger Lines

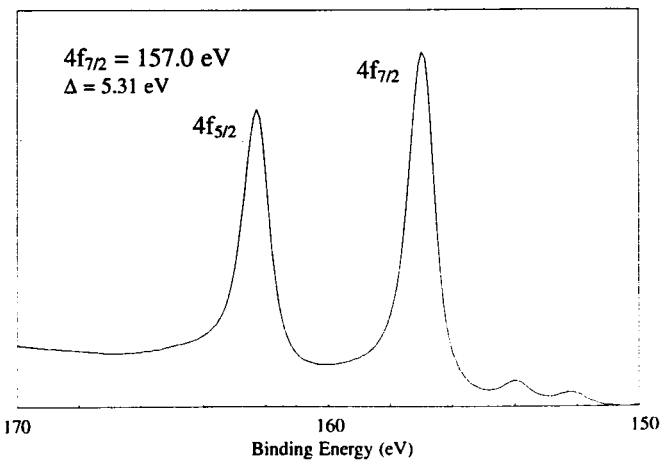
$N_7O_{45}O_{45}$	$N_6O_{45}O_{45}$	
1387	1383	(Al)
1154	1150	(Mg)

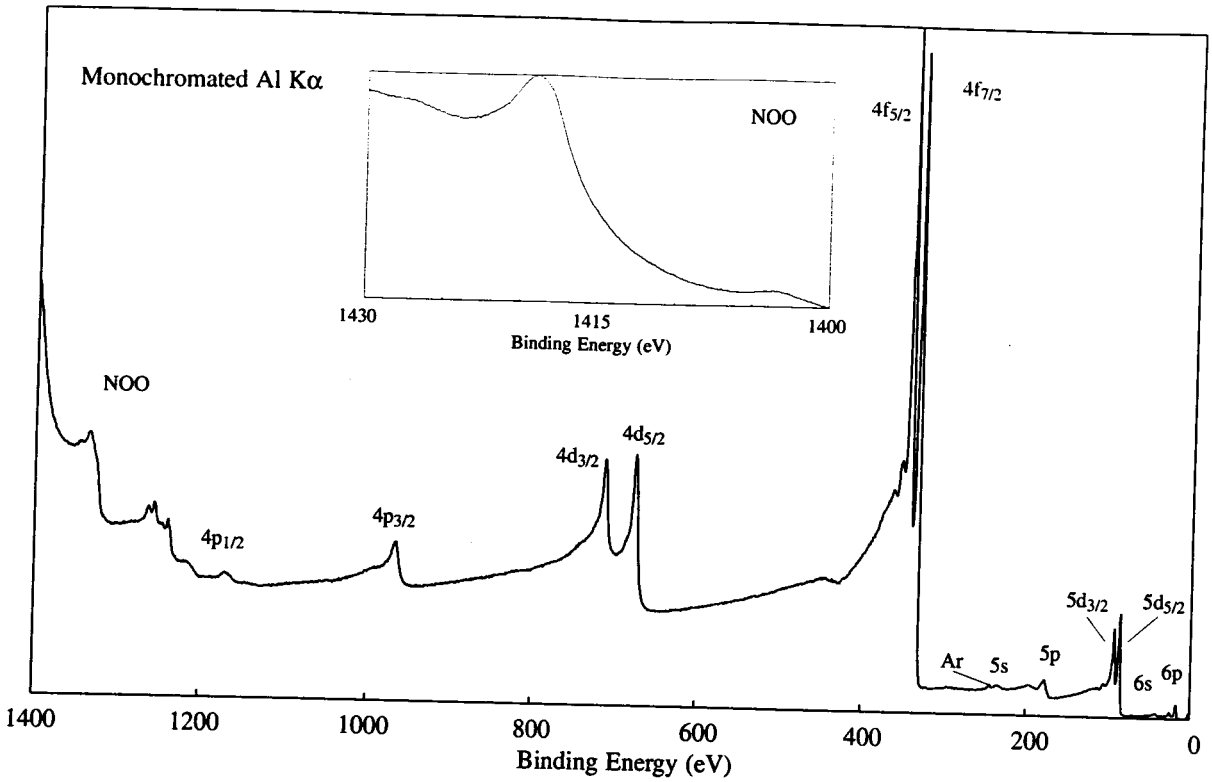
*Estimate

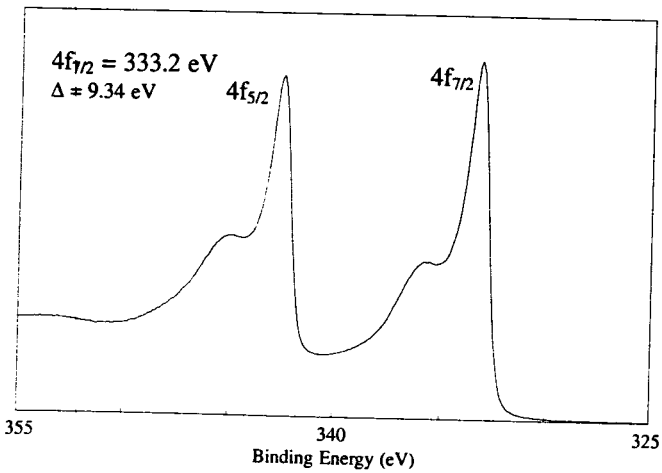
Bismuth Bi
Atomic Number 83











Line Positions (eV)

Photoelectron Lines

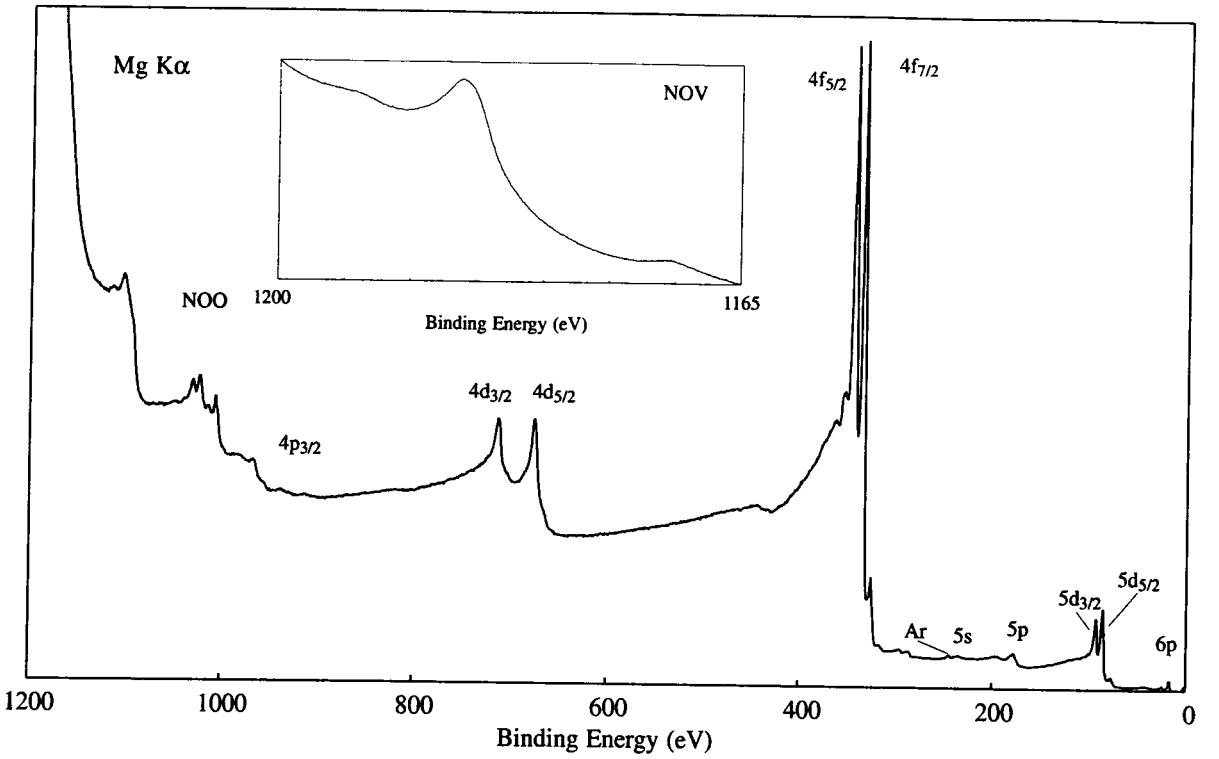
4s*	4p1/2	4p3/2	4d3/2	4d5/2	4f5/2	4f7/2	
1330	1170	965	713	676	342	333	
5s	5p1/2	5p3/2	5d3/2	5d5/2	6s	6p1/2	6p3/2
294	234	177	93	85	42	25	17

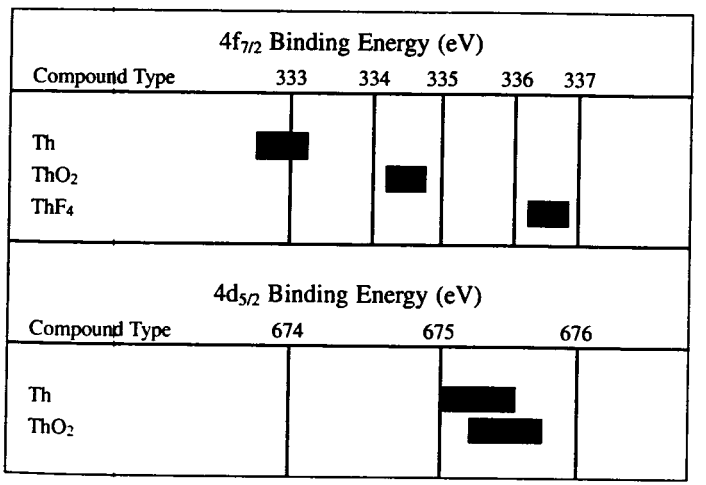
Auger Lines

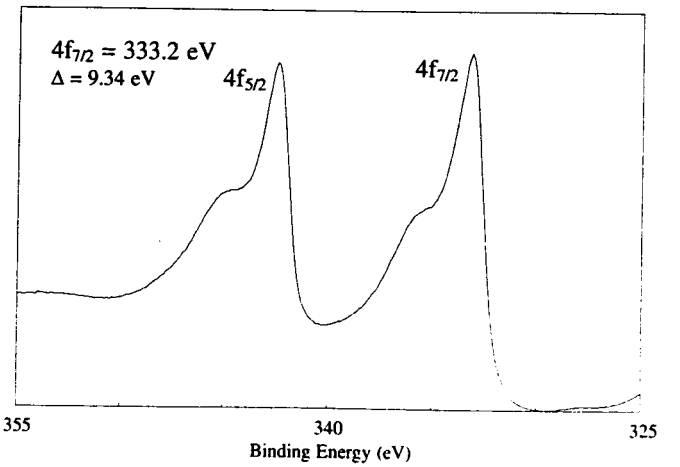
$N_6O_{23}V$	$N_{67}O_{45}O_{45}$	$N_7O_4O_5$	$N_{67}O_{45}V$	
1419	1404	1335	1239	(Al)
1186	1171	1102	1006	(Mg)

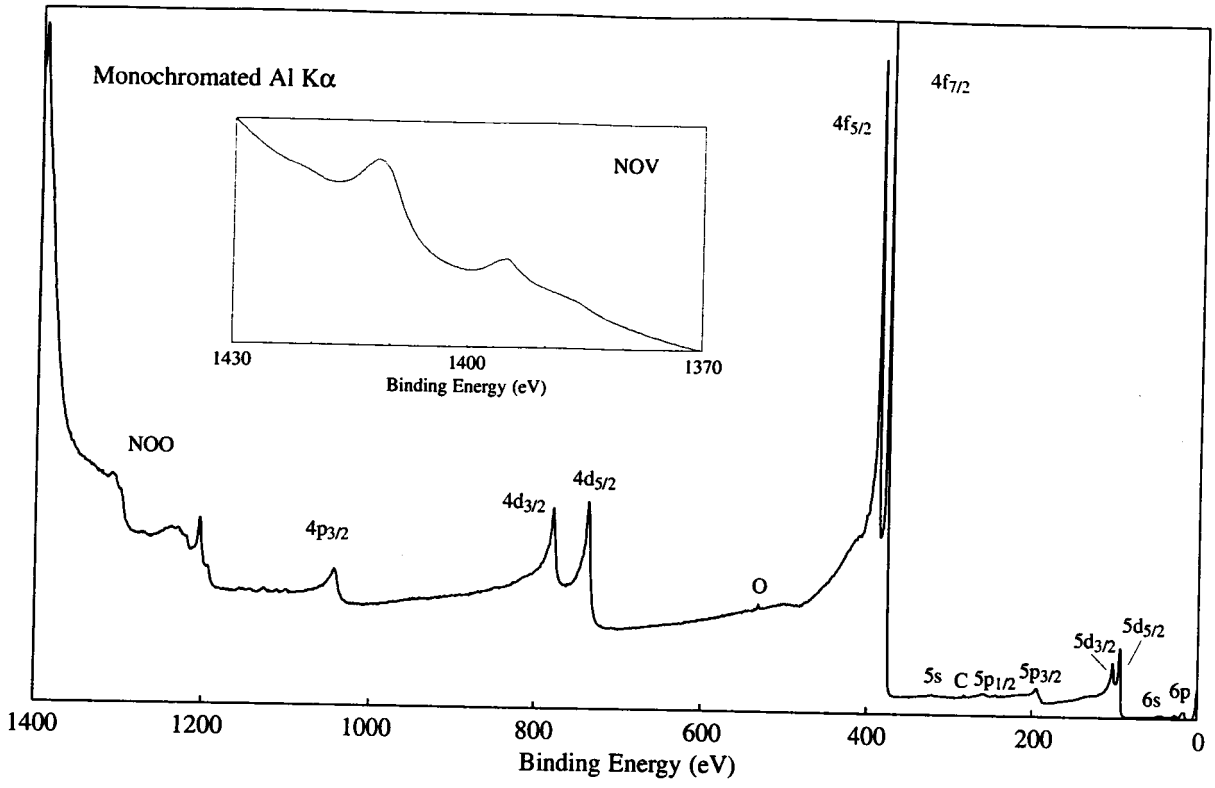
*Estimate

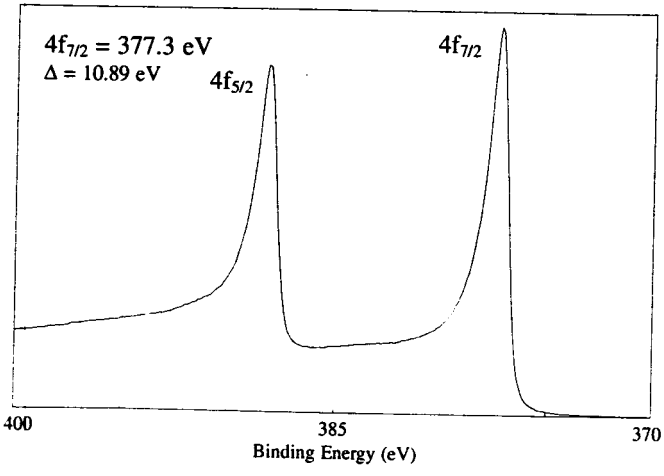
Thorium Th
Atomic Number 90











Line Positions (eV)

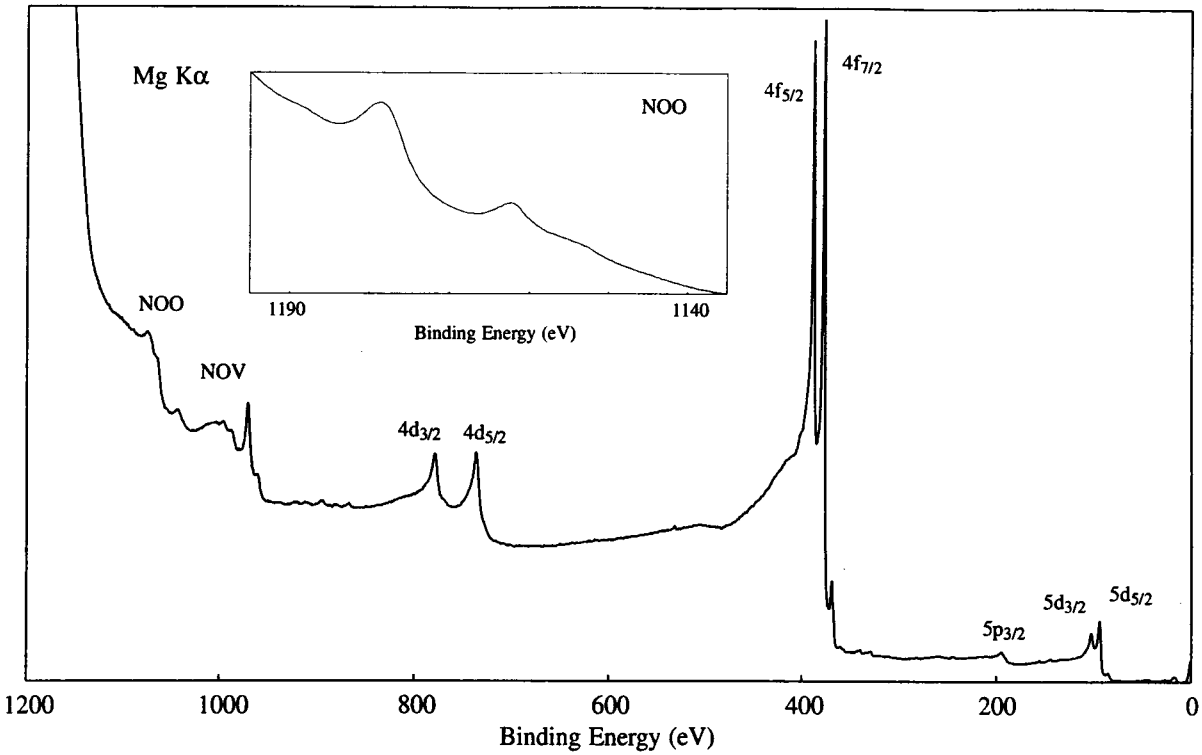
Photoelectron Lines

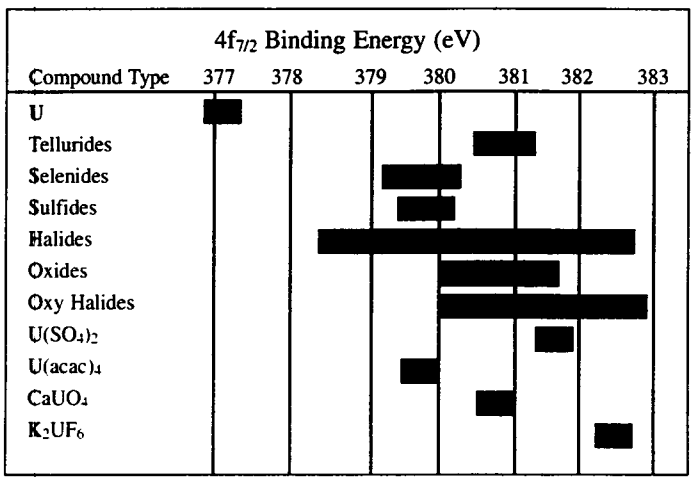
4p1/2	4p3/2	4d3/2	4d5/2	4f5/2	4f7/2		
1272	1043	779	736	388	377		
5s	**5p1/2**	**5p3/2**	**5d3/2**	**5d5/2**	**6s**	**6p1/2**	**6p3/2**
322	260	195	103	94	44	26	17

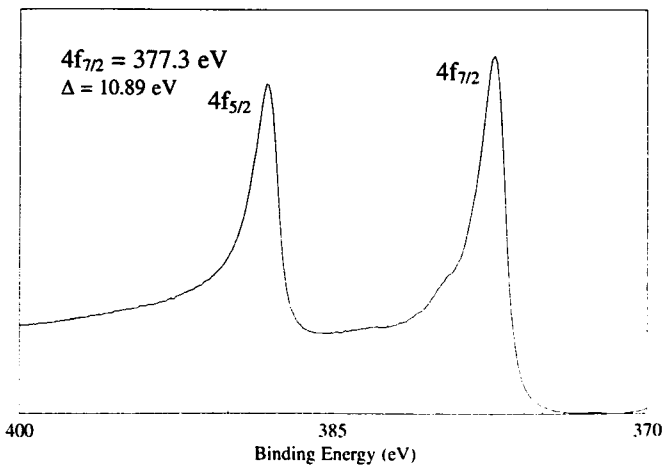
Auger Lines

$N_6O_{23}V$	$N_7O_{23}O_5$	$N_6O_{45}O_{45}$	$N_{67}O_{45}V$	
1412	1396	1386	1204	(Al)
1179	1163	1153	971	(Mg)

Uranium U
Atomic Number 92







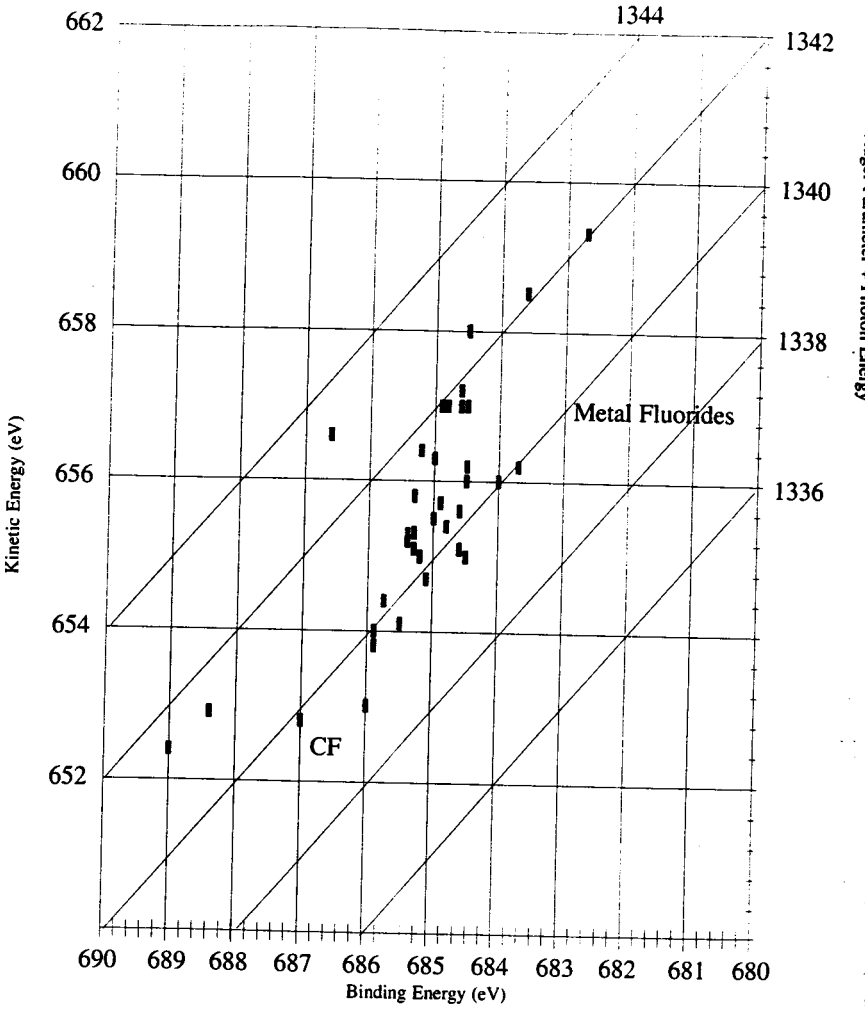
III. Appendix

Appendix A. Auger Parameters

The following tables plot the binding energy of the most intense photoelectron line versus the kinetic energy of the most intense Auger transition. The Auger parameter plots are useful for further separation of the chemical states.

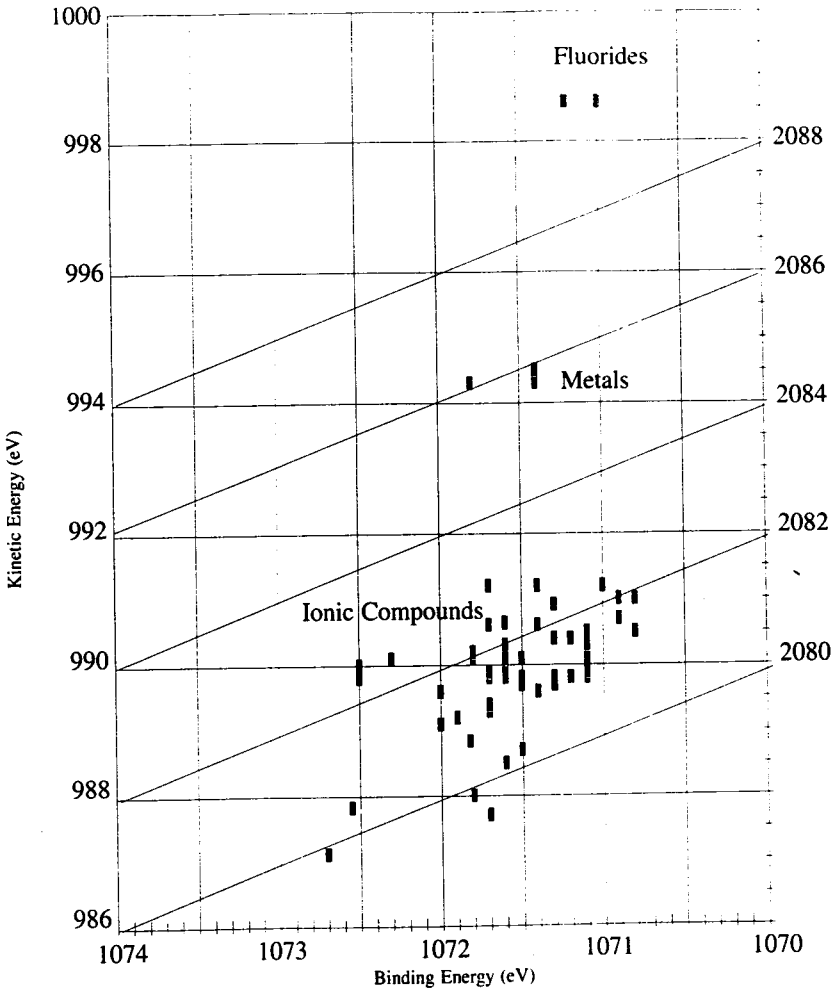
Fluorine

Compound	F 1s Binding Energy (eV)	F KLL Kinetic Energy (eV)
AgF	682.7	659.3
PbF_2	683.6	658.5
BaF_2	683.7	656.2
K_3FeF_6	684.0	656.0
NaF	684.5	655.0
CdF_2	684.5	656.0
CuF_2	684.5	657.0
CuF_2	684.5	656.2
CuF_2	684.5	656.2
LaF_3	684.5	658.0
ZnF_2	684.6	655.6
PrF_3	684.6	657.2
SmF_3	684.6	657.0
K_2ZrF_6	684.6	655.1
CaF_2	684.8	655.4
NdF_3	684.8	657.0
ThF_4	684.9	657.0
K_2TiF_6	684.9	655.7
SrF_2	685.0	656.3
NiF_2	685.0	655.5
LiF	685.1	654.7
InF_3	685.2	656.4
K_2TaF_7	685.2	655.0
YF_3	685.3	655.8
Na_2TiF_6	685.3	655.1
$NaSnF_3$	685.3	655.3
HfF_4	685.4	655.3
K_2NbF_7	685.4	655.2
Na_3AlF_6	685.5	654.1
MgF_2	685.8	654.4
CsF	685.9	653.8
Na_2GeF_6	685.9	654.0
Na_2SiF_6	686.0	653.0
$KSbF_6$	686.6	656.6
$NaBF_4$	687.0	652.8
$NiOOCCF_3$	688.4	652.9
p-(CF_2=CF_2)	689.0	652.4



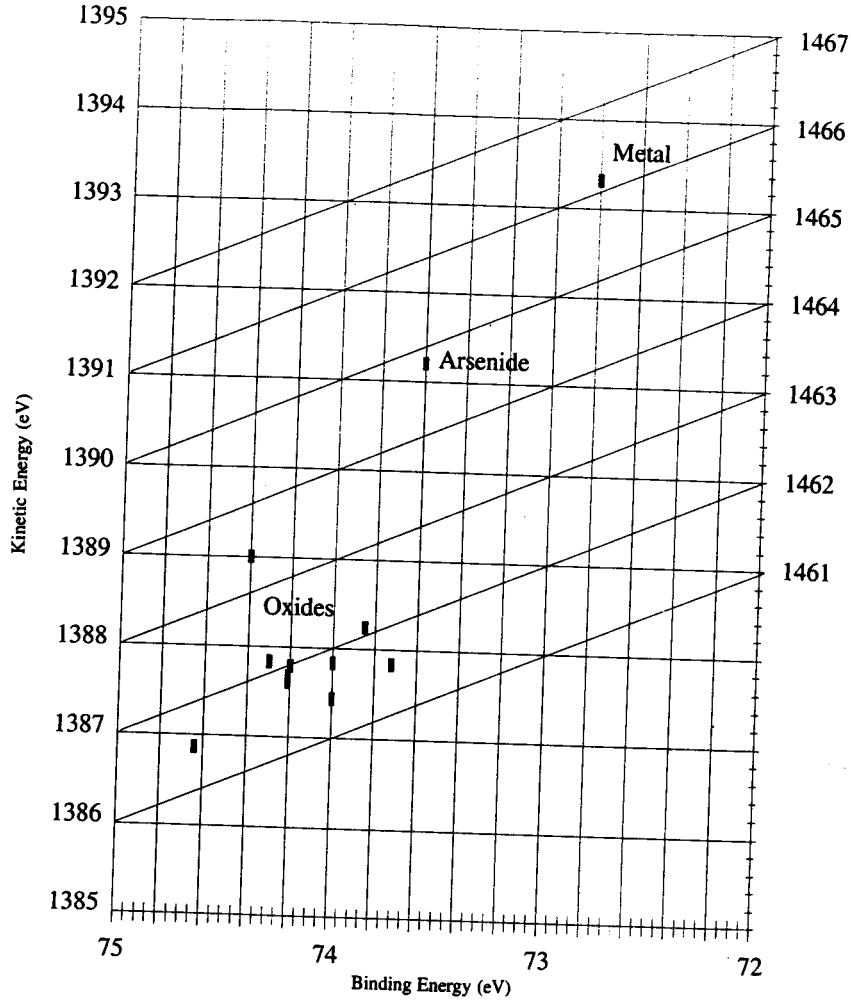
Sodium

Compound	Na 1s Binding Energy (eV)	Na KLL Kinetic Energy (eV)
Na_2SeO_3	1070.8	991.0
$Na_2C_2O_4$	1070.8	990.5
Na_2MoO_4	1070.9	991.0
$NaAsO_2$	1070.9	990.7
NaF	1071.0	998.6
Na_2CrO_4	1071.0	991.2
Na_3PO_4	1071.1	990.1
NaH_2PO_2	1071.1	989.8
$Na_2SnO_3 \cdot 3H_2O$	1071.1	990.3
NaOAc	1071.1	989.9
NaF	1071.2	998.6
Na_2SO_4	1071.2	989.8
$NaOOCCH_2SH$	1071.2	990.4
Na_2SO_3	1071.3	990.4
Na	1071.4	994.3
Na	1071.4	994.5
NaBr	1071.4	990.6
$NaNO_3$	1071.4	989.6
Na_2CrO_4	1071.4	991.2
NaCl	1071.5	990.1
Na_2CO_3	1071.5	989.8
Na_2HPO_4	1071.5	989.7
$Na_2S_2O_3$	1071.6	990.1
$NaNO_2$	1071.6	989.8
$Na_2Cr_2O_7$	1071.6	990.6
NaI	1071.7	991.2
NaBr	1071.7	990.6
Na_2CO_3	1071.7	989.8
NaOAc	1071.7	989.9
Na	1071.8	994.3
NaCl	1071.8	990.1
NaCl	1072.5	990.0
Na_2O	1072.5	989.8
Mol Sieve Y	1072.6	987.8
$NaBF_4$	1072.7	987.1



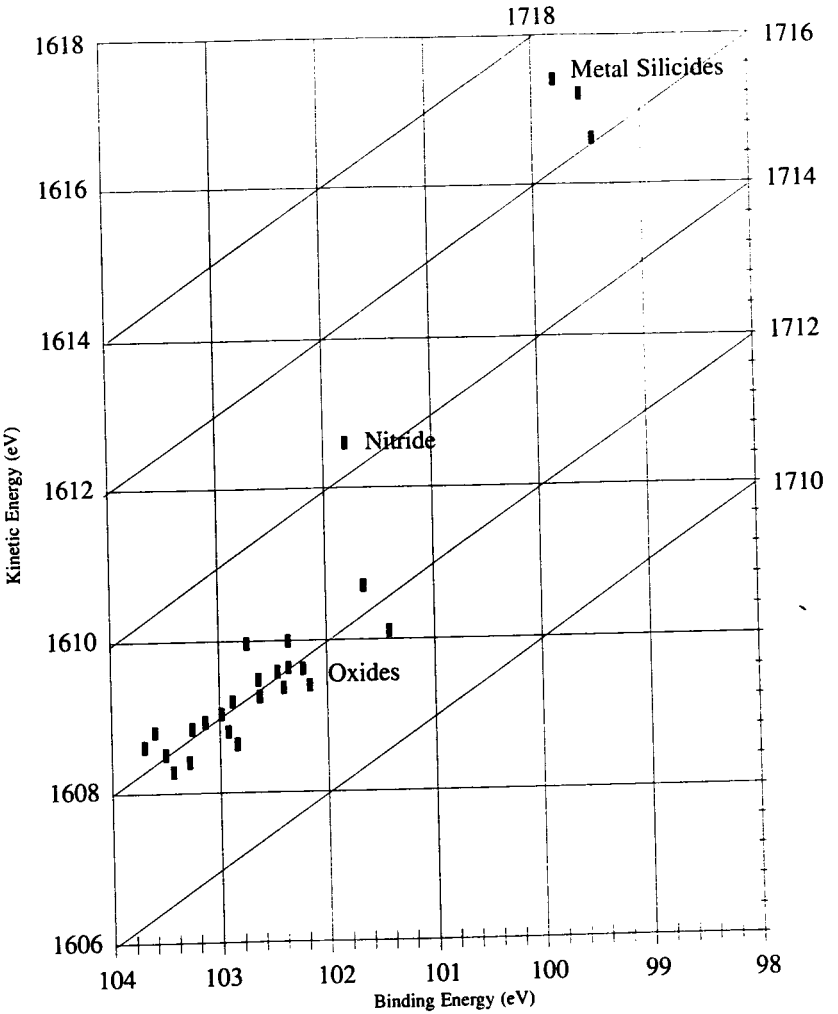
Aluminum

Compound	Al 2p Binding Energy (eV)	Al KLL Kinetic Energy (eV)
Al	72.8	1393.3
AlAs	73.6	1391.2
Al_2O_3, gamma	73.7	1387.8
Al_2O_3, alpha	73.9	1388.2
Al_2O_3, gamma	74.0	1387.8
$Al(OH)_3$, gibbsite	74.0	1387.4
Al_2O_3, sapphire	74.2	1387.8
AlOOH, boehmite	74.2	1387.6
$Al(OH)_3$, bayerite	74.2	1387.7
Al_2O_3, gamma	74.3	1387.8
AlN	74.4	1389.0
Al_2SiO_5, sillimanite	74.6	1386.9



