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XAP, A program for deconvolution and analysis of
complex x-ray spectra

by

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CONTENTS

LIST OF ILLUSTRATIONS

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James E. Quick and Abdul Malik Helaby

ABSTRACT

The X-ray analysis program (XAP) is a spectral-deconvolution program written in BASIC and specifically designed to analyze complex spectra produced by energy-dispersive X-ray analytical systems (EDS). XAP compensates for spectrometer drift, utilizes digital filtering to remove background from spectra, and solves for element abundances by least-squares, multiple-regression analysis. Rather than base analyses on only a few channels, broad spectral regions of a sample are reconstructed from standard reference spectra. The effects of this approach are (1) elimination of tedious spectrometer adjustments, (2) removal of background independent of sample composition, and (3) automatic correction for peak overlaps. Although the program was written specifically to operate a KEVEX 7000 X-ray fluorescence analytical system, it could be adapted (with minor modifications) to analyze spectra produced by scanning electron microscopes, electron microprobes, and probes, and X-ray defractometer patterns obtained from whole-rock powders.

INTRODUCTION

Energy-dispersive X-ray analytical systems (EDS) perform simultaneous data acquisition over wide spectral ranges. In X-ray fluorescence spectrometry and electron microprobe analysis, this method allows measurement of many elemental abundances simultaneously and without movement of crystal spectrometers as is required when using wavelength dispersive X-ray analytical systems (WDS). However, the energy resolution of EDS is low relative to WDS and, as a result, EDS spectra are characterized by complex peak overlaps that make analysis difficult. Conventional approaches to spectral analysis subtract model backgrounds from spectra and measure peak intensities by utilizing counts in only a few channels of the spectrum. Unfortunately, background shapes are dependent on sample composition, and so methods that utilizes counts in only a few channels ignores much of the spectral information that is provided by EDS.

The X-ray Analysis Program (XAP) is a spectral-deconvolution program written in BASIC. XAP removes background by digital filtering of spectra and calculates contributions of reference spectra by least-squares, multiple-regression analysis. XAP is designed to compensate for spectrometer drift, remove the background continuum from spectra, suppress noise, and remove peak-overlap effects. Although XAP is an entirely new program, it is based on proven methods (Schamber, 1973; Schamber and others, 1977; McCarthy and Schamber, 1981) of analyzing complex EDS spectra.

XAP was written to perform on-line semiquantitative analysis of energy-dispersive X-ray fluorescence spectra produced by a KEVEX 7000 analyzer. As presently configured, the program handles spectra composed of as many as 1,024

1

channels and can analyze for as many as 20 elements at a time. The program can be modified to handle larger or smaller spectra or to analyze for more than 20 elements. Spectra produced by other analytical systems, such as electron microprobes or X-ray defractometers, could be deconvoluted by XAP with minor modification of the program code that controls data input. XAP could be extended to produce true quantitative analyses by applying rigorous absorption and fluorescence corrections.

Analytical results are output to a dot matrix printer and consist of abundances in terms of weight percent or parts per million (ppm), as appropriate. The output also includes estimates of precision for each element in each analysis based on the volume of characteristic peaks and the local intensity of the background. Abundances and precisions may be stored on computer disks in DATASAVE (Quick, 1987) files for later use in graphical or statistical analysis. Entire spectra may be output to the printer or may be stored on disk for recall and analysis at a later time.

SYSTEM AND SOFTWARE REQUIREMENTS

XAP is written in IBM BASICA. The program must be compiled to execute because the program length and variables collectively exceed the 64 kilobytes addressed by that language. The program will run on any IBM or IBM-compatible microcomputer using DOS 1.1 or higher and that has a minimum of 128 kilobytes of memory, one disk drive, graphics capability, and a serial communications port. XAP is specifically written to print formatted results on an EPSON FX dot-matrix printer. Substitution of another printer may require modification of printer-control escape sequences. Similarly, minor modifications (to baud rate, etc.) may have to be made to adapt the program for serial communication with a system other than the KEVEX 7000.

TERMINOLOGY

Discussion of XAP requires some usage of specialized terms. An "unknown" spectrum is one that will be analyzed as if its composition is not documented. A "reference" spectrum is one containing spectral features that are used to create a standard for subsequent least-squares analysis of an unknown spectrum. A "region of interest" is the actual part of a reference spectrum that is used in least-squares analysis. A region of interest typically contains all of the major characteristic X-ray peaks for the element being standardized. An "internal region of interest" is a part of a region of interest that defines a single dominant X-ray peak to be used for estimation of precision.

APPROACH

Analysis of any EDS X-ray spectrum requires (1) correction for detector drift, (2) subtraction of the background continuum from the spectrum, (3) measurement of X-ray peak intensities, and (4) calculation of element abundances and estimation of precision using peak intensities. XAP subtracts the background continuum from the spectrum and determines peak intensity values by least-squares, multiple-regression analysis of filtered spectra. Justification for this

2

approach is presented in detail by McCarthy and Schamber (1981); programs using similar calculations have been tested by Tracor Northern X-ray analytical systems for more than 10 years. The calculation of elemental abundance is based on a method outlined by Elsass and du Bray (1982) using calibration curves and estimating the X-ray absorption of the sample matrix from the intensity of Compton-scattered source radiation.

BACKGROUND SUBTRACTION

In XAP, background subtraction is accomplished by use of a digital filtering proceedure. An X-ray spectrum may be considered in terms of three frequency components: (1) a background continuum characterized by low-frequency variations, (2) low-amplitude, high-frequency variations from channel to channel that result from random counting errors, and (3) characteristic X-ray peaks, which may be thought of as high-amplitude, intermediate-frequency components. McCarthy and Schamber (1981) demonstrate that it is possible to mathematically construct a linear, digital filter that suppresses the low- and high-frequency components of the spectrum but preserves the mid frequency information (i.e., the characteristic X-ray peaks). The advantage of this approach lies in the fact that background subtraction is independent of the shape of the background continuum and the composition of the sample.

Figure 1 illustrates the effects of digital filtering on an artificial spectrum composed of a single gaussian peak and a background continuum. Random "counting noise" has been introduced into the individual channels. The digital filter is a simple algorithm that replaces the counts at each channel with a weighted average of the nearby channels. In the specific case of figure 1, the filtered contents of the nth channel, $F(n)$ are calculated by

$$
(1) \quad F(n) = 1/12 \left[-\sum_{i=4}^{6} C(n-i) + \sum_{i=1}^{3} C(n-i) + \sum_{i=1}^{3} C(n+i) - \sum_{i=4}^{6} C(n+i) \right]
$$

where $C(n)$ is the number of counts in the nth channel before filtering. The results of the calculation are shown in Figure 1B. The background continuum is removed, the counting noise is reduced, and the original gaussian peak is replaced by a sinusoidal structure, that has a shape and magnitude that is characteristic of the original peak(s). Note that the sinusoidal structure in the filtered spectrum (fig. 1B) has been shifted to the right relative to the peak in the original spectrum (fig. 1A). This does not influence subsequent calculations because all reference and unknown spectra are shifted equally.

PEAK INTENSITY

XAP calculates peak intensities by least-squares fitting of filtered reference spectra to a filtered unknown spectrum. Least-squares fitting of unfiltered spectra would require additional consideration of a background continuum in the analysis. However, McCarthy and Schamber (1981) demonstrate that filtered spectra may be subjected to least-squares analysis without consideration of the background continuum and without loss of significant spectral information.

3

Figure 2 illustrates the analysis of a filtered spectrum. The spectrum was synthesized using U, Rb, Sr, and Y spectra that were measured with a KEVEX 7000 X-ray fluorescence analyzer and combined in the ratio 0.1/0.5/0.3/0.1. The left side of the figure shows the unfiltered spectra for U, Rb, Sr, Y and the synthesized "unknown". The right side of the figure shows the same spectra after digital filtering. Least-squares fitting of the four filtered "reference" spectra to the filtered unknown spectrum yields 10.0000 percent U, 50.0000 percent Rb, 30.0000 percent Sr, and 10.0000 percent Y. The result accurately reproduces the original ratios to six significant figures, demonstrating the validity of least-squares fitting of filtered spectra. Note that the result was obtained in spite of a serious overlap between Rb K_α and U L_α peaks, between Rb K_β and Y K_α peaks, and between Y K_β and U L_β peaks.