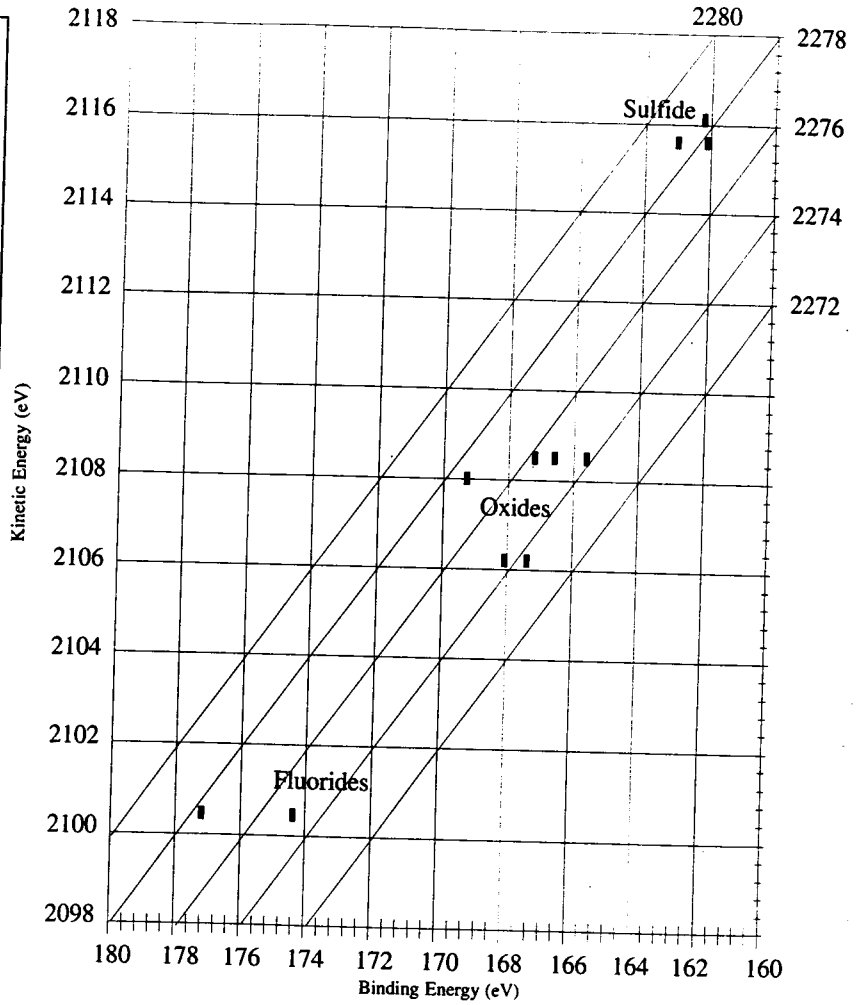
Silicon

Compound	Si 2p Binding Energy (eV)	Si (KLL) Kinetic Energy (eV)
Si	99.5	1616.6
$MoSi_2$	99.6	1617.2
PdSi	99.8	1617.4
Mol Sieve A	101.4	1610.1
Hydroxysodalite	101.7	1610.7
Si_3N_4	101.8	1612.6
Mol Sieve X	102.2	1609.4
Natrolite	102.2	1609.6
Mica, muscovite	102.4	1609.6
Wollastonii, $Ca_3Si_3O_9$	102.4	1610.0
p-Methylsil. (linear)	102.4	1609.4
$LiAlSi_2O_6$, spodumene	102.5	1609.6
$NaAlSi_3O_8$, albite	102.6	1609.2
$AlSiO_5$, sillimanite	102.6	1609.5
p-Phenylsil. (resin)	102.7	1610.0
Mol Sieve Y	102.8	1608.7
Pyrophyllite	102.9	1609.2
p-Methylsil. (resin)	102.9	1608.8
Kaolinite	103.0	1609.0
Talc, $Mg_3Si_4O_{10}(OH)_2$	103.1	1608.9
SiO_2, alpha cristobal	103.3	1608.8
H Zeolon	103.3	1608.4
SiO_2, gel	103.4	1608.3
SiO_2, Vycor	103.5	1608.5
SiO_2	103.6	1608.8
SiO_2, quartz	103.7	1608.6



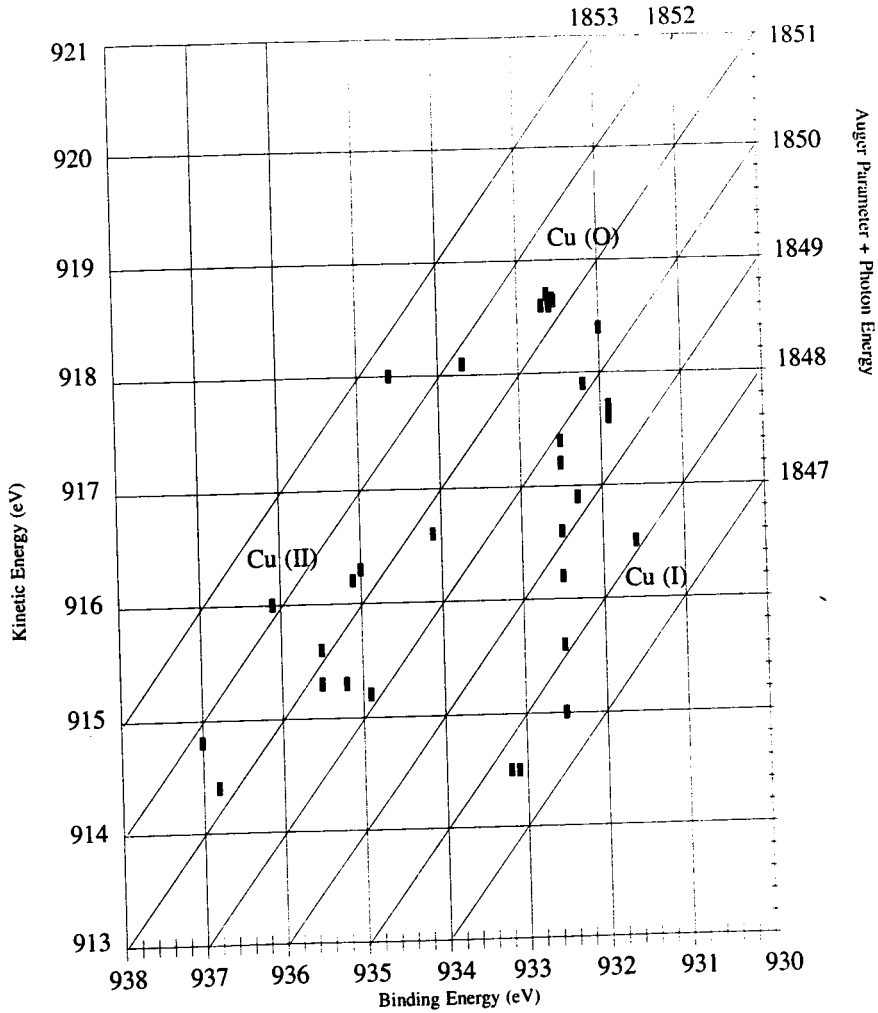
Sulfur

Compound	S 2p Binding Energy (ev)	S KLL Kinetic Energy (eV)
WS_2	162.1	2115.6
NiS	162.2	2116.1
WS_2	163.0	2115.6
Na_2SO_3	165.6	2108.5
Na_2SO_3	166.6	2108.5
Na_2SO_3	167.2	2108.5
SO_2	167.4	2106.2
SO_2	168.1	2106.2
$CuSO_4$	169.3	2108.0
SF_6	174.4	2100.5
SF_6	177.2	2100.5



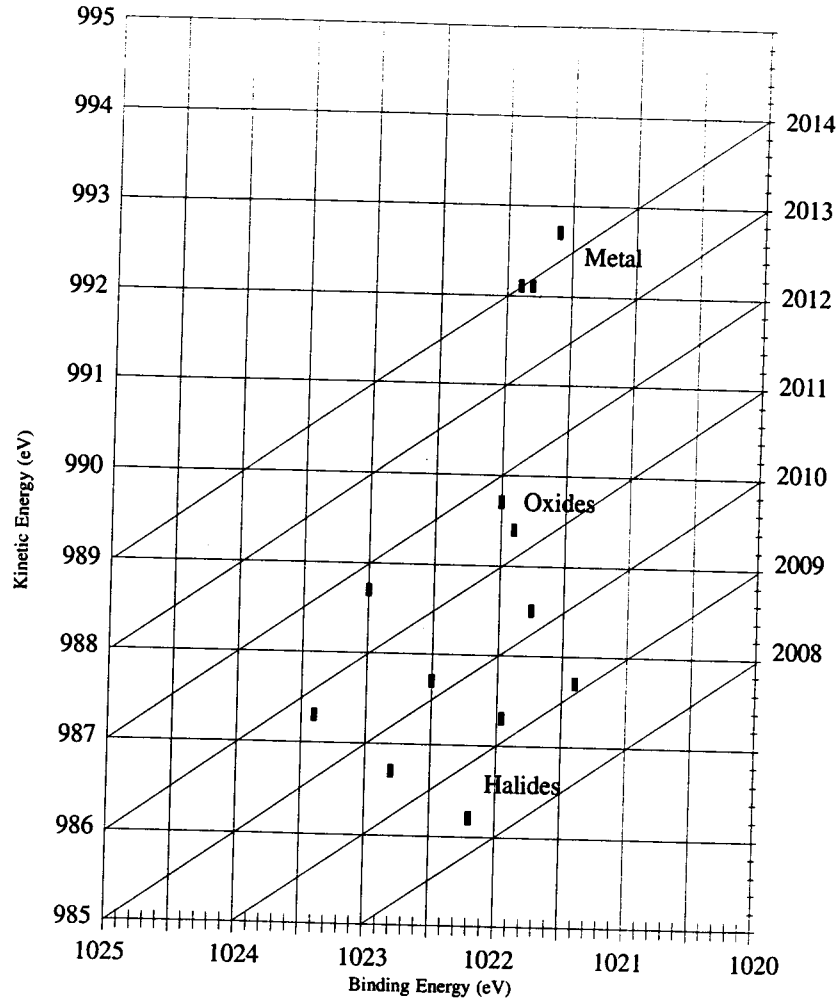
Copper

Compound	Cu 2p Binding Energy (eV)	Cu LMM Kinetic Energy (eV)
$Cu_2Mo_3O_{10}$	931.6	916.5
Cu_2Se	931.9	917.6
CuAgSe	931.9	917.7
CuSe	932.0	918.4
CuS	932.2	917.9
$CuBr_2$	932.3	916.9
Cu_2S	932.5	917.4
CuCl	932.5	915.0
CuCl	932.5	915.6
Cu_2O	932.5	916.2
Cu_2O	932.5	916.2
Cu_2O	932.5	916.6
Cu_2O	932.5	917.2
Cu	932.6	918.6
Cu	932.6	918.7
$Cu_{64}Zn_{36}$	932.6	918.6
Cu	932.6	918.6
Cu	932.6	918.7
Cu	932.7	918.6
CuCN	933.1	914.5
$CuC(CN)_3$	933.2	914.5
CuO	933.7	918.1
$Cu_3Mo_2O_9$	934.1	916.6
$CuMoO_4$	934.1	916.6
$CuCr_2O_4$	934.6	918.0
$CuSiO_3$	934.9	915.2
$CuCO_3$	935.0	916.3
$Cu(OH)_2$	935.1	916.2
$CuCl_2$	935.2	915.3
$Cu(NO_3)_2$	935.5	915.3
$CuSO_4$	935.5	915.6
CuF_2	936.1	916.0
CuF_2	936.8	914.4
CuF_2	937.0	914.8



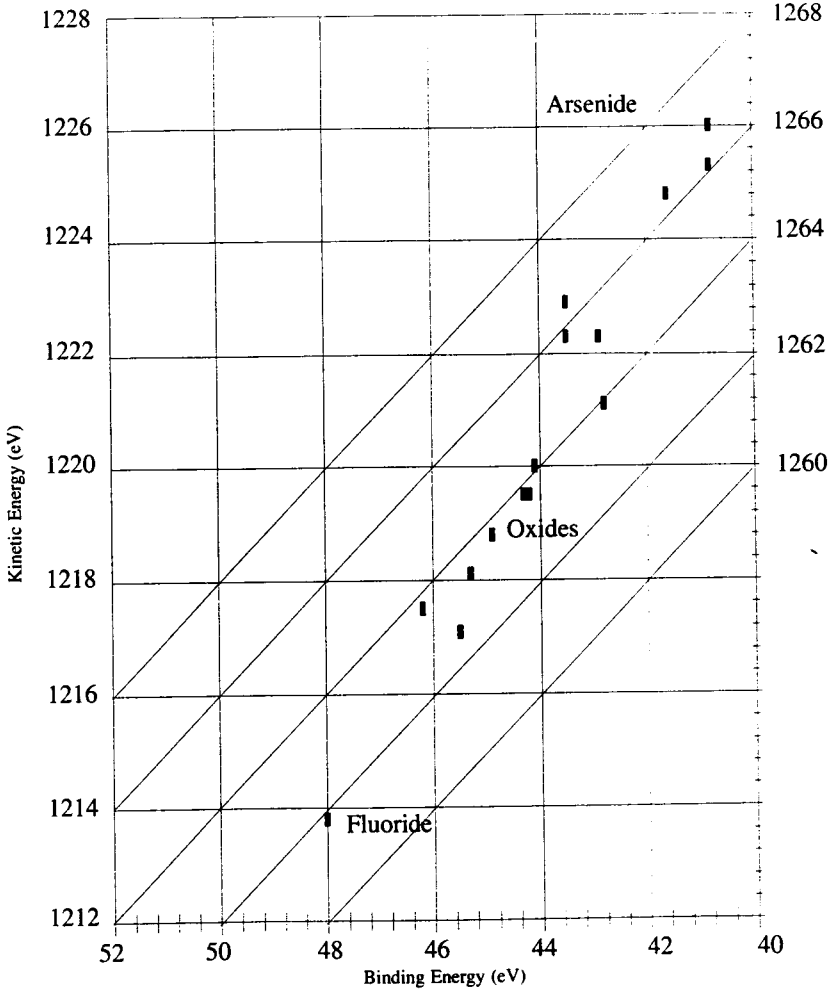
Zinc

Compound	Zn $2p_{3/2}$ Binding Energy (eV)	Zn LMM Kinetic Energy (eV)
$Zn(acac)_2$	1021.4	987.7
$Cu_{64}Zn_{36}$	1021.6	992.7
ZnO	1021.75	988.5
Zn	1021.8	992.1
Zn	1021.89	992.1
$ZnCl_2$	1021.9	989.4
$Zn_4Si_2O_7(OH)_2 \cdot 2H_2O$	1021.96	987.3
ZnS	1022	989.7
ZnF_2	1022.2	986.2
ZnO	1022.5	987.7
ZnF_2	1022.8	986.7
ZnI_2	1023	988.7
$ZnBr_2$	1023.4	987.3



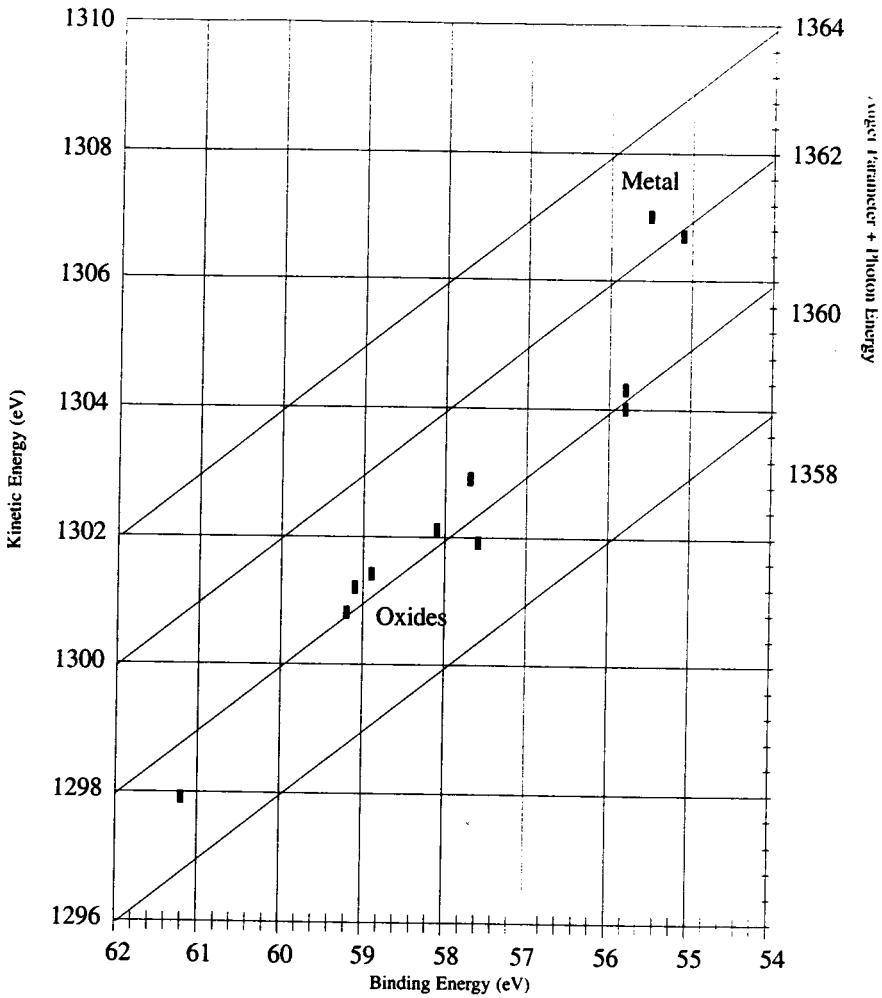
Arsenic

Compound	As 3d Binding Energy (eV)	As LMM Kinetic Energy (eV)
NbAs	40.8	1226.0
GaAs	40.8	1225.3
As	41.6	1224.8
Ph_3As	42.8	1221.1
As_2Se_3	42.9	1222.3
AsI_3	43.5	1222.9
$MeAsI_2$	43.5	1222.3
Ph_3AsS	44.1	1220.0
$NaAsO_2$	44.2	1219.5
Ph_3AsO	44.3	1219.5
As_2O_3	44.9	1218.8
$AsBr_3$	45.3	1218.1
NaH_2AsO_4	45.5	1217.1
As_2O_5	46.2	1217.5
$KAsF_6$	48.0	1213.8



Selenium

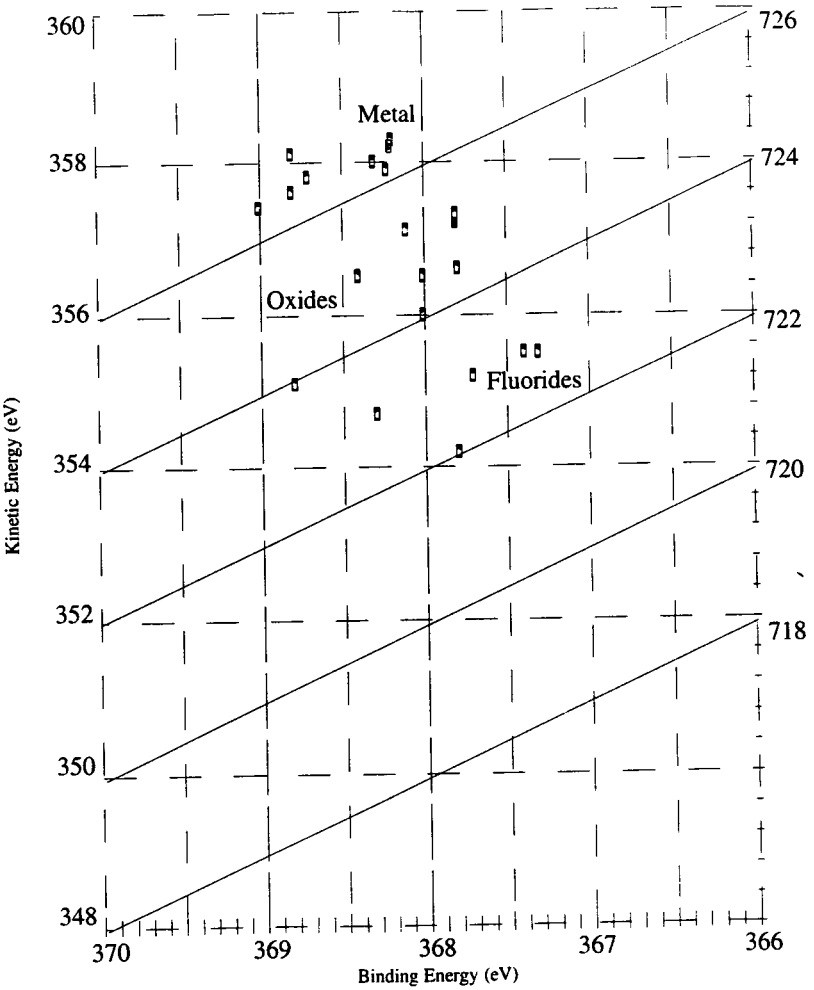
Compound	Se 3d Binding Energy (eV)	Se LMM Kinetic Energy (eV)
Se	55.1	1306.7
Se	55.5	1307.0
Ph_2Se	55.8	1304.0
Ph_2Se_2	55.8	1304.3
Ph_2SeO	57.6	1301.9
Cl_2SePh_2	57.7	1302.9
I_2SePh_2	58.1	1302.1
SeO_2	58.9	1301.4
Na_2SeO_3	59.1	1301.2
H_2SeO_3	59.2	1300.8
H_2SeO_4	61.2	1297.9



Silver

Compound	Ag 3d Binding Energy (eV)	Ag $M_4N_5N_5$ Kinetic Energy (eV)
AgF_2	367.3	355.6*
AgO	367.4	355.5
AgF	367.7	355.3*
CuAgSe	367.8	357.3*
Ag_2Se	367.8	357.4*
Ag_2O	367.8	356.6
Ag_2SO_4	367.8	354.2
AgI	368.0	356.1*
AgO	368.0	356.6*
Ag_2S	368.1	357.2*
Ag	368.2	358.2
Ag	368.2	357.9
$Mg_{21}Ag_{79}$	368.3	358.1*
Ag_2SO_4	368.3	354.7
Ag_2O	368.4	356.6*
$Mg_{30}Ag_{50}$	368.7	357.9*
$Al_{40}Ag_{60}$	368.8	357.7*
$Mg_{97}Ag_3$	368.8	358.2*
$AgOOCCF_3$	368.8	355.1
$Al_{95}Ag_5$	369.0	357.5*

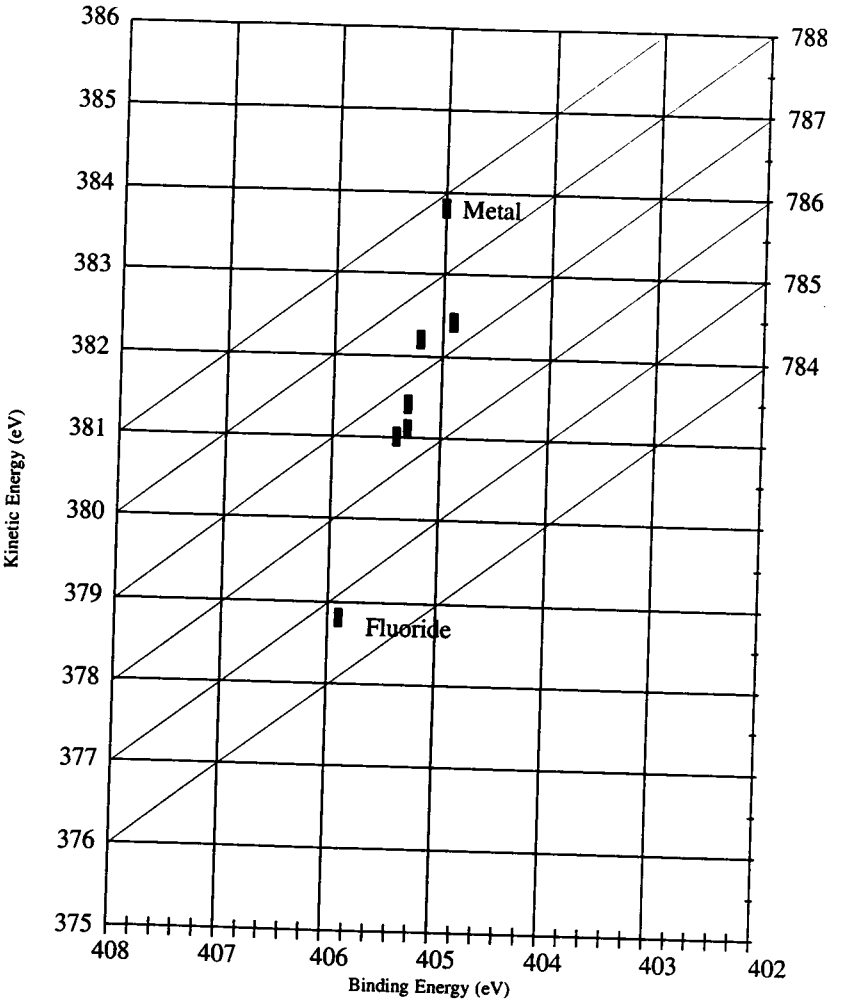
* 6.0 eV added to the kinetic energy data on $M_5N_5N_5$ to obtain kinetic energy of $M_4N_5N_5$ line.



Auger Parameter + Photon Energy

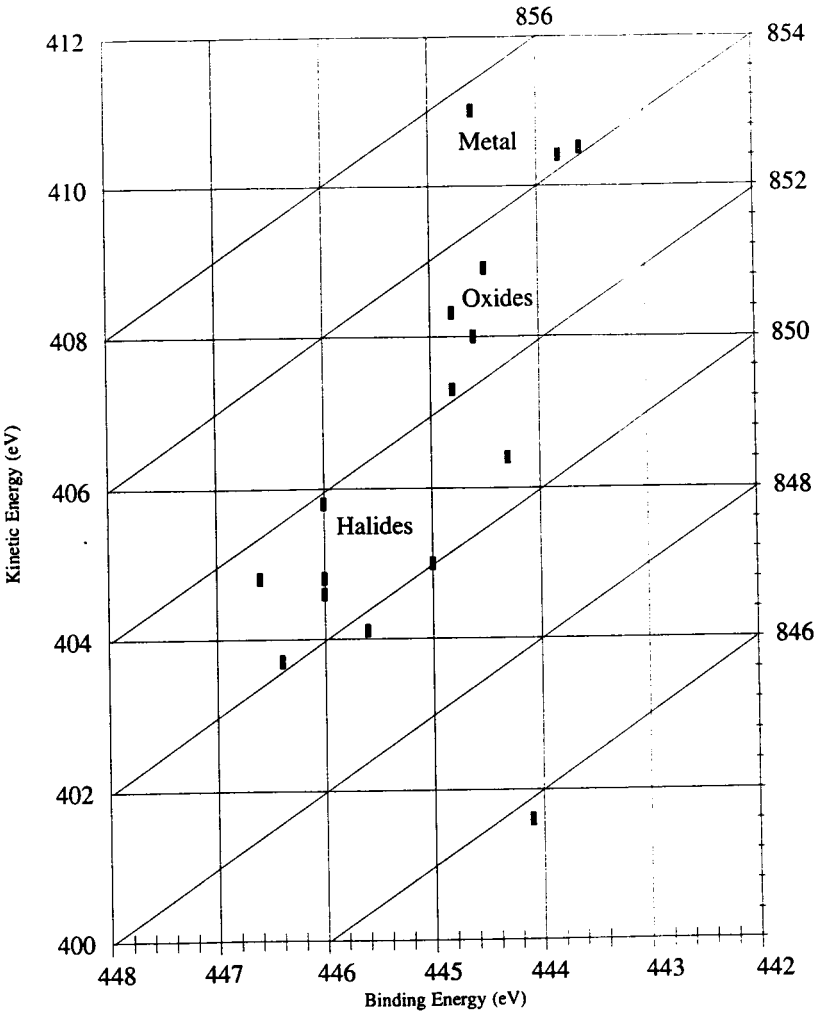
Cadmium

Compound	Cd $3d_{5/2}$ Binding Energy (eV)	Cd MNN Kinetic Energy (eV)
CdTe	404.9	382.4
Cd	405.0	383.8
CdO	405.2	382.2
CdSe	405.3	381.4
CdS	405.3	381.1
CdI_2	405.4	381.0
CdF_2	405.9	378.8



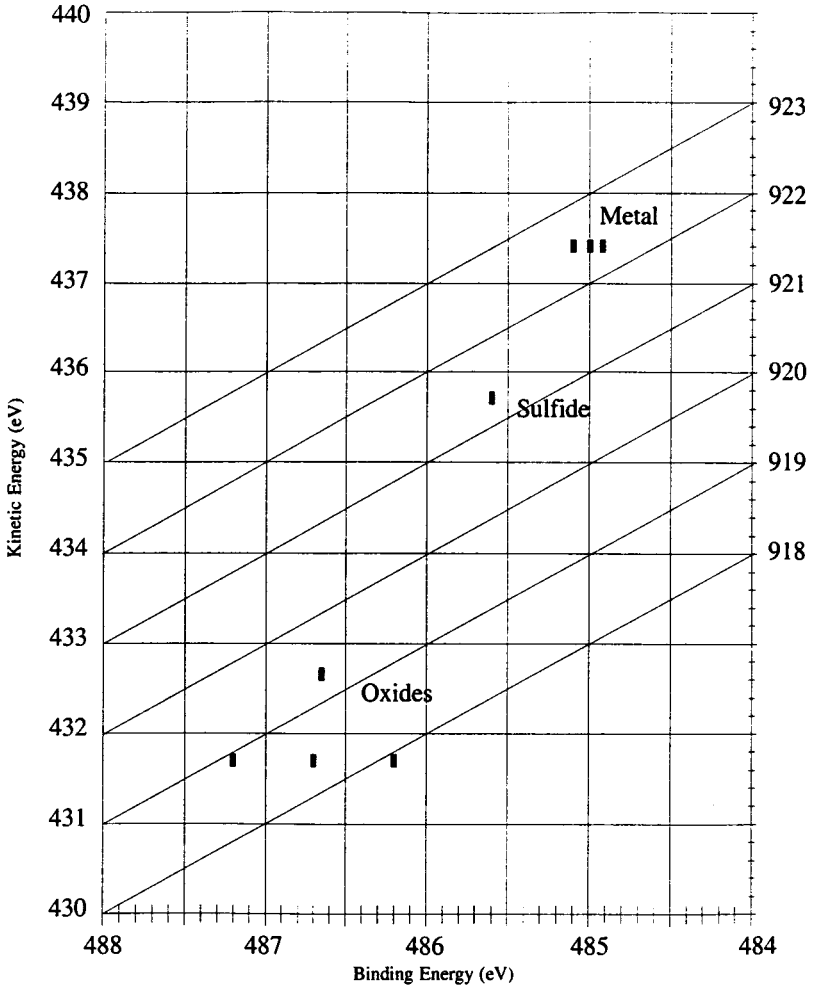
Indium

Compound	In 3d5/2 Binding Energy (eV)	In MNN Kinetic Energy (eV)
$In_{95}Sn_5$	443.6	410.5
In	443.8	410.4
InSb	444.1	401.6
In_2O_3	444.3	406.4
In_2Te_3	444.5	408.9
InP	444.6	408.0
InP	444.6	411.0
In_2Se_3	444.8	408.3
In_2S_3	444.8	407.3
$In(OH)_3$	445.0	405.0
$(NH_4)_3InF_6$	445.6	404.1
InI_3	446.0	405.8
$InBr_3$	446.0	404.8
$InCl_3$	446.0	404.6
InF_3	446.4	403.7
$InBr_3$	446.6	404.8



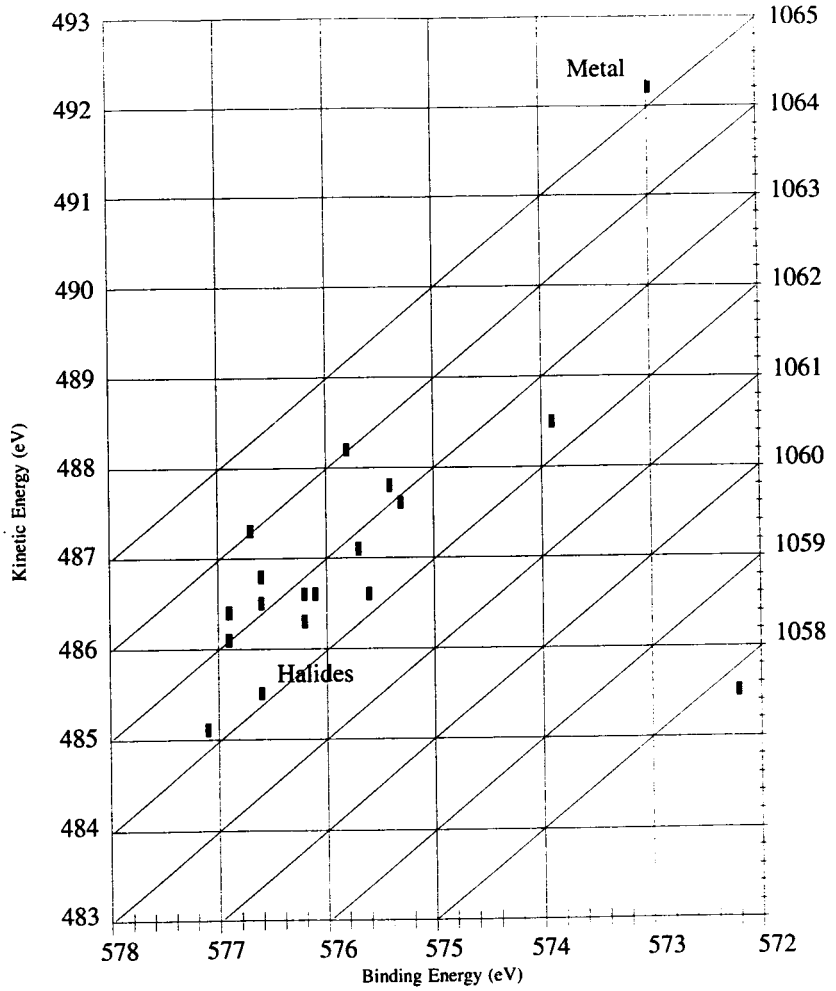
Tin

Compound	Sn 3d5/2 Binding Energy (eV)	Sn MNN Kinetic Energy (eV)
Sn	484.9	437.4
Sn	485.0	437.4
Sn	485.1	437.4
SnS	485.6	435.7
Na_2SnO_3	486.2	431.7
SnO_2	486.7	432.7
Na_2SnO_3	486.7	431.7
Na_2SnO_3	487.2	431.7
$NaSnF_3$	487.4	430.8



Tellurium

Compound	Te $3d_{5/2}$ Binding Energy (eV)	Te MNN Kinetic Energy (eV)
Na_2Te	572.2	485.5
Te	573.0	492.2
Ph_2Te_2	573.9	488.5
I_2TeEt_2	575.3	487.6
I_2TePh_2	575.4	487.8
I_2TeMe_2	575.6	486.6
TeO_2	575.7	487.1
I_3TePh	575.8	488.2
p-tolylTeOOH	576.1	486.6
Cl_2TePh_2	576.2	486.3
Br_2TePh_2	576.2	486.6
TeO_3	576.6	485.5
Br_3TePh	576.6	486.8
Br_3TeBu	576.6	486.5
$TeBr_2$	576.7	487.3
$TeCl_4$	576.9	486.1
$(NH_4)_2TeCl_6$	576.9	486.4
$Te(OH)_6$	577.1	485.1



Appendix B. Chemical States Tables

This compilation of all the elements, listed alphabetically, provides specific binding energies of various compounds and pure elements, and a reference in abbreviated notation. When Auger lines are listed, they are in kinetic energy. For compounds with more than one chemical state, an asterisk denotes the atom whose binding energy is listed. The references are expanded in Appendix C. Any listing with a Φ refers to the work contained in this handbook.

This appendix, most of which was compiled by Dr. Charles Wagner for Physical Electronics, is part of the chemical state identification algorithm of the PHI software and is also the basis for the XPS database SRD-20 of the National Institute for Standards and Technology (NIST). Further references may also be found in the journal Surface Science Spectra *published by the American Vacuum Society.*

Ag 3d

Ag	368.3	Φ
Ag	368.2	Asam76
Ag	368.2	BiSw80
Ag	368.1	BiSw80
Ag	368.2	BiSw80
Ag	368.2	JHBK73
Ag	368.2	NyMa80
Ag	368.2	HGW75, Scho73, WRDM79, GaWi77, SFS77, Wagn75
Ag	368.2	RRD78, Scho72
$Ag_{95}Sn_5$	368.0	HSBS81
$Al_{40}Ag_{60}$	368.8	WeAn80
$Al_{95}Ag_5$	369.0	WeAn80
$Mg_{21}Ag_{79}$	368.3	WeAn80
$Mg_{30}Ag_{50}$	368.7	WeAn80
$Mg_{97}Ag_3$	368.8	WeAn80
Ag_2Yb	368.8	WWC78
CuAgSe	367.8	RRD78
Ag_2Se	367.8	RRD78
Ag_2S	368.1	RRD78
AgI	368.0	GaWi77
AgF	367.7	GaWi77
AgF_2	367.3	GaWi77
Ag_2O	367.8	HGW75, GaWi77, Scho73
Ag_2O	368.4	RRD78
AgO	367.4	HGW75, GaWi77, Scho73
AgO	368.0	WRDM79
Ag_2CO_3	367.5	HGW75
Ag_2SO_4	367.8	TMR80
Ag_2SO_4	368.3	Wagn75
$AgOOCCF_3$	368.8	Wagn75
Ag(OAc)	368.4	HHDD81
$Ag(3\text{-Cl-pyridin})_2NO_3$	368.6	SmWa77

Ag $M_4N_5N_5$

Ag	357.9	WRDM79
Ag	358.2	Wagn75
Ag ($M_5N_5N_5$)	351.9	RRD 78, PWA 79
Ag ($M_5N_5N_5$)	351.6	GaWi77
Ag	358.3	Scho73, FKWF77
Al_4OAg_{60} ($M_5N_5N_5$)	351.7	WeAn80
$Al_{95}Ag_5$ ($M_5N_5N_5$)	351.5	WeAn80
$Mg_{21}Ag_{79}$ ($M_5N_5N_5$)	352.1	WeAn80
$Mg_{30}Ag_{50}$ ($M_5N_5N_5$)	351.9	WeAn80
$Mg_{97}Ag_3$ ($M_5N_5N_5$)	352.2	WeAn80
CuAgSe ($M_5N_5N_5$)	351.3	RRD78
Ag_2Se($M_5N_5N_5$)	351.4	RRD78
Ag_2S($M_5N_5N_5$)	351.2	RRD78
AgI($M_5N_5N_5$)	350.1	GaWi77
AgF($M_5N_5N_5$)	349.3	GaWi77
AgF_2($M_5N_5N_5$)	349.6	GaWi77
Ag_2O	356.6	Scho73
Ag_2O($M_5N_5N_5$)	350.6	RRD78, GaWi77
AgO	355.5	WRDM79
AgO($M_5N_5N_5$)	350.6	GaWi77
Ag_2SO_4	354.2	Wagn75
Ag_2SO_4	354.7	TMR80
$AgOOCCF_3$	355.1	Wagn75

Al 2p

Al	72.9	Φ
Al_2O_3, sapphire	74.4	Φ
Al	72.8	LMKJ75, Tayl82, WPHK82, WRDM79, WaTa80
AlB_2	71.9	MECC73
AlAs	73.6	Tayl82
AlGaAs	73.6	Tayl82
Fe_3Al	73.4	ShTr75
$LiAlH_4$	75.6	MSC73
AlN	74.4	MSC73
Al_2S_3	74.6	MSC73
AlI_3	74.6	MSC73
$AlBr_3$	75.2	MSC73
$AlCl_3$	74.7	MSC73
AlF_3	76.3	MSC73
$Al_2(MoO_4)_3$	74.2	PCLH76
$Al_2(WO_4)_3$	74.3	NgHe76
$CoAl_2O_4$	73.6	PCLH76
$MgAl_2O_4$	74.7	HNUW78
$NiAl_2O_4$	74.2	LFWS79, NgHe76
Al_2O_3	74.3	Nefe82, MSC73, NSLS77
Al_2O_3	74.7	KlHe83, NGDS75
Al_2O_3, sapphire	74.2	Tayl82, WPHK82
Al_2O_3, alpha	73.9	WPHK82
Al_2O_3, gamma	73.7	WPHK82
Al_2O_3, gamma	74.0	Barr83
Al_2O_3, gamma	74.3	NgHe76
AlO_2H, boehmite	74.2	Tayl82, WPHK82
$Al(OH)_3$, bayerite	74.2	Tayl82, WPHK82
$Al(OH)_3$, gibbsite	74.0	WPHK82
Al_2SiO_5, kyanite	74.7	AnSw74
Al_2SiO_5, mullite	74.8	AnSw74
Al_2SiO_5, sillimanite	74.6	AnSw74, WPHK82
Albite, $NaAlSi_3O_8$	74.3	WPHK82

Bentonite	75.0	Barr83
Kaolinite	74.6	Barr83, WPHK82
Mica, muscovite	74.3	WPHK82
Natrolite	74.3	WPHK82
Pyrophyllite	74.7	WPHK82
Spodumene	74.3	WPHK82
H Zeolon	74.8	WPHK82
Hydroxysodalite	75.0	WPHK82
Mol Sieve A	73.6	WPHK82, Barr83
$Al(acac)_3$	72.9	MSC73

Al KLL

Al	1393.3	WPHK82, WaTa80
AlAs	1391.2	Tayl82
AlN	1389.0	TaRa81
Al_2O_3, sapphire	1387.8	Tayl82, WPHK82
Al_2O_3, alpha	1388.2	WPHK82
Al_2O_3, gamma	1387.8	WPHK82
AlOOH	1387.6	WPHK82, Tayl82
$Al(OH)_3$, bayerite	1387.7	WPHK82, Tayl82
$Al(OH)_3$, gibbsite	1387.4	WPHK82
Al_2SiO_5, sillimanite	1386.9	WPHK82
Albite, $NaAlSi_3O_8$	1386.5	WPHK82
Kaolinite	1386.7	WPHK82
Mica, muscovite	1387.1	WPHK82
Natrolite	1386.5	WPHK82
Pyrophyllite	1386.8	WPHK82
Spodumene	1387.1	WPHK82
H Zeolon	1385.5	WPHK82
Hydroxysodalite	1386.4	WPHK82
Mol Sieve	1386.9	WPHK82

Ar 2p

Ar in Si	241.9	Φ
Ar in Ag	241.2	CiHa74
Ar in Ag	241.9	KiWi75
Ar in Au	240.3	CiHa74
Ar in Au	240.7	KiWi75
Ar in Cu	241.1	CiHa74
Ar in Pt	240.4	KiWi75
Ar in graphite	241.8	KiWi75
Ar in graphite	241.5	WRDM79

As 3d

As	41.6	Φ
As	41.6	Bert81, BWWI76, MINN78, SMAV72, UeOd81
NbAs	40.8	BWWI76
AlAs	41.0	Tayl82
AlGaAs	41.0	Tayl82
GaAs	40.8	LPMK74
GaAs	40.9	GGVL79, WRDM79, Tayl82, MINN78, IMNN79
InAs	40.6	LPMK74
As_2Se_3	42.9	BWWI76, UeOd82
As_4S_4	43.1	BWWI76
As_2S_3	43.4	BWWI76
As_2S_5	44.4	SMAV72
AsI_3	43.5	BWWI76
$AsBr_3$	45.3	BWWI76
As_2O_3	44.9	LPGC77, MINN78, Tayl82, WRDM79
As_2O_5	46.2	Bert81, BWWI76, MINN78, SMAV72
KH_2AsO_4	46.7	SMAV72
NaH_2AsO_4	45.5	WRDM79
$NaAsO_2$	44.2	Tayl82, WRDM79
K_3AsO_4	44.4	SMAV72
Na_3AsO_4	44.9	SMAV72
$Na_4As_2O_7$	45.4	SMAV72
$KAsF_6$	48.0	SMAV72, WRDM79
$LiAsF_6$	49.4	SMAV72
Ph_3As	42.8	HVV79, SMAV72
Ph_3AsS	44.1	BWWI76, HVV79
Ph_3AsO	44.3	BWWI76, SMAV72, HVV79
$Ph_3As(OH)_2$	44.5	SMAV72
$MeAsI_2$	43.5	BWWI76
Ph_4AsI	44.6	HVV79
Ph_4AsBr	44.6	HVV79, SMAV72

As LMM

As	1224.8	Wagn75, BWWI76
NbAs	1226.0	BWWI76
GaAs	1225.3	Tayl82, WRDM79
As_2Te_3	1225.0	BWWI76
As_2Se_3	1223.3	BWWI76
As_2S_3	1222.1	BWWI76
AsI_3	1222.9	BWWI76
$AsBr_3$	1218.1	BWWI76
As_2O_3	1218.8	Tayl82, WRDM79, BWWI76
As_2O_5	1217.5	BWWI76
NaH_2AsO_4	1217.1	WRDM79
$NaAsO_2$	1219.5	Tayl82, WRDM79
K_2AsF_6	1213.8	WRDM79
Ph_3As	1221.1	BWWI76
Ph_3AsS	1220.0	BWWI76
Ph_3AsO	1219.5	BWWI76
$MeAsI_2$	1222.3	BWWI76

Au 4f

Au	84.0	Φ
Au	84.1	Asam76
Au	84.0	BiSw80
Au	84.0	BiSw80
Au	83.9	BiSw80
Au	84.1	PEJ 82
Au	84.2	ALMP82
AuSn	84.5	FHPW73
$AuSn_4$	85.1	FHPW73
$YbAu_2$	84.6	WWC 78
$ClAuPh_3P$	85.4	BMCK77, VVSW77

$ClAu(Ph_3P)_2$	85.4	BMCK77
Cl_3AuPh_3P	87.3	BMCK77
$(Ph_3P)AuNO_3$	85.4	BMCK77
$ClAu(Ph_3As)$	85.2	VVSW77
$(-AuSPEt_2S-)_2$	84.8	VVSW77
$(-AuCH_2PEt_2CH_2-)_2$	84.0	VVSW77

Au $M_5N_7N_7$

Au	2015.8	PEJ82
$Au(M_4N_7N_7)$	2101.6	WaTa80
Au	2015.7	WaTa80

B 1s

B	189.4	Φ
B	187.3	HHJ70
B_4C	186.5	HHJ70
AlB_2	188.5	MECC73
Co_2B	189.1	MECC73
CoB	188.1	MECC73
Fe_2B	188.4	MECC73
FeB	187.9	MECC73
HfB_2	188.3	MECC73
MnB_2	187.2	MECC73
Mo_2B_5	187.7	BrWh78
MoB_2	188.4	MECC73
TiB_2	187.5	MECC73
VB_2	188.3	MECC73
W_2B_5	187.9	MECC73
CrB_2	188.0	MECC73
BN	190.5	HJGN70, KOK83, WRDM79
Na_3BO_6	192.0	HHJ70
B_2O_3	192.0	BrWh78
B_2O_3	193.3	NGDS75
$NaBF_4$	194.9	HHJ70, RNS73
NF_4BF_4	195.2	RNS73
$NaBH_4$	187.2	HHJ70
H_3BO_3	193.0	HHJ70
$Na_2B_4O_7 \cdot 10H_2O$	192.6	HHJ70
$B_{10}H_{14}$	187.8	HHJ70
$Me_4NB_3H_8$	187.2	HHJ70
$NaBPh_4$	187.5	HHJ70
NH_3BF_3	194.9	BCGH73
$C_5H_5NBF_3$	194.3	BCGH73
$EtNH_2BF_3$	194.6	BCGH73
Me_3NBF_3	193.6	HHJ70
$NaBH(OMe)_3$	192.1	HHJ70
Ph_3PBF_3	193.3	HHJ70
Ph_3POBF_3	193.8	HHJ70
Ph_3POBCl_3	192.6	HHJ70
Ph_3PBCl_3	192.7	HHJ70
CH_3CNBF_3	195.5	BCGH73
$ClC_6H_4B(OH)_2$	191.7	HHJ70
$FC_6H_4B(OH)_2$	191.7	HHJ70
$(Et_3P)_2PtB_{10}H_{12}$	188.9	Rigg72
$(Ph_3P)_2PtB_{10}H_{12}$	188.5	Rigg72

Ba $3d_{5/2}$

Ba	780.6	Φ
Ba	779.3	VaVe80
BaS	779.8	SiWo80
BaO	779.9	WRDM79
BaO	779.6	SiWo80
BaO	779.1	VaVe80
$Ba(NO_3)_2$	780.7	CLSW83
$BaCO_3$	779.9	CLSW83
$BaSO_4$	780.8	Wagn77
$BaSO_4$	780.4	CLSW83
$BaSO_4$	779.9	SiWo80
$BaCrO_4$	778.9	ACHT73
$BaMoO_4$	779.1	NFS82
$BaRh_2O_4$	779.6	NFS82

Ba MNN

Ba	602.0	VaVe80
BaO	597.5	WRDM79
BaO	598.4	VaVe80
$BaSO_4$	596.1	Wagn77

Be 1s

Be	111.8	Φ
Be	111.7	HJGN70, SMKM77, WRDM79
BeO	113.8	HJGN70, KOK83, NFS82
$BeMoO_4$	113.7	NFS82
$BeRh_2O_4$	113.8	NFS82
BeF_2	115.3	NKBP73
BeF_2	116.1	HJGN70
$NaBeF_3$	115.3	NKBP73
Na_2BeF_4	114.7	NKBP73

Bi 4f

Bi	157.0	Φ
Bi	156.9	SFS77
Bi	157.0	LKMP73
Bi	157.0	WRDM79, MSV73
Bi_2S_3	158.9	MSV73
BiI_3	159.3	MSV73
BiF_3	160.8	MSV73
Bi_2O_3	158.8	NGDS75
Bi_2O_3	159.3	MSV73
Bi_2O_3	159.8	DSBG82
BiOCl	159.9	MSV73
$NaBiO_3$	159.1	MSV73
Bi_2MoO_6	158.3	MaWo75
$Bi_2Ti_2O_7$	159.7	MSV73
$(BiO)_2Cr_2O_7$	159.6	MSV73
$Bi_2(SO4)_3 \cdot H_2O$	161.2	MSV73

Br 3d

KBr	68.8	Φ
CsBr	68.1	MVS73
CsBr	69.6	Shlq78

RbBr	68.4	MVS73
KBr	68.8	MVS73, WaTa80
NaBr	68.8	MVS73, ShIq78
LiBr	69.2	MVS73
$CdBr_2$	69.2	SATD73
$CuBr_2$	68.9	VWHS81
$HgBr_2$	69.0	SATD73
$PbBr_2$	68.7	Nefe82
$ZnBr_2$	70.0	SATD73
$Co(NH_3)_6SbBr_6$	68.9	Tric74
$Ni(NH_3)_6Br_2$	68.7	NZB 78
$Pt(NH_3)_4Br_2$	68.4	SNMK78
K_2PtBr_4	69.3	SNMK78
K_2PtBr_6	69.2	SNMK78
$Cs_3Sb_2Br_9$	70.8	Tric74
$Rb_3Sb_2Br_9$	70.1	Tric74
Bromanil	70.1	OYK74
Ph_4AsBr	66.7	HVV79
Ph_4SbBr	68.0	HVV79
$(Me_4N)_2ZnBr_4$	67.8	EMGK74
$(Et_4N)_2MnBr_4$	67.9	EMGK74
$(Et_4N)_2NiBr_4$	68.9	EMGK74
H_3POBBr_3	69.3	HVV79
H_3PBBr_3	69.6	HVV79
$Br_2Pt(CH_3CONH)_4$	68.7	NeSa78

Br LMM

LiBr	1389.2	Wagn78
NaBr	1388.3	Wagn78
KBr	1388.0	WaTa80
$KBrO_3$	1384.4	Wagn78
$C_6H_{13}Me_3NBr$	1390.1	Wagn78

C 1s

Graphite	284.5	Φ
Graphite	284.3	JHBK73
Cr_3C_2	282.8	RHJF69
Fe_3C	283.9	ShTr75
HfC	280.8	RHJF69
Mo_2C	282.7	RHJF69
NbC	281.9	RHJF69
Ni_3C	283.9	SiLe78
TaC	281.9	RHJF69
TiC	281.6	RHJF69, IKIM73
VC	282.2	RHJF69
WC	282.8	RHJF69, CoRa76
ZrC	281.1	RHJF69
KCN	286.1	Vann76
NaCN	286.2	Vann76
$K_3Co(CN)_6$	285.9	Vann76
$K_3Cr(CN)_6$	283.9	Vann76, ZeHa71
$K_3Fe(CN)_6$	283.9	Vann76, ZeHa71
$K_4Fe(CN)_6$	283.5	Vann76
$K_3Mn(CN)_6$	284.0	Vann76
$Na_4Mn(CN)_6$	284.0	Vann76
$K_4V(CN)_6$	285.5	Vann76
$Cr(CO)_6$	287.9	BCGH72, BCHM72, KTWY76, PFD73
$Co(CO)_3NO$	288.2	BCGH72
$Fe(CO)_5$	288.0	BCGH72
$Fe(CO)_2(NO)_2$	288.2	BCGH72
$Mn_2(CO)_{10}$	287.5	VWVB77
$Ni(CO)_4$	288.2	BCGH72
$(Mn(CO)_4Br)_2$	287.6	VWVB77
$BrMn(CO)_5$	288.0	VWVB77
Ag_2CO_3	288.4	HGW 75
$BaCO_3$	289.4	CLSW83
$CaCO_3$	289.6	CLSW83
$CdCO_3$	289.3	HGW 75
Li_2CO_3	289.8	CSFG79
Na_2CO_3	289.4	GHHL70, HHDD81
$NaHCO_3$	290.0	GHHL70
$SrCO_3$	289.5	CLSW83
CS_2	287.0	GHHL70
CO_2	291.9	GHHL70
CCl_4	292.4	GHHL70
COF_2	293.9	GHHL70
CF_4	296.7	GHHL70
Cyclohexane	285.2	GHHL70
Benzene	284.7	GHHL70, LaFo76, CKAM72
$C_6H_5C^*H_3$	284.7	CKM71
$C_6H_5CH_3$ (C^*CH_3)	285.1	CKM71
$C_6H_5CH_3$ (C^*-H)	285.0	CKM71
$Fe(C_5H_5)_2$	284.5	BCDH73
$Cr(C_6H_6)_2$	284.4	KTWY76
$CH_3C^*H_2OH$	286.3	GHHL70
$CH_3COOC^*H_2CH_3$	286.9	GHHL70
C_6F_6	289.5	CKAM72
Inositol	286.7	GHHL70
Hydroquinone	286.4	OYK74
$(C^*HCOH)_3$	284.8	GHHL70
$(CHC^*OH)_3$	286.6	GHHL70
$(CH_3C^*H_2)_2O$	286.5	GHHL70, ClTh78
HCHO	287.7	GHHL70
$(CH_3C^*HO)_3$	287.6	GHHL70
$CH_3C^*OCH_3$	287.9	GHHL70
$CF_3C^*OCH_3$	288.5	GHHL70
$C^*F_3COCH_3$	292.6	GHHL70
$(CO)_6$	288.3	GHHL70
CH_3C^*OOH	289.3	GHHL70
CH_3C^*OONa	288.2	HHDD81
CH_3C^*OONa	288.8	GHHL70
CH_3C^*OOAg	288.3	HHDD81
HOOCCOOH	289.9	GHHL70
$(COONa)_2$	289.0	GHHL70
CF_3C^*OOEt	290.4	GHHL70
C^*F_3COOEt	292.9	GHHL70
Cl_3C^*COONa	289.5	GHHL70
Cl_3CC^*OONa	288.3	GHHL70
F_3C^*COONa	292.1	GHHL70
F_3CC^*OONa	288.9	GHHL70
p-Benzoquinone	287.4	OYK74

$Cr(acac)_3$	286.0	ZeHa71
$CH_3C^*H_2OCOCl$	287.1	GHHL70
$EtOC^*OCl$	290.8	GHHL70
$(PhO)_2CO$	290.7	ClTh78
$HC^*(OCH_3)_3$	289.7	GHHL70
$HCOONH_4$	238.4	GHHL70
$OC^*(OCH_3)_2$	291.2	GHHL70
$O(C^*H_2COOH)_2$	286.7	GHHL70
$O(CH_2C^*OOH)_2$	289.5	GHHL70
$CH_3C^*H_2Cl$	286.1	GHHL70
CH_2Br_2	287.1	GHHL70
CH_2Cl_2	287.8	GHHL70
HCF_3	294.7	GHHL70
$HCCl_3$	289.6	GHHL70
C_6H_5Cl (C^*Cl)	287.1	CKM71
$C_6H_5Cl(C^*H)$	285.7	CKM71
C_6H_5Br	285.1	LaFo76
$C_6H_5F(C^*F)$	287.8	CKM71
$C_6H_5F(C^*H)$	285.6	CKM71
C_6HCl_5	286.1	CKAM75
$C_6HF_5(C^*H)$	286.9	CKAM72
$C_6HF_5(C^*F)$	289.2	CKAM72
C_6F_6	288.7	GHHL70
$Cl_2FCCFCl_2$	291.7	GHHL70
$ClF_2C^*CFCl_2$	292.9	GHHL70
C^*H_3CN	286.3	BCGH73
CH_3C^*N	287.2	BCGH73
CH_3CONH_2	288.4	SNMK78
$EtNH_2$	285.6	BCGH73, GHHL70
$EtNH_2BF_3$	286.8	BCGH73
$PhNH_2$	284.6	LaFo76
$C(NH_2)_3Cl$	289.4	LeRa77
$(CH_2)_6N_4$	286.9	GHHL70
C_5H_5N	285.5	BCGH73
PhCN	285.4	LaFo76
$C^*H_3CNBF_3$	287.3	BCGH73
$CH_3C^*NBF_3$	289.1	BCGH73
Triazole	286.3	GHHL70
$NC^*N=C(NH_2)_2$	286.4	LeRa77
$NCN=C^*(NH_2)_2$	288.2	LeRa77
$H_2NCH_2C^*OONa$	287.9	GHHL70
H_2NCONH_2	288.7	GHHL70, LeRa77
H_2NCSNH_2	288.0	LeRa77, SrWa77
$H_2NCONHCONH_2$	289.3	YYS78
$PhNO_2$	285.3	LaFo76
Ph_3P	284.9	LMF80
Ph_3PO	284.6	LMF80
Ph_3PBr	285.4	LMF80, LaFo76
Ph_4Sn	284.6	BALS76
$p(CH_2=CHCl)$	286.3	PRCV77
$p(CH_2=CHOH)$	286.3	PRCV77
$p(HOCOCH=CH_2)$	289.0	HHDD81
$p(NaOCOCMe=CH_2)$	288.1	HHDD81
$p(C^*H_3OCOCH=CH_2)$	286.4	ClTh78
$p(CH_3OC^*OCH=CH_2)$	288.6	ClTh78
$p(MeOCOCMe=CH_2)$	289.0	HHDD81
PVA ($-CH_2C^*HOH-$)n	286.1	PRCV77
Cellulose	286.2	Wagn81
PEO ($-CH_2C^*H_2O-$)n	286.1	Wagn81
poly ($-CH_2CH_2C=O-$)n	287.4	Wagn81
$C_6H_4(C^*OOH)_2$	288.9	Wagn81
$HOOC^*(CH_2)_4C^*OOH$	288.9	Wagn81
Sodium Stearate	288.3	Wagn81
Mylar Polyester C*-H	284.85	Φ
Mylar Polyester C*-O	286.3	Wagn81
Mylar Polyester C^*O_2	288.7	Wagn81
Polycarbonate-OC^*O_2-	290.4	Wagn81
Teflon ($-CF_2CF_2-$)n	292.2	CFK73
($-C^*FHCF_2-$)n	289.3	CFK73
($-CFHC^*F_2-$)n	291.6	CFK73
($-CFHCFH-$)n	288.4	CFK73
($-C^*H_2CF_2-$)	286.3	CFK73
($-CH_2C^*F_2-$)n	290.8	CFK73
($-C^*H_2CFH-$)n	285.9	CFK73
($-CH_2C^*FH-$)n	288.0	CFK73
PVC ($-C^*H_2CHCl-$)	284.9	PRCV77
PVC ($-CH_2C^*HCl-$)	286.5	PRCV77

Ca 2p

Ca	346.3	Φ
$CaCO_3$	346.6	Φ
Ca	345.9	VaVe80
Ca	346.8	SMKM77
CaH_2	346.7	FMUK77
CaSe	345.9	FMUK77
CaS	346.5	FMUK77
$CaCl_2$	348.3	Wagn77
CaF_2	347.8	Wagn77, NSLS77
CaO	346.1	InYa81
CaO	346.7	FMUK77
CaO	347.3	VaVe80
$CaCO_3$	346.9	Wagn77, CLSW83, WRDM79
$Ca(NO_3)_2$	348.7	CLSW83
$CaCrO_4$	346.3	ACHT73
$CaMoO_4$	347.2	NFS82
$CaRh_2O_4$	345.7	NFS82
$CaSO_4$	348.0	CLSW83
$CaWO_4$	346.5	Nefe82
$Ca_3Si_3O_9$	347.0	WPHK82

Ca LMM

Ca	298.2	VaVe80
CaO	292.5	VaVe80
$CaCO_3$	291.9	WRDM79, Wagn77
$CaCl_2$	291.9	Wagn77
CaF_2	289.1	Wagn77

Cd $3d_{5/2}$

Cd	405.1	Φ
Cd	405.0	GaWi77, HSBS81,WRDM79, Wagn75
$Cd_{99.6}Sn_4$	404.9	HSBS81

$Hg_{0.8}Cd_{0.2}Te$	404.6	SBB80
CdTe	404.9	SBB80, GaWi77
CdSe	405.3	GaWi77
CdS	405.3	GaWi77
CdI_2	405.4	GaWi77
$CdBr_2$	406.0	SATD73
$CdCl_2$	406.1	SATD73
CdF_2	405.9	GaWi77, SATD73, Wagn77
CdO	405.2	GaWi77, NGDS75, NFS82, SBB80
CdO_2	403.6	HGW75
$Cd(OH)_2$	405.0	WRDM79, HGW75
$CdCO_3$	405.1	HGW75
$CdRh_2O_4$	404.7	NFS82

Cd MNN

Cd	383.8	WRDM79, Wagn75, GaWi77
CdTe	382.4	GaWi77
CdSe	381.4	GaWi77
CdS	381.1	GaWi77
CdI_2	381.0	GaWi77
CdF_2	378.8	GaWi77
CdO	382.2	GaWi77

Ce 3d

Ce	883.8	Φ
Ce	883.9	ScOs82
$CeAl_2$	883.5	LFBC80
$CePd_3$	884.3	LFBC80
CeSe	884.3	LFBC80
$CeCu_2Si_2$	883.6	LFBC80
CeO_2	881.8	WRDM79
CeO_2	882.4	NGDS75, SaRa80
CeH_3	886.0	ScOs82

Cl 2p

KCl	198.5	Φ
CsCl	196.3	MVS73
KCl	198.2	MVS73, NSLS77, YYS78
NaCl	198.4	MVS73, NSLS77, SGSO70
LiCl	198.5	MVS73, CSFG79
RbCl	197.9	MVS73
$CuCl_2$	200.0	VWHS81
$NiCl_2$	199.4	KlHe83, TRLK73, YYS 78
$PdCl_2$	198.9	NKBP73
$RhCl_3$	199.3	OIIT79
$RhCl_3 \cdot 12H_2O$	199.2	CMHL77
$SbCl_5$	199.7	BCH 75
$ZnCl_2$	198.5	KlHe83
K_2IrCl_6	198.6	NSBN77, LeBr72, CoHe72
K_2MoCl_6	198.4	CoHe72
K_2OsCl_6	198.6	CoHe72, LeBr72
K_2PdCl_4	198.8	NKBP73
K_2PtCl_4	198.8	CMHL77, SNMK78
K_2PtCl_6	198.8	CoHe72, LeBr72, SNMK78
K_2ReCl_6	198.4	CoHe72
K_2ReCl_6	199.3	LeBr72
K_2SnCl_6	198.4	CoHe72
K_2WCl_6	199.0	LeBr72
K_3IrCl_6	198.7	NSBN77
K_3RhCl_6	198.4	SNMK78
$K_4Mo_2Cl_8$	198.8	HUGH79
Na_2PdCl_4	199.3	SeTs76
$Co(NH_3)_6SbCl_6$	198.9	Tric74
$Pt(NH_3)_2Cl_2$	198.8	CMHL77, Nefe78
$Pt(NH_3)_4Cl_2$	197.8	SNMK78
$Pt(NH_3)_6Cl_4$	197.8	SNMK78
$Rh(NH_3)_6Cl_3$	198.1	Nefe78
$Cs_3Sb_2Cl_9$	198.0	BCH75, Tric74
$CsSbCl_6$	199.2	Tric74
$KIrCl_5NO$	198.9	NSBN77
ICl	200.1	Sher76
$CsClO_4$	208.2	MVS73
$KClO_3$	206.5	MVS73
$KClO_4$	208.8	MVS73
$LiClO_4$	209.0	MVS73
$NaClO_4$	208.5	MVS73
$Ni(NH_3)_6(ClO_4)_2$	208.2	NZB78
$NiClO_4 \cdot 6H_2O$	208.6	NZB78
$RbClO_4$	208.4	MVS73
Me_4NCl	196.2	EMGK74
Et_4NCl	196.4	EMGK74
Ph_4NCl	196.1	HVV79
NH_4Cl	197.9	EMGK74
Chlorobenzene	200.1	CKAM75
Pentachlorobenzene	200.0	CKAM75
$ClRh(Ph_3P)_3$	198.0	Nefe78, OIIT79, MMRC72
$(Et_3P)_2PtHCl$	198.0	Rigg72
$(Ph_3P)_2PtHCl$, trans	197.1	CBA73
$(Et_3P)_2PtCl_4$	199.2	LeBr72, Nefe78, Rigg72
$(Et_3P)_2PtCl_2$	198.1	Rigg72
$(Ph_3P)_2NiCl_2$	199.0	BNSA70, STHU76
$(Ph_3P)_2NiCl_2$	198.3	NZB78
Ph_3PBCl_3	199.4	HVV79
Ph_3POBCl_3	198.9	HVV79
$(Nb_6Cl^*_{12})Cl_6(Et_4N)_3$	199.4	BeWa79
$(Nb_6Cl_{12})Cl^*_6(Et_4N)_3$	197.5	BeWa79
$CdCl_2$	199.0	SATD73
$CuCl_2$	199.2	YYS78
$HgCl_2$	198.7	SATD73
InCl	198.4	FHT77
$InCl_3$	199.0	FHT77
$TiCl_4$	198.2	MRV83
UCl_3	198.1	TBVL82
UCl_4	197.7	TBVL82
UCl_5	197.7	TBVL82
UOCl	198.5	TBVL82
$UOCl_2$	198.3	TBVL82
$ZnCl_2$	199.7	SATD73
$(NH_4)_2PtCl_4$	198.2	KaEl79
$OPCl_3$	201.7	FlWe75

$KClO_3$	206.5	NZK77
$KClO_4$	208.7	NZK77
$HClPt(Ph_3P)_2$	197.9	AL77
$HClPt(Et_3P)_2$	198.0	AL77
$Cl_2Pt(Ph_3P)_2$	198.0	AL77
Ph_4PCuCl_2	198.9	FSJL83
Ph_4PCuCl_3	199.0	FSJL83
C_6H_5Cl	201.0	CKM71
$C_6H_5CCl_3$	201.0	CKM71
$C(NH_2)_3Cl$	198.0	LeRa77
$p(CH_2{=}CHCl)$	200.0	PRCV77, WRDM79

Co 2p

Co	778.3	Φ
CoO	780.4	Φ
Co	778.3	LANM81
Co	778.1	WRDM79
Co_2OSn_{80}	777.9	ThSh78
Co_2B	778.1	MECC73
CoB	778.0	MECC73
CoS	781.9	Limo81
CoF_2	783.0	CSC72
$CoF_2 \cdot 4H_2O$	782.6	NBMO73
CoF_3	782.4	CSC72
CoO	780.2	WRDM79
CoO	780.4	Kim75, NGDS75, NFS82, CBR76
Co_3O_4	780.2	NGDS75, OkHi76
Co_3O_4	779.5	GPDG79
Co_2O_3	779.9	McCo75
CoOOH	780.0	McCo75
$Co(OH)_2$	781.0	McCo75
$CoAl_2O_4$	780.8	OkHi76
$CoAl_2O_4$	781.9	PCLH76
$CoCr_2O_4$	780.2	OkHi76
$CoFe_2O_4$	779.7	OkHi76
$CoMn_2O_4$	780.0	OkHi76
$CoMoO_4$	780.9	GPDG79
$CoMoO_4$	782.8	PCLH76
$CoRh_2O_4$	781.2	NFS82
$CoSO_4$	784.0	Limo81
$ZnCo_2O_4$	780.4	OkHi76
Cs_2CoI_4	780.5	NBMO73
Cs_2CoBr_4	780.8	NBMO73
Cs_2CoCl_4	781.0	NBMO73
$K_3Co(C_2O_4)_3$	780.9	CSC72
$K_3Co(NO_2)_6$	781.8	NBMO73
$Co(CO)_3NO$	780.7	BCGH72
$K_3Co(CN)_6$	781.2	OkHi76
$K_3Co(CN)_6$	782.1	Vann76
$Co(NH_3)_3Cl_3$	781.4	NBMO73
$Co(NH_3)_5Cl_3$	781.9	YNAB77
$Co(NH_3)_6Cl_3$	781.1	CSC72
$Co(NH_3)_6Cl_3$	781.8	NBMO73
$Co(C_5H_5)_2$	779.1	BCDH73
$Co(C_5H_5)_2$	781.3	ClAd71
$Br_4Co(Et_4N)_2$	780.1	EMGK74
$Cl_4Co(Et_4N)_2$	780.6	EMGK74
$Cl_2Co(thiourea)_2$	780.9	NBMO73