The least-squares analysis used by XAP is a simple multiple-regression calculation described in numerous texts on data analysis (e.g. Davis, 1973). The solution is given by solving for the "b" coefficients in the following matrix equation:

(2)

$$
\begin{vmatrix}
\Sigma N & \Sigma R1 & \Sigma R2 & \Sigma R3 \dots \Sigma RN \\
\Sigma R1 & \Sigma R1{*}R1 & \Sigma R1{*}R2 & \Sigma R1{*}R3 \dots \Sigma R1{*}RN \\
\Sigma R2 & \Sigma R2{*}R1 & \Sigma R2{*}R2 & \Sigma R2{*}R3 \dots \Sigma R2{*} \\
\Sigma R3 & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot \\
\Sigma RN & \Sigma RN{*}R1 & \Sigma RN{*}R2 & \dots \Sigma RN{*}RN
\end{vmatrix}
\cdot
\begin{vmatrix}
\Sigma b0 \\
\Sigma b1 \\
\Sigma b2 \\
\cdot \\
\cdot \\
\cdot \\
\cdot \\
\Sigma bN
\end{vmatrix}
=
\begin{vmatrix}
\Sigma F \\
\Sigma F{*}R1 \\
\Sigma F{*}R2 \\
\cdot \\
\cdot \\
\cdot \\
\cdot \\
\Sigma F{*}RN
\end{vmatrix}
$$

In Equation 2, N is the total number of channels, Rj is the number of counts in a given channel of the jth filtered reference spectrum, bj is the contribution of the jth reference spectrum to the observed spectrum, and F is the number of counts in a given channel of the filtered observed spectrum. The summation indicated for each matrix element is performed over the spectral region(s) under consideration. For example, if the entire observed spectrum is being analyzed, R1 would be the sum of the counts in each channel of the entire filtered spectrum of reference number 1. Similarly, R1*R2 would be given by the product of the counts in each channel in reference 1 and reference 2 summed over the entire spectrum. The b coefficients correspond to the residual error (b0) and the fraction (b1, b2, etc.) of each reference spectrum present in the optimum fit to the observed spectrum.

Equation 2 may be abbreviated using standard matrix notation to:

(3) $$\overline{R} \bullet \overline{B} = \overline{F}$$

The contents of $\overline{R}$ depend only on the references and, therefore, need to be calculated only once for a given set of references during an analytical run. This calculation is most conveniently performed at the time that the references are recalled from disk.
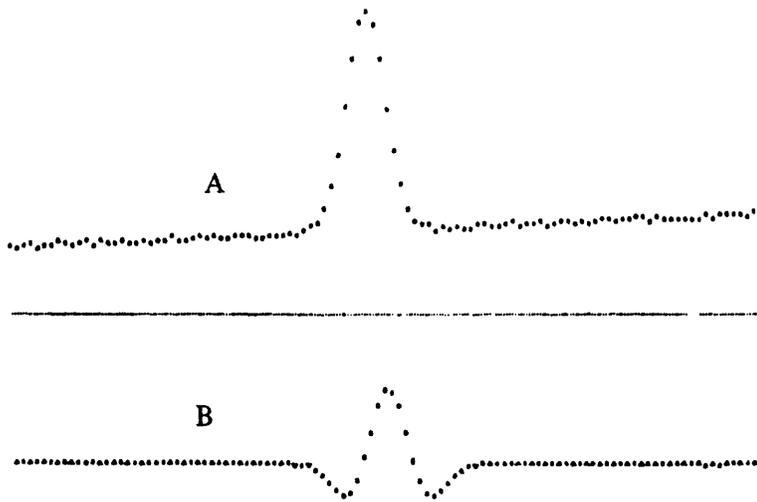
Figure 1.--Effects of digital filtering on a synthetic spectrum. (A) Spectrum is constructed of single gaussian peak superimposed on background continuum. Random "counting noise" introduced into each channel. (B) Filtered spectrum is composed of a sinusoidal shape characteristic of original gaussian peak. Background has been removed and counting noise has been reduced. Fine dotted line in A and B is zero-count base line. Dots in dark dotted line represent count in each channel.
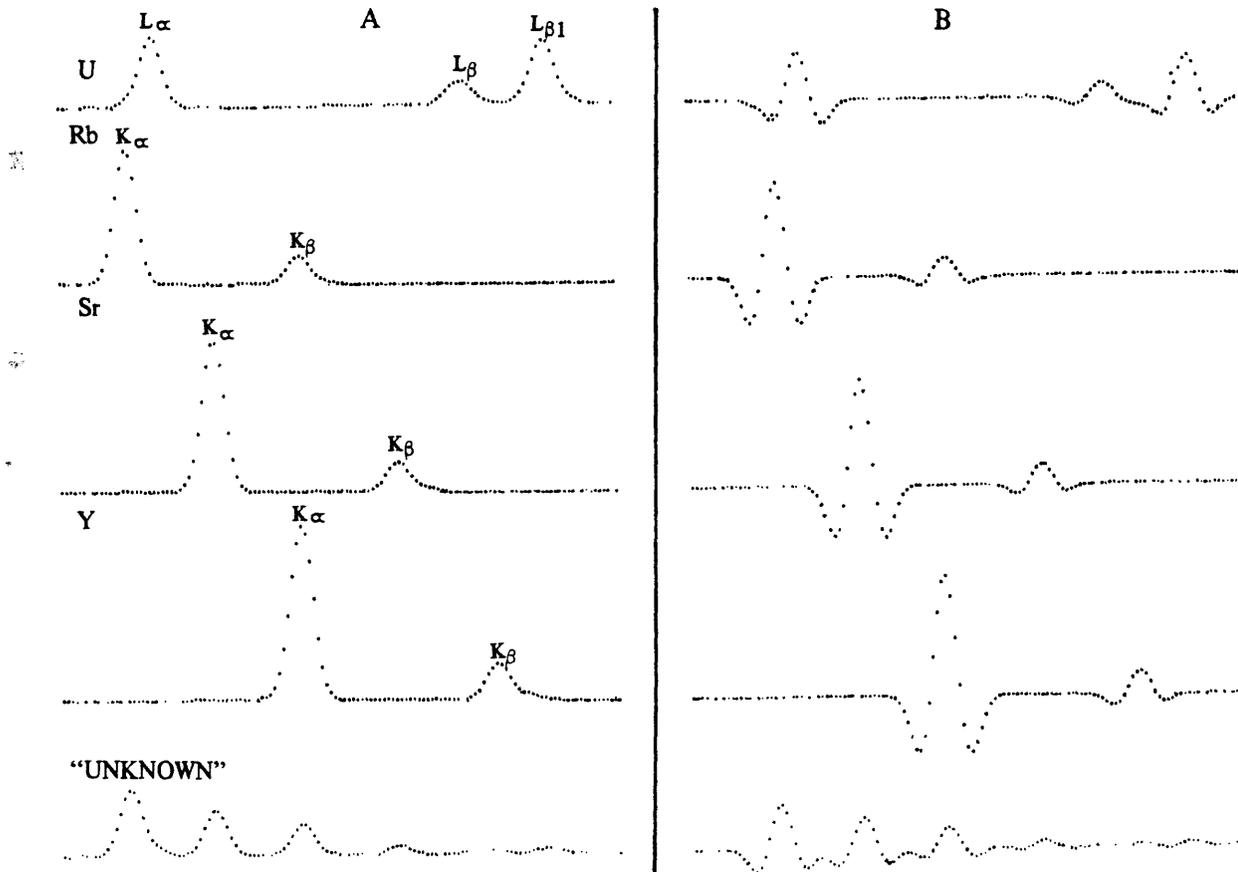
Figure 2.--Effects of digital filtering on least-squares analysis. (A) Reference spectra for U, Rb, Sr, and Y, and a synthetic spectrum composed by combining those spectra in the ratio 0.1/0.5/0.3/0.1. (B) Digitally filtered synthetic and reference spectra. Least-squares analysis of filtered reference spectrum returns values of 10.0000 percent U, 50.0000 percent Rb, 30.0000 percent Sr, and 10.0000 percent Y. Fine dotted line in each spectrum is zero-count base line.