Cr 2p

Cr	574.4	Φ
Cr_2O_3	576.9	Φ
Cr	574.3	LANM81
Cr	574.3	WRDM79
Cr_2N	576.1	RoRo76
CrN	575.8	STAB76
CrB_2	574.3	MECC73
Cr_2S_3	574.8	CSC72
CrI_3	576.7	CSC72
$CrBr_3$	576.2	CSC72
$CrCl_3$	577.4	CSC72
Cr_2O_3	576.8	BDFP81, CDFM82, CSC72, WRDM79, NGDS75
CrO_2	576.3	IIKK76
CrO_3	578.3	ACHT73
CrF_3	580.3	CSC72
CrO_3	579.8	CDFM82
$Cr(OH)_3$	577.3	CDFM82
CrOOH	577.0	IIKK76
$Cr(CO)_6$	576.3	BCGH72, BCHM72
$Cr(CO)_6$	577.0	PFD73
Cs_2CrO_4	579.8	AT76
$Cs_2Cr_2O_7$	579.5	AT76
$CuCrO_2$	576.4	ACHT73
$CuCr_2O_4$	577.1	CDFM82
$K_2Cr_2O_7$	579.9	NSSP80
$LaCrO_3$	575.8	HoTh80
Li_2CrO_4	579.8	ACHT73
$LiCrO_2$	577.0	ACHT73
Na_2CrO_4	579.8	ACHT73
Na_2CrO_4	580.5	LaKe76
$Na_2Cr_2O_7$	579.4	ACHT73
Na_3CrO_4	578.5	LaKe76
Na_4CrO_4	577.9	LaKe76
$NaCrO_2$	577.1	LaKe76, ACHT73
$ZnCr_2O_4$	577.2	BDFP81
$BaCrO_4$	579.1	AlTu76
$CaCrO_4$	578.9	ACHT73
$(NH_4)_3CrF_6$	579.5	AlTu76
$Cr(NH_3)_6Cl_3$	578.5	AlTu76
$K_3Cr(CN)_6$	576.3	Vann76, ZeHa71
K_3CrF_6	583.0	AlTu76
$Cr(acac)_3$	577.7	AlTu76
$Cr(acac)_3$	576.1	ZeHa71
$Cl_3Cr(urea)_6$	579.9	AlTu76
$Cr(C_5H_5)_2$	574.8	BCDH73, CDH 74, GSMJ74
$Cr(C_5H_5)_2$	576.3	ClAd71
$Cr(C_5H_5)(C{\cdot}H_5)$	574.4	CDH74, GSMJ74
$Cr(C_6H_6)_2$	574.1	CDH74
$Cr(C_6H_6)_2$	575.4	PFD73
$Cr(CO)_5PH_3$	575.3	BCGH72

$Cr(CO)_5NH_3$	575.5	BCGH72, BCHM72
$Cr(CO)_3C_6H_6$	575.7	CDH74
$Cr(CO)_3C_6H_6$	576.3	PFD73
$Cr(CO)_5(Me_3P)$	575.2	BCGH72, BCHM72
$Cl_3Cr(C_5H_5)$	576.1	GSMJ74
$ICr(C_6H_6)$	576.4	CDH74
Cr LMM		
Cr	527.2	WRDM79
Cs 3d5/2		
Cs	726.4	Φ
C	726.0	KDR77
CsI	723.9	MVS73
CsBr	724.0	MVS73
CsCl	723.7	MVS73
CsF	724.0	MVS73
CsN_3	723.6	SGRS72
Cs_2SO_4	723.9	Wagn77
Cs_3PO_4	723.9	MVS73
$Cs_4P_2O_7$	723.8	MVS73
$CsClO_4$	724.2	MVS73
Cs_2CrO_4	724.5	ACHT73
$Cs_2Cr_2O_7$	723.9	ACHT73
CsOH	724.5	WRDM79
Cs MNN		
Cs_2SO_4	568.4	Wagn77
CsOH	586.7	WRDM79
Cu 2p		
Cu	932.7	Φ
CuO	933.6	Φ
Cu	932.6	ALMP82
Cu	932.6	LANM81
Cu	932.6	BiSw80
Cu	932.6	BiSw80
Cu	932.7	BiSw80
Cu	932.7	PEJ82
Cu	932.6	Asam76, GaWi77, KPML73, WRDM79, Wagn75
$Cu_{64}Zn_{36}$	932.6	VanO77
$Cu_{95}Sn_5$	932.5	Hegd82
Cu_3P	932.2	NSDU75
Cu_3P	932.2	NSDU75
Cu_2Se	931.9	RRD78
CuSe	932.0	RRD78
CuAgSe	931.9	RRD78
$CuInSe_2$	931.9	KJID81
Cu_2S	932.5	Wagn75
CuS	932.2	RRD78
CuS	933.2	Limo81
CuS	931.9	BSRR81
CuS	935.0	NSSP80
CuBr	932.1	BrFr74
$CuBr_2$	932.3	VWHS81
CuCl	932.5	GaWi77, Wagn75
$CuCl_2$	934.4	GaWi77
$CuCl_2$	935.2	WRDM79
$CuCl_2$	934.8	VWHS81
$CuCl_2$	935.6	YYS78
CuF_2	936.1	GaWi77
CuF_2	937.0	WRDM79
CuF_2	936.8	VWHS81
Cu_2O	932.5	CDFM82, GaWi77, Wagn75, HMUZ78, MSSS81, Scho73b
CuO	933.7	HMUZ78, GaWi77, WRDM79, MSSS81
$Cu(OH)_2$	935.1	MSSS81
$Cu(NO_3)_2$	935.5	NZK77
CuCN	933.1	Wagn75
$CuC(CN)_3$	933.2	NZK77
$CuCO_3$	935.0	WRDM79
$CuSO_4$	934.9	Limo81
Cu_3O_4	935.5	NZK77
$C SiO_3$	934.9	WRDM79
$Cu_2Mo_3O_{10}$	931.6	HMUZ78
$Cu_3Mo_2O_9$	934.1	HMUZ78
$CuCr_2O_4$	934.6	CDFM82
$CuCrO_2$	932.3	ACHT73
$CuFe_2O_4$	933.8	LDDB80
$CuFeO_2$	932.6	LDDB80
$CuMoO_4$	934.1	HMUZ78
$CuRh_2O_4$	934.4	NFS82
$Cu(OAc)_2$	931.8	BrFr74
$Cu(OAc)_2$	935.0	YYS79
$Cu(acac)_2$	934.5	BrFr74
Cu(8-Hydrozyquinol.)	935.0	BrFr74
Cu Salicylaldoxime	934.0	BuBu74
$Cu_4Cu(Et_4N)_2$	932.5	EMGK74
$Cu_2Cu(H_2NCONHCONH_2)_{20}$	935.8	YYS78
Cu LMM		
Cu	918.6	BiSw80
Cu	918.7	BiSw80
Cu	918.6	BiSw80
Cu	918.7	PEJ82
Cu	918.6	KPML73, WRDM79, Wagn75, Asam76, GaWi77
$Cu_{64}Zn_{36}$	918.6	VanO77
Cu_2Se	917.6	RRD78
CuSe	918.4	RRD78
CuAgSe	917.7	RRD78
Cu_2S	917.4	RRD78
CuS	917.9	Wagn75
$CuBr_2$	916.9	RRD78
CuCl	915.0	VWHS81
CuCl	915.6	Wagn75
$CuCl_2$	915.3	GaWi77
CuF_2	916.0	WRDM79, VWHS81, GaWi77
CuF_2	914.8	GaWi77
		WRDM79

CuF_2	914.4	VWHS81
Cu_2O	916.2	CDFM82, HMUZ78
Cu_2O	916.2	CDFM82, GaWi77, Wagn75, HMUZ78, MSSS81, Scho73b
Cu_2O	916.6	MSSS81, Wagn75
Cu_2O	917.2	GaWi77
CuO	918.1	GaWi77, MSSS81, Scho73b
$Cu(OH)_2$	916.2	MSSS81
$Cu(NO_3)_2$	915.3	NZK77
CuCN	914.5	Wagn75
$CuC(CN)_3$	914.5	NZK77
$CuCO_3$	916.3	WRDM79
$CuSO_4$	915.6	NZK77
$CuSiO_3$	915.2	WRDM79
$Cu_2Mo_2O_{10}$	916.5	HMUZ78
$Cu_2Mo_2O_9$	916.6	HMUZ78
$CuCr_2O_4$	918.0	CDFM82
$CuMoO_4$	916.6	HMUZ78
Dy 4d		
Dy	152.4	Φ
Dy_2O_3	167.7	SaRa80
Dy $3d_{5/2}$		
Dy	1295.5	Φ
Dy_2O_3	1298.9	SaRa80
Er 4d		
Er	167.3	Φ
Er	169.4	WRDM79
Er_2O_3	168.7	WRDM79
Eu $3d_{5/2}$		
Eu	1125.6	Φ
Eu 4d		
Eu	128.2	NNBF68
Eu_2O_3	135.9	NNBF68
F 1s		
LiF	684.9	Φ
CsF	685.9	WRDM79
KF	683.9	NBK74, MVS73
KF	684.4	PMDS77
LiF	685.1	WRDM79
LiF	685.0	MVS73, NBK74
NaF	684.5	WRDM79
NaF	684.5	NBK74, NSLS77
NaF	683.7	MVS73
RbF	683.6	MVS73
RbF	682.9	NBK74
BaF_2	683.7	WRDM79
BaF_2	684.3	NBK74
CaF_2	684.8	WRDM79
CaF_2	684.8	NBK74, NSLS77
MgF_2	685.8	Wagn80
MgF_2	685.7	NBK74
SrF_2	685.0	WRDM79
SrF_2	684.5	NBK74
AgF	682.7	GaWi77
BeF_2	685.8	NBK74, NKBP73
CdF_2	684.5	GaWi77, WRDM79
CdF_2	684.8	NBK74, SATD73
CdF_2	684.2	NSLS77
CuF_2	684.5	GaWi77, WRDM79
CuF_2	685.9	VWHS81
HgF_2	686.0	SATD73
MnF_2	684.8	WRDM79
NiF_2	685.0	GaWi77, WRDM79
$NiF_2 \cdot 4H_2O$	684.7	NSLS77
PbF_2	683.6	WRDM79
ZnF_2	684.6	GaWi77, Wagn77
ZnF_2	685.1	NBK74
$AlF_3 \cdot 3H_2O$	686.3	NBK74, NKBP73
$GaF_3 \cdot 3H_2O$	685.2	NBK74, NKBP73
GdF_3	684.8	McTh76
InF_3	685.2	WRDM79
$InF_3 \cdot 3H_2O$	685.3	NBK74, NKBP73
LaF_3	684.5	WRDM79
NdF_3	684.8	WRDM79
PrF_3	684.6	WRDM79
SmF_3	684.6	WRDM79
YF_3	685.3	WRDM79
UF_3	685.3	TBVL82
UF_4	684.8	TBVL82, PMDS77
UF_5	684.8	TBVL82
ThF_4	684.9	WRDM79
HfF_4	685.4	WRDM79
ZrF_4	685.1	NKBP73
$NaBeF_3$	685.7	NKBP73
Na_2BeF_4	685.2	NKBP73
$NaBF_4$	687.0	WRDM79
NF_4BF_4	694.2	RNS73
Na_3AlF_6	685.5	WRDM79
Na_2SiF_6	686.0	Wagn77
Na_2SiF_6	686.4	NSLS77
K_2SiF_6	686.6	NBK74
K_2TiF_6	685.0	WRDM79
K_2TiF_6	684.9	NBK74
Na_2TiF_6	685.3	Wagn77
K_3FeF_6	684.0	WRDM79
K_2NiF_6	687.6	TRLK73
K_2GeF_6	685.2	NBK74
Na_2GeF_6	685.9	WRDM79
K_2ZrF_6	684.6	NBK74, NKBP73
Na_2ZrF_6	685.0	WRDM79
$KZrF_5 \cdot H_2O$	684.8	NKBP73
K_3ZrF_7	684.3	NKBP73
$NaSnF_3$	685.3	WRDM79
$K_2SnF_6 \cdot H_2O$	685.1	NBK74
$CsSbF_4$	683.6	BCH75

K_2SbF_5	683.9	Tric74
$KSbF_6$	686.6	Wagn77
KSb_2F_7	684.3	Tric74
Na_2SbF_5	683.4	Tric74
$NaSbF_6$	685.1	BCH75
K_3RhF_6	685.7	Nefe78
K_2NbF_7	685.4	WRDM79
K_2NbF_7	685.2	NBK74
K_2TaF_7	685.2	WRDM79
K_2TaF_7	685.1	NBK74
$NaTaF_6$	685.2	NKBP73
Na_2TaF_7	685.6	NKBP73
Na_3TaF_8	685.5	NKBP73
K_2UF_6	684.7	PMDS77
EuOF	685.3	PGBH80
LaOF	685.2	RGBH80
NdOF	685.1	RGBH80
PrOF	685.0	RGBH80
YOF	685.5	RGBH80
$Cs_2MoO_2F_4$	684.7	NKBP73
$Cs_2WO_2F_4$	684.7	NKBP73
UO_2F_2	685.6	TBVL82
p-(CF_2=CF_2)	689.0	Wagn77
$NiOOCCF_3$	688.4	WRDM79
CH_3CNBF_3	687.0	BCGH73
NH_3BF_3	686.6	BCGH73
$C_5H_5NBF_3$	685.6	BCGH73
$EtNH_2BF_3$	686.6	BCGH73
Et_4NSbF_6	684.7	BCH 75
Ph_3PBF_3	685.7	HVV79
Ph_3POBF_3	685.8	HVV79

F KLL

CsF	653.8	WRDM79
LiF	654.7	WRDM79
NaF	655.0	Wagn77
BaF_2	656.2	WRDM79
CaF_2	655.4	WRDM79
MgF_2	654.4	Wagn77
SrF_2	656.3	WRDM79
AgF	659.3	GaWi77
CdF_2	656.0	GaWi77, WRDM79
CuF_2	657.0	GaWi77
CuF_2	656.2	WRDM79
CuF_2	656.2	WRDM79
NiF_2	655.5	GaWi77, WRDM79
PbF_2	658.5	WRDM79
ZnF_2	655.6	GaWi77, WRDM79
InF_3	656.4	WRDM79
LaF_3	658.0	WRDM79
NdF_3	657.0	WRDM79
PrF_3	657.2	WRDM79
SmF_3	657.0	WRDM79
YF_3	655.8	WRDM79
ThF_4	657.0	WRDM79
HfF_4	655.3	WRDM79
$NaBF_4$	652.8	WRDM79
Na_3AlF_6	654.1	WRDM79
Na_2SiF_6	653.0	Wagn77
K_2TiF_6	655.7	WRDM79
Na_2TiF_6	655.1	Wagn77
K_3FeF_6	656.0	WRDM79
Na_2GeF_6	654.0	WRDM79
Na_2ZrF_6	655.1	WRDM79
$NaSnF_3$	655.3	WRDM79
$KSbF_6$	656.6	Wagn77
K_2NbF_7	655.2	WRDM79
K_2TaF_7	655.0	WRDM79
p-(CF_2=CF_2)	652.4	Wagn77
$NiOOCCF_3$	652.9	WRDM79

Fe 2p

Fe	707.0	Φ
Fe_2O_3	710.9	Φ
Fe	706.7	LANM81
Fe	706.8	Asam76
Fe	707.0	WRDM79, McZe77
Fe_3Al	707.6	ShTr75
Fe_3Si	707.5	ShTr75
Fe_2B	706.9	MECC73
FeB	707.1	MECC73
Fe_3C	708.1	ShTr75
FeS	710.3	CSC72
FeS	712.2	Bind73, Limo81
FeS_2 (markasite, pyr)	706.7	Bind73
$KFeS_2$	708.7	Bind73
$FeBr_2$	710.3	CSC72
$FeBr_3$	710.1	CSC72
$FeCl_2$	710.6	CSC72
$FeCl_3$	711.3	CSC72
FeF_2	711.3	CSC72
FeF_3	714.2	CSC72
FeO	709.4	McZe77
Fe_3O_4	708.2	McZe77
Fe_3O_4	710.4	OkHi76
Fe_2O_3	710.8	WRDM79, NGDS75
Fe_2O_3, alpha	710.9	McZe77
Fe_2O_3, gamma	710.9	McZe77
FeOOH, alpha	711.8	McZe77
FeOOH, gamma	711.3	KoNa80
$CoFe_2O_4$	710.5	McZe77
$Fe(C_2O_4)_3 \cdot 6H_2O$	713.6	Kilk73
$FeSO_4$	712.1	Limo81
K_3FeF_6	714.4	CSC72
$NiFe_2O_4$	710.5	McZe77
$K_3Fe(CN)_6$	709.6	Vann76
$K_4Fe(CN)_6$	707.1	Vann76
$K_4Fe(CN)_6$	708.5	YNNA77
$Na_2Fe(CN)_5(NO)$	709.7	YNNA77
$Na_3Fe(CN)_5(N_2O)$	707.4	YNNA77
$Na_3Fe(CN)_5(NO_2)$	706.8	YNNA77
$Na_3Fe(CN)_5NH_3$	707.6	YNNA77

$Na_3Fe(CN)_5N_2H_4$	707.7	YNNA77
$Fe(CO)_5$	709.6	BCGH72
$Fe(CO)_2(NO)_2$	709.5	BCGH72
$KFe_4(NO)_7S_3 \cdot 2H_2O$	708.9	Nefe78
$Fe(SMe)(CO)_3$	708.6	BBFR77
$Fe(C_5H_5)_2$	707.7	FWUM79, BCDH73, CDH74, Nefe78
$I_8Fe(C_5H_5)_2$	709.9	CDH74
$Fe(C_5H_4COOH)_2$	708.4	FWUM79
Fe(phthalocyanine)	709.1	MSV79
Fe LMM		
Fe	702.4	WRDM79
Ga 2p3/2		
Ga	1116.7	Φ
Ga	1116.5	Scho73a
GaP	1116.8	N[illegible]75
Ga_2O_3	1116.9	[illegible]
Ga_2O_3	1117.8	Scho73a
Ga LMM		
Ga	1068.2	WRDM79, MINN78, Scho73a
GaAs	1066.3	MINN78
GaAs	1067.1	MINN78
GaP	1065.6	MINN78, MIN81
GaP	1066.8	MIN81
GaN	1064.5	HeMa80
Ga_2Se_3	1065.2	ITI82
Ga_2Se_3	1065.6	ITI82
Ga_2O_3	1061.6	MINN78
$Ga2O_3$	1062.4	ITI82
Ga_2O_3	1062.9	Scho72a
Ga 3d		
Ga	18.6	MINN78, LBHK73, Scho73a, WRDM79
GaSb	20.2	LBHK73
GaAs	18.8	LPMK74
GaAs	19.2	IMNN79, MINN78, Tayl82,
GaP	18.8	MIN81
GaP	19.3	NIMN78, IMNN79
GaP	19.9	LBHK73, MIN81
GaP	18.7	LPMK74
GaN	19.5	HeMa80
AlGaAs	19.0	Tayl82
Ga_2Se_3	19.7	ITI82
Ga_2Se_3	19.9	ITI82
Ga_2O_3	20.5	GGVL79
Ga_2O_3	20.2	LBHK73, Scho73a
Ga_2O_3	20.5	ITI82
Ga_2O_3	21.0	MINN78
Gd 4d		
Gd	140.4	Φ
Gd_2O_3	143.8	SaRa80
Gd 3d		
Gd	1187.0	Φ
Gd_2O_3	1189.0	SaRa80
Ge 2p3/2		
Ge	1217.2	McWe76
Ge	1217.4	TLR78, MoVa73, Wagn75
GeS_2	1219.8	MoVa73
GeS_2	1219.8	MoVa73
GeN_4	1218.8	TLR78
GeI_2	1218.2	MoVa73
GeF_2	1220.7	MoVa73
GeO_2	1220.4	MoVa73, Wagn75
Na_2GeO_3	1218.9	MoVa73
Na_2GeF_6	1221.3	Wagn75
K_2GeF_6	1220.7	MoVa73
Ph_4Ge	1218.9	MoVa73
Ge LMM		
Ge	1146.2	McWe76
Ge	1145.4	SFS77
Ge	1145.1	Wagn75, WRDM79
GeTe	1144.8	SFS77
GeSe	1143.8	SFS77
GeS	1143.7	SFS77
GeO_2	1137.7	Wagn75
Na_2GeF_6	1135.7	Wagn75
Ge 3d		
Ge	29.4	Φ
Ge	29.3	McWe76
Ge	29.0	SFS77
Ge	29.1	HKMP74, UeOd82, WRDM79
$GeAs_2$	29.7	HKMP74
$GeTe_3As_2$	29.9	HKMP74
GeS_2TeAs_2	30.2	HKMP74
GeS_3As	30.4	HKMP74
$GeTe_2$	30.1	HKMP74
GeTe	30.0	SFS77
GeTe	29.7	HKMP74
$GeSe_2$	31.0	UeOd82
GeSe	30.9	SFS77
GeS_2	30.4	HKMP74
GeS	30.5	SFS77
GeS	29.5	HKMP74
GeO_2	32.5	HKMP74
Ph_4Ge	31.2	HWVV74
Ph_3GeI	31.8	HWVV74
Ph_3GeBr	31.8	HWVV74
Ph_3GeCl	31.8	HWVV74
Hf 4f		
Hf	14.3	Φ

Hf	14.4	WRDM79
HfO_2	16.7	SaRa80
Hf 4d		
HfO_2	213.2	SaRa80, NGDS75
Hg 4f		
HgS (cinnabar)	101.0	Φ
Hg	99.8	BrMc72, SATD73, SMBM76, WRDM79
$Hg_{0.8}Cd_{0.2}Te$	100.2	SBB80
HgS	100.8	NSSP80
HgI_2	100.7	SATD73
$HgBr_2$	101.0	SATD73
$HgCl_2$	101.4	SATD73
HgF_2	101.2	SATD73
HgO	100.8	NSSP80
$Et_2NC_6H_4HgOAc$	101.3	NSSP80
$Cl_2Hg(H_2NCONHCONH_2)_2$	101.3	YYS78
$Hg(thiodibenzoylme)_2$	101.3	TBHH77
$(Ph_4P)_2Hg(SCN)_4$	101.4	FoLa82
Ho 4d		
Ho	159.6	Φ
I $3d_{5/2}$		
KI	619.3	Φ
I_2	619.9	Sher76
CsI	618.2	MVS73
RbI	618.2	MVS73
KI	618.8	MVS73
NaI	618.6	MVS73, Sher76
LiI	619.7	WRDM79
LiI	618.9	MVS73
AgI	619.4	GaWi77
CdI	619.2	GaWi77
CdI	619.4	SATD73
CuI	619.0	GaWi77
HgI_2	619.4	SATD73
InI	619.0	FHT77
InI_3	619.1	FHT77
NiI_2	619.0	GaWi77
$NiI_2 \cdot 6H_2O$	619.7	NZB78
ZnI_2	619.8	GaWi77
ZnI_2	619.7	SATD73
$NaIO_3$	623.5	Sher76
$NaIO_4$	624.0	Sher76
HIO_3	623.1	Sher76
H_5IO_6	623.0	Sher76
I_2O_5	623.3	Sher76
ICl	621.5	Sher76
ICl_3	622.5	Sher76
$Cs_3Sb_2I_9$	618.5	BCH75
$Rb_3Sb_2I_9$	620.8	Tric74
$Na(NiIO_6) \cdot H_2O$	624.4	NZB78
$I_2Ni(Ph_3P)_2$	619.3	NZB78
$I_2Pt(Et_3P)_2$	619.2	Rigg72
$I_4In(Pr_4N)$	619.6	FHT77
$I_2Pt(Me_3P)_2$ cis	621.1	CAB71
$I_2Pt(Me_3P)_2$ tran	621.9	CAB71
$I_4(Mo_6I^*_8)$	620.6	BeWa79
$I^*_4(Mo_6I_8)$	619.3	BeWa79
I MNN		
LiI	517.0	WRDM79
AgI	506.8	GaWi77
CdI	507.0	GaWi77
CuI	507.1	GaWi77
NiI_2	507.3	GaWi77
ZnI_2	506.0	GaWi77
In $3d_{5/2}$		
In	443.9	Φ
In	443.8	Bert81, Hegd82, WRDM79, PVVA79, LAK77
$In_{95}Sn_5$	443.6	Hegd82
InSb	444.1	IMNN79
InP	444.6	Bert81, CFRS80
In_2Te_3	444.5	WRDM79
In_2Se_3	444.8	WRDM79
In_2S_3	444.8	Wagn77, MSC 73
InI_3	446.0	Wagn77, MSC 73
InI	443.9	FHT77
$InBr_3$	446.0	Wagn77
$InBr_3$	446.6	MSC73
InBr	445.1	FHT77
$InCl_3$	446.0	Wagn77
$InCl_3$	446.9	MSC73
InCl	444.9	MSC73
InF_3	446.4	Wagn75, MSC73
In_2O_3	444.3	Wagn77, NGDS75, Bert81
In_2O_3	444.6	CFRS80
In_2O_3	444.9	LAK77, MSC73
$In(OH)_3$	445.0	WRDM79
$(NH_4)_3InF_6$	445.6	Wagn77
$CuInSe_2$	444.7	KJID81
$In(acac)_3$	445.4	MSC73
Br_2InEt_4N	445.7	FHT77
Cl_2InEt_4N	445.2	FHT77
Br_4InPr_4N	445.9	FHT77
I_4InPr_4N	445.4	FHT77
Cl_4InPr_4N	445.8	FHT77
In MNN		
In	410.4	WRDM79
$In_{95}Sn_5$	410.5	PVVA79, KISC80, LAK77
InSb	401.6	IMNN79
InP	408.0	Bert81
InP	411.0	KISC80
In_2Te_3	408.9	WRDM79

In_2Se_3	408.3	WRDM79
In_2S_3	407.3	Wagn77
InI_3	405.8	Wagn77
$InBr_3$	404.8	Wagn77
$InCl_3$	404.6	Wagn77
InF_3	403.7	Wagn75
In_2O_3	406.4	Wagn77
$In(OH)_3$	405.0	WRDM79
$(NH_4)_3InF_6$	404.1	Wagn77

Ir 4f

Ir	60.9	Φ
Ir	60.8	WRDM79, BHHK70, EPC75
$IrCl_3$	62.7	Folk73
K_2IrBr_6	62.6	Nefe78$K_3IrBr_6$61.8Nefe78
K_2IrCl_6	63.0	CoHe72, LeBr72
K_2IrCl_6	63.6	KSPB76, NSBN77
K_3IrCl_6	62.5	NSBN77
$(NH_4)_2IrCl_6$	63.7	EPC75
$(NH_4)_3IrCl_6$	63.0	EPC75
$Ir(CO)_3Cl$	63.4	KSPB76
$KIrCl_5NO$	65.0	NSBN77
$KIr_2(CO)_4Cl_4$	62.7	KSPB76
$K_2Ir_2(CO)_4Cl_5$	63.0	KSPB76
$IrCl_4(EtcP)_2$	63.6	LeBr72
$IrClN_2(Ph_3P)_2$	60.7	Folk73
$IrI_3(H_2NCH_2CH_2NH_2)_3$	63.1	NeBa72
$IrCl_3(H_2NCH_2CH_2NH_2)_3$	63.2	NeBa72
$IrCl_6(H_2NCH_2CH_2NH_2)_3$	63.2	Nefe78

K 2p

K	294.4	Φ
KCl	292.9	Φ
K	294.6	SMKM77, PeKa77
KI	292.8	MVS73
KBr	293.0	MVS73, WRDM79
KCl	292.8	MVS73, NSLS77
KF	292.5	Wagn75
KF	292.8	PMDS77
KF	293.1	MVS73
KCN	294.7	Vann76
KN_3	292.5	SGRS72
KNO_2	292.9	NSLS77
$KClO_3$	293.2	MVS73
$KClO_4$	293.4	MVS73
K_3PO_4	293.5	MVS73
$K_4P_2O_7$	292.2	MVS73
K_2CrO_4	292.6	ACHT73
$K_2Cr_2O_7$	292.1	ACHT73
$K_2Cr_2O_7$	292.8	NSSP80
K_2MoO_4	292.6	NFS82
$KRhO_2$	292.5	NFS82
$KAl_2(AlSi_3O_{10})_2(OH)_2$	293.0	WPHK82
K_2IrCl_6	292.8	NSBN77, LeBr72, CoHe72
K_2MoCl_6	292.7	CoHe72
K_2OsCl_6	293.0	CoHe72, LeBr72
K_2PtCl_6	292.8	CoHe72, LeBr72
K_2ReCl_6	292.8	CoHe72
K_2ReCl_6	293.7	LeBr72
K_2SnCl_6	292.8	CoHe72
K_2WCl_6	293.3	LeBr72
K_3IrCl_6	293.0	NSBN77
$K_4Mo_2Cl_8$	293.2	HUGH79
$KSbFF_6$	293.7	Wagn77
$KZrFF_5 \cdot H_2O$	292.7	NKBP73
K_2NiF_6	294.2	TRLK73
K_2UF_6	293.1	PMDS77
K_2ZrF_6	292.6	NKBP73
K_3ZrF_7	292.8	NKBP73
$K_3Co(CN)_6$	293.7	Vann76
$K_3Cr(CN)_6$	292.2	ZeHa7
$K_3Fe(CN)_6$	291.9	Vann76
$K_3Mn(CN)_6$	291.9	Vann76
$K_4Fe(CN)_6$	291.9	Vann76
$K_4V(CN)_6$	293.7	Vann76
$KIrCl_5NO$	293.1	NSBN77
$K_2Pt(CN)_4 \cdot 3H_2O$	293.3	CaLe73
$K_2Pt(CN)_4Cl_2 \cdot 3H_2O$	292.9	CaLe73
$K_3Co(SCH_2CHNH_2COO)_3$	292.8	SSEW79

K LMM

KBr	250.7	WRDM79
KF	250.1	Wagn77
$KSbF_6$	249.3	Wagn77

Kr 3d

Kr in graphite	87.0	Φ

La 3d

La	835.8	Φ
La	835.9	ScSc82
LaH_2	838.8	ScSc82
La_2O_3	835.1	WRDM79
La_2O_3	833.7	SaRa80

La 4d

La	103.9	NIS72, KEML74
La_2O_3	101.3	SaRa80, NGDS75, HoTh80
$LaCrO_3$	101.7	HoTh80

Li 1s

LiF	55.6	Φ
Li	54.7	KLMP73, CSFG79
LiN_3	55.2	SGRS72
LiBr	56.8	MVS73
LiCl	56.0	CSFG79, MVS73
LiF	55.7	MVS73, WRDM79
Li_2O	55.6	CSFG79
LiOH	54.9	CSFG79
Li_2CO_3	55.2	CSFG79
Li_3PO_4	55.4	MVS73

$Li_4P_2O_7$	55.6	MVS73
$LiClO_4$	57.2	MVS73
Li_2CrO_4	57.1	ACHT73
$LiCrO_2$	55.6	ACHT73
$LiNbO_3$	54.8	StHo79
Lu 4f		
Lu	7.3	Φ
Lu 4d		
Lu	196.2	KEML74, LPWF75
Lu_2O_3	196.0	SaRa80, NGDS75
Mg 2p		
Mg	49.8	Φ
Mg	49.6	HAS75, LMKJ75, HFV 77, Fugg77, WRDM79
Mg_2Cu	49.8	FWFA75
Mg_3Bi_2	50.6	FWFA75
MgF_2	51.0	Wagn80
MgO	50.8	InYa81
$Mg(OH)_2$	49.5	HNUW78a
$MgAl_2O_4$	50.4	HNUW78b
Talc, $Mg_3Si_4O_1O(OH)_2$	50.5	WPHK82
Mg 1s		
Mg	1303.1	HAS75, LMKJ75, Fugg77
Mg_2Cu	1303.0	FWFA75
Mg_3Bi_2	1304.0	FWFA75
MgF_2	1305.0	Wagn80
$Mg(OH)_2$	1302.7	HNUW78a
$MgAl_2O_4$	1304.0	HNUW78b
Mg KLL		
Mg	1185.5	LMKJ75, SRHH78, WRDM79, Fugg77, HFV 77
Mg_2Cu	1185.7	FWFA75
Mg_3Bi_2	1184.6	FWFA75
MgF_2	1178.2	Wagn80
Talc, $Mg_3Si_4O_1O(OH)_2$	1180.3	WPHK82
Mn 2p		
Mn	639.0	Φ
MnO_2	642.1	Φ
Mn	638.8	LANM81
Mn	639.0	WRDM79
MnN	641.3	CSC72
MnS	640.3	CSC72
MnS, beta	640.8	Aoki76
MnS, alpha	641.9	Aoki76
MnS	642.1	Limo81
MnI_2	641.9	Aoki76, CSC72
$MnBr_2$	642.0	Aoki76, CSC72
$MnCl_2$	642.0	Aoki76, CSC72
MnF_2	642.6	Aoki76, CSC72
MnF_3	642.6	CSC72
MnO	640.7	OHI75
MnO	640.5	OkHi76
MnO	641.4	Aoki76, CSC72
Mn_2O_3, alpha	641.2	OHI75
Mn_2O_3	641.6	CSC72
Mn_2O_3, alpha	641.7	OkHi76
Mn_2O_3, gamma	641.5	OkHi76
Mn_3O_4	641.4	OHI75
MnO_2	642.4	WRDM79
MnO_2, beta	641.1	OHI75
MnO_2	642.3	Aoki76, CSC72, NGDS75
MnOOH	641.7	OHI75
$CoMn_2O_4$	641.5	OkHi76
$CuMn_2O_4$	641.0	OkHi76
$MnCr_2O_4$	640.6	OkHi76
$MnSO_4$	644.9	Limo81
$KMnO_4$	647.0	UmRe78
$Mn_2(CO)_{10}$	641.6	VWVB77
$BrMn(CO)_5$	641.9	VWVB77
$(BrMn(CO)_4)_2$	641.7	VWVB77
$BrMn(CO)_4(Ph_3P)$	641.5	VWVB77
$BrMn(CO)_3(P(OMe)_3)_2$	641.0	VWVB77
$Mn_2(CO)_8(Ph_3P)_2$	640.7	VWVB77
$K_3Mn(CN)_6$	639.7	Vann76
$Na_4Mn(CN)_6$	638.3	Vann76
$Mn(C_5H_5)_2$	638.5	BCDH73, CDH74
$Mn(CO)_3(C_5H_5)$	640.6	CDH74
$Mn(CO)_3(C_5H_5)$	641.8	ClAd71
Mn LMM		
Mn	617.6	Vayr81
Mo 3d		
Mo	228.0	Φ
Mo	227.9	NyMa80
Mo	228.0	CiDe75, WRDM79, CGR 78, GrMa75, KBAW74, WaTa80
MoB_2	227.9	MECC73
Mo_2B_5	227.3	BrWh78
Mo_2C	227.8	BrWh78
$MoSi_2$	227.7	WPHK82
$MoSe_2$	228.3	GrMa75
MoS_2	229.0	PCLH76, GrMa75
MoS_2	229.6	SSOT81, StEd75
$MoCl_3$	230.0	GrMa75
$MoCl_4$	230.6	GrMa75
$MoCl_5$	231.0	GrMa75, SwHe71
MoO_2	229.3	SaRa80, CGR78, CiDe75, KBAW74
MoO_3	232.6	GPDG79, KBAW74, SaRa80, CiDe75, CGR78, GrMa75
MoO_3	232.6	WRDM79
$(NH)_{42}MoO_4$	232.1	SwHe71
$Al_2(MoO_4)_3$	232.5	PCLH76
$Al_2(MoO_4)_3$	233.3	NFS82

$CaMoO_4$	232.8	NFS82
$CoMoO_4$	232.4	GPDG79, CiDe75, AMFL74
$CrMoO_4$	232.2	TVG76
$CuMoO_4$	232.7	HMUZ78
K_2MoO_4	232.1	NFS82
Na_2MoO_4	232.1	CiDe75, NFS82, SwHe71, NSLS77
$Na_2MoO_4 \cdot 2H_2O$	232.5	GrMa75
$(NH_4)_2Mo_2O_7$	232.5	AMFL74
$(NH_4)_2Mo_7O_{24} \cdot 4H_2O$	232.7	GrMa75
$Cu_2Mo_3O_{10}$	232.4	HMUZ78
$Cu_3Mo_2O_9$	232.8	HMUZ78
Rh_2MoO_6	231.8	NFS82
$Cl_2Mo(NO)_2$	230.4	Nefe78
$K_4Mo_2Cl_8$	229.2	HUGH79
$I_4(Mo_6I_8)$	228.8	BeWa79
$Br_4(Mo_6Br_8)$	229.3	BeWa79
$Cl_4Mo(Ph_3P)_2$	231.9	HuBa74
$Cl_4Mo_2(Et_3P)_4$	228.7	Walt77
$Cl_3Mo(PhPMe_2)_3$ mer	229.4	LeBr72
$Cl_4Mo_2(PhPMe_2)_4$	228.7	Walt77
$(CO)_5Mo(Ph_3P)$	228.3	HVV79
$(CO)_4Mo(Ph_3P)_2$	227.8	HuBa74
$(CO)_5Mo(Ph_3P)_3$	227.4	HuBa74
$Cl_2Mo(CO)_2(Ph_3P)_2$	229.3	Nefe78
$Cl_2Mo(CO)_3(Ph_3P)_2$	228.8	HuBa74
$Cl_2Mo(NO)_2(Ph_3P)_2$	230.3	HuBa74
$Cl_3Mo(NO)_2(MeCN)_2$	231.5	Nefe78
$Cl_3Mo(pyridyl)_3$	229.5	CELC76
$Cl_4Mo_2(pyridyl)_4$	228.9	Walt77
$Cl_4Mo(pyridyl)_2$	230.8	SwHe71
$Br_4(Mo_6Br_8)(pyridyl)_2$	229.7	BeWa79
$Cl_{12}Mo_6(pyridyl)$	229.6	HaWa74
$Cl_4Mo(bipyridyl)$	232.0	CELC76
$Cl_3MoO(bipyridyl)$	231.9	CELC76
$Cl_2MoO_2(bipyridyl)$	232.3	CELC76
$(CO)_4Mo(bipyridyl)$	226.3	GrMa75
$Cl_{12}Mo_6(Ph_3P)_2$	229.6	HaWa74
$Cl_6(Mo_6Br_8)(Et_4N)_2$	229.2	BeWa79
$Br_6(Mo_6Br_8)(Et_4N)_2$	229.3	BeWa79
$(Bu_3N)_2Mo(CO)_4$	227.4	GrMa75
$(Bu_4N)_2Mo_4I_{11}$	229.0	BeWa79
$(Bu_4N)_3Mo_2Cl_9$	229.5	Walt77
$(C_5H_5)Mo(CO)_3$	227.4	GrMa75
$MoO_2(acac)_2$	232.0	GrMa75

N 1s

BN	398.1	Φ
NH_3	399.6	HHJ69
NH_3	398.7	LaLu79, RNS73
Cr_2N	397.4	RoRo76
CrN	396.7	STAB76
GaN	397.0	HeMa80
Ge_3N_4	397.4	TLR78
ScN	396.2	STAB76
TiN	396.9	STAB76
VN	397.4	STAB76
BN	398.1	WRDM79, HJGN70
Si_3N_4	397.4	TLR78
S_2N_2	398.9	SDIO77
$SP(NH_3)_3$	398.8	FlWe75
S_4N_3Cl	400.4	HHJ69
$(NPCl_2)_3$	400.3	HHJ69
Cs(N*NN*)	397.9	SGRS72
Cs(NN*N)	402.2	SGRS72
K(N*NN*)	398.5	SGRS72
K(NN*N)	402.8	SGRS72
Li(N*NN*)	398.7	SGRS72
Li(NN*N)	403.1	SGRS72
Na(N*NN*)	398.5	SGRS72
Na(N*NN*)	400.1	HHJ69
Na(NN*N)	402.9	SGRS72
Na(NN*N)	404.5	HHJ69
Rb(N*NN*)	398.1	SGRS72
Rb(NN*N)	402.4	SGRS72
K3Co(CN)$_6$	399.6	Vann76
K3Cr(CN)$_6$	397.6	Vann76, ZeHa71
$K_3Fe(CN)_6$	398.1	Vann76
$K_3Mn(CN)_6$	398.3	Vann76
$K_4Fe(CN)_6$	398.0	Vann76
$K_4Fe(CN)_6$	397.8	YNNA77
$K_4V(CN)_6$	398.5	Vann76
$Na_4Mn(CN)_6$	397.6	Vann76
$Na_2Fe(CN)_3(N*O)$	402.7	YNNA77
$Na_2Fe(CN*)_3(NO)$	397.4	YNNA77
$Na_4Fe(CN)_5N*O_2$	404.3	YNNA77
$Na_4Fe(CN*)_5NO_2$	396.6	YNNA77
KCN	399.8	HHJ69
KCN	398.3	YNNA74
KCN	400.6	Vann76
NaCN	400.2	Vann76
$(NH_4)_2PtCl_4$	400.3	KaEl79
$(NH_4)_2SO_4$	401.3	SwAl74
$N*H_4NO_3$	401.9	SwAl74, BCM78
$N*H_4NO_3$	402.3	BTE77
$N*H_4NO_3$	403.1	HHJ69
$N_2H_6SO_4$	403.3	HHJ69
$N_2H_6SO_4$	401.7	Folk73
NH_3OHCl, ionic	402.9	HHJ69
NH_3OHCl, ionic	401.4	Folk73
NH_3SO_3	402.6	HHJ69
NaN_2O_2	402.1	HHJ69
KSCN	399.3	HHJ69
KOCN	399.1	HHJ69
KOCN	397.9	Folk73
NF_4BF_4	417.1	RNS73
$NaNO_2$	404.9	HHJ69, LiHe75
$NaNO_2$	403.9	BTE77
$Ba(NO_3)_2$	407.5	CLSW83
$Ca(NO_3)_2$	408.0	CLSW83
KNO_3	407.2	NSLS77
NH_4N*O_3	407.3	BTE77

$NH_4N^*O_3$	408.0	HHJ69
$NH_4N^*O_3$	405.8	BCM78
$NaNO_3$	408.1	HHJ69, LiHe75
$NaNO_3$	407.4	BTE77
$Ni(NO_3)_2$	407.0	TRLK73
$Ni(NO_3)_2 \cdot 6H_2O$	407.6	NZB78
$Pb(NO_3)_2$	407.2	TLR78
$Sr(NO_3)_2$	408.1	CLSW83
$K_2Pt(NO_2)_4$	404.7	SNMK78
$K_2Pt(NO_2)_6$	404.7	SNMK78
$K_3Co(NO_2)_6$	404.2	NBMO73
$K_3Rh(NO_2)_6$	404.1	SNMK78
$K_3Rh(NO_3)_6$	407.3	SNMK78
$MoCl_2(NO)_2$	401.4	Nefe78
$K_2Os(NO)Cl_5$	402.8	Nefe78
$K_2Ru(NO)I_5$	402.5	Nefe78
$K_2Ru(NO)Br_5$	403.30	Nefe78
$Rh_2(NO)_6Cl_3$	401.90	Nefe78
$Co(CO)_3NO$	402.20	BCGH72
$Fe(CO)_2(NO)_2$	401.80	BCGH72
$Co(NH_3)_5Cl_3$	400.10	YNAB77
$Ni(NH_3)_6Br_2$	399.60	NZB 78
$Ni(NH_3)_6(ClO_4)_2$	399.90	NZB 78
$Pt(N^*H_3)_2(NO_2)_2$	400.40	Nefe78, CMHL77
$Pt(NH_3)_2(N^*O_2)_2$	404.40	Nefe78, CMHL77
$Pt(NH_3)_2Cl_2$	400.20	Nefe78, CMHL77
$Rh(NH_3)_6Cl_3$	400.10	Nefe78
Me_4NBr	401.40	SGCT74
Me_4NCl	401.50	EMGK74
Me_4NCl	402.30	LiHe75
Et_4NCl	401.40	EMGK74
Et_3NHCl	401.20	LiHe75
Et_3NHHSO_4	401.80	EvRe81
Bu_3N	398.90	LiHe75
$BuNH_3HSO_4$	401.00	EvRe81
Bu_4NHSO_4	402.20	EvRe81
$EtNH_2$	398.90	BCGH73
$EtNH_2BF_3$	401.40	BCGH73
NH_4Cl	400.80	SwAl74
NH_4Cl	401.50	EMGK74, BTE 77
NH_4BF_3	401.90	BCGH73
C_5H_5N	398.80	LiHe75
C_5H_5N	399.30	BCGH73
C_5H_5NHCl	401.00	HHJ 69
$C_5H_5NBF_3$	401.40	BCGH73
Hexamethylenetetramn	399.40	LiHe75
PhC^*N	399.20	LiHe75
$C(NH_2)_3Cl$	400.10	LeRa77
$PhNH_2$	399.40	LiHe75
Me_3NO	403.00	LiHe75
$OP(NMe_3)_3$	399.10	FlWe75
$P(NMe_2)_3$	398.30	GBMP79
Cysteine HCl Hydrate	401.20	SSEW79
Cysteine	400.00	LlMa79
$H_3N(CH_2)_3COOH$ ionic	400.80	YoSa74
$HN(CH_2COOH)_3$ ionic	400.70	YoSa74
$N(CH_2COOH)_3$	398.70	YoSa74
H_2NCH_2COOH	398.70	YoSa74
H_3NCH_2COO ionic	400.60	YoSa74
$EtCHNH_2COOH$	400.60	YNAB77
$H_2N(CH_2)_3COOH$	398.80	YoSa74
CH_3CHNH_2COOH	401.00	YNAB77, KNPP74
H_2NCONH_2	399.50	LeRa77
H_2NCSNH_2	399.80	SrWa77, NBMO73
H_2NCSNH_2	399.20	LeRa77
CH_3CONH_2	399.60	SNMK78
$PhCONH_2$	399.50	LBNN78, HHJ 69
PhN=NPh	399.60	BrFe76
PhN=NPh	400.10	LiHe75
PhCH=NPh	399.10	SZNS77
1,1'-azonaphthalene	400.00	Yosh80
$NCN=C(N^*H_2)_2$	399.20	LeRa77
AmONO	404.5	LiHe75
PhC=NOHC=NOHPh	400.6	Yosh78
MeC=NOHC=NOHMe	399.8	Yosh78
Ni(dimethylglyoxime)$_2$	400.4	NZB78
Cu Salicylaldoxime	400.3	BuBu74
Cu(8-hydroxyquinol)$_2$	399.5	YoSa74
8-Quinolinol	398.9	Yosh80
$Cr(CO)_5NH_3$	399.5	BCGH72
$N(EtO)_3SiCl$	400.5	GrHe77
$N(EtO)_3SiH$	399.8	GrHe77
Morphine	398.5	SCKK75
Morphine H_2SO_4	401.2	SCKK75

Na 1s

Na	1071.8	Φ
NaCl	1072.1	Φ
Na	1071.8	BaSt75
Na	1071.4	KLMP73
NaI	1071.7	WRDM79
NaBr	1071.7	Wagn75
NaBr	1071.4	MVS73
NaCl	1071.6	Wagn75
NaCl	1072.5	SGSO70
NaCl	1071.5	KOK83
NaCl	1071.8	NSLS77
NaCl	1072.3	HHDD81
NaF	1071.2	Wagn75
NaF	1071.0	MVS73, NSLS77
Na_2CO_3	1071.5	WRDM79
Na_2CO_3	1071.7	HHDD81
Na_2HPO_4	1071.6	WRDM79
Na_2HPO_4	1071.5	Swif82
$Na_2S_2O_3$	1071.6	Wagn75
Na_2SO_3	1071.3	Wagn75
Na_2SO_4	1071.2	Wagn75
Na_2SeO_3	1070.8	Wagn75
Na_2TeO_4	1071.1	Wagn75
Na_3PO_4	1071.1	MVS73, Swif82, GMD79
$Na_4P_2O_7$	1070.8	MVS73
$Na_4P_2O_7$	1071.6	GMD79

$NaClO_4$	1071.8	MVS73
NaH_2PO_2	1071.1	Swif82
NaH_2PO_4	1072.0	Swif82
$NaHCO_3$	1071.3	WRDM79
NaN_3	1070.8	SGRS72
$NaNO_2$	1071.6	Wagn75
$NaNO_3$	1071.4	Wagn75
$NaPO_3$	1071.7	Wagn75
$NaPO_3$	1071.7	Swif82, GMD 79
$Na_2Cr_2O_7$	1071.6	WRDM79
Na_2CrO_4	1071.4	Wagn75
Na_2CrO_4	1071.0	ACHT73
Na_2IrCl_6	1071.9	Wagn75
Na_2MoO_4	1070.9	Wagn75
Na_2MoO_4	1071.8	NSLS77
Na_2PdCl_4	1071.8	Wagn75
$Na_2SnO_3 \cdot 3H_2O$	1071.1	WRDM79
Na_2WO_4	1072.0	Wagn75
$NaAsO_2$	1070.9	Wagn75
$NaBiO_3$	1071.3	WRDM79
$NaCrO_2$	1072.4	ACHT73
Na_2BeF_4	1071.8	NKBP73
Na_2GeF_6	1071.7	Wagn75
Na_2SiF_6	1071.7	Wagn75
Na_2SiF_6	1072.1	NSLS77
Na_2TaF_7	1071.9	NKBP73
Na_2TiF_6	1071.6	Wagn75
Na_2ZrF_6	1071.5	Wagn75
Na_3AlF_6	1071.8	Wagn75
Na_3TaF_8	1071.8	NKBP73
$NaBF_4$	1072.7	Wagn75
$NaBeF_3$	1071.9	NKBP73
$NaTaF_6$	1071.7	NKBP73
Na_2O	1072.5	BaSt75
NaOOCH	1071.1	WRDM79
$Na_2C_2O_4$	1070.8	WRDM79
$NaAlSi_3O_8$, albite	1072.2	WPHK82
Hydroxysodalite	1070.5	WPHK82
Natrolite	1072.4	WPHK82
Mol Sieve A	1071.8	WPHK82
Mol Sieve X	1072.3	WPHK82
Mol Sieve Y	1072.6	WPHK82
NaOAc	1071.1	Wagn75
NaOAc	1071.7	HHDD81
$NaOOCCH_2SH$	1071.2	WRDM79
NaO_3SPh	1071.3	WRDM79
p-($NaOCOCMe=CH_2$)	1072.2	HHDD81

Na KLL

Na	994.3	BaSt75
Na	994.3	KLMP73
Na	994.5	SRHH78
NaI	991.2	WRDM79
NaBr	990.6	Wagn75
NaCl	990.3	Wagn75
NaCl	990.0	SGSO70
NaCl	990.1	KOK83
NaF	998.6	Wagn75
Na_2CO_3	989.8	WRDM79
Na_2HPO_4	989.9	WRDM79
Na_2HPO_4	989.7	Swif82
$Na_2S_2O_3$	990.1	Wagn75
Na_2SO_3	990.4	Wagn75
Na_2SO_4	989.8	Wagn75
Na_2SeO_3	991.0	Wagn75
Na_2TeO_4	990.5	Wagn75
Na_3PO_4	990.1	Swif82
NaH_2PO_2	989.8	Swif82
NaH_2PO_4	989.1	Swif82
$NaHCO_3$	989.8	WRDM79
$NaNO_2$	989.8	Wagn75
$NaNO_3$	989.6	Wagn75
$NaPO_3$	989.3	Wagn75
$NaPO_3$	989.4	Swif82
$Na_2Cr_2O_7$	990.6	WRDM79
Na_2CrO_4	991.2	Wagn75
Na_2IrCl_6	989.2	Wagn75
Na_2MoO_4	991.0	Wagn75
Na_2PdCl_4	990.2	Wagn75
$Na_2SnO_3 \cdot 3H_2O$	990.3	WRDM79
Na_2WO_4	989.6	Wagn75
$NaAsO_2$	990.7	Wagn75
$NaBiO_3$	990.9	WRDM79
Na_2GeF_6	998.1	Wagn75
Na_2SiF_6	987.7	Wagn75
Na_2TiF_6	988.5	Wagn75
Na_2ZrF_6	988.7	Wagn75
Na_3AlF_6	988.0	Wagn75
$NaBF_4$	987.1	Wagn75
Na_2O	989.8	BaSt75
NaOOCH	989.8	WRDM79
$Na_2C_2O_4$	990.5	WRDM79
Mol Sieve A	988.8	WPHK82
Mol Sieve X	988.4	WPHK82
Mol Sieve Y	987.8	WPHK82
NaOAc	989.9	Wagn75
$NaOOCCH_2SH$	990.4	WRDM79
NaO_3SPh	989.7	WRDM79

Nb 3d

Nb	202.4	Φ
Nb	202.3	NyMa80
Nb	202.2	MSC73, NSCP74, WRDM79
Nb	201.8	Bahl75
Nb_3Te_4	202.8	Bahl75
$NbTe_4$	203.8	Bahl75
Nb_3Se_4	203.0	Bahl75
$NbSe_2$	203.4	Bahl75
NbS_2	207.7	MSC73
NbN	203.8	Bahl75
$NbBr_5$	207.1	MSC73
$NbCl_5$	208.0	MSC73

NbO	202.8	SPB76
NbO	203.7	Bahl75
NbO	204.7	FCFG77
Nb_2O_5	207.5	SPB76, MSC73, FCFG77, NFS82, NGDS75
$LiNbO_3$	207.1	StHo79
$KNbO_3$	206.5	MSC73
$CaNb_2O_6$	206.8	Bahl75
$CdNb_2O_6$	207.0	Bahl75
$Ca_2Nb_2O_7$	206.7	Bahl75
$RhNbO_4$	206.5	NFS82
$Cl_2Nb_6Cl_{12}(H_2O)_4 \cdot 4H_2O$	204.7	BeWa79
$Cl_6(Nb_6Cl_{12})(Et_4N)_3$	204.7	BeWa79
$Br_6(Nb_6Cl_{12})(Bu_4N)_2$	204.7	BeWa79
$Cl_2(Nb_6Cl_{12})(Pr_3P)_4$	204.6	BeWa79
$Cl_2(Nb_6Cl_{12})(Me_2SO)_4$	204.6	BeWa79

Nd 3d

Nd	980.8	Φ
Nd_2O_3	982.0	SaRa80

Nd 4d

Nd_2O_3	120.8	SaRa80

Ne 1s

Ne in graphite	863.1	Φ
Ne in Ag	862.4	CiHa74
Ne in Au	861.6	CiHa74
Ne in Cu	862.2	CiHa74
Ne in Fe	863.4	Wagn75

Ne KLL

Ne in Fe	818.0	Wagn75

Ni 2p

Ni	852.7	Φ
NiO	853.8	Φ
Ni	852.7	LANM81
Ni	852.7	ALMP82
Ni	852.8	PEJ82
Ni	852.7	WRDM79, ShRe79
Ni_5Yb	852.7	WWC78
Ni_2Si	853.0	GGM82
NiSi	853.5	GGM82
NiS	852.8	ShRe79
NiS	853.2	DPS77
NiS	855.1	NgHe76
$NiI_2 \cdot 6H_2O$	855.3	NZB78
$NiCl_2$	856.7	TRLK73, KlHe83, YYS78
$NiF_2 \cdot 4H_2O$	857.5	NSLS77
NiO	853.5	WRDM79
NiO	854.3	DPS77, KlHe83, LFWS79, NFS82, NZB78, SRD79
NiO	854.3	KiWi74, McCo75
Ni_2O_3	857.3	NgHe76
Ni_2O_3	855.8	KiWi74
$Ni(OH)_2$	855.6	DPS77, LFWS79, McCo75
$Ni(NO_3)_2$	857.1	TRLK73
$Ni(NO_3)_2 \cdot 6H_2O$	856.9	NZB78
$NiAl_2O_4$	855.8	SDR 80, LFWS79
$NiAl_2O_4$	857.4	NgHe76
Ni_2SiO_4	856.1	LFWS79
$NiClO_4 \cdot 6H_2O$	857.2	NZB78
$NiFe_2O_4$	855.4	McCo75
$NiRh_2O_4$	855.9	NFS82
$NiSO_4$	856.8	ShRe79
$NiSiO_3$	856.5	SRD79
$NiWO_4$	857.7	NgHe76
$NaNiIO_6 \cdot H_2O$	856.4	NZB78
K_2NiF_6	861.0	TRLK73
$Ni(CO)_4$	854.8	BCGH72
$Br_2Ni(NH_3)_6$	855.9	NZB78
$Ni(NH_3)_6(ClO_4)_2$	856.5	NZB78
$Ni(acac)_2$	855.9	NZB78, TRLK73
$Ni(OAc)_2 \cdot 4H_2O$	856.5	NZB78
$Ni(C_5H_5)$	854.2	BCDH73
$Ni(C_5H_5)$	856.8	ClAd71, TRLK73
$Cl_2Ni(Ph_3P)_2$	855.0	BNSA70
$Cl_2Ni(Ph_3P)_2$	854.4	NZB78
$Cl_2Ni(Ph_3P)_2$	857.0	STHU76
Ni(dimethylglyoxim)$_2$	855.0	NZB78,YoYa81
Cl_2Ni(bipyridyl)	855.7	NSWU77, NZB78
$Ni(SPh)_2$	854.6	BBFR77
$Cl_2Ni(NH_2CONHCONH_2)_2$	856.7	YYS78
Ni(2-aminobenzoate)$_2$	855.9	YoYa81
$Ni(P(OEt)_3)_4$	853.8	TRLK73
$Cl_2Ni(Et_3P)_2$	854.7	FaBa79
$Br_4Ni(Et_4N)_2$	855.2	EMGK74

Ni LMM

Ni	846.1	PEJ82
Ni	846.2	WRDM79
Ni	846.1	KiWi74, KGW76

O 1s

Al_2O_3, sapphire	531.0	Φ
Ag_2O	529.2	Scho73
AgO	528.6	Scho73, SRD80
Al_2O_3	531.3	Nefe82, SDR80, BGD75, ZSOS79
Al_2O, sapphire	531.0	Tayl82, WPHK82
Al_2O_3, alpha	531.8	WPHK82
Al_2O_3, gamma	530.9	Barr83, WPHK82
As_2O_3	531.7	Tayl82, MINN78
As_2O_5	531.6	WZR80
B_2O_3	533.0	NGDS75
BaO	528.3	InYa81
BeO	531.7	NGDS75, NFS75, HJGN70
Bi_2O_3	530.0	NGDS75, DSBG82
CaO	529.4	InYa81

CaO	531.3	WZR80
CdO	529.2	NFS75, NGDS75, SBB80
CdO_2	530.3	HGW75
Ce_2O_3	530.3	PKHL80
CeO_2	529.2	NGDS75
Co_2O_3	529.9	McCo75
Co_3O_4	530.2	NGDS75, WZR80
Co_3O_4	529.6	BGD75
Co_3O_4	529.7	CBR76, GPDG79, HSU76
CoO	530.1	BGD75, NFS82, NGDS75
Cr_2O_3	531.0	HoTh80, DPS76, WZR80, BDFP81
Cr_2O_3	531.5	NGDS75
CrO_2	529.3	IIKK76
CrO_3	530.2	DPS76
CsO_2	527.5	YaBa80
Cs_2O_4	530.5	YaBa80
Cu_2O	530.3	HMUZ78, MSSS81, RBO72, Scho73b
CuO	529.6	MSSS81, McCo75, HMUZ78, RBO72, Scho73b
Fe_2O_3	530.2	NGDS75, WZR80, Kilk73, Limo81
Fe_2O_3	529.6	HSU76, NSLS77
Fe_2O_3, alpha	529.6	McZe77
Fe_2O_3, gamma	529.8	McZe77
Fe_3O_4	530.0	McZe77
FeO	529.8	McZe77
Ga_2O_3	530.8	NGDS75, Scho73a, WZR80, ZSOS79
GeO_2	520.0	NGDS75, WZR80
H_2O	533.2	NGDS75, WZR80
HfO_2	530.4	NGDS75
I_2O_5	529.9	Sher76
In_2O_3	529.8	NGDS75
In_2O_3	530.3	CFRS80
In_2O_3	530.5	LAK77
La_2O_3	528.6	NGDS75
Li_2O	531.3	CSFG79
Lu_2O_3	529.5	NGDS75
MgO	530.0	NFS82, NGDS75
MgO	531.2	InYa81
MgO	532.1	WZR80
MnO	529.7	OHI75
Mn_3O_4	529.6	OHI75
Mn_2O_3	529.6	OHI75
MnO_2	530.0	NGDS75, WZR80
MnO_2, beta	529.6	OHI75
MoO_2	531.1	PCLH76
MoO_2	530.7	CGR78, KBAW74
MoO_2	529.9	SaRa80
MoO_3	530.9	NGDS75, NFS82
MoO_3	531.6	PCLH76
MoO_3	530.4	SaRa80, KBAW74, HMUZ78, CGR78
Na_2O	529.7	BaSt75
Nb_2O_5	529.6	GBP81
Nb_2O_5	530.6	NGDS75, NFS82
Nb_2O_5	531.3	SaRa80
NbO_2	530.7	SaRa80
Nd_2O_3	530.6	SaRa80
Ni_2O_3	531.8	KiWi74, NgHe76
NiO	529.6	DPS77, LFWS79, NFS82, NGDS75, SRD79, WZR80
P_2O_5 (bridging O)	532.2	NGDS75
P_2O_5 (bridging O)	532.6	GMD79
P_2O_5 (nonbridging O)	533.6	NGDS75
P_2O_5 (nonbridging O)	534.3	GMD79
PbO	528.9	NFS82
PbO	531.6	WZR80
PbO, rhombic	529.4	KOW73
PbO, rhombic	530.9	ZiHe78
PbO, tetragonal	527.5	KOW73
PbO, tetragonal	528.9	ZiHe78
PbO_2	527.4	KOW73
PbO_2	529.0	TLR78
PdO	529.3	KGW74
Pr_2O_3	529.3	SaRa80
PrO_2	528.6	SaRa80
PtO_2	531.4	CMHL77
ReO_2	530.1	BHU81
ReO_3	531.9	BHU81
Rh_2O_3	530.4	CMHL77, NFS82
RuO_2	529.4	MWLF78
RuO_2	529.4	KiWi74, McGi82, SaRa80
RuO_3	530.7	KiWi74
Sb_2O_3	530.0	WZR80
Sc_2O_3	530.0	NGDS75, WZR80
SiO_2	533.0	Barr83, KMH78, NGDS75
SiO_2	534.3	Kilk73
SiO_2	532.5	NSLS77, SRD79
SiO_2, gel	532.8	WPHK82
SiO_2, Vycor	532.9	WPHK82
SiO_2, alpha cristobal	532.5	WPHK82
SiO_2, alpha quartz	532.7	WPHK82
SiO_2, alpha quartz	533.2	TLR78
SnO	530.1	ADPS77
SnO_2	530.6	ADPS77, LAK77, MWLF78, NGDS75, TLR78
SrO	530.5	VaVe80
Tb_2O_3	528.8	SaRa80
TbO_2	528.8	SaRa80
TeO_2	530.2	GBP81, SBB80
ThO_2	530.0	NGDS75
TiO_2	529.9	MWLF78, WZR80, NGDS75
UO_2	530.4	MSSS81
UO_3	529.9	MSSS81
V_2O_3	530.5	CGR78
V_2O_4	530.0	KKL83
V_2O_5	529.9	BCM78, KKL83
V_2O_5	530.5	NSLS77, NGDS75, NFS82
WO_2	530.4	CoRa76

WO_3	530.6	CoRa76, KMH78, NFS82, NGDS75, NSLS77
ZnO	530.4	NFS82, NGDS75, NSLS77, Scho73, WZR80, ZSOS79
ZrO_2	530.2	NGDS75
ZrO_2	530.9	WZR80
$Al(OH)_3$, bayerite	531.4	WPHK82
$Al(OH)_3$, gibbsite	531.5	WPHK80
AlOOH, boehmite	531.5	Tayl82
$Co(OH)_2$	531.2	HSU76
$Cr(OH)_3$	531.2	DPS76
$Cu(OH)_2$	531.2	MSSS81
$Fe(OH)_2$	531.3	HSU76
FeO*OH	530.1	McZe77
FeOO*H	531.2	McZe77
$In(OH)_3$	531.8	WZR80
KOH	531.8	Kilk73
LiOH	531.2	CSFG79, WZR80
$Mg(OH)_2$	530.9	HNUW78
NaOH	532.8	BaSt75
$Ni(OH)_2$	531.3	LFWS79
$AlPO_4$	532.8	CFRS80
Cs_3PO_4	530.1	MVS73
$Cs_4P_2O_7$	530.2	MVS73
K_3PO_4	530.4	MVS73
$K_4P_2O_7$	530.1	MVS73
Li_3PO_4	531.5	MVS73
$Li_4P_2O_7$	531.7	MVS73
Na_3PO_4	530.4	MVS73, GMD79
$Na_4P_2O_7$ (bridging O)	531.1	GMD79
$Na_4P_2O_7$ (nonbridging O)	532.9	GMD79
$NaPO_3$ (bridging O)	531.5	GMD79
$NaPO_3$ (nonbridging O)	533.4	GMD79
$Ba(NO_3)_2$	533.0	CLSW83
$Ca(NO_3)_2$	533.6	CLSW83
KNO_3	532.7	NSLS77
$Pb(NO_3)_2$	532.7	TLR78
$BaSO_4$	531.8	CLSW83
$BaSO_4$	532.5	WZR80
$CaSO_4$	532.0	CLSW83, WZR80
$Cr_2(SO_4)_3$	532.1	DPS76
$FeSO_4$	532.4	Limo81
K_2SO_4	531.2	WZR80
$NiSO_4$	532.1	NSLS77, Nefe82
$PbSO_4$	531.5	ZiHe78
$ZnSO_4$	532.5	Nefe82
Na_2SO_3	531.2	WZR80
$Na_2S_4O_3$	531.8	WZR80
$PbSO_3$	530.8	ZiHe78
PbS_2O_3	531.1	ZiHe78
Ag_2CO_3	530.6	HGW75
$BaCO_3$	531.3	CLSW83
$CaCO_3$	531.4	CLSW83, WZR80
$CdCO_3$	531.4	HGW75
$CuCO_3$	531.5	WZR80
Li_2CO_3	531.5	CSFG79
Na_2CO_3	531.6	HHDD81, WZR80
$PbCO_3$	531.2	WZR80
$CsClO_4$	532.7	MVS73
$KClO_4$	532.2	MVS73
$KClO_3$	532.3	MVS73
$LiClO_4$	533.4	MVS73
$NaClO_4$	533.0	MVS73
$RbClO_4$	532.8	MVS73
Al_2SiO_5, kyanite	531.3	AnSw74
Al_2SiO_5, mullite	531.6	AnSw74
Al_2SiO_5, sillimanite	531.3	AnSw74
Al_2SiO_5, sillimanite	531.9	WPHK82
$Ca_3(HSiO_4)_2$	531.2	ClRi76
Co_2SiO_4	531.6	WZR80
$Na_2SiO^*_3 \cdot 5H_2O$	530.6	ClRi76
$Na_2SiO_3 \cdot 5H_2O^*$	532.5	ClRi76
Ni_2SiO_4	531.9	LFWS79
$NiSiO_3$	532.3	SRD79
$MgSiO^*_3 \cdot 2H_2O$	532.0	ClRi76
$MgSiO_3 \cdot 2H_2O^*$	532.8	ClRi76
$Al_2(MoO_4)_3$	531.0	PCLH76
$Al_2(WO_4)_3$	532.0	NgHe76
$CaCrO_4$	529.5	ACHT73
$CaMoO_4$	530.6	NFS82
$CaWO_4$	529.9	NFS82
p-Benzoquinone	532.2	OYK74
Hydroquinone	533.5	OYK74
PhCOONa	531.4	LBNN78
$p(Me_2Si(O))$	532.5	WPHK82
Methylsilicone Resin	532.7	WPHK82
Phenylsilicone Resin	532.6	WPHK82
$PhCONH_2$	532.2	LBNN78

Os 4f

Os	50.7	Φ
Os	50.6	Folk73, BNMN79
Os	50.2	BHHK70
$OsCl_3$	53.1	Nefe78
OsO_2	52.0	SaRa80
OsO_2	52.7	Folk73
$Os(HSO_3)_2$	52.2	Nefe78
K_2OsI_6	51.9	Nefe78
K_2OsBr_6	52.9	Nefe78
K_2OsCl_6	53.0	Folk73
K_2OsCl_6	53.2	CoHe72
K_2OsCl_6	53.5	LeBr72
K_2OsCl_6	53.9	Nefe78
$K_2OsO_2(OH)_4$	55.2	Nefe78
$Os(NH_3)_5N_2I_2$	50.9	Folk73
$Os(NH_3)_5N_2Br_2$	52.0	Folk73
$Os(NH_3)_4(N_2)_2Br_2$	51.6	Folk73
$Os(NH_3)_5N_2Cl_2$	52.2	Folk73
$K_2Os(NO)Br_5$	53.3	Nefe78
$K_2Os(NO)Cl_5$	53.4	Nefe78
$HOs(Ph_3P)Cl(CO)$	51.1	Nefe78
$OsCl_4(Et_3P)_2$	52.6	LeBr72

$OsCl_4(PhPMe_2)_2$ trans	53.0	LeBr72
$OsCl_3(PhPMe_2)_3$ mer	51.7	LeBr72
$OsCl_2(PhPMe_2)_4$ trans	50.5	LeBr72

P 2p

P	129.9	Φ
P	130.0	NSDU75
P (red)	130.0	ScBr81
Cu_3P	129.6	NSDU75
CuP_2	129.7	NSDU75
GaP	128.8	WaTa80, IMNN79, NIMN78
GaP, anodically oxid.	128.5	MIN81
GaP, thermally oxid.	129.7	MIN81
InP	128.3	CFRS80
InP	129.4	Bert81
Zn_3P_2	128.3	NSDU75
ZnP_2	129.8	NSDU75
$AlPO_4$	132.9	CFRS80
Cs_3PO_4	132.1	MVS73
K_2HPO_4	132.8	Bert81
K_3PO_4	133.2	MVS73
Li_3PO_4	133.6	MVS73
Na_2HPO_4	133.1	Swif82, WRDM79, WaTa80
Na_3PO_4	132.4	MVS73, GMD79, Swif82
NaH_2PO_4	134.2	Swif82
$NaPO_3$	134.2	Swif82,GMD79
Rb_3PO_4	132.5	MVS73
NaH_2PO_2	132.6	Swif82
$Cs_4P_2O_7$	132.6	MVS73
$K_4P_2O_7$	132.6	MVS73
$Li_4P_2O_7$	134.3	MVS73
$Na_4P_2O_7$	133.2	MVS73, GMD79, Bert81
$Rb_4P_2O_7$	133.1	MVS73
P_4O_{10}	135.3	NIMN78, NGDS75, CFRS80, Bert81, GMD79
$OPCl_3$	135.7	FlWe75
$SPCl_3$	135.3	FlWe75
$SP(NH_3)_3$	133.4	FlWe75
Ph_3P	130.9	Dale76, NSMS79, TRLK73, GBMP79
Ph_3P	130.9	HVV79, LMF80, SRH72
Ph_3P	130.9	MSAV71, GZF73
Ph_3PS	132.5	HVV79, STA74, FlWe75, MSAV71
Ph_3PSe	132.6	HVV79, MSAV71
Ph_3PO	132.5	GZF73, STA74, FlWe75, MSAV71, HVV79, BNSA70
Ph_3PBI_3	132.2	HVV79
Ph_3PBBr_3	132.1	HVV79
Ph_3PBCl_3	132.2	HVV79
Ph_3PBF_3	132.0	HVV79
Ph_2PSH	132.3	NSWM80
Ph_2PSeH	132.3	NSWM80
$(PhS)_3P$	134.3	MSAV71
$(PhS)_3PS$	133.1	MSAV71
$(PhO)_3P$	134.7	MSAV71
$(PhO)_3PS$	134.7	MSAV71
$(PhO)_3PSe$	134.3	MSAV71
$(PhO)_3PO$	133.6	CFRS80
$(PhO)_3PO$	134.8	FlWe75
Ph_3POBBr_3	133.7	HVV79
Ph_3POBCl_3	133.4	HVV79
Ph_3POBF_3	133.3	HVV79
$Ph_2PO(OH)$	133.3	MSAV71
$OPCl(OEt)_2$	134.8	FlWe75
OPF_2NPh_2	135.8	FlWe75
$OPCl_2OEt$	135.2	FlWe75
$OP(NMe_3)_3$	133.4	FlWe75
Ph_4PI	133.0	HVV79
Ph_4PBr	133.5	LMF80, SRH72
Ph_4PCl	132.8	HVV79
$MePPh_3Br$	133.0	SRH 2
$(Ph_3P)_3P^*F_6$	136.7	LMF80
$(Ph_3P^*)_3PF_6$	133.5	LMF80
$Pt(Ph_3P)_4$	131.2	Rigg72
Ph_3P=CHCOPh	132.2	Dale76, STA74
Ph_3P=CHCOOMe	132.5	STA74
$Cl_2Ni(Ph_3P)_2$	132.4	BNSA70
$Ni(CO)_2(Ph_3P)_2$	131.4	TRLK73