Equation 2 (or 3) is solved for the b coefficients using the Gauss method by which the matrix is manipulated to set all elements to the left of the Rii diagonal equal to zero. This approach is slower than inverting R and solving directly by

$$(4) \qquad \overline{B} = \overline{R}^{-1} \bullet \overline{F}$$

However, the Gauss method is used because it is less susceptible to round-off errors and because elements may be eliminated from analysis at any time by omitting an appropriate row and column from consideration.

ELEMENT ABUNDANCE

Calculation of element abundances from the b coefficients in Equation 2 requires absorption and fluorescence corrections. The KEVEX 7000 X-ray fluorescence analyzer is used primarily to measure minor and trace abundances (<10,000 ppm) of elements heavier than Fe. The matrix of most powdered rock samples is composed of more than 99 percent Fe and lighter elements. Therefore, fluorescence corrections may be ignored in semiquantitative analysis for elements heavier than Fe in most samples. An absorption-correction coefficient may be estimated based on the observation that absorption is inversely proportional to the intensity of the Compton-scattered source peaks (Giauque and others, 1977). Using this approximation and ignoring fluorescence corrections, XAP calculates an approximate concentration (or K-value) for each element using the following equation:

$$(5) \qquad Ki = Ci \times bi \times Ui \; / \; Us.$$

In Equation 5, Ki is the K-value for element i, Ci is the concentration of element i in the ith reference, bi is the fraction of the ith reference spectrum in the sample spectrum, Ui is the intensity of a preselected Compton-scattered source peak in the ith reference spectrum, and Us is the intensity of the same Compton-scattered source peak in the sample. Elsass and du Bray (1982) point out that this correction procedure provides the additional advantage of correcting for steadily reducing peak intensities due to progressive decay of the radioactive source.

K-values are converted to actual elemental abundances in XAP by fitting first- or second-order regression equations to working curves established with samples of known composition. This procedure is necessary because the rate of variation differs for different parts of the spectrum, despite the fact that the absorption correction varies inversely with the intensity of Compton scatter. The Compton scatter is also an inadequate indicator of absorption for a given element in samples where the element is present in high concentrations (>>10,000 ppm). XAP calculates elemental abundances from K-values by the the following equation:

$$(6) \qquad Csi = A0i + A1i \times Ki + A2i \times Ki^2$$

where Csi is the concentration of element i in the sample, and $A0i$, $A1i$, and $A2i$ are the solutions to the second-order regression calculation for element i. $A0i$ may be thought of as the absolute detection limit of of element i and, for most elements that are measured with K-series peaks, it is in the range of 0 to 20 ppm. $A1$ is close to 1 for most elements, typically falling between 0.85 and 1.15. $A2$ is zero for most elements in the range of 0 to 10,000 ppm and is used in XAP only to

6

extend measurements into ranges of high concentration where marked nonlinear relationships between concentration and K-value are found. For example, Fe measured as FeO displays a strongly nonlinear relationship above 7 weight percent FeO but can be measured in that range with a second-order correction.

ZERO AND GAIN CORRECTION

Amplifier output on EDS detectors varies with time. As a result, spectra may be shifted to lower or higher apparent energy and(or) there may be spectral telescoping, causing distances between peaks to contract or expand. These variations can be minimized on most EDS detectors by adjustment of zero and gain amplifier controls until two known, widely spaced X-ray peaks are located perfectly with respect to their predicted energies. This can be a time-consuming task but, in the absence of another solution, could be essential on a daily basis because the least-squares deconvolution of filtered spectra requires precise amplifier drift correction.

XAP corrects for amplifier drift so that manual correction is not required unless drift produces extreme shifts of peaks from their theoretical positions. The XAP correction is made by calculating theoretical gain- and zero-correction factors that are required to adjust a standard reference spectrum so that two widely spaced peaks are moved into perfect theoretical position. These correction factors are then used to telescope and shift each subsequent spectra so that they are adjusted in the same manner as the standard reference. This procedure reduces the offset of spectral elements from their theoretical positions by approximately one order of magnitude.

The calculation and use of theoretical gain and zero corrections is based on a procedure outlined by Tracor Northern, Inc. in descriptions for their subroutines "Calibrate Lines" and "Recalibrate" that appear in an unpublished manual for the TN2000 energy-dispersive analytical system. Measurement of two X-ray peaks, which should be centered at energies E1 and E2, with an EDS will return measured peak locations at E1' and E2', which are not necessarily equal to E1 and E2. The offset of these peaks from their theoretical positions may be expressed in terms of gain and zero parameters that are defined according to

$$(7) \quad g = 10^5 \times ((E2' - E2) - (E1' - E1)) / (E2 - E1)$$

and

$$(8) \quad z = (E2 \times (E1' - E1) - E1 \times (E2' - E2)) / (E2 - E1)$$

where g is the gain, z is the zero, and the values for E1, E1', E2, and E2' are in electron volts (eV).

The observed spectrum may be corrected for these offsets according to

$$(9) \quad Ec = z + Eo \times (1 + (g / 10^5))$$

where Eo is the energy of a given channel in the observed spectrum and Ec is the energy of the same channel in the corrected spectrum. EDS spectra are normally expressed in terms of uniformly separated channels, each of which is located at precisely the same energy in all spectra. For example, the 20th channel may be

located at 800 eV and separated from its neighbors by 40 eV. This uniform data presentation is another strict requirement for least-squares analysis of filtered spectra, and, although Eo values are always located at appropriate and uniformly spaced energies, the calculated Ec values are generally not. Therefore, new channels with proper spacing must be calculated from the Ec values. Following the approach of Tracor Northern, Inc., this is accomplished in XAP by parabolic interpolation to calculate counts in appropriately spaced channels.

ESTIMATION OF PRECISION

XAP estimates the precision of each element abundance measurement individually in each spectrum. During standardization, the user defines internal regions of interest that consist of single, isolated peaks for each element. Ideally, the most intense characteristic peak should be chosen since the most intense peaks will dominate the least-squares fit. XAP saves the background-subtracted counts for each of these peaks and uses this information to calculate the background-subtracted counts for each element according to the equation

$$(10) \qquad\qquad Pi = Pir \times bi.$$

Pi represents the background-subtracted counts for the internal region of interest for element i in the unknown, Pir represents the background-subtracted counts for the same region in the reference spectrum for element i, and bi is the contribution of the ith reference spectrum to the unknown spectrum as defined in Equation 2. The precision for element abundance measurement i is then estimated as a 2-sigma percent standard deviation given by

$$(11) \qquad\qquad s.d. \ \% = 2 \times 100 \times (\ \sqrt{Pi + Ri} \ / \ Pi \ )$$

where Ri represents the residual counts (or "background") after Pi is subtracted. In cases of peak overlap, Ri would equal true background plus the counts contributed by another X-ray peak and thus would be much greater than true background.

It is emphasized that Equation 11 gives only an estimate of precision. It is a reasonable approximation for elements whose reference spectra are dominated by one large peak, such as a K-alpha peak. However, when L-peaks are used, a reference spectrum could consist of as many as 5 peaks, several of which will be similar in intensity. In such cases, the actual precision will be less than the value estimated by Equation 11.

QUALITY OF FIT

Any least-squares spectral deconvolution should be tested by comparing the observed spectrum to the sum of the calculated components. Following the suggestions of McCarthy and Schamber (1981), XAP calculates a measurement of the quality of fit in terms of a Chi-squared value that is given by:

$$(12) \qquad X^2 = (c - n)^{-1} \times \left[\sum_{i=1}^{c} \left(Fi - \sum_{j=1}^{n} bj \times Rij \right)^2 / \ Fi \right]$$

where Fi represents the counts in the ith channel of the unknown spectrum, bj is the contribution of the jth reference spectrum to the "unknown" spectrum, Rij is the counts in the ith channel of the jth reference spectrum, c is the number of channels, and n is the number of degrees of freedom. A perfect fit would yield a chi-squared value of zero. A solution that is, on the average, within the statistical limits of uncertainty for each channel would yield a chi-squared value of zero to one. Chi-squared values that are much greater than one indicate a failure to fit a significant part of the spectrum. This is typically due to either uncorrected detector drift or failure to analyze for one or more major peaks. The first source of error can be eliminated by recalibrating the zero- and gain-correction factors; the second source of error would require addition of one or more appropriate references to the analysis.

PROGRAM DESCRIPTION

XAP is menu driven and designed to allow maximum flexibility. It is possible to manipulate, store, and recall spectra, change standards, and modify run conditions while new spectra are being accumulated by an interfaced EDS. The general structure of the program is outlined in flow diagrams in figures 3 through 6. A complete program listing is presented in the appendix.

MAIN MENU

XAP is run from two menus: a main menu that controls data transfer and analysis and an initialization submenu that is used to set up run conditions. Functions that can be addressed by the main menu are summarized in figure 3 and illustrated in detail in figures 4 and 5. Upon entry, the program presents a logo and proceeds to the main menu. The operator may elect to (1) exit the program, (2) put the program on hold by returning to the logo, (3) initialize an analytical run, (4) transfer spectra from an EDS to the computer for manipulation, (5) perform on-line analysis to run sequential spectra, or (6) recall spectra from either computer memory or disk. Selecting "transfer spectrum" (fig. 4) allows the operator to transfer a spectrum from an EDS, display it on the computer screen, and then (optionally) store the spectrum on disk, use the spectrum to create one or more references, print the spectrum on a dot-matrix printer, or expand and contract the vertical scale. Figure 7 is an example of the computer-display output to a dot-matrix printer. Selecting "on-line analysis" (fig. 4) directs the program into a loop that waits for data transfer from an EDS. The spectrum is analyzed without graphical display and calculated elemental abundances are then displayed on the screen and output to a printer (fig. 8). The program then waits for transfer of another spectrum from the EDS, but the last transferred spectrum is resident in memory until a new spectrum is received. During this waiting period, the operator may exit the loop and return to the main menu by pressing <ESC>. Selecting "recall spectrum" allows the operator to recall either the last spectrum transferred from the EDS or a spectrum from disk for graphical display. Once the spectrum is displayed on the computer screen, the same options are provided as in the "transfer spectrum" subroutine. This gives the operator an opportunity to examine a spectrum after it was analyzed on line and then store it on disk, change standards and reanalyze it, or output a copy to the printer.

Control is transferred to the initialization submenu by selecting the "initialization" option of the main menu. Functions provided by this submenu are illustrated in figure 6. Selection of "calibration check" establishes the gain- and zero-correction factors and stores them on disk. The locations of the two peaks used in the zero and gain calculation are displayed relative to their theoretical positions, and the operator is advised on how to manually adjust the EDS amplifier (fig. 9). The "recover calibration" command recalls these correction factors from disk allowing the operator to exit XAP and return without recalibrating gain and zero. The "recall standards" command recalls a standard file from disk and calculates the contents of matrix R in Equation 2. The "edit standards" command allows modification of standard names, concentration factors, and A values (see Eq. 6). Standards may be erased or stored on disk, and the standard file may be listed on a printer. The "flag abundances" command allows the operator to define a minimum abundance for a selected element above which the results will be printed in bold characters (fig. 9). The "prepare forms" command establishes the top of the page for output and prints the heading "USGS SEMI-QUANT XRF ANALYSES". The "datasave file" command allows the operator to establish a file for disk storage of data. The program returns to the submenu until the operator chooses to return to the main menu.
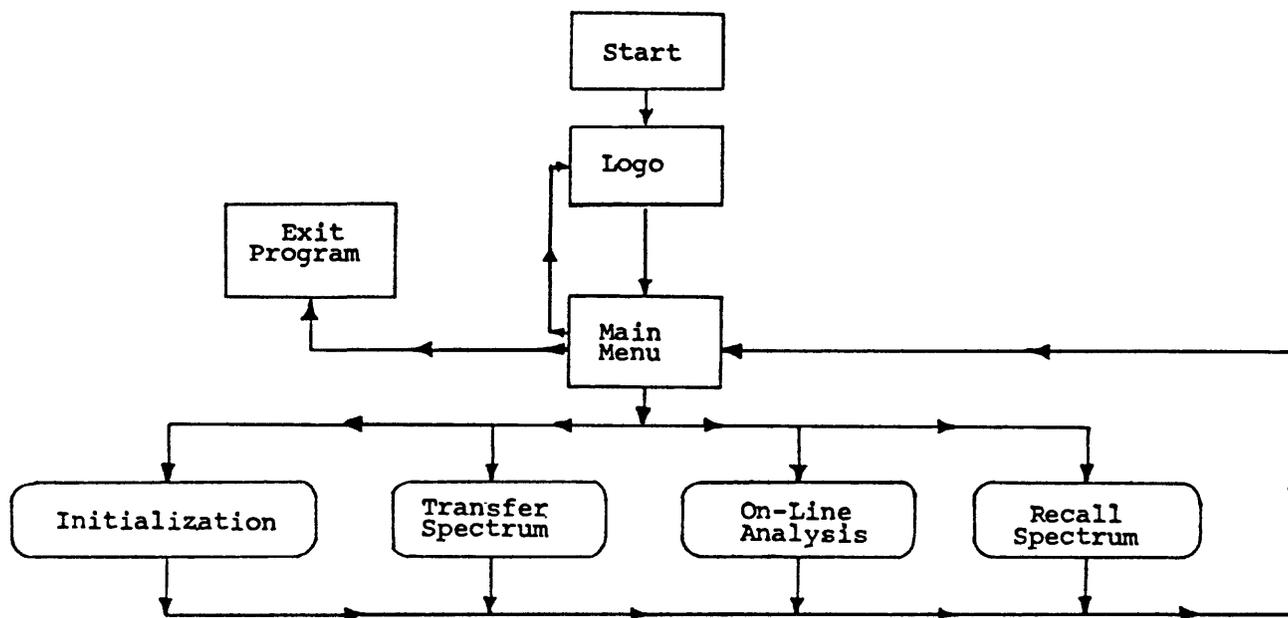

Figure 3.--Flow diagram illustrating basic structure of XAP.
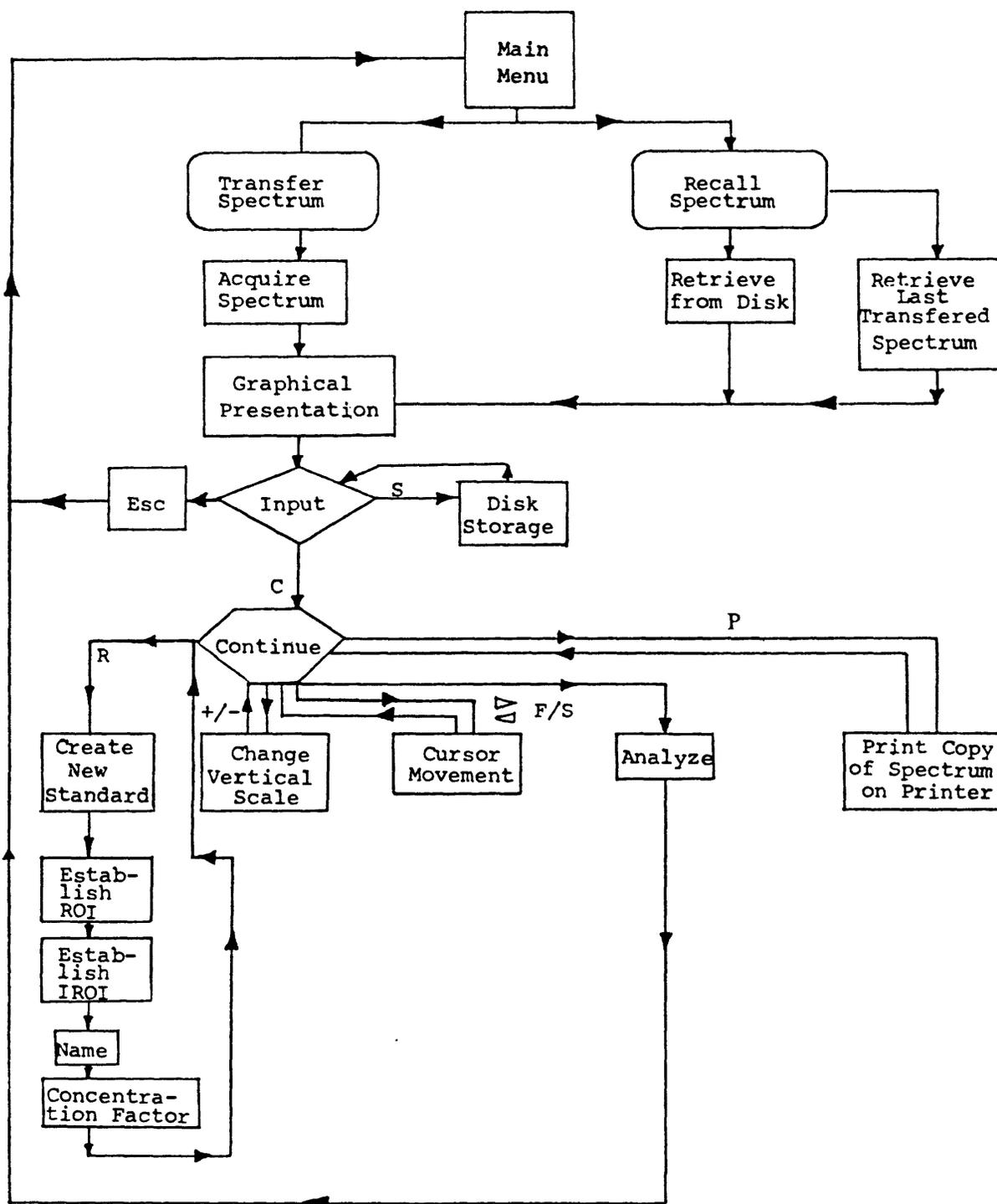
Figure 4.--Flow diagram illustrating in detail two options provided by XAP main menu "transfer spectrum" and "recall spectrum".