Pb 4f

Pb	136.9	Φ
Pb	136.4	LKMP73
Pb	136.8	SFS77
Pb	136.8	BeFl80, KOW73, KiWi73, TLR78, WRDM79, WaTa80
Pb	136.8	HSBS81, OCH79
$Pb_{98}Sn_2$	136.8	HSBS81
PbTe	137.4	SFS77
PbSe	137.4	SFS77
PbS	137.6	MoVa73, SFS77, ZiHe78
PbI_2	138.7	MoVa73
$PbBr_2$	138.8	NeFe82
PbF_2	139.0	MoVa73
PbO	138.9	KOW73, ZiHe78, WRDM79, NFS82, NSSP80, MoVa73
PbO	138.9	MoVa73, BeFl80
Pb_3O_4	138.0	MoVa73
PbO_2	137.4	BeFl80, KOW73, TLR78, MoVa73
$Pb(OH)_2$	138.4	NSSP80
$Pb(NO_3)_2$	139.3	BeFl80, TLR78, NSSP80
$PbSO_3$	138.6	ZiHe78
$PbSO_4$	139.4	NSSP80, ZiHe78
PbS_2O_3	138.4	ZiHe78
$PbRh_2O_4$	137.3	NFS82
Ph_4Pb	138.2	MoVa73
Ph_3PbCl	138.9	MoVa73
Ph_2PbCl_2	139.4	MoVa73
$Pb(OAc)_2$	138.5	BeFl80
$Pb(OAc)_4$	137.2	BeFl80

Pd 3d		
Pd	335.1	Φ
Pd	335.1	NyMa80
Pd	335.2	BiSw80
Pd	335.2	BiSw80
Pd	335.5	BiSw80
Pd	335.2	JHBK73, Asam76
Pd	335.3	WRDM79, WeAn80, BHHK70, Scho72, GGM82, KBAM72
Ag_3OPd_5O	334.6	WeAn80
Ag_8OPd_2O	334.9	WeAn80
Ag_9OPd_1O	334.9	WeAn80
Al_8OPd_2O	337.4	WeAn80
$Mg_{75}Pd_{25}$	336.2	WeAn80
Pd_2Si	336.8	GGM82
Pd_3Si	336.2	AWL80
PdI_2	336.4	KBAM72
$PdBr_2$	337.1	KBAM72
$PdCl_2$	337.8	KBAM72, NKBP73
PdO	336.3	KGW74
PdO_2	337.9	KGW74
Na_2PdCl_4	338.0	SeTs76
K_2PdCl_4	338.2	KBAM72, NKBP73
K_2PdBr_4	337.3	KBAM72
$K_2Pd(NO_2)_4$	339.0	KBAM72
K_2PdCl_6	340.2	KBAM72, Nefe78
$Br_2Pd(Ph_3P)_2$	337.8	KBAM72
$Cl_2Pd(Ph_3P)_2$	337.8	KBAM72, NSMS79
$I_2Pd(Ph_3P)_2$	337.5	KBAM72
$(CN)_2Pd(Ph_3P)_2$	338.2	KBAM72
$Pd_2(Ph_3P)_2$	336.6	NSMS79
$Cl_2Pd(Ph_3P)_3$	342.9	BNSA70
$Pd(Ph_3P)_4$	336.0	NSMS79
$Pd(OAc)_2$	338.6	NSMS79
$Pd(SPh)_2$	337.7	BBFR77
Pd MNN		
Pd	327.8	WeAn80, WRDM79
Ag_3OPd_5O	328.8	WeAn80
Ag_8OPd_2O	329.8	WeAn80
Ag_9OPd_1O	329.7	WeAn80
Al_8OPd_2O	325.5	WeAn80
$Mg_{75}Pd_{25}$	326.4	WeAn80
Pm 3d		
$PmCl_3$	1033.5	MNTB70
Pm 4d		
$PmCl_3$	128.3	MNTB70
Pr 3d		
Pr	931.8	Φ
Pr_2O_3	933.2	SaRa80
PrO_2	935.3	SaRa80
Pr 4d		
Pr_2O_3	116.1	SaRa80
PrO_2	116.2	SaRa80
Pt 4f		
Pt	71.2	Φ
Pt	71.0	JHBK73
Pt	71.2	BHHK70, KWD71, Nefe78, Scho72, WRDM79, Wagn75
Pt	71.2	CMHL77, CaLe73, HaWi77, BACB75
PtSi	73.0	GGM82
Pt_2Si	72.5	GGM82
$PtCl_2$	73.6	EPCC75
$PtCl_4$	75.5	EPCC75
PtO	73.8	KWD71
PtO	74.2	EPCC75
PtO_2	74.6	KWD71
PtO_2	75.0	EPCC75
$Pt(OH)_2$	72.6	HaWi77
K_2PtI_6	73.4	SNMK78
K_2PtBr_4	72.6	SNMK78
K_2PtBr_6	74.6	SNMK78
K_2PtCl_4	73.0	CMHL77, EPCC75, SNMK78
K_2PtCl_4	73.4	Wagn75
K_2PtCl_6	75.4	CoHe72, EPCC75, LeBr72, SNMK78
K_2PtF_6	77.6	SNMK78
$Pt(NH_3)_4Br_2$	73.4	Nefe78
$Pt(NH_3)_2Cl_2$	73.2	CMHL77, Nefe78
$Pt(NH_3)_4Cl_2$	73.4	SNMK78
$Pt(NH_3)_6Cl_4$	76.3	SNMK78
$Pt(NH_3)_2(NO_2)_2$	73.7	Nefe78
$Pt(NH_3)_2(NO_2)_2$	74.4	CMHL77
$K_2Pt(OH)_6$	75.1	SNMK78
$K_2Pt(NO_2)_4$	74.1	SNMK78
$K_2Pt(NO_2)_6$	75.9	SNMK78
$(NH_4)_2PtCl_4$	72.4	KaEl79
$Pt(Ph_3P)_3$	71.4	Nefe78
$Pt(Ph_3P)_4$	71.4	Rigg72
$Cl_2Pt(Ph_3P)_2$ cis	72.3	CAB71
$Cl_2Pt(Ph_3P)_2$ cis	73.0	Rigg72
$Cl_4Pt(Et_3P)_2$	75.3	LeBr72
$Cl_4Pt(Et_3P)_2$	75.9	Nefe78, Rigg72
$HClPt(Et_3P)_2$	72.6	Rigg72
$O_2Pt(Ph_3P)_2$	73.0	Rigg72
$Pt(SPh)_2$	72.8	BBFR77
$Ph_3PPt(SPPh_2)$	71.8	NeSa78
$Cl_2Pt(Et_3P)_2$	73.1	Rigg72
$I_2Pt(Et_3P)_2$	72.5	Rigg72
$I_2Pt(Me_3P)_2$ cis	72.6	CAB71
$I_2Pt(Me_3P)_2$ trans	72.7	CAB71
$I_2Pt(CH_3CONH)_4$	74.6	NeSa78
$Br_2Pt(CH_3CONH)_4$	74.9	NeSa78
$Cl_2Pt(CH_3CONH)_4$	74.8	NeSa78

$Cl_2Pt(H_2NCH_2CH_2NH_2)_2$	73.0	YMK78
Cl_2Pt(cyclooctadien)	73.9	CMHL77
K_2PtCl_6	318.1	EPCC75
Pt $M_5N_7N_7$		
Pt	1960.7	Wagn78
$Pt(M_4N_7N_7)$	2041.1	Wagn78
Rb 3d		
Rb	111.5	Φ
RbCl	109.9	Φ
RbN_3	109.8	SGRS72
RbI	110.4	MVS 73
RbBr	110.0	MVS 73
RbCl	109.9	MVS 73
RbF	109.8	MVS 73
Rb_3PO_4	110.0	MVS 73
$Rb_4P_2O_7$	110.0	MVS 73
$RbClO_4$	110.4	MVS73
Re 4f		
Re	40.3	Φ
Re	40.5	FHR80
Re	40.5	SSHU83, WRDM79
Re	41.0	BHU81
ReO_2	43.6	BHU81
ReO_3	46.8	BHU81
K_2ReCl_6	44.2	CoHe72, LeBr72
$Cl_3ReO(Ph_3P)_2$	43.9	Folk73, Nefe78
$Cl_2ReN(Ph_3P)_2$	42.7	Nefe78
$Cl_4Re(Et_3P_2$	43.3	LeBr72
$Cl_4Re(PMe_2Ph)_2$	43.6	LeBr72
$Cl_3Re(PMe_2Ph)_3$, mer	41.8	LeBr72
$Cl_2Re(PMe_2Ph)_4$, trans	40.5	LeBr72
$ClReN_2(PMe_2Ph)_4$, trans	40.3	LeBr72, Folk73
Rh 3d		
Rh	307.2	Φ
Rh	307.2	NyMa80
Rh	307.2	OIIT79, WRDM79, FHPW73
RhI_3	308.6	Nefe78
$RhCl_3$	310.1	OIIT79
$RhCl_3 \cdot 3H_2O$	310.0	CWH82
$RhCl_3 \cdot 12H_2O$	310.1	CMHL77
Rh_2O_3	308.8	NFS82, CMHL77
Rh_2O_3	308.2	OIIT79
$BaRh_2O_4$	308.4	NFS82
$BeRh_2O_4$	308.9	NFS82
$CaRh_2O_4$	308.8	NFS82
$CoRh_2O_4$	308.8	NFS82
$PbRh_2O_4$	308.6	NFS82
$KRhO_2$	308.5	NFS82
$LiRhO_2$	308.9	NFS82
$ZnRh_2O_4$	308.7	NFS82
Rh_2MoO_6	309.2	NFS82
Rh_2WO_6	309.4	NFS82
$RhNbO_4$	309.2	NFS82
$RhTaO_4$	309.5	NFS82
$RhVO_4$	309.2	NFS82
K_3RhCl_6	309.8	SNMK78
K_3RhF_6	312.2	Nefe78
$K_3Rh(NO_2)_6$	310.5	SNMK78
$K_3Rh(NO_3)_6$	311.1	SNMK78
$Rh(NH_3)_6Cl_3$	310.5	Nefe78
$Rh(NO)_6Cl_3$	309.8	Nefe78
$ClRh(Ph_3P)_3$	307.4	CWH82, Nefe78, OIIT79
$Cl_3Rh(Ph_3P)_3$	309.7	CWH82
$Cl_6Rh(Ph_3P)_3$	309.7	Nefe78
$Br_6Rh(Ph_3P)_3$	307.9	Nefe78
$NORh(Ph_3P)_3$	308.2	Nefe78
$Cl_3Rh(Ph_3P)_2MeCN$	309.6	GlWa79
$H(CO)Rh(Ph_3P)_2$	308.5	OIIT79
$Cl(CO)_2Rh(Ph_3P)$	308.7	Nefe78
$Cl(CO)Rh(Ph_3P)_2$	308.6	CWH82, OIIT79
Cl_2Rh_2(cyclooctadi)$_2$	308.7	CMHL77, CWH82
$Rh_2(OAc)_4 \cdot 2H_2O$	309.0	Nefe78
$Rh(NH_2CH_2COO)_3 \cdot H_2O$	310.3	NPBS74
Ru 3d		
Ru	280.1	Φ
Ru	280.0	NyMa80
Ru	280.1	Folk73, BHHK70, KiWi74, FEMY77, WRDM79
$RuCl_3$	281.8	Folk73
RuO_2	280.7	SaRa80, KiWi74, McGi82
RuO_3	282.5	KiWi74
RuO_4	283.3	KiWi74
$Ru(NH_3)_5N_2I_2$	282.2	Folk73
$Ru(NH_3)_5N_2Br_2$	280.5	Folk73
$Ru(NH_3)_5N_2Cl_2$	282.5	Folk73
$Cl_3Ru(PhPMe_2)_3$ mer	276.6	LeBr72
S 2p		
S	164.0	Φ
S	164.1	SNRS76, WRDM79, RiVe83, LHJG70
BaS	160.1	SiWo80
CdS	161.7	BSRR81
CoS	162.0	Limo81
Cu_2S	161.3	BSRR81
Cu_2S	162.4	NSSP80
CuS	162.0	Limo81, NSSP80
CuS	161.3	BSRR81
FeS	161.6	Bind73, Limo81
FeS_2	162.9	Bind73, Limo81
Ga_2S_3	162.2	TJWB72
GeS	161.8	SFS77
GeS_2	161.7	HKMP74
HgS	162.0	NSSP80
MnS	162.5	Limo81

MoS_2	162.5	SSOT81, StEd75, PCLH76
Na_2S	160.6	SWH71
Na_2S	161.8	LHJG70
NiS	162.2	ShRe79, NgHe76, DPS77
PbS	160.8	SFS77
Sb_2S_3	161.8	BCH75
SnS	161.1	SFS77
US	161.5	SNRS76
US_3	162.6	SNRS76
WS_2	162.1	NgHe76
WS_2	163.0	Wagn75
ZnS	164.0	Limo81
GeS_2TeAs_2	161.5	HKMP74
GeS_3As_2	161.6	HKMP74
$KFeS_2$	161.6	Bind73
$Na_2(S*SO_3)$	162.5	Wagn75
$Na_2(S*SO_3)$	161.7	LHJG70
$Na_2(SS*O_3)$	167.7	LHJG70
K_2SO_3	167.5	TMR80
Na_2SO_3	165.6	SWH71
Na_2SO_3	166.6	WaTa82, LHJG70
Na_2SO_3	167.2	TMR80
Ag_2SO_4	168.6	TMR80
$Al_2(SO_4)_3$	168.8	LHJG70
$BaSO_4$	168.8	SiWo80, CLSW83
$CaSO_4$	169.0	CLSW83
$CoSO_4$	169.7	Limo81
$CuSO_4$	169.3	WaTa80, NSSP80, Limo81
$FeSO_4$	168.8	Limo81, LHJG70
$Fe_2(SO_4)_3$	169.1	LHJG70
K_2SO_4	169.1	TMR80
$MnSO_4$	171.0	Limo81
Na_2SO_4	168.8	TMR80
$NiSO_4$	169.2	Limo81, NSLS77, Nefe82, ShRe79
$PbSO_4$	168.6	NSSP80
$SrSO_4$	169.1	CLSW83
$U(SO_4)_2$	169.1	Chad73
$ZnSO_4$	169.5	Nefe82
NO_2SO_3	166.8	BCM78
S_2N_2	164.6	SDIO77
SF_6	174.4	WaTa82
SF_6	177.2	LHJG70
SO_2	167.4	WaTa82
SO_2	168.1	LHJG70
$SOCl_2$	168.1	LHJG70
SOF_2	170.0	LHJG70
$SP(NH_3)_3$	162.3	FlWe75
$SPCl_3$	163.7	FlWe75
S_2Cl_2	163.5	LHJG70
S_2Cl_{10}	174.4	LHJG70
CS_2	163.7	LHJG70
$(CH_2COOH)_2S$	163.7	LHJG70
$(CH_2Ph)_2$$	163.3	LHJG70
PhSH	163.1	LHJG70
Ph_2S	163.2	LHJG70
Thiophene	164.3	LHJG70
Ph_3PS	162.4	FlWe75, MSAV71
Ph_3PS	161.8	HVV79
Ph_3AsS	161.7	HVV79
PhSSPh	164.4	RiVe83, LHJG70
$PhCH_2SSCH_2Ph$	164.2	RiVe83
$(PhS)_3P$	163.6	MSAV71
$(PhS)_3PS$	163.5	MSAV71
BuSSBu	164.1	RiVe83
MeSSMe	164.3	RiVe83
NH_2CSNH_2	162.1	LeRa77, NBMO73, SrWa77
2-Mercaptobenzimidaz	162.2	YYS79
2-Mercaptobenzimidaz	162.8	ChHa79
$BuNH_3HSO_4$	167.3	EvRe81
Bu_4NHSO_4	168.0	EvRe81
Et_3NHHSO_4	168.5	EvRe81
$PhSCMe_3$	162.4	PiLu72
Tetrathionaphthalene	164.4	RiVe83
Cysteine	163.2	LlMa79, LHJG70
Cysteine HCl hydrate	163.1	SSEW79
Cysteine HCl hydrate	163.6	LHJG70
Methionine	162.8	BBFR77
$NH_2C_6H_4SO_{33}H$	167.8	HaSh73
$(MeOS)_2$	164.5	LHJG70
Me_2SO	166.5	LHJG70
$(PhCH_2)_2SO$	165.9	LHJG70
Ph_2SO	166.0	LHJG70
Me_2SO_2	169.0	LHJG70
$CH_3OS(O)OCH_3$	168.4	LHJG70
$MeSO_2Cl$	169.3	LHJG70
$ClC_6H_4CH_2SO_2Cl$	168.5	LHJG70
$PhSO_2Na$	166.3	LHJG70
$p\text{-}NH_2C_6H_4SO_2C_6H_4NH_2$-	167.9	LHJG70
$p\text{-}NH_2C_6H_4SO_2NH_2$	168.4	LHJG70
$p\text{-}CH_3C_6H_4SO_2Cl$	168.4	LHJG70
$p\text{-}NH_2C_6H_4SO_3Na$	168.1	LHJG70
$p\text{-}O_2NC_6H_4SNa$	161.0	LHJG70
$CO_2NC_6H_4SH$	163.5	LHJG70
$o\text{-}O_2NC_6H_4SH$	163.9	LHJG70
$p\text{-}O_2NC_6H_4SMe$	163.5	LHJG70
$o\text{-}O_2NC_6H_4SNH_2$	164.1	LHJG70
$o\text{-}O_2NC_6H_4SCl$	163.9	LHJG70
$p\text{-}O_2NC_6H_4SO_2F$	169.6	LHJG70
$o\text{-}O_2NC_6H_4SO_2F$	170.0	LHJG70
$PhCH_2SSCH_2Ph$	163.6	LHJG70
$PhCH_2S*SOCH_2Ph$	163.7	LHJG70
$PhCH_2SS*OCH_2Ph$	165.9	LHJG70
$PhCH_2S*SO_2CH_2Ph$	163.9	LHJG70
$PhCH_2SS*O_2CH_2Ph$	168.0	LHJG70
$(CH_3)_3S+I-$	165.8	LHJG70
$(CH_3)_3S+(O)I-$	168.2	LHJG70
$(HOOCCH_2)_2S+CH_2COO-$	166.2	LHJG70

S KLL

NiS	2116.1	WaTa80
NiW_2S	2115.9	Wagn78

WS_2	2115.6	Wagn78
Na_2SO_3	2108.5	WaTa82
$Na_2(SS^*O_3)$	2107.8	Wagn75
$Na_2(S^*SO_3)$	2112.5	Wagn75
$CuSO_4$	2108.0	WaTa80
SO_2	2106.2	WaTa82
SF_6	2100.5	WaTa82

Sb 3d5/2

Sb	528.3	Φ
Sb	528.2	HSBS81,MSV 73,PVVA79, SFS77,WRDM79,Wagn75
AlSb	528.6	MSV73
$Sb_{95}Sn_5$	528.0	HSBS81
Sb_2S_3	529.5	MSV73,Wagn75
Sb_2S_5	529.2	MSV73,Wagn75
SbI_3	530.4	MSV73
$SbCl_5$	530.9	BCH75
SbF_3	531.7	MSV73
Sb_2O_3	530.0	MSV73,Wagn75
Sb_2O_5	530.8	MSV73
$Rb_3Sb_2Br_9$	529.9	Tric74
$Rb_3Sb_2I_9$	529.9	Tric74
$Cs_3Sb_2I_9$	529.2	BCH75
$Cs_3Sb_2Br_9$	530.0	BCH75,Tric74
$Cs_3Sb_2Cl_9$	529.3	BCH75
$Cs_2Sb_2Cl_9$	530.5	Tric74
C_3SbCl_6	530.9	Tric74
$Co(NH_3)_6SbBr_6$	530.1	Tric74
$Co(NH_3)_6SbCl_6$	530.8	Tric74
$KSbF_6$	532.3	MSV73
$KSbF_6$	532.9	Wagn75
$NaSbF_6$	532.1	BCH75
$CsSbF_4$	530.6	BCH75
KSb_2F_7	531.2	Tric74
K_2SbF_5	531.0	Tric74
Na_2SbF_5	531.3	Tric74
$BuNH_3SbI_4$	529.6	BCH75
$BuNH_3Sb_2I_9$	529.9	BCH75
Et_4NSbF_6	532.4	BCH75
Ph_3Sb	528.9	BCH75
Bu_3Sb	528.1	BCH75
Ph_3SbBr_2	529.8	BCH75
Me_3SbBr_2	530.3	BCH75
Ph_3SbS	528.7	BCH75
$(C_{12}H_{25})_3SSb$	529.8	MSV73
Ph_4PSbCl_6	531.7	MSV73

Sb MNN

Sb	464.1	WRDM79, PVVA79, Wagn75
Sb_2S_3	462.1	Wagn75
Sb_2S_5	462.2	Wagn75
Sb_2O_3	462.1	Wagn75
$KSbF_6$	454.4	Wagn75

Sc 2p

Sc	398.6	Φ
Sc_2O_3	401.8	Φ
Sc	398.7	SMKM77
ScN	400.7	STAB76
Sc_2O_3	401.9	NGDS75,WRDM79
$ClSc(C_5H_5)_2$	401.4	WeMe78
$Sc(C_5H_5)(C_8H_8)$	400.2	WeMe78

Se 3d

Se	55.6	Φ
Se	55.5	SFS77, BWI80, UeOd82, WRDM79, WSP77, MTHB71
Se	55.1	BWI80
As_2Se_3	55.1	UeOd82, WSP77
Ga_2Se_3	54.6	ITI82, TIWB72
GeSe	54.8	SFS77
$GeSe_2$	54.5	UeOd82
$CuInSe_2$	54.0	KJID81
In_2Se_3	54.8	KJID81
Nb_2Se_4	54.9	Bahl75
$NbSe_2$	53.7	Bahl75
PbSe	53.4	SFS77
PbSe	54.1	WSP7
SnSe	53.7	SFS77
SnSe	55.0	WSP77
$MoSe_2$	54.6	BWI79
$FeSe_2$	54.9	BWI79
SeO_2	58.9	BWI81, ITI82
SeO_2	59.8	MTHB71, WSP77
H_2SeO_3	59.2	BWI81
H_2SeO_3	59.9	MTHB71
H_2SeO_4	61.2	BWI81
Na_2SeO_3	59.1	WSP77
Na_2SeO_4	61.6	WSP77
$Na_2SeS_4O_6$	56.9	WSP77
Ph_2Se	55.8	BWI81
$(BrC_6H_4)_2Se$	56.4	MTHB71
Ph_2Se_2	55.8	BWI81
$(BrC_6H_4)_2Se_2$	56.0	BWI81
$(C_{14}H_{29}Se)_2$	56.1	MTHB71
I_2SePh_2	58.1	BWI81
Br_2SePh_2	57.8	BWI81
Cl_2SePh_2	57.7	BWI81
Cl_2SePh_2	58.8	MTHB71
$C_{16}H_{33}SeCN$	57.7	MTHB71
$HSePh_2P$	54.5	NSWM80
$SePh_3P$	54.3	HVV79
Ph_2SeO	57.6	BWI81
$(PhCH_2)_2SeO$	58.2	MTHB71
$(BrC_6H_4)_2SeO$	58.4	MTHB71
$(C_4H_8COOH)_2SeO$	58.5	MTHB71
PhSeO(OH)	58.8	MTHB71
$ClC_6H_4SeO(OH)$	59.3	MTHB71

$FC_6H_4SeO(OH)$	59.3	MTHB71
$ClC_6H_3SeO_2(OH)$	60.2	MTHB71
$(MeOC_6H_4)_2SeO_2$	60.0	MTHB71
$(HOC_2H_4S)_2Se$	56.2	WSP77
Se LMM		
Se	1307.0	BWI81
Se	1306.7	Wagn75
SeO_2	1301.4	BWI81
H_2SeO_3	1300.8	BWI81
H_2SeO_4	1297.9	BWI81
Na_2SeO_3	1301.2	Wagn75
Ph_2Se	1304.0	BWI81
Ph_2Se_2	1304.3	BWI81
I_2SePh	1302.1	BWI81
Cl_2SePh_2	1302.9	BWI81
Ph_2SeO	1301.9	BWI81
Si 2p		
Si	99.3	Φ
SiO_2	103.3	Φ
Si	99.5	AWL80, PADS78, WRDM79, WPHK82, Tayl81, KBHN74
Si, p-type	99.0	HBBK72
Si, n-type	100.0	HBBK72
Si, (100)	99.7	TLR78
Fe_3Si	99.5	ShTr75
$MoSi_2$	99.6	WPHK82
$MoSi_2$	99.1	BrWh78
Ni_2Si	98.9	GGM82
NiSi	98.8	GGM82
NiSi	98.4	AWL80
Pd_2Si	99.7	GGM82
Pd_3Si	99.6	AWL80
PdSi	99.8	WaTa80
Pt_2Si	100.5	GGM82
PtSi	100.5	GGM82
Si_3N_4	101.8	WHMC78, WaTa80, Tayl81, TLR78
SiS_2	103.4	MoVa73
SiO_2	103.6	KBHN74, NGDS75, MoVa73, Barr83
SiO_2, Vycor	103.5	WPHK82
SiO_2, quartz	103.7	WPHK82, TLR 78
SiO_2, alpha cristobal	103.3	WPHK82
SiO_2 gel	103.4	WPHK82
Ni_2SiO_4	102.9	LFWS79
$NiSiO_3$	103.3	SRD79
Al_2SiO_5, kyanite	102.8	AnSw74
Al_2SiO_5, mullite	103.0	AnSw74
Al_2SiO_5, sillimanite	102.6	AnSw74
$NaAlSi_3O_8$, albite	102.6	WPHK82
Bentonite	102.9	Barr83
H Zeolon	103.3	WPHK82
$Zn_4Si_2O_7(OH)_2 \cdot 2H_2O$	102.0	WPHK82
Hydroxysodalite	101.7	WPHK82
Kaolinite	102.7	Barr83
Kaolinite	103.0	WPHK82
Mica, Muscovite	102.4	WPHK82
Natrolite	102.2	WPHK82
Pyrophyllite	102.9	WPHK82
$AlSiO_5$, sillimanite	102.7	WPHK82
$LiAlSi_2O_6$, spodumene	102.5	WPHK82
Talc, $Mg_3Si_4O_{10}(OH)_2$	103.1	WPHK82
Wollastonii,$Ca_3Si_3O_9$	102.4	WPHK82
Mol Sieve A	101.4	WPHK82
Mol Sieve A	101.3	Barr83
Mol Sieve A, Ca form	101.8	Barr83
Mol Sieve X	102.2	WPHK82
Mol Sieve X	102.2	Barr83
Mol Sieve X, Ca form	102.7	Barr83
Mol Sieve Y	102.8	WPHK82
Mol Sieve Y	102.8	Barr83
Mol Sieve Y, Ca form	102.8	Barr83
K_2SiF_6	104.6	MoVa73
Na_2SiF_6	104.3	NSLS77
p-Methylsil. (linear)	102.4	WPHK82
p-Methylsil. (resin)	102.9	WPHK82
p-Phenylsil. (resin)	102.7	WPHK82
Me_4Si	100.5	GCH76
Ph_4Si	100.7	MoVa73
Ph_4Si	101.2	GCH76
Et_3SiH	100.7	GCH76
Et_3SiOH	101.1	GCH76
Et_3SiBr	101.0	GCH76
Et_3SiCl	101.4	GCH76
Et_3SiF	101.8	GCH76
Et_2SiCl_2	102.1	GCH76
$EtSiCl_3$	102.9	GCH76
$(CH_2{=}CH)_4Si$	100.7	GCH76
$Me_3SiSiMe_3$	100.5	GCH76
$Me_3SiOSiMe_3$	100.9	GCH76
$Ph_3SiSiPh_3$	100.7	GCH76
$Ph_3SiOSiPh_3$	101.3	GCH76
Si (KLL)		
Si	1616.6	WPHK82, CDN 77
$MoSi_2$	1617.2	WPHK82
PdSi	1617.4	WaTa80
Si_3N_4	1612.6	WaTa80
SiO_2	1608.8	KBHN74
SiO_2, Vycor	1608.5	WPHK82
SiO_2, quartz	1608.6	WPHK82
SiO_2, alpha cristobal	1608.8	WPHK82
SiO_2 gel	1608.3	WPHK82
$NaAlSi_3O_8$, albite	1609.3	WPHK82
H Zeolon	1608.4	WPHK82
Hemimorphite	1610.5	WPHK82
Hydroxysodalite	1610.7	WPHK82
Kaolinite	1609.0	WPHK82
Mica, Muscovite	1609.6	WPHK82

Natrolite	1609.6	WPHK82
Pyrophyllite	1609.2	WPHK82
$AlSiO_5$, sillimanite	1609.5	WPHK82
$LiAlSi_2O_6$, spodumene	1609.6	WPHK82
Talc, $Mg_3Si_4O_{10}(OH)_2$	1608.9	WPHK82
Wollastonii, $Ca_3Si_3O_9$	1610.0	WPHK82
Mol Sieve A	1610.1	WPHK82
Mol Sieve X	1609.4	WPHK82
Mol Sieve Y	1608.6	WPHK82
p-Methylsil. (linear)	1609.4	WPHK82
p-Methylsil. (resin)	1608.8	WPHK82
p-Phenylsil. (resin)	1610.0	WPHK82

Sm 3d5/2

Sm	1081.1	Φ
Sm	1081.2	DKMB76
Sm_2O_3	1083.4	WRDM79

Sn 3d5/2

Sn	485.0	Φ
Sn	484.9	NyMa80
Sn	485.1	SFS77
Sn	485.0	WRDM79, PVVA79, LAK 77, Wagn75, OCH 79
Sn alpha	485.0	Hegd82
Sn beta	484.6	Hegd82, HSBS81
$Ag_{95}Sn_5$	485.6	HSBS81, Hegd82
AuSn	485.2	FHPW73
$AuSn_4$	484.9	FHPW73
$Cd_{99} \cdot 5Sn \cdot OO_5$	485.3	Hegd82
$Cd_{95}Sn_5$	485.6	Hegd82
$In_{95}Sn_5$	485.2	Hegd82
$Pb_{95}Sn_5$	486.4	Hegd82
$Sb_{95}Sn_5$	485.2	Hegd82
SnTe	485.6	SFS77
SnSe	485.7	SFS77
SnS	485.6	SFS77
$SnBr_2$	486.9	GZF73
$SnCl_2$	486.7	WVV79
SnF_2	487.0	MoVa73
SnF_2	487.0	MoVa73
SnO	486.0	ADPS77
SnO	486.9	WVV79, MoVa73
SnO_2	486.7	LAK 77, MoVa73, WRDM79, NGDS75, WVV79
$(NH_4)_2SnCl_6$	486.7	GZF73
$BaSnCl_4$	486.8	WVV79
$Ba(SnCl_3)_2$	486.8	WVV79
$KSnF_3$	486.7	GZF73
K_2SnF_6	487.6	MoVa73
$NaSnF_3$	487.4	Wagn75
Na_2SnO_3	486.2	MoVa73
Na_2SnO_3	486.7	Wagn75
Na_2SnO_3	487.2	ADPS77
Ph_4Sn	485.1	WVV79
Ph_4Sn	486.3	MoVa73
Ph_4Sn	487.1	HWVV74
Ph_3SnI	486.3	WVV79
Ph_3SnI	487.5	HWVV74
Ph_3SnBr	487.5	HWVV74
Ph_3SnCl	486.3	WVV79
Ph_3SnCl	487.0	MoVa73
Ph_3SnCl	487.6	HWVV74
Ph_3SnF	486.2	WVV79
Ph_3SnF	487.3	HWVV74
Ph_3SnOH	485.6	WVV79
$Cl_4Sn(pyridine)_2$	487.3	WVV79
$Cl_3SnEt(pyridine)_2$	487.2	WVV79
$Cl_3SnPh(pyridine)_2$	487.2	WVV79
Me_3SnF	486.7	WVV79
Me_2SnF_2	487.1	WVV79
Me_2SnSO_4	487.0	WVV79
Bu_2SnO	485.6	WVV79
$Br_6Sn(Et_4N)_2$	487.0	WVV79
$Cl_3Sn(Me_4N)$	486.1	GZF73
$Cl_4Sn(Me_2SO)_2$	487.0	GZF73, WVV79

Sn MNN

Sn	437.4	PVVA79, Wagn75, WRDM79, LAK 77
SnS	435.7	Wagn75
SnO_2	432.7	LAK77
$NaSnF_3$	430.8	Wagn75
Na_2SnO_3	431.7	Wagn75

Sr 3d

Sr	134.3	Φ
Sr	134.4	VaVe80
SrO	135.3	VaVe80
SrF_2	133.8	WRDM79
$SrCO_3$	133.2	CLSW83
$SrSO_4$	134.3	CLSW83
$Sr(NO_3)_2$	134.7	CLSW83
$SrMoO_4$	133.5	NFS82
$SrRh_2O_4$	133.0	NFS82

Ta 4f

Ta	21.9	Φ
Ta	21.6	VHE82
Ta	21.6	MSC73
Ta	21.9	WRDM79, WaTa80
TaS	26.6	MSC73
TaS_2	26.7	MSC73
$TaBr_5$	26.9	MSC73
$TaCl_5$	27.3	MSC73
TaF_5	27.8	MSC73
Ta_2O_5	26.7	SaRa80, MSC 73, NFS82, NGDS75
$KTaO_4$	25.9	MSC73
$RhTaO_4$	25.8	NFS82
K_2TaF_7	29.4	MSC73