11
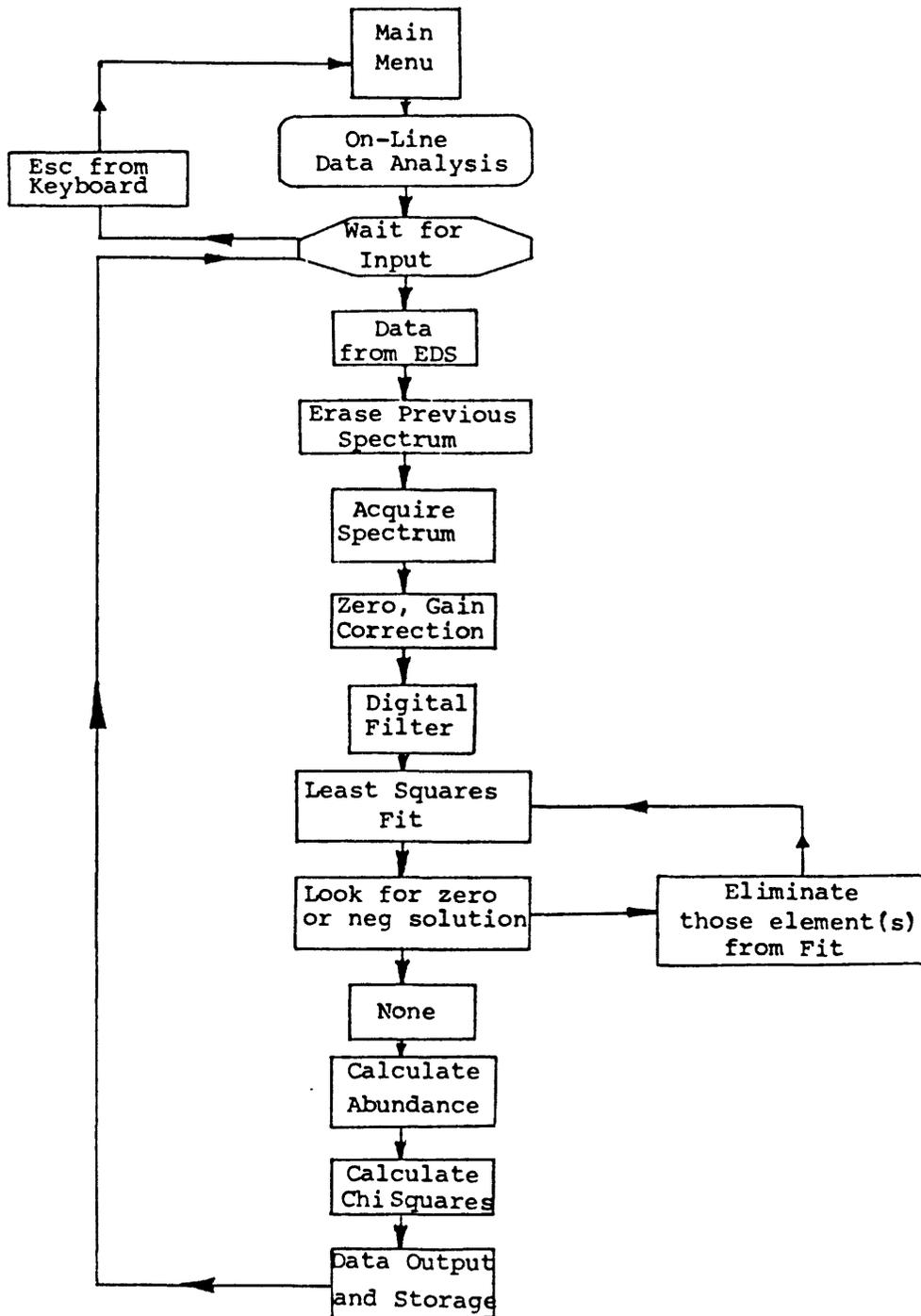
Figure 5.--Flow diagram illustrating in detail "on-line data analysis" option provided by XAP main menu.
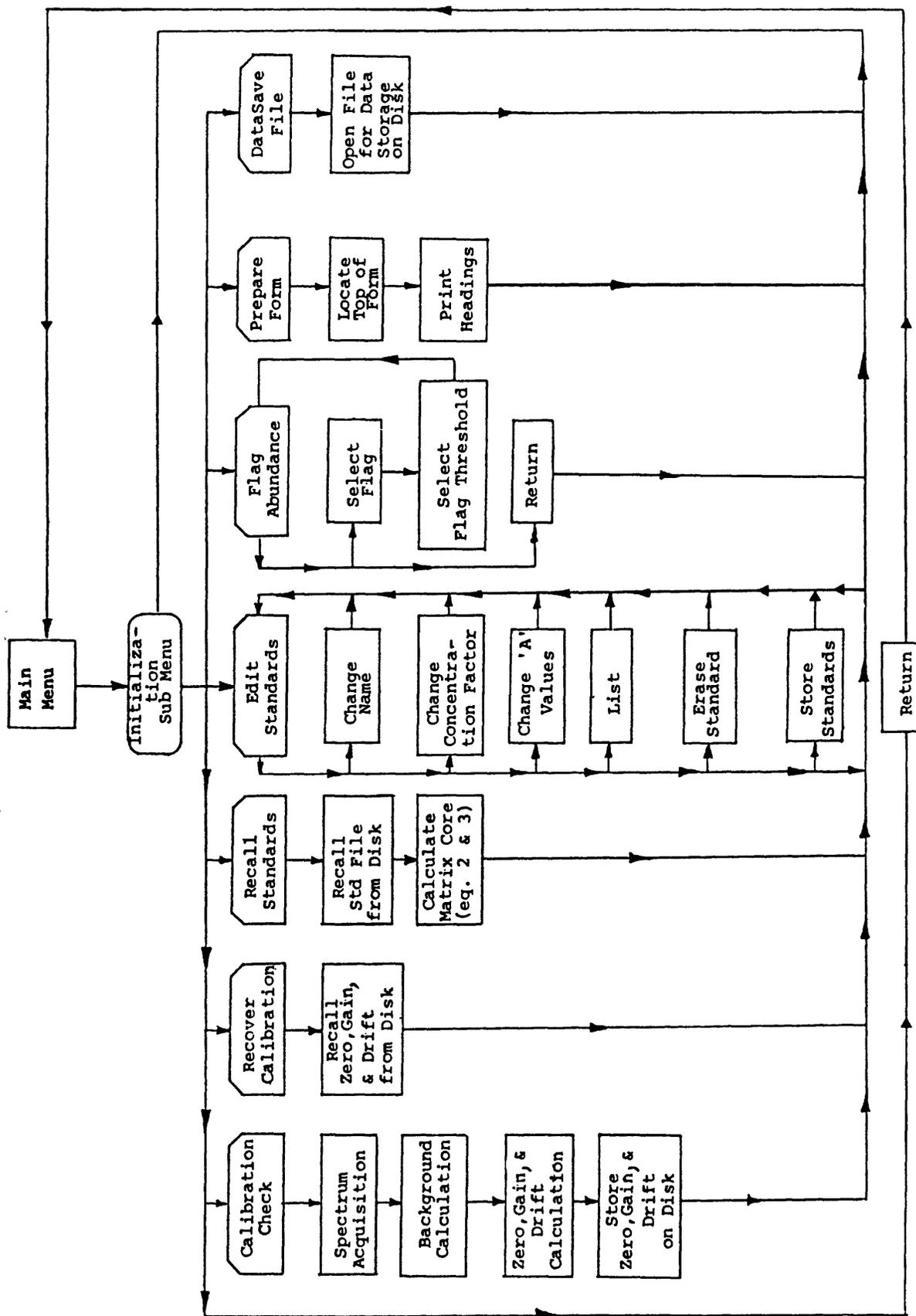
Figure 6.--Flow diagram illustrating in detail options provided by XAP initialization submenu.
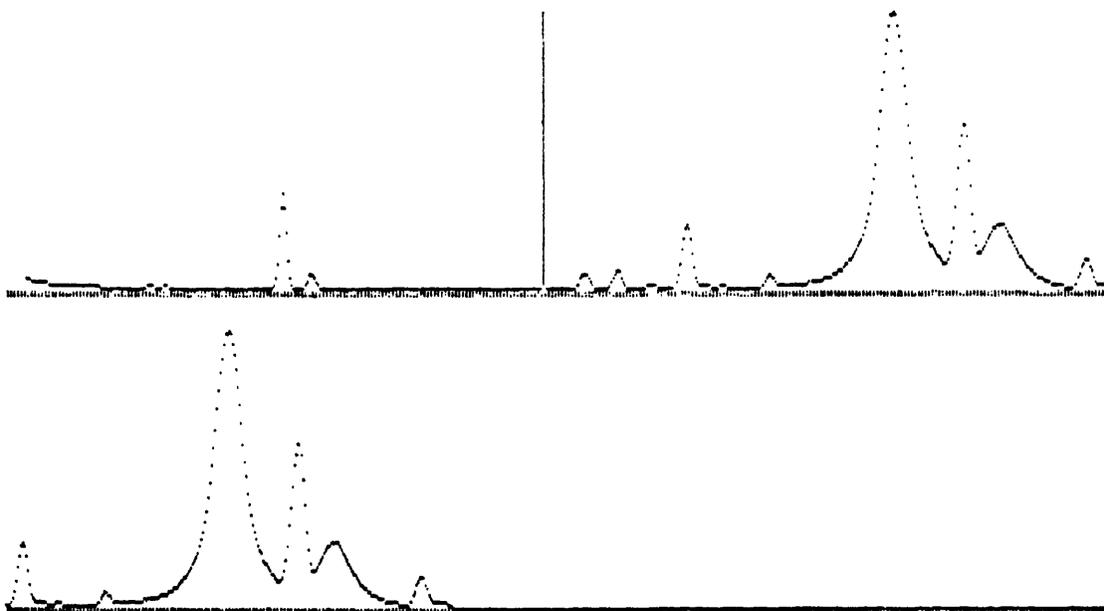
Figure 7.--XAP screen display of a representative spectrum. The spectrum is divided into two sections (top and bottom) with overlapping ranges because of the screen limitations of the IBM PC.

Center 6402.18 ev

Offset   2.18 ev

Peak max 22247

Center 14144.35 ev

Offset   2.35 ev

Peak max 5073
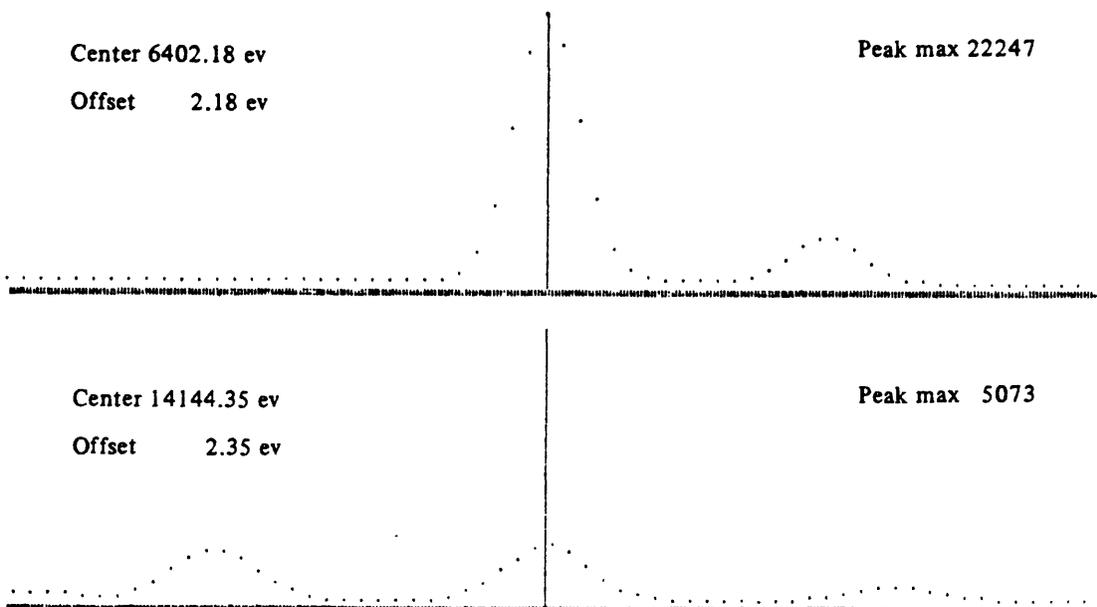
Figure 8.--Sample of calibration display using Fe and Sr K peaks of standard GSP-1. Fe K is shown in top spectral [a] region and Sr K is shown in [c] the bottom spectral region. The theoretical centers for both peaks are indicated with vertical lines. Departure from the theoretical positions are reported to left of each region in eV. Calculated theoretical gain and zero corrections and suggested manual adjustments to detector amplifier are reported at bottom of display. "Drift" value, giving height of a Compton-scatter peak, is reported in lower left corner of display and is proportional to intensity of source radiation.

14

U.S.G.S. SEMI-EQUANT XRF ANALYSES

Sample: RFB   Counting time 200 sec

Ele	Conc	% s.d.	Ele	Conc	% s.d.
FEO%	4.5	0.35	CU	69.9	34.81
ZN	2258.4	1.39	GA	67.7	19.77
AS	150.8	6.48	RB	902.0	0.82
SR	21.2	18.32	Y	36.5	9.53
ZR	69.5	6.43	NB	58.2	5.53
PB	129.0	8.60	TH	35.2	46.48
U	20.1	67.57	W	861.4	5.07
BI	99.1	41.77	BN	4060.6	9.35

Chi squared   0.060

Figure 9.--Sample printer output of an XAP analysis. Fe is reported in weight percent (indicated by "%") and all other elements are reported in parts per million. Precisions are 2-sigma standard deviations given as percent of the reported abundance.

STANDARDIZATION

Standard files may be created or modified using the main menu. A reference spectrum is displayed on the computer screen by either direct transfer from the EDS or by recall from disk. The operator then selects option "R" to establish a region of interest. The program leads the operator through the creation of (1) a region of interest used for least-squares analysis, (2) an internal region of interest used to estimate precision of elemental-abundance measurements, (3) a standard name used for reporting results, and (4) a concentration factor equal to the abundance of the element of interest in the reference spectrum. The program automatically stores the new standard in the standard file currently resident in memory. If there is no file in memory, a new file is automatically created. The standard file may be stored on disk after creation of a new standard or at any time by selecting the "edit standards" option of the initialization submenu.

The standard name may be any alpha-numeric string as much as 5 characters long. A string beginning with any character other than "*" or "(" will be reported as a weight-percent value in subsequent analyses. If the string begins with "*", concentrations of that element will be reported in parts per million. If the string

begins with "(", the standard will be used in the least-squares analysis, but a concentration will not be reported. This is potentially useful for dealing with K-series and L-series peaks of the same element when both are present. Normally, K-series peaks would be used to measure the abundance of the element but L-series peaks could be overlapping with peaks of other elements. Unfortunately, the relative intensity of K- and L-series peaks depends on the composition of the sample; therefore, the contribution of L-series peaks to another part of a spectrum cannot be calculated accurately by taking a ratio of the K-series intensities. However, the L-series peaks could be included in the least-squares fit by creating a standard such as "STD)", which would not be reported in the final results. The "(" option is also useful for subtracting local spectral features that originate from the radioactive source. For example, a small Sn peak is present in all spectra regardless of sample composition. The intensity of this feature is directly related to the intensity of Rayleigh-scattered peaks from the Cd^{109} radioactive source and, therefore, appears to be produced by excitation in either the source or the housing of the source. However, Sn may be analyzed (fig. 11) using the following procedure. First, using a Sn-free sample, a standard called (BKG) is created that has a region of interest including the anomalous Sn peak and the Rayleigh-scattered peak. Second, using a Sn-rich sample, a standard called "*SN" is created that has a region of interest including only the Sn peak. During least-squares analysis, the contribution of (BKG) to the spectrum will be controlled by the intensity of the Rayleigh-scattered peak, and contribution of *SN will be controlled by the residual Sn-peak intensity after (BKG) is accounted for.

The A-values in Equation 6 are defined initially as A0=0, A1=1, and A2=0 when a new standard is created. Although this is a reasonable first approximation, these values generally require refinement. A series of standards, for which the element in question is well documented, should be analyzed using the default A-values. A-values are then calculated graphically or by simple first- or second-order regression analysis of peak intensity versus composition. New A-values are entered into the standard file by selecting the "edit standards" option of the initialization submenu.

ANALYTICAL RESULTS

Figures 10-12 display XAP analytical results for 15 elements in a suite of samples of known compositon. The samples are a combination of international and U.S. Geological Survey standards, samples analyzed by commercial laboratories, and synthetic standards prepared by Elsass and du Bray (1982) by mixing carefully measured amounts of pure elements and oxides. All samples were powders ground to 200 mesh and lightly compressed in teflon cylinders. Spectra were obtained with a nonevacuated KEVEX 7000 EDS X-ray fluorescence analyzer using a Cd^{109} radioactive source and counting times of 200 or 300 seconds live time. Detector dead time ranged between 50 and 60 percent total time.

For semiquantitative analyses, the XAP results in figures 10-12 are in excellent agreement with the accepted abundances. Major departures from agreement are attributable to poor counting statistics at low elemental abundances or to failure to properly estimate absorption corrections. Counting statistics could be improved with longer counting times and analysis under vacuum. XAP could be modified to yield true quantitative results by minor additions to the code to calculate absorption corrections based on measured major-element abundances.

In general, elements analyzed using K-series peaks appear to be measurable down to the 50-ppm range. Some of these, notably Zn, Rb, Sr, Zr and Y, appear to be measurable down to the 10-20-ppm range. The Cu values show considerable scatter at less than 150 ppm abundance, which is attibuted to the small size (due to strong absorption by Fe) size of the Cu K-series peaks. Using the analytical conditions described above, Sn is not detectable below about 500 ppm because the Sn peak is excited by a high-energy gamma ray from the Cd^{109} source that is significantly less intense than its emitted X-rays. Despite the results shown in figure 11, Sn measurements cannot be considered reliable using the Cd^{109} source because the relative scatter and absorption of source X- and gamma-rays will vary with the composition of the sample. The strong linear correlation for Sn in figure 11 probably reflects the similar bulk compositions in the analyzed samples.

Results for elements measured with L-series peaks show more scatter due to the lower intensity of those peaks relative to K-series peaks. The U and Th value display significant scatter below about 200-250 ppm. The Pb values show significant scatter below about 150 ppm.