$Cl_2Ta_6Cl_{12}(H_2O)_4 \cdot 4H_2O$	25.8	BeWa79
$Br_6(Ta_6Cl_{12})(Bu_4N)_2$	26.3	BeWa79
$Cl_6(Ta_6Cl_{12})(Et_4N)_2$	26.2	BeWa79
Ta MNN		
Ta	1674.8	WaTa80
Tb 4d		
Tb	146.0	Φ
Tb_2O_3	148.7	SaRa80
TbO_2	149.2	SaRa80
Tb 3d		
Tb	1242.0	Φ
Tb_2O_3	1241.5	SaRa80
TbO_2	1241.4	SaRa80
Te 3d5/2		
Te	573.1	Φ
Te	573.0	NyMa80
Te	573.0	SFS77
Te	573.0	PVVA79, WRDM79, BWI77, Bahl75
Te	572.7	SNRS76, SWH71
CdTe	572.3	SBB80
GeTe	572.7	SFS77
$Hg_{0.8}Cd_{0.2}Te$	572.3	SBB80
Na_2Te	572.2	SWH71
Nb_3Te_4	572.6	Bahl75
$NbTe_4$	572.8	Bahl75
PbTe	572.0	SFS77
SnTe	572.3	SFS77
U_2Te_3	572.9	SNRS76
UTe_3	573.0	SNRS76
ZnTe	572.9	SWH71
TeI_4	575.8	BWI77
$TeBr_2$	576.7	BWI77
$TeCl_4$	576.9	BWI77
TeO_2	575.7	GBP81, SBB80
TeO_3	576.6	SWH71
$Te(OH)_6$	577.1	BWI77
$(NH_4)_2TeCl_6$	576.9	BWI77
$(NH_4)_2TeO_4$	576.5	SWH71
K_2TeO_3	575.5	SWH71
Na_2TeO_3	576.8	Wagn75
Cl_2TePh_2	576.2	BWI77
Br_2TePh_2	576.2	BWI77
I_2TePh_2	575.4	BWI77
I_2TeEt_2	575.3	BWI77
Ph_2Te_2	573.9	BWI77
Br_3TePh	576.6	BWI77
I_3TePh	575.8	BWI77
I_2TeMe_2	575.6	BWI77
p-tolylTeOOH	576.1	BWI77
Br_3TeBu	576.6	BWI77
Te MNN		
Te	492.2	WRDM79
$TeBr_2$	487.3	BWI78
$TeCl_4$	486.1	BWI78
TeO_2	487.1	BWI78
TeO_3	485.5	BWI78
$Te(OH)_6$	485.1	BWI78
$(NH_4)_2TeCl_6$	486.4	BWI78
Na_2TeO_4	485.5	Wagn75
Cl_2TePh_2	486.3	BWI78
Br_2TePh_2	486.6	BWI78
I_2TePh_2	487.8	BWI78
I_2TeEt_2	487.6	BWI78
Ph_2Te_2	488.5	BWI78
Br_3TePh	486.8	BWI78
I_3TePh	488.2	BWI78
I_2TeMe_2	486.6	BWI78
p-tolylTeOOH	486.6	BWI78
Br_3TeBu	486.5	BWI78
Th 4f7/2		
Th	333.2	Φ
Th	333.2	WRDM79
ThO_2	334.4	VLDH77
ThF_4	336.5	WRDM79
Th 4d5/2		
Th	675.3	FBWF74
ThO_2	675.5	VLDH77
Ti 2p		
Ti	454.1	Φ
TiO_2	458.8	Φ
Ti	453.7	ALMP82
Ti	453.9	LANM81
Ti	453.9	NSCP74, WRDM79
TiB_2	454.4	MECC73
TiN	455.8	STAB76
$TiCl_4$	458.5	MRV83
TiO	455.1	SPB76a
TiO_2	458.7	NSCP74, SPB76a, WRDM79, NGDS75
TiO_2 (anatase, rutile)	459.2	MWI75
$BaTiO_3$ (cubic, tetra.)	458.5	MWI75
$CaTiO_3$	458.9	MWI75
$PbTiO_3$	458.6	MWI75
$SrTiO_3$	458.8	MWI75
$Cl_2Ti(C_5H_5)_2$	457.1	GSMJ74
$ClTi(C_5H_5)_2$	455.8	GSMJ74
$Ti(C_5H_5)(C_7H_7)$	455.4	GSMJ74
Ti LMM		
Ti	419.1	WRDM79

Tl 4f		
Tl	117.7	Φ
Tl	117.8	MBN80, WRDM79
TlI	118.5	MSC73
TlBr	119.2	MSC73
TlCl	119.0	MSC73
TlF	119.2	MSC73
Tl_2S	118.7	MSC73
Tl_2S_3	118.7	MSC73
Tl_2O_3	117.5	MSC73
$Cl_3Tl(pyridine)_2$	118.5	Walt77
$Cl_3Tl_2(PhPEt_2)_5$	117.9	Walt77
Tm 4d		
Tm	175.4	Φ
U 4f7/2		
U	377.3	Φ
U	377.2	VRPC74, Chad73, WRDM79
U_2Te_3	380.5	SNRS76
UTe_3	381.3	SNRS76
USe	380.3	SNRS76
USe_3	379.1	SNRS76
US	380.1	SNRS76
US_3	379.4	SNRS76
UBr_3	378.4	TBVL82
UBr_4	379.9	TBVL82
UCl_3	378.3	TBVL82
UCl_4	380.2	TBVL82
UCl_5	381.9	TBVL82
UF_3	380.1	TBVL82
UF_4	382.2	TBVL82
UF_5	382.7	Chad73
UF_6	382.6	TBVL82
UO_2	380.0	VRPC74, Chad73, MSSS81
U_3O_8	381.0	Chad73, ChGr72
U_2O_9	379.9	HoTh79
UO_3	381.7	MSSS81, Chad73, ChGr72
UOBr	380.1	TBVL82
$UOBr_2$	380.4	TBVL82
UOCl	380.0	TBVL82
$UOCl_2$	380.3	TBVL82
UO_2Br	380.5	TBVL82
UO_2Br_2	381.1	TBVL82
UO_2Cl_2	381.6	TBVL82
UO_2F_2	382.9	TBVL82,Chad73
$U(SO_4)_2$	381.6	Chad73
$UO_2(NO_3)_2 \cdot 6H_2O$	382.0	Chad73
$U(acac)_2$	379.7	Chad73
$UO_2(AcO)_2 \cdot 2H_2O$	381.0	Chad73
$CaUO_4$	380.7	Chad73
Li_2UO_3	381.4	Chad73
K_2UF_6	382.4	PMDS77

V 2p		
V	512.2	Φ
V_2O_5	517.4	Φ
V	512.1	LANM81
V	512.3	WRDM79, NSCP74
V	512.9	KKL83
V	513.4	SMKM77
V	512.4	RoRo76, LFS 73, FrSa75
VB_2	513.2	MECC73
VN	514.4	RoRo76, STAB76
V_2O_3	515.7	CGR78
VO_2	516.3	KKL83
V_2O_5	517.6	NSLS77, NSCP74, WRDM79, NGDS75, NFS82
$VOCl_2$	516.4	LFS73
$VOSO_4$	515.9	LFS73
Cs_3VO_4	516.9	NFS82
Rb_3VO_4	516.9	NFS82
Na_3VO_4	517.3	NFS82
Li_3VO_4	517.5	NFS82
Rh_3VO_4	516.9	NFS82
$K_4V(CN)_6$	513.3	Vann76
$V(acac)_3$	514.2	LFS73
$VO(acac)_2$	515.1	LFS73
$ClV(C_5H_5)_2$	513.8	GSMJ74
$V(C_5H_5)_2$	512.9	GSMJ74, BCDH73
$V(C_5H_5)(C_7H_7)$	513.3	GSMJ74
V LMM		
V	472.0	WRDM79
VO_2	468.6	KKL83
V_2O_5	468.0	KKL83
W 4f		
W	31.4	Φ
W	31.4	VHE82
W	31.4	WRDM79, CoRa76, CGR 78, BiPo73, NSLS77
WC	31.5	CoRa76
WC	32.2	MSC73
WS_2	33.2	Wagn75
WBr_5	36.3	MSC73
WBr_6	35.9	MSC73
WCl_6	36.9	MSC73
$WOCl_4$	37.2	MSC73
WO_2	32.8	CGR78, CoRa76, NgHe76
$W_{18}O_{49}$	34.3	BiPo73
WO_3	35.8	SaRa80, CoRa76, CGR 78, BiPo73, KMH 78
WO_3	35.8	NFS82, NGDS75
$Al_2(WO_4)_3$	36.1	BiPo73
$CaWO_4$	35.0	Nefe82, NFS 82
H_2WO_4	35.3	CGR78
H_2WO_4	36.2	BiPo73
K_2WO_4	36.0	NFS82

Li_2WO_4	36.0	NFS 82, MSC 73
Na_2WO_4	36.3	Wagn75
$Na_{0.6}WO_3$	35.8	BiPo73
$Na_{0.1}WO_3$	35.6	BiPo73
$NiWO_4$	35.4	NgHe76
Rh_2WO_6	35.6	NFS82
$(NH_4)_6W_7O_{24} \cdot 4H_2O$	36.3	BiPo73
K_2WCl_6	34.9	LeBr72
$Cl_4W(Et_3P)_2$	34.6	LeBr72
$Cl_3SnW(CO)_3(C_5H_5)$	32.4	WWVV77
$Ph_3PW(CO)_5$	31.6	HVV79

Xe 3d5/2

Xe in graphite	669.7	Φ
Xe in Ag	669.6	CiHa74
Xe in Au	668.9	CiHa74
Xe in Cu	669.6	CiHa74
Xe in Fe	670.2	Wagn75
Xe in graphite	669.7	WRDM79
Na_4XeO_6	674.1	Wagn77

Xe MNN

Xe in Fe	544.8	Wagn75
Xe in graphite	545.2	WRDM79
Na_4XeO_6	541.4	Wagn77

Y 3d

Y	156.0	Φ
Y	155.8	NyMa80
Y_2O_3	156.8	WRDM79, NGDS75

Yb 4d

Yb	182.4	Φ
Yb	181.3	HHL70, KEML74
Yb	182.7	LPWF75
Yb_2O_3	185.4	HHL70

Zn 2p3/2

Zn	1021.8	Φ
Zn	1021.9	LANM81, LKMP73
Zn	1021.8	GaWi77, KLMP74, MaDu77, Scho73a, KPML73, KlHe83
Zn	1021.8	WRDM79, Wagn75, SMKM77
$Cu_{64}Zn_{36}$	1021.6	VanO77
ZnS	1022.0	GaWi77
Zn_3P_2	1020.6	NSDU75
ZnP_2	1020.9	NSDU75
ZnI_2	1023.0	GaWi77, SATD73
$ZnBr_2$	1023.4	Wagn75, SATD73
$ZnCl_2$	1021.9	KlHe83
$ZnCl_2$	1023.1	SATD73
ZnF_2	1022.2	GaWi77
ZnF_2	1022.8	Wagn75
ZnO	1021.8	Scho73a, WRDM79
ZnO	1022.5	GaWi77
$Zn(acac)_2$	1021.4	Wagn75
$(Me_4N)_2ZnBr_4$	1020.9	EMGK74
$ZnSO_4$	1023.1	Nefe82
$Zn_4Si_2O_7(OH)_2 \cdot 2H_2O$	1022.0	WPHK82
$ZnCr_2O_4$	1022.1	BDFP81
$ZnRh_2O_4$	1021.7	NFS82

Zn LMM

Zn	992.1	GaWi77, KLMP74, MaDu77, Scho73a, KPML73, KlHe83
Zn	992.1	WRDM79, Wagn75
$Cu_{64}Zn_{36}$	992.7	VanO77
ZnS	989.7	GaWi77
ZnI_2	988.7	GaWi77
$ZnBr_2$	987.3	Wagn75
$ZnCl_2$	989.4	KlHe83
ZnF_2	986.2	GaWi77
ZnF_2	986.7	Wagn75
ZnO	988.5	Scho73a
ZnO	987.7	GaWi77
ZnO	988.2	KlHe83
$Zn(acac)_2$	987.7	Wagn75
$Zn_4Si_2O_7(OH)_2 \cdot 2H_2O$	987.3	WPHK82

Zr 3d

Zr	178.9	Φ
Zr	178.8	NyMa80
Zr	178.3	NSCP74
Zr	178.9	WRDM79
ZrO_2	182.2	SaRa80, NGDS75, NSCP74
ZrF_5	185.3	NKBP73
K_2ZrF_6	184.2	NKBP73
K_3ZrF_7	183.7	NKBP73
$KZrF_5 \cdot H_2O$	184.7	NKBP73
$Br_2Zr(OH)_2CH_3CHNH_2C$	182.9	KNPP74
$Cl_2Zr(OH)_2CH_3CHNH_2C$	183.0	KNPP74

Appendix C. Chemical States Tables References

Note: The references in the Chemical States Tables are made with three or four letters which represent the authors' initials. Three or four capital letters indicate three or more authors; alternating upper- and lower-case letters represent two authors (the letters are the first two letters of each last name); and a capital letter followed by three lower case letters indicates a single author. The initials are followed by two digits, which represent 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.

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BiSw80 Bird, R.J., Swift, P. *J. Electron Spectrosc. Relat. Phenom.* **21**, 227 (1980).

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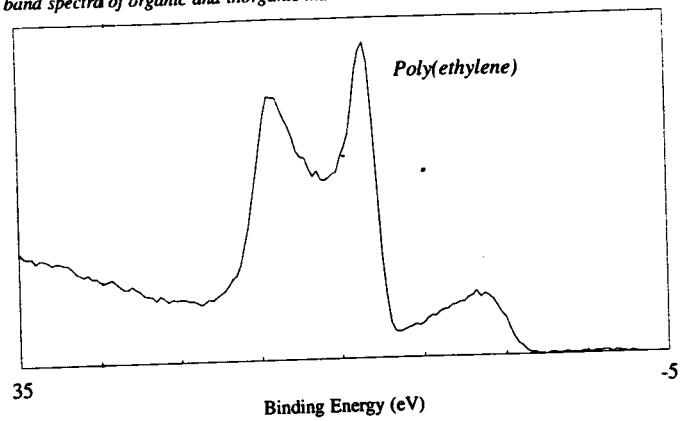
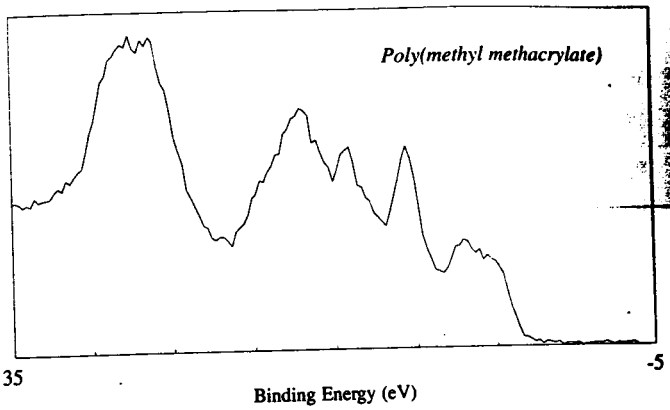
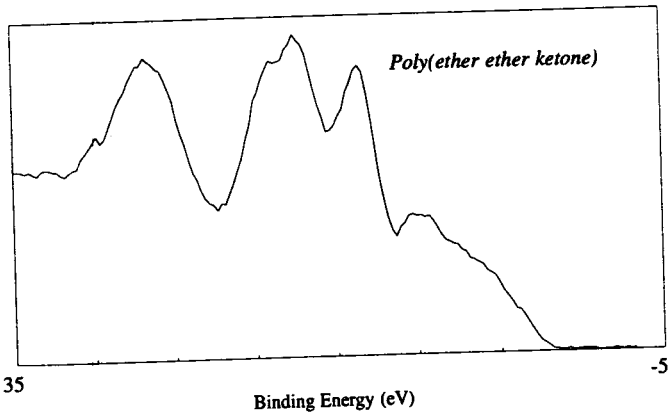
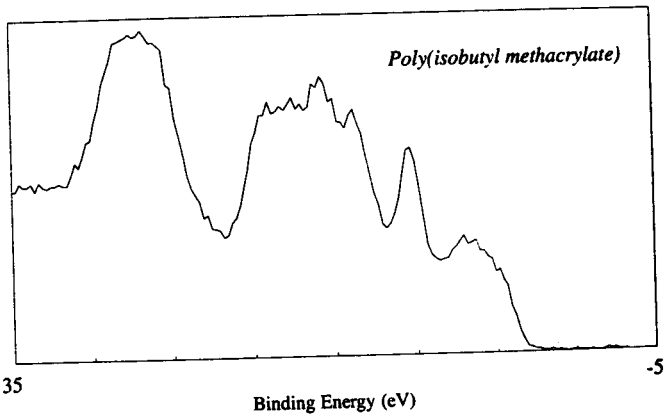
Appendix D. Valence Band Spectra

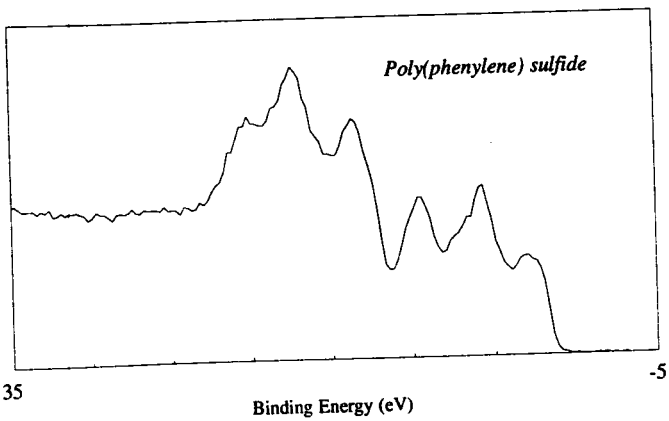
In some cases, the chemical shifts observed in core level XPS are not sufficient to identify the surface chemistry of a particular sample. In the case of XPS analysis of polymers, the changes in carbon chemistry may be quite subtle in core level XPS or the chemical shifts may be only a secondary or tertiary effect. With the routine use of monochromators in XPS and the high counting rates made possible by current spectrometer technologies, many analysts use valence bands for identification of materials. In many cases, the valence bands are used as fingerprints for a sample or a surface treatment, rather than for identifying specific molecular orbitals. The fingerprints of the valence bands may then be used to aid in both the identification of polymers and the quantification of polymer mixtures by using methods such as linear least squares fitting. The following is a small compilation of valence band spectra of organic and inorganic materials to illustrate the utility of valence band data.

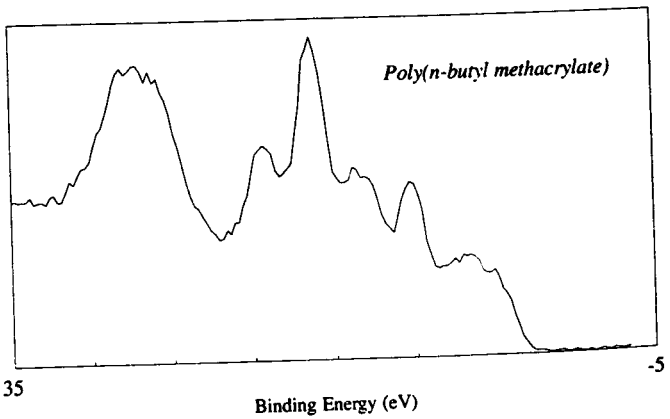


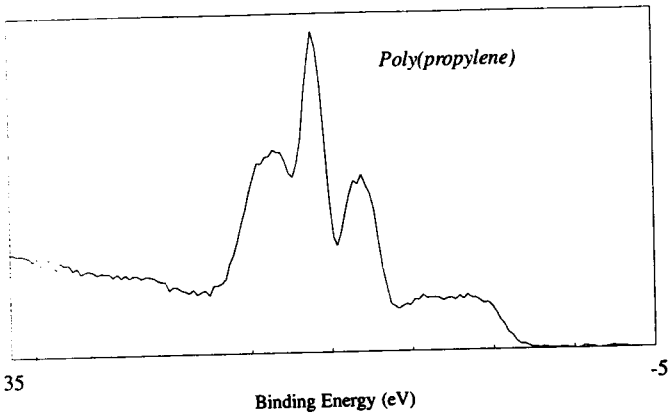


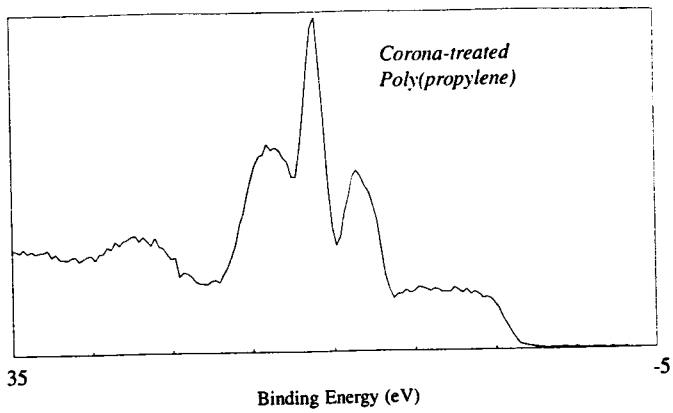


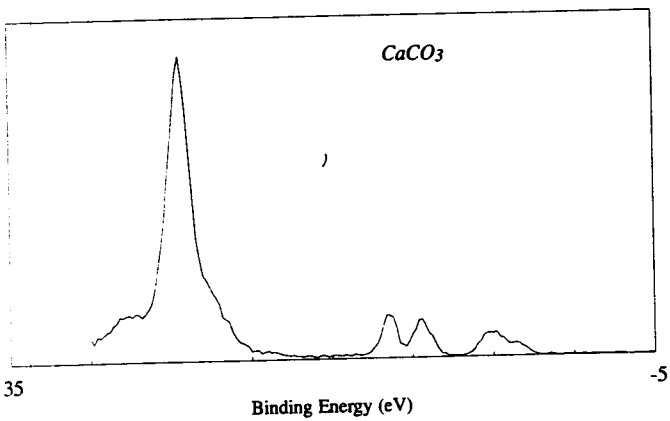


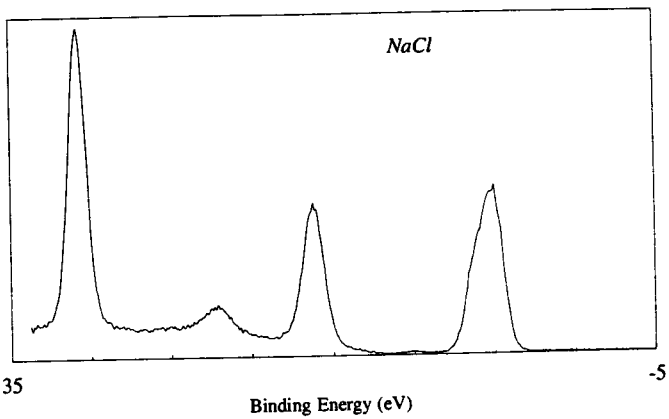


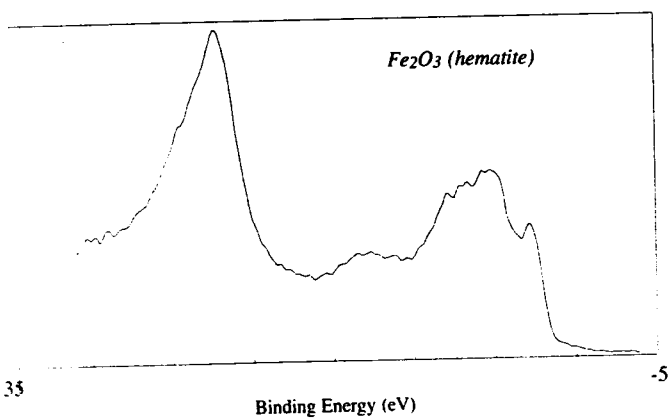


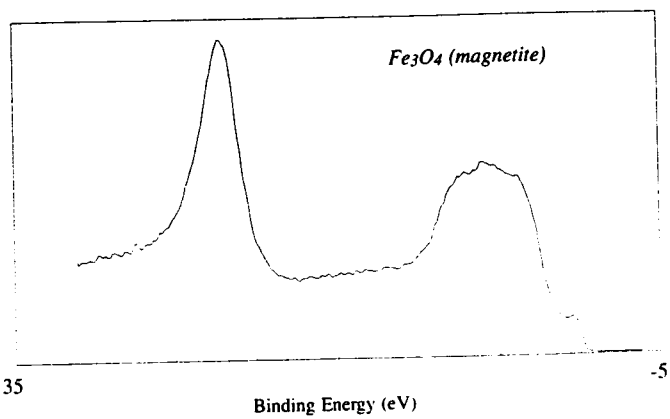

Poly(propylene)
35
-5
Binding Energy (eV)


Corona-treated
Poly(propylene)
35
-5
Binding Energy (eV)


CaCO3
35
-5
Binding Energy (eV)


NaCl
35
-5
Binding Energy (eV)


Fe2O3 (hematite)
35
-5
Binding Energy (eV)


Fe3O4 (magnetite)
35
-5
Binding Energy (eV)

Appendix E. Atomic Sensitivity Factors for X-ray Sources at 90°

This table is based upon empirical peak area values corrected for the system's transmission function. The values are only valid for and should only be applied when the electron energy analyzer used has the transmission characteristics of the spherical capacitor type analyzer equipped with an Omni Focus III lens supplied by Physical Electronics. The data are calculated for x-rays at 90° relative to the analyzer.*

Element	Line	ASF
Ag	3d	5.198
Al	2p	0.193
Ar	2p	1.011
As	3d	0.570
Au	4f	5.240
B	1s	0.159
Ba	4d	2.627
Be	1s	0.074
Bi	4f	7.632
Br	3d	0.895
C	1s	0.296
Ca	2p	1.634
Cd	$3d_{5/2}$	3.444
Ce	3d	7.399
Cl	2p	0.770
Co	2p	3.255
Cr	2p	2.201
Cs	$3d_{5/2}$	6.032
Cu	2p	4.798
Dy	4d	2.198
Er	4d	2.184

Element	Line	ASF
Eu	4d	2.210
F	1s	1.000
Fe	2p	2.686
Ga	$2p_{3/2}$	3.341
Gd	4d	2.207
Ge	$2p_{3/2}$	3.100
Hf	4f	2.221
Hg	4f	5.797
Ho	4d	2.189
I	$3d_{5/2}$	5.337
In	$3d_{5/2}$	3.777
Ir	4f	4.217
K	2p	1.300
Kr	3d	1.096
La	3d	7.708
Li	1s	0.025
Lu	4d	2.156
Mg	2s	0.252
Mn	2p	2.420
Mo	3d	2.867
N	1s	0.477

Element	Line	ASF
Na	1s	1.685
Nb	3d	2.517
Nd	3d	4.697
Ne	1s	1.340
Ni	2p	3.653
O	1s	0.711
Os	4f	3.747
P	2p	0.412
Pb	4f	6.968
Pd	3d	4.642
Pm	3d	3.754
Pr	3d	6.356
Pt	4f	4.674
Rb	3d	1.316
Re	4f	3.327
Rh	3d	4.179
Ru	3d	3.696
S	2p	0.570
Sb	$3d_{5/2}$	4.473
Sc	2p	1.678
Se	3d	0.722

Element	Line	ASF
Si	2p	0.283
Sm	$3d_{5/2}$	2.907
Sn	$3d_{5/2}$	4.095
Sr	3d	1.578
Ta	4f	2.589
Tb	4d	2.201
Tc	3d	3.266
Te	$3d_{5/2}$	4.925
Th	$4f_{7/2}$	7.498
Ti	2p	1.798
Tl	4f	6.447
Tm	4d	2.172
U	$4f_{7/2}$	8.476
V	2p	1.912
W	4f	2.959
Xe	$3d_{5/2}$	5.702
Y	3d	1.867
Yb	4d	2.169
Zn	$2p_{3/2}$	3.354
Zr	3d	2.216

*C.D Wagner, et al. *Surf. Interface Anal.* **3**, 211 (1981).

Appendix F. Atomic Sensitivity Factors for X-ray Sources at 54.7°

This table is based upon empirical peak area values corrected for the system's transmission function. The values are only valid for and should only be applied when the electron energy analyzer used has the transmission characteristics of the spherical capacitor type analyzer equipped with an Omni Focus III lens supplied by Physical Electronics. The data are calculated for x-rays at 54.7° relative to the analyzer.*

Element	Line	ASF
Ag	3d	5.987
Al	2p	0.234
Ar	2p	1.155
As	3d	0.677
Au	4f	6.250
B	1s	0.159
Ba	$3d_{5/2}$	7.469
Be	1s	0.074
Bi	4f	9.140
Br	3d	1.053
C	1s	0.296
Ca	2p	1.833
Cd	$3d_{5/2}$	3.974
Ce	3d	8.808
Cl	2p	0.891
Co	2p	3.590
Cr	2p	2.427
Cs	$3d_{5/2}$	7.041
Cu	2p	5.321
Dy	4d	2.474
Er	4d	2.463

Element	Line	ASF
Eu	4d	2.488
F	1s	1.000
Fe	2p	2.957
Ga	$2p_{3/2}$	3.720
Gd	4d	2.484
Ge	$2p_{3/2}$	3.457
Hf	4f	2.639
Hg	4f	6.915
Ho	4d	2.469
I	$3d_{5/2}$	6.206
In	$3d_{5/2}$	4.359
Ir	4f	5.021
K	2p	1.466
Kr	3d	1.287
La	3d	9.122
Li	1s	0.025
Lu	4d	2.441
Mg	2s	0.252
Mn	2p	2.659
Mo	3d	3.321
N	1s	0.477

Element	Line	ASF
Na	1s	1.685
Nb	3d	2.921
Nd	3d	5.671
Ne	1s	1.340
Ni	2p	4.044
O	1s	0.711
Os	4f	4.461
P	2p	0.486
Pb	4f	8.329
Pd	3d	5.356
Pm	3d	4.597
Pr	3d	7.627
Pt	4f	5.575
Rb	3d	1.542
Re	4f	3.961
Rh	3d	4.822
Ru	3d	4.273
S	2p	0.666
Sb	$3d_{5/2}$	5.176
Sc	2p	1.875
Se	3d	0.853

Element	Line	ASF
Si	2p	0.339
Sm	$3d_{5/2}$	3.611
Sn	$3d_{5/2}$	4.725
Sr	3d	1.843
Ta	4f	3.082
Tb	4d	2.477
Tc	3d	3.776
Te	$3d_{5/2}$	5.705
Th	$4f_{7/2}$	9.089
Ti	2p	2.001
Tl	4f	7.691
Tm	4d	2.454
U	$4f_{7/2}$	10.315
V	2p	2.116
W	4f	3.523
Xe	$3d_{5/2}$	6.64
Y	3d	2.175
Yb	4d	2.451
Zn	$2p_{3/2}$	3.726
Zr	3d	2.576

*C.D Wagner, et al. *Surf. Interface Anal.* **3**, 211 (1981).