Bi was not tested between 10 and 500 ppm due to an absence of standards. W appears to be measurable down to the 50-100-ppm range. Again, analytical precision at low concentrations could be improved with longer counting times.
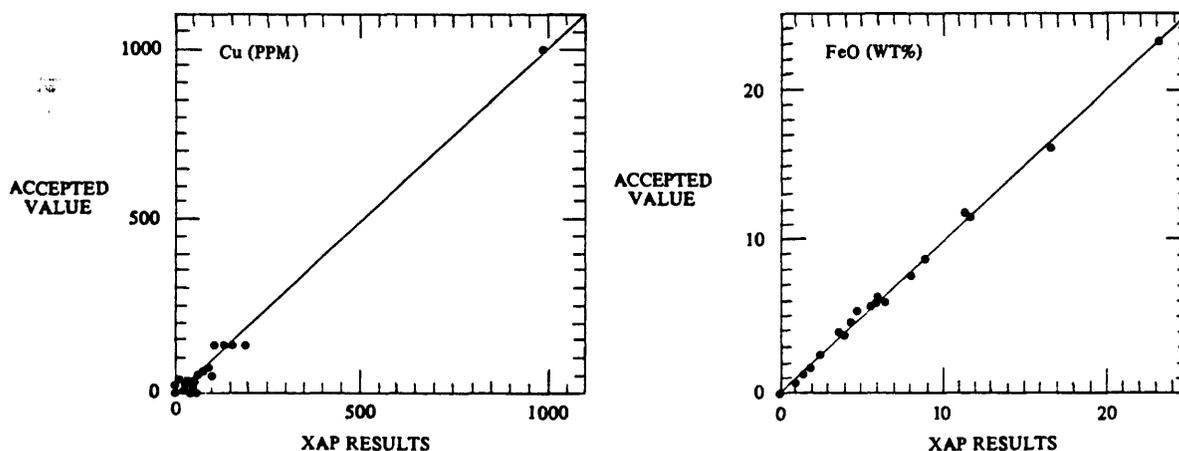
Figure 10.--XAP analytical results for Fe (in weight percent FeO) and Cu (in parts per million Cu). Both elements were measured using K-series peaks and counting times of 200 to 300 seconds.
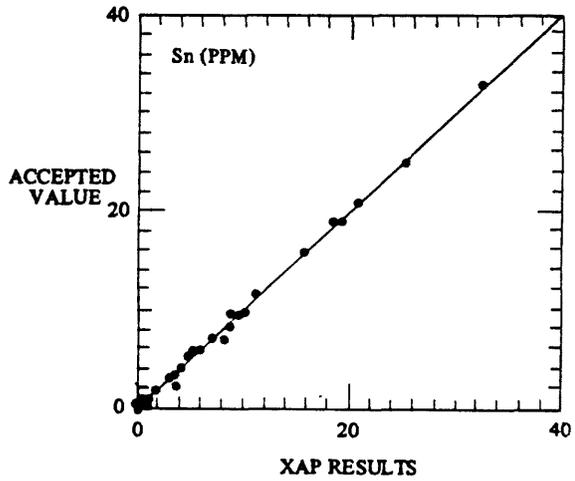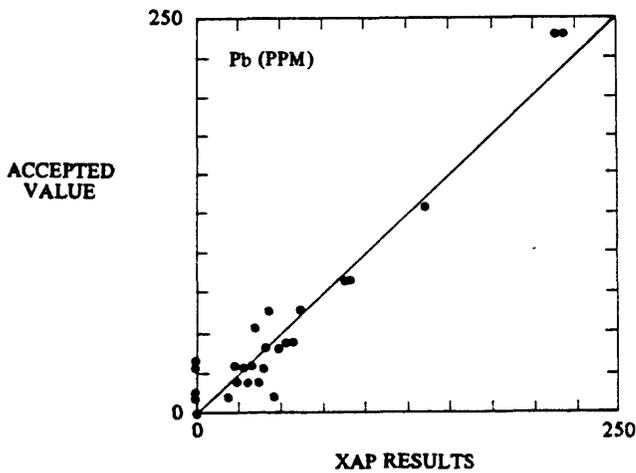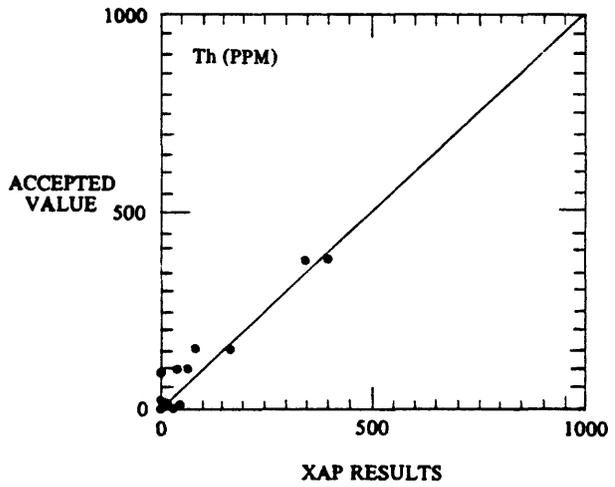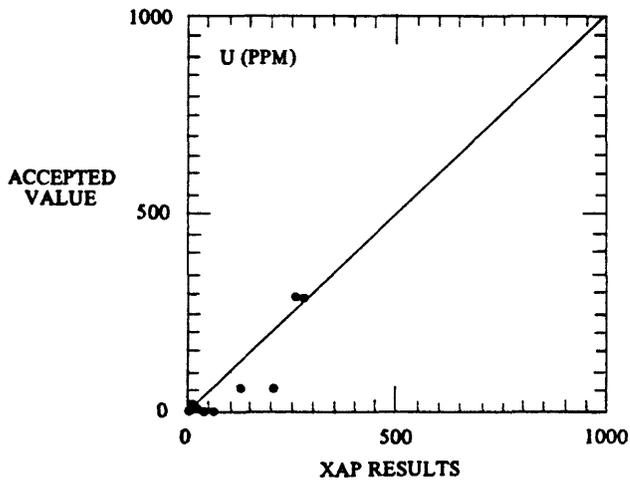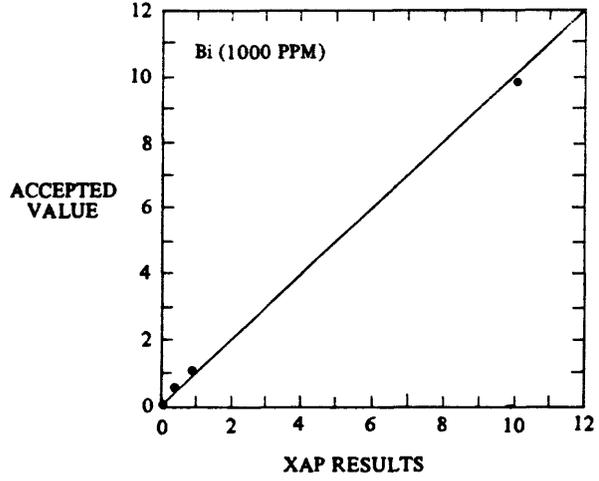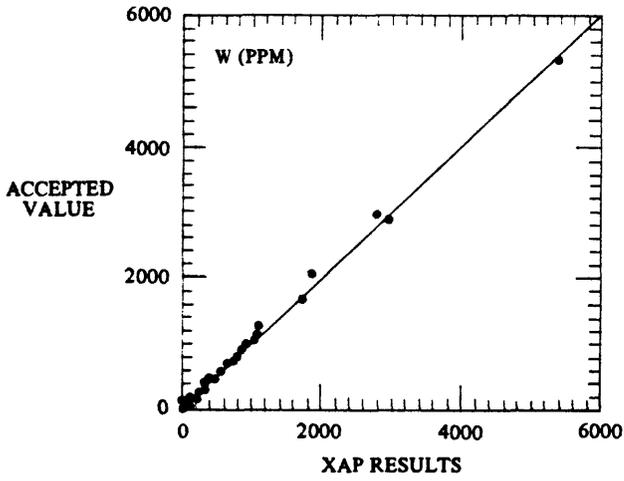
Figure 11.--XAP analytical results for W, Bi, U, Th, Pb, and Sn. Sn was measured using a K peak. All other elements were measured using L-series peaks. Counting times were 200 to 300 seconds. All values in parts per million. Accepted value corresponds to published values for standards or value determinations in proven laboratory.
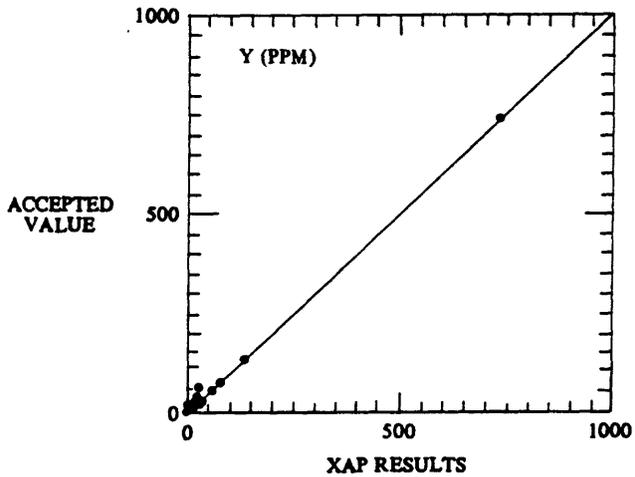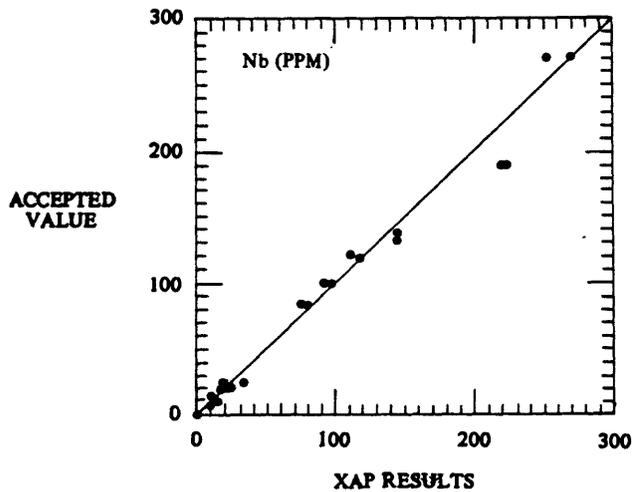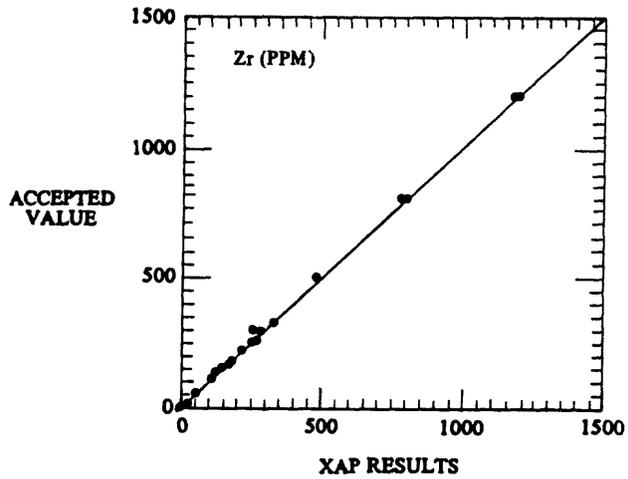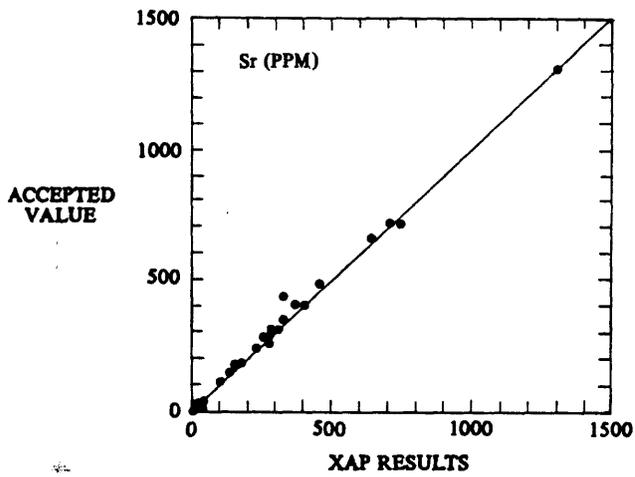