Appendix G. Line Positions[a)] by Element for Al Kα X-rays

Photoelectron Lines

<table>
<tr><th>Atomic Number</th><th>Element</th><th>1s</th><th>2s</th><th>$2p_{1/2}$</th><th>$2p_{3/2}$</th><th>3s</th><th>$3p_{1/2}$</th><th>$3p_{3/2}$</th><th>$3d_{3/2}$</th><th>$3d_{5/2}$</th><th>4s</th><th>$4p_{1/2}$</th><th>$4p_{3/2}$</th></tr>
<tr><td>3</td><td>Li</td><td>56</td><td></td><td colspan="2"></td><td></td><td colspan="2"></td><td colspan="2"></td><td></td><td colspan="2"></td></tr>
<tr><td>4</td><td>Be</td><td>112</td><td></td><td colspan="2"></td><td></td><td colspan="2"></td><td colspan="2"></td><td></td><td colspan="2"></td></tr>
<tr><td>5</td><td>B</td><td>189</td><td></td><td colspan="2"></td><td></td><td colspan="2"></td><td colspan="2"></td><td></td><td colspan="2"></td></tr>
<tr><td>6</td><td>C</td><td>285</td><td></td><td colspan="2"></td><td></td><td colspan="2"></td><td colspan="2"></td><td></td><td colspan="2"></td></tr>
<tr><td>7</td><td>N</td><td>398</td><td></td><td colspan="2"></td><td></td><td colspan="2"></td><td colspan="2"></td><td></td><td colspan="2"></td></tr>
<tr><td>8</td><td>O</td><td>531</td><td>23</td><td colspan="2"></td><td></td><td colspan="2"></td><td colspan="2"></td><td></td><td colspan="2"></td></tr>
<tr><td>9</td><td>F</td><td>685</td><td>30</td><td colspan="2"></td><td></td><td colspan="2"></td><td colspan="2"></td><td></td><td colspan="2"></td></tr>
<tr><td>10</td><td>Ne</td><td>863</td><td>41</td><td colspan="2">14</td><td></td><td colspan="2"></td><td colspan="2"></td><td></td><td colspan="2"></td></tr>
<tr><td>11</td><td>Na</td><td>1072</td><td>64</td><td colspan="2">31</td><td></td><td colspan="2"></td><td colspan="2"></td><td></td><td colspan="2"></td></tr>
<tr><td>12</td><td>Mg</td><td>1303</td><td>89</td><td colspan="2">50</td><td></td><td colspan="2"></td><td colspan="2"></td><td></td><td colspan="2"></td></tr>
<tr><td>13</td><td>Al</td><td></td><td>118</td><td colspan="2">73</td><td></td><td colspan="2"></td><td colspan="2"></td><td></td><td colspan="2"></td></tr>
<tr><td>14</td><td>Si</td><td></td><td>151</td><td>100</td><td>99</td><td></td><td colspan="2"></td><td colspan="2"></td><td></td><td colspan="2"></td></tr>
<tr><td>15</td><td>P</td><td></td><td>188</td><td>131</td><td>130</td><td>14</td><td colspan="2"></td><td colspan="2"></td><td></td><td colspan="2"></td></tr>
<tr><td>16</td><td>S</td><td></td><td>228</td><td>165</td><td>164</td><td>18</td><td colspan="2"></td><td colspan="2"></td><td></td><td colspan="2"></td></tr>
<tr><td>17</td><td>Cl</td><td></td><td>271</td><td>201</td><td>199</td><td>17</td><td colspan="2">6</td><td colspan="2"></td><td></td><td colspan="2"></td></tr>
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<tr><td>19</td><td>K</td><td></td><td>380</td><td>297</td><td>294</td><td>35</td><td colspan="2">19</td><td colspan="2"></td><td></td><td colspan="2"></td></tr>
<tr><td>20</td><td>Ca</td><td></td><td>440</td><td>351</td><td>347</td><td>45</td><td colspan="2">26</td><td colspan="2"></td><td></td><td colspan="2"></td></tr>
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<tr><td>22</td><td>Ti</td><td></td><td>561</td><td>460</td><td>454</td><td>59</td><td colspan="2">33</td><td colspan="2"></td><td></td><td colspan="2"></td></tr>
<tr><td>23</td><td>V</td><td></td><td>626</td><td>520</td><td>512</td><td>66</td><td colspan="2">37</td><td colspan="2"></td><td></td><td colspan="2"></td></tr>
<tr><td>24</td><td>Cr</td><td></td><td>696</td><td>583</td><td>574</td><td>75</td><td colspan="2">43</td><td colspan="2"></td><td></td><td colspan="2"></td></tr>
<tr><td>25</td><td>Mn</td><td></td><td>769</td><td>650</td><td>639</td><td>83</td><td colspan="2">48</td><td colspan="2"></td><td></td><td colspan="2"></td></tr>
<tr><td>26</td><td>Fe</td><td></td><td>845</td><td>720</td><td>707</td><td>92</td><td colspan="2">53</td><td colspan="2"></td><td></td><td colspan="2"></td></tr>
<tr><td>27</td><td>Co</td><td></td><td>925</td><td>793</td><td>778</td><td>101</td><td colspan="2">60</td><td colspan="2"></td><td></td><td colspan="2"></td></tr>
<tr><td>28</td><td>Ni</td><td></td><td>1009</td><td>870</td><td>853</td><td>111</td><td colspan="2">67</td><td colspan="2"></td><td></td><td colspan="2"></td></tr>
<tr><td>29</td><td>Cu</td><td></td><td>1097</td><td>953</td><td>933</td><td>123</td><td>77</td><td>75</td><td colspan="2"></td><td></td><td colspan="2"></td></tr>
<tr><td>30</td><td>Zn</td><td></td><td>1195</td><td>1045</td><td>1022</td><td>140</td><td>91</td><td>89</td><td colspan="2">10</td><td></td><td colspan="2"></td></tr>
<tr><td>31</td><td>Ga</td><td></td><td>1301</td><td>1144</td><td>1117</td><td>160</td><td>107</td><td>104</td><td colspan="2">19</td><td></td><td colspan="2"></td></tr>
<tr><td>32</td><td>Ge</td><td></td><td></td><td>1248</td><td>1217</td><td>181</td><td>126</td><td>122</td><td>30</td><td>29</td><td></td><td colspan="2"></td></tr>
<tr><td>33</td><td>As</td><td></td><td></td><td>1359</td><td>1324</td><td>205</td><td>146</td><td>141</td><td>43</td><td>42</td><td></td><td colspan="2"></td></tr>
<tr><td>34</td><td>Se</td><td></td><td></td><td></td><td></td><td>232</td><td>169</td><td>163</td><td>57</td><td>56</td><td></td><td colspan="2"></td></tr>
<tr><td>35</td><td>Br</td><td></td><td></td><td></td><td></td><td>256</td><td>189</td><td>182</td><td>70</td><td>69</td><td>15</td><td colspan="2">5</td></tr>
<tr><td>36</td><td>Kr</td><td></td><td></td><td></td><td></td><td>287</td><td>216</td><td>208</td><td>88</td><td>87</td><td>21</td><td colspan="2">8</td></tr>
<tr><td>37</td><td>Rb</td><td></td><td></td><td></td><td></td><td>325</td><td>249</td><td>240</td><td>113</td><td>111</td><td>31</td><td colspan="2">16</td></tr>
<tr><td>38</td><td>Sr</td><td></td><td></td><td></td><td></td><td>360</td><td>281</td><td>270</td><td>136</td><td>134</td><td>39</td><td colspan="2">21</td></tr>
<tr><td>39</td><td>Y</td><td></td><td></td><td></td><td></td><td>394</td><td>311</td><td>299</td><td>158</td><td>156</td><td>45</td><td colspan="2">24</td></tr>
<tr><td>40</td><td>Zr</td><td></td><td></td><td></td><td></td><td>430</td><td>343</td><td>330</td><td>181</td><td>179</td><td>51</td><td colspan="2">28</td></tr>
</table>

Auger Lines

Atomic Number	Element	KL_1L_1	KL_1L_{23}	$KL_{23}L_{23}$ [b)]
4	Be			1384
5	B			1310
6	C			1223
7	N			1107
8	O	1013	999	978
9	F	878	859	832
10	Ne	725	702	669
11	Na	561	532	493
12	Mg	381	347	301

<table>
<tr><th>Atomic Number</th><th>Element</th><th>$L_3M_{23}M_{23}$ [c)]</th><th>$L_2M_{23}M_{23}$ [c)]</th><th>$L_3M_{23}M_{45}$ (^1P)</th><th>$L_3M_{23}M_{45}$ (^3P)</th><th>$L_2M_{23}M_{45}$ (^1P)</th><th>$L_3M_{45}M_{45}$ [d)]</th><th>$L_2M_{45}M_{45}$</th></tr>
<tr><td>13</td><td>Al</td><td colspan="2">1419</td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>14</td><td>Si</td><td colspan="2">1394</td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>15</td><td>P</td><td colspan="2">1367</td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>16</td><td>S</td><td colspan="2">1336</td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>17</td><td>Cl</td><td colspan="2">1304</td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>18</td><td>Ar</td><td colspan="2">1272</td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>19</td><td>K</td><td colspan="2">1239</td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>20</td><td>Ca</td><td colspan="2">1197</td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>21</td><td>Sc</td><td colspan="2">1149</td><td>1118</td><td></td><td></td><td></td><td></td></tr>
<tr><td>22</td><td>Ti</td><td colspan="2">1098</td><td>1068</td><td></td><td></td><td></td><td></td></tr>
<tr><td>23</td><td>V</td><td colspan="2">1048</td><td>1014</td><td></td><td></td><td>977</td><td></td></tr>
<tr><td>24</td><td>Cr</td><td colspan="2">997</td><td>959</td><td></td><td></td><td>917</td><td></td></tr>
<tr><td>25</td><td>Mn</td><td colspan="2">944</td><td>900</td><td></td><td></td><td>852</td><td></td></tr>
<tr><td>26</td><td>Fe</td><td colspan="2">888</td><td>839</td><td></td><td></td><td>784</td><td></td></tr>
<tr><td>27</td><td>Co</td><td>838</td><td>831</td><td>777</td><td>771</td><td></td><td>713</td><td>698</td></tr>
<tr><td>28</td><td>Ni</td><td>778</td><td>772</td><td>712</td><td>706</td><td></td><td>641</td><td>624</td></tr>
<tr><td>29</td><td>Cu</td><td>719</td><td>712</td><td>648</td><td>640</td><td>628</td><td>568</td><td>548</td></tr>
<tr><td>30</td><td>Zn</td><td>660</td><td>652</td><td>582</td><td>573</td><td>559</td><td>495</td><td>472</td></tr>
<tr><td>31</td><td>Ga</td><td>597</td><td>589</td><td>514</td><td>504</td><td>487</td><td>419</td><td>392</td></tr>
<tr><td>32</td><td>Ge</td><td>534</td><td>525</td><td>444</td><td>433</td><td>412</td><td>342</td><td>310</td></tr>
<tr><td>33</td><td>As</td><td></td><td></td><td>371</td><td>360</td><td>336</td><td>262</td><td>226</td></tr>
<tr><td>34</td><td>Se</td><td colspan="2">$M_{23}M_{45}N_{23}$</td><td>299</td><td>287</td><td>257</td><td>181</td><td>140</td></tr>
<tr><td>35</td><td>Br</td><td colspan="2">1386</td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>36</td><td>Kr</td><td colspan="2"></td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>37</td><td>Rb</td><td colspan="2">1385</td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>38</td><td>Sr</td><td colspan="2"></td><td>$M_{45}N_{23}V$</td><td>$M_{45}N_{45}N_{45}$</td><td></td><td></td><td></td></tr>
<tr><td>39</td><td>Y</td><td colspan="2"></td><td colspan="2">1356</td><td></td><td></td><td></td></tr>
<tr><td>40</td><td>Zr</td><td colspan="2"></td><td>1368</td><td>1337</td><td></td><td></td><td></td></tr>
</table>

a) Lines enclosed in boxes are the ones which are most useful for identifying chemical states.
b) Includes KVV designation when L_{23} is not a core level.
c) Designation is oversimplified.
d) Includes LVV when M levels are not in core and MVV when N levels are not in core.
e) No simple $4p_{1/2}$ line exists for this group of elements.
f) The 4d doublet for these elements is complex and is variable with chemical state because of multiplet splitting and multi-electron processes.
g) The 5s is of low intensity and is often in the shake-up structure of the 4f lines. These values are estimates of the energy.

Atomic Number/Element		Photoelectron Lines																	Auger Lines					
		3s	$3p_{1/2}$	$3p_{3/2}$	$3d_{3/2}$	$3d_{5/2}$	4s	$4p_{1/2}$	$4p_{3/2}$	$4d_{3/2}$	$4d_{5/2}$	$4f_{5/2}$	$4f_{7/2}$	5s	$5p_{1/2}$	$5p_{3/2}$	$5d_{3/2}$	$5d_{5/2}$	6s	$6p_{1/2}$	$6p_{3/2}$	$M_4N_{23}V$	$M_5N_{45}N_{45}$[d]	$M_4N_{45}N_{45}$[d]	$M_4N_{45}V$	M_5VV	M_4VV
41	Nb	467	376	361	205	202	56	31														1319		1287			
42	Mo	506	412	394	231	228	63	36														1299		1264			
43	Tc	544	445	425	257	253	68	39														1280		1241			
44	Ru	586	484	462	284	280	75		43[c]													1256		1212			
45	Rh	629	521	497	312	307	81		48													1234		1185			
46	Pd	671	560	533	340	335	88		52													1211		1159			
47	Ag	719	604	573	374	368	98		60													1191	1135		1129		
48	Cd	772	652	618	412	405	110		69	11													1110		1103		
49	In	828	703	665	452	444	123		78	17													1084		1076		
50	Sn	885	757	715	493	485	137		89	25													1058		1049		
51	Sb	944	813	767	537	528	153		99	33													1032		1022		
52	Te	1009	871	820	583	573	170		111	42	41			12									1005		995		
53	I	1071	930	875	630	619	187		123	51	49			17									982		971		
54	Xe	1141	996	934	683	670	207		139	63	61			17									955		942		
55	Cs	1219	1069	1002	740	726	234	173	161	80	77			25									931		918		
56	Ba	1292	1138	1064	796	781	254	193	179	93	90			31	15								900		886		
57	La		1208	1128	853	836	275	213	197	106	103			34	17								867		854		
58	Ce		1272	1184	902	884	290	223	207	112	109			36	18									833			
59	Pr		1339	1242	952	932	305	234	218		115[f]			38	18									797			
60	Nd			1301	1003	981	320	245	228		121			39	19									758			
61	Pm				1060	1034	337	264	242		129			38	22									714			
62	Sm				1108	1081	349	283	250		129			41	19									682			
63	Eu				1155	1126	363	289	255		128			39	19									637			
64	Gd				1218	1186	378	291	272		140		8	43	21									602			
65	Tb				1276	1241	396	322	285		146		8	45	22									559		411	260	230
66	Dy				1333	1296	417	337	297		152		8	48	23									526		368		
67	Ho				1393	1352	435	353	309		160		9	49	30	24								488		314		117
68	Er						451	368	321		167		9	52	31	24								440		273	98	56
69	Tm						470	384	333		175		8	53	32	25								398				
70	Yb						482	389	341		182		3	51	30	24												
71	Lu						509	413	360	206	196	9	7	57	34	27						$N_5N_{67}N_7$	$N_4N_{67}N_7$				
72	Hf						534	437	380	222	211	16	14	63	38	30						1317	1306				
73	Ta						563	463	401	238	226	24	22	69	43	33						1316	1306				
74	W						594	491	424	256	243	33	31	75	47	37						1320	1307				
75	Re						625	518	446	274	260	42	40	99								1322	1309				
76	Os						658	548	471	293	279	54	51	89[g]		44						1326	1311				
77	Ir						692	578	495	312	297	64	61	96[g]		48						1329	1314				
78	Pt						725	609	520	332	315	74	71	103[g]		52						1334	1317	$N_5N_{67}O$	N_4N_6O	$N_7O_{45}O_{45}$	$N_6O_{45}O_{45}$
79	Au						763	643	547	353	335	88	84	110[g]	57	74						1342	1324	1247	1231	1416	
80	Hg						805	682	579	381	361	105	101	125[g]	85	67	12	10					1336	1246	1230	1412	1406
81	Tl						847	720	610	406	385	122	118	133[g]	95	74	15	13				1364	1343	1241	1222	1401	1399
82	Pb						893	762	644	434	412	142	137	150[g]	107	84	21	18				1369	1354			1394	1391
83	Bi						940	806	679	464	440	162	157	161[g]	119	93	27	24				$N_6O_{23}V$	$N_{67}O_{45}V$			1387	1383
90	Th						1330	1170	965	713	676	342	333	294	234	177	93	85	42	25	17	1419	1239			1335	1404
92	U							1272	1043	779	736	388	377	322	260	195	103	94	44	26	17	1412	1204				1386
93	Np							1327	1086	816	771	414	402			206		101		29	18						
94	Pu								1121	850	802	439	427			216		105		31	18						
95	Am									883	832	463	449	351		216	119	109		31	18						
96	Cm									919	865	487	473			232		113		32	18						
97	Bk									958	901	514	498			246		120		34	18						
98	Cf									994	933	541	523					124		35	19						

Appendix H. Line Positions[a] by Element for Mg Kα X-rays

Atomic Number	Element	Photoelectron Lines											Auger Lines						
		1s	2s	$2p_{1/2}$	$2p_{3/2}$	3s	$3p_{1/2}$	$3p_{3/2}$	$3d_{3/2}$	$3d_{5/2}$	4s	$4p_{1/2}$	$4p_{3/2}$	KL_1L_1	KL_1L_{23}	$KL_{23}L_{23}$[b]	$L_3M_{23}M_{23}$[c]	$L_2M_{23}M_{23}$[c]	$L_3M_{23}M_{45}$ (^1P)	$L_3M_{23}M_{45}$ (^3P)	$L_2M_{23}M_{45}$ (^1P)	$L_3M_{45}M_{45}$[d]	$L_2M_{45}M_{45}$
3	Li	56														1151							
4	Be	112														1077							
5	B	189														990							
6	C	285														874							
7	N	398																					
8	O	531	23											780	766	745							
9	F	685	30											645	626	599							
10	Ne	863	41	14										492	469	436							
11	Na	1072	64	31										328	299	260							
12	Mg	1303	89	50										148	114	68							
13	Al		118	73																			
14	Si		151	100	99													1186					
15	P		188	131	130	14												1161					
16	S		228	165	164	18												1134					
17	Cl		271	201	199	17	6											1103					
18	Ar		320	244	242	24												1071					
19	K		380	297	294	35	19											1039					
20	Ca		440	351	347	45	26											1006					
21	Sc		499	404	399	51	29											964					
22	Ti		561	460	454	59	33											916		895			
23	V		627	520	512	66	37											865		835			
24	Cr		696	583	574	75	43											815		781		744	
25	Mn		769	650	639	83	48											764		726		684	
26	Fe		845	720	707	92	53											711		667		619	
27	Co		925	793	778	101	60											655		606		551	
28	Ni		1009	870	853	111	67										605	598		544	538	480	465
29	Cu		1097	953	933	123	77	75									545	539		479	473	408	391
30	Zn		1195	1045	1022	140	91	89		10							486	479		415	407	335	315
31	Ga			1144	1117	160	107	104		19							427	419		349	340	262	239
32	Ge			1248	1217	181	126	122	30	29							364	356		281	271	186	159
33	As					205	146	141	43	42							301	292		211	200	109	77
34	Se					232	169	163	57	56													
35	Br					256	189	182	70	69	15	5											
36	Kr					287	216	208	88	87	21	8											
37	Rb					325	249	240	113	111	31	16											
38	Sr					360	281	270	136	134	39	21											
39	Y					394	311	299	158	156	45	24											
40	Zr					430	343	330	181	179	51	28											

$M_{23}M_{45}N_{23}$	$M_{45}N_{23}V$	$M_{45}N_{45}N_{45}$
1153		
1152	1123	
	1160	1104

a) Lines enclosed in boxes are the ones which are most useful for identifying chemical states.
b) Includes KVV designation when L_{23} is not a core level.
c) Designation is oversimplified.
d) Includes LVV when M levels are not in core and MVV when N levels are not in core.
e) No simple $4p_{1/2}$ line exists for this group of elements.
f) The 4d doublet for these elements is complex and is variable with chemical state because of multiplet splitting and multi-electron processes.
g) The 5s is of low intensity and is often in the shake-up structure of the 4f lines. These values are estimates of the energy.

Atomic Number/Element		Photoelectron Lines																			Auger Lines					
		3s	$3p_{1/2}$	$3p_{3/2}$	$3d_{3/2}$	$3d_{5/2}$	4s	$4p_{1/2}$	$4p_{3/2}$	$4d_{3/2}$	$4d_{5/2}$	$4f_{5/2}$	$4f_{7/2}$	5s	$5p_{1/2}$	$5p_{3/2}$	$5d_{3/2}$	$5d_{5/2}$	6s	$6p_{1/2}$	$6p_{3/2}$	$M_4N_{23}V$	$M_5N_{45}N_{45}$[d]	$M_4N_{45}N_{45}$[d]	$M_4N_{45}V$	M_5VV	M_4VV
41	Nb	467	376	361	205	202	56	31														1086		1054			
42	Mo	506	412	394	231	228	63	36														1066		1031			
43	Tc	544	445	425	257	253	68	39														1047		1008			
44	Ru	586	484	462	284	280	75		43[e]													1023		979			
45	Rh	629	521	497	312	307	81		48													1001		952			
46	Pd	671	560	533	340	335	88		52													978		926			
47	Ag	719	604	573	374	368	98		60													958	902		896		
48	Cd	772	652	618	412	405	110		69		11												877		870		
49	In	828	703	665	452	444	123		78		17												851		843		
50	Sn	885	757	715	493	485	137		89		25												825		816		
51	Sb	944	813	767	537	528	153		99		33												799		789		
52	Te	1009	871	820	583	573	170		111	42	41				12								772		762		
53	I	1071	930	875	630	619	187		123	51	49				18								749		738		
54	Xe	1141	996	934	683	670	207		139	63	61				17								722		709		
55	Cs	1219	1069	1002	740	726	234	173	161	80	77				25								698		685		
56	Ba		1138	1064	796	781	254	193	179	93	90				31		15						667		653		
57	La		1208	1128	853	836	275	213	197	106	103				34		17						634		621		
58	Ce			1184	902	884	290	223	207	112	109				36		18							600			
59	Pr			1242	952	932	305	234	218		115[f]				38		18							564			
60	Nd				1003	981	320	245	228		121				39		19							525			
61	Pm				1060	1034	337	264	242		129				38		22							481			
62	Sm				1108	1081	349	283	250		129				41		19							449			
63	Eu				1155	1126	363	289	255		128				39		19							404			
64	Gd				1218	1186	378	291	272		140	8			43		21							369			
65	Tb					1241	396	322	285		146	8			45		22							326		170	
66	Dy						417	337	297		152	8			48		23										
67	Ho						435	353	309		159	9			49	30		24									
68	Er						451	368	321		167	9			52	31		24									
69	Tm						470	384	333		175	8			53	32		25									
70	Yb						482	389	341		182	3			51	30		24									
71	Lu						509	413	360	206	196	9	7		57	34		27				$N_5N_{67}N_7$	$N_4N_{67}N_7$				
72	Hf						534	437	380	222	211	16	14		63	38		30				1084	1073				
73	Ta						563	463	401	238	226	24	22		69	43		33				1085	1073				
74	W						594	491	424	256	243	33	31		75	47		37				1087	1075				
75	Re						625	518	446	274	260	42	40		99							1089	1076				
76	Os						658	548	471	293	279	54	51		89		44					1093	1078				
77	Ir						692	578	495	312	297	64	61		96[g]		48					1096	1081				
78	Pt						725	609	520	332	315	74	71		103[g]		52					1101	1084	N_5N_7O	N_4N_6O	$N_7O_{45}O_{45}$	$N_6O_{45}O_{45}$
79	Au						763	643	547	353	335	88	84		110[g]		74					1109	1091	1014	998	1183	
80	Hg						805	682	579	381	361	107	103		125[g]	85	67	12	10			1119	1103	1013	997	1179	1173
81	Tl						847	720	610	406	385	122	118		133[g]	95	74	15	13			1131	1110	1008	989	1168	1166
82	Pb						893	762	644	434	412	142	137		150[g]	107	84	21	18			1136	1121			1161	1158
83	Bi						940	806	679	464	440	162	157		161[g]	119	93	27	24			$N_6O_{23}V$	$N_6O_{45}V$			1154	1150
90	Th							1170	965	713	676	342	333		294	234	177	93	85	42	25	17	1186	1006			1102	1171
92	U							1272	1043	779	736	388	377		322	260	195	103	94	44	26	17	1179	971				1153
93	Np								1086	816	771	414	402				206		101		29	18						
94	Pu								1121	850	802	439	427				216		105		31	18						
95	Am									883	832	463	449		351		216	119	109		31	18						
96	Cm									919	865	487	473				232		113		32	18						
97	Bk									958	901	514	498				246		120		34	18						
98	Cf									994	933	541	523						124		35	19						

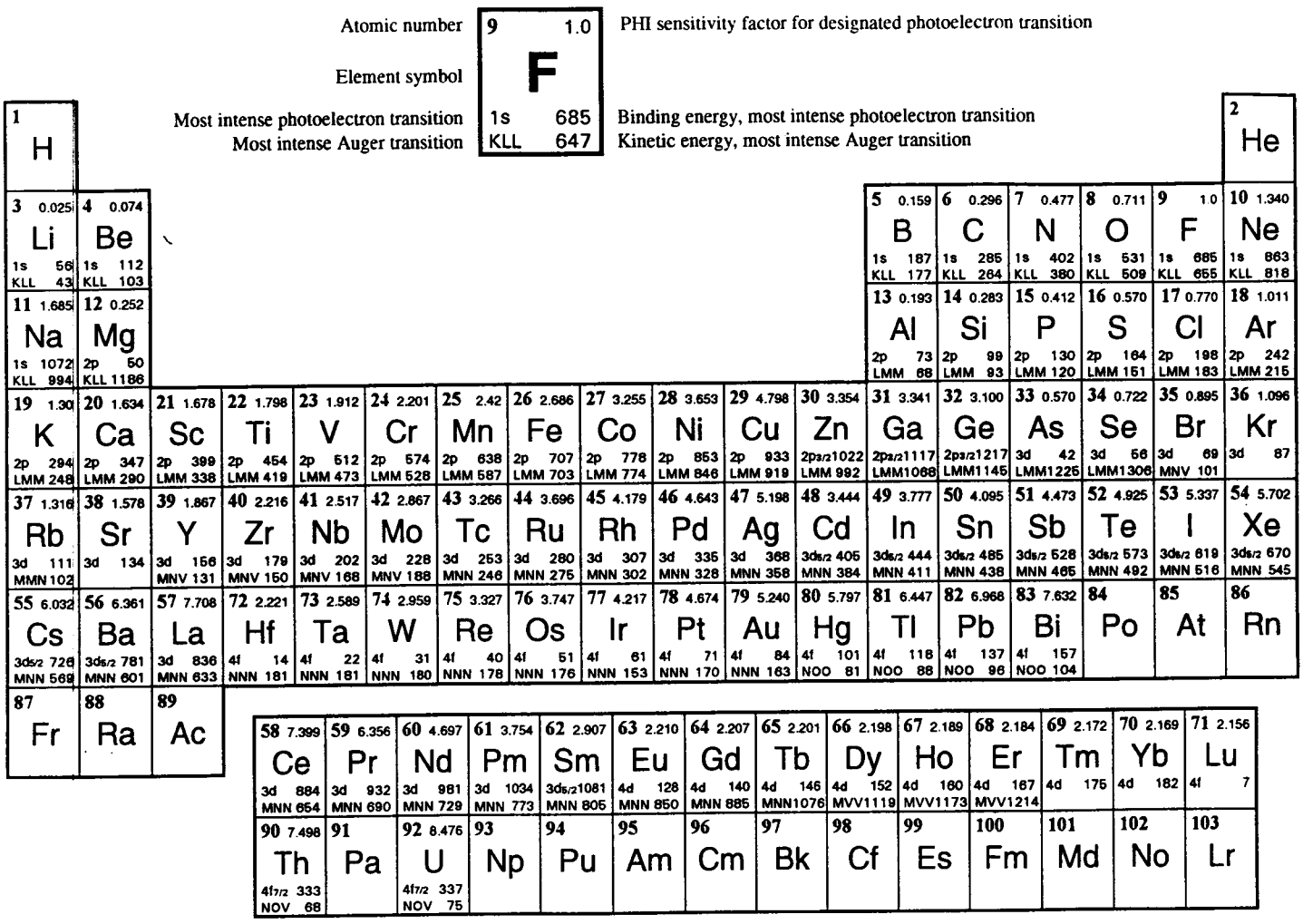
Appendix J. Line Positions in Numerical Order

For photoelectron lines, the spin orbit splitting is indicated in parentheses. Auger lines are in italics, and the photon source for the Auger excitation is indicated in parentheses.

7	Lu $4f_{7/2}$	(2)	89	Mg 2s		175	Tm 4d		299	Y $3p_{3/2}$	(12)
14	Hf $4f_{7/2}$	(2)	90	Ba $4d_{5/2}$	(3)	179	Zr $3d_{5/2}$	(2)	301	*Mg*	*(Al)*
23	O 2s		98	*Er*	*(Al)*	181	*Se*	*(Al)*	307	Rh $3d_{5/2}$	(5)
22	Ta 4f	(2)	99	Si $2p_{3/2}$	(1)	182	Yb 4d		309	Ho $4p_{3/2}$	(44)
25	Sn 4d		101	Hg $4f_{7/2}$	(4)		Br $3p_{3/2}$	(7)	315	Pt $4d_{5/2}$	(17)
29	Ge $3d_{5/2}$	(1)	103	La $4d_{5/2}$	(3)	186	*Ga*	*(Mg)*	320	Ar 2s	
30	F 2s		104	Ga $3p_{3/2}$	(3)	188	P 2s		321	Er $4p_{3/2}$	(47)
31	W $4f_{7/2}$	(2)	109	Ce $4d_{5/2}$	(3)	189	B 1s		330	Zr $3p_{3/2}$	(14)
37	V 3p			*Ge*	*(Mg)*	196	Lu $4d_{5/2}$	(10)	333	Th $4f_{7/2}$	(9)
40	Re $4f_{7/2}$	(2)	112	Rb $3d_{5/2}$	(1)	199	Cl $2p_{3/2}$	(2)		Tm $4p_{3/2}$	(51)
41	Ne 2s			Be 1s		202	Nb $3d_{5/2}$	(3)	335	Pd $3d_{5/2}$	(5)
42	As $3d_{5/2}$	(1)	115	Pr 4d		208	Kr $3p_{3/2}$	(8)		Au $4d_{5/2}$	(18)
43	Cr 3p		117	*Ho*	*(Al)*	211	Hf $4d_{5/2}$	(11)		*Cu*	*(Mg)*
48	Mn 3p		118	Tl $4f_{7/2}$	(4)	226	Ta $4d_{5/2}$	(12)	341	Yb $4p_{3/2}$	(48)
49	I $4d_{5/2}$	(2)		Al 2s		228	S 2s		342	*Ge*	*(Al)*
50	Mg 2p		121	Nd 4d			Mo $3d_{5/2}$	(3)	347	Ca $2p_{3/2}$	(3)
51	Os $4f_{7/2}$	(3)	122	Ge $3p_{3/2}$	(4)	240	Rb $3p_{3/2}$	(9)	360	Lu $4p_{3/2}$	(53)
53	Fe 3p		128	Eu 4d		242	Ar $2p_{3/2}$	(2)	361	Hg $4d_{5/2}$	(20)
56	Li 1s		129	Sm 4d		243	W $4d_{5/2}$	(13)		Nb $3p_{3/2}$	(15)
	Se $3d_{5/2}$	(1)	131	P $2p_{3/2}$	(1)	260	Re $4d_{5/2}$	(14)	368	Ag $3d_{5/2}$	(6)
60	Co 3p		134	Sr $3d_{5/2}$	(2)		*Na*	*(Mg)*	369	*Gd*	*(Mg)*
61	Ir $4f_{7/2}$	(3)	137	Pb $4f_{7/2}$	(5)		*Tb*	*(Al)*	377	U $4f_{7/2}$	(11)
	Xe $4d_{5/2}$	(2)	140	Gd 4d		262	*Zn*	*(Mg)*	380	K 2s	
64	Na 2s		141	As $3p_{3/2}$	(5)		*As*	*(Al)*	385	Tl $4d_{5/2}$	(21)
67	Ni 3p		146	Tb 4d		270	Sr $3p_{3/2}$	(11)	394	Mo $3p_{3/2}$	(17)
69	Br $3d_{5/2}$	(1)	151	Si 2s		271	Cl 2s		398	N 1s	
71	Pt $4f_{7/2}$	(3)	152	Dy 4d		279	Os $4d_{5/2}$	(14)	399	Sc $2p_{3/2}$	(5)
73	Al 2p		156	Y $3d_{5/2}$	(2)	280	Ru $3d_{5/2}$	(4)	404	*Eu*	*(Mg)*
75	Cu $3p_{3/2}$	(2)	157	Bi $4f_{7/2}$	(5)	285	Tb $4p_{3/2}$	(37)	405	Cd $3d_{5/2}$	(7)
77	Cs $4d_{5/2}$	(3)	160	Ho 4d			C 1s		408	*Ni*	*(Mg)*
84	Au $4f_{7/2}$	(4)	163	Se $3p_{3/2}$	(6)	294	K $2p_{3/2}$	(3)	412	Pb $4d_{5/2}$	(22)
87	Kr $3d_{5/2}$	(1)	164	S $2p_{3/2}$	(1)	297	Dy $4p_{3/2}$	(40)	419	*Ga*	*(Al)*
89	Zn $3p_{3/2}$	(2)	167	Er 4d			Ir $4d_{5/2}$	(15)	436	*Ne*	*(Mg)*

440	Ca 2s		669	*Ne*	*(Al)*	874	*N*	*(Mg)*	1103	*Cd*	*(Al)*
449	*Sm*	*(Mg)*	670	Xe $3d_{5/2}$	(13)	884	Ce $3d_{5/2}$	(18)	1107	*N*	*(Al)*
441	Bi $4d_{5/2}$	(24)	676	Th $4d_{5/2}$	(37)	886	*Ba*	*(Al)*	1117	Ga $2p_{3/2}$	(27)
444	In $3d_{5/2}$	(8)	682	*Sm*	*(Al)*	896	*Ag*	*(Mg)*	1126	Eu $3d_{5/2}$	(30)
454	Ti $2p_{3/2}$	(6)	685	F 1s		900	*Mn*	*(Al)*	1129	*Ag*	*(Al)*
462	Ru $3p_{3/2}$	(22)		*Cs*	*(Mg)*	916	*Sc*	*(Mg)*	1149	*Sc*	*(Al)*
480	*Co*	*(Mg)*	696	Cr 2s		918	*Cs*	*(Al)*	1154	*Bi*	*(Mg)*
485	Sn $3d_{5/2}$	(8)	707	Fe $2p_{3/2}$	(13)	926	*Pd*	*(Mg)*	1159	*Pd*	*(Al)*
493	*Na*	*(Al)*	709	*Xe*	*(Mg)*	932	Pr $3d_{5/2}$	(20)	1161	*Pb*	*(Mg)*
495	*Zn*	*(Al)*	713	*Co*	*(Al)*	933	Cu $2p_{3/2}$	(20)	1168	*Tl*	*(Mg)*
497	Rh $3p_{3/2}$	(24)	715	Sn $3p_{3/2}$	(42)	942	*Xe*	*(Al)*	1179	*Hg*	*(Mg)*
499	Sc 2s		726	Cs $3d_{5/2}$	(14)	952	*Rh*	*(Mg)*	1183	*Au*	*(Mg)*
512	V $2p_{3/2}$	(8)		*Cr*	*(Mg)*	959	*Cr*	*(Al)*	1185	*Rh*	*(Al)*
525	*Nd*	*(Mg)*	736	U $4d_{5/2}$	(42)	964	*Ca*	*(Mg)*	1186	Gd $3d_{5/2}$	(32)
526	*Dy*	*(Al)*	738	*I*	*(Mg)*	971	*U*	*(Mg)*	1197	*Ca*	*(Al)*
528	Sb $3d_{5/2}$	(9)	745	*O*	*(Mg)*		*I*	*(Al)*	1204	*U*	*(Al)*
531	O 1s		758	*Nd*	*(Al)*	978	*O*	*(Al)*	1212	*Ru*	*(Al)*
533	Pd $3p_{3/2}$	(27)	767	Sb $3p_{3/2}$	(46)	979	*Ru*	*(Mg)*	1217	Ge $2p_{3/2}$	(31)
551	*Fe*	*(Mg)*	772	*Te*	*(Mg)*	981	Nd $3d_{5/2}$	(21)	1223	*C*	*(Al)*
561	Ti 2s		778	Co $2p_{3/2}$	(15)	990	*C*	*(Mg)*	1239	*Th*	*(Al)*
564	*Pr*	*(Mg)*	781	Ba $3d_{5/2}$	(15)	1005	*Te*	*(Al)*		*K*	*(Al)*
568	*Cu*	*(Al)*		*V*	*(Mg)*	1006	*K*	*(Mg)*	1241	Tb $3d_{5/2}$	(35)
573	Ag $3p_{3/2}$	(31)	784	*Fe*	*(Al)*		*Th*	*(Mg)*	1272	*Ar*	*(Al)*
	Te $3d_{5/2}$	(10)	797	*Pr*	*(Al)*	1014	*V*	*(Al)*	1296	Dy $3d_{5/2}$	(37)
574	Cr $2p_{3/2}$	(9)	799	*Sb*	*(Mg)*	1022	Zn $2p_{3/2}$	(23)	1299	*Mo*	*(Al)*
599	*F*	*(Mg)*	816	*Sn*	*(Mg)*	1032	*Sb*	*(Al)*	1303	Mg 1s	
600	*Ce*	*(Mg)*	820	Te $3p_{3/2}$	(51)	1039	*Ar*	*(Mg)*	1304	*Cl*	*(Al)*
602	*Gd*	*(Al)*	832	*F*	*(Al)*	1049	*Sn*	*(Al)*	1310	*B*	*(Al)*
619	Cd $3p_{3/2}$	(34)	833	*Ce*	*(Al)*	1068	*Ti*	*(Al)*	1319	*Nb*	*(Al)*
	I $3d_{5/2}$	(12)	835	*Ti*	*(Mg)*	1071	*Cl*	*(Mg)*	1324	As $2p_{3/2}$	(35)
634	*La*	*(Mg)*	836	La $3d_{5/2}$	(17)	1072	Na 1s		1336	*S*	*(Al)*
637	*Eu*	*(Al)*	843	*In*	*(Mg)*	1076	*In*	*(Al)*	1387	*Bi*	*(Al)*
639	Mn $2p_{3/2}$	(11)	853	Ni $2p_{3/2}$	(18)	1077	*B*	*(Mg)*	1394	*Pb*	*(Al)*
641	*Ni*	*(Al)*	863	Ne 1s		1081	Sm $3d_{5/2}$	(27)	1401	*Tl*	*(Al)*
653	*Ba*	*(Mg)*	867	*La*	*(Al)*	1086	*Nb*	*(Mg)*	1412	*Hg*	*(Al)*
665	In $3p_{3/2}$	(38)	870	*Cd*	*(Mg)*	1103	*S*	*(Mg)*	1416	*Au*	*(Al)*
667	*Mn*	*(Mg)*									

Appendix K. Periodic Table



*The values are for area measurements of the designated transitions and are only valid when the electron energy analyzer used has the transmission characteristics of the spherical capacitor type analyzer equipped with an Omni Focus III lens supplied by Physical Electronics and with x-rays at 90° relative to the analyzer. When a spin-orbit splitting is not designated, the value is for a measurement including both spin-orbit components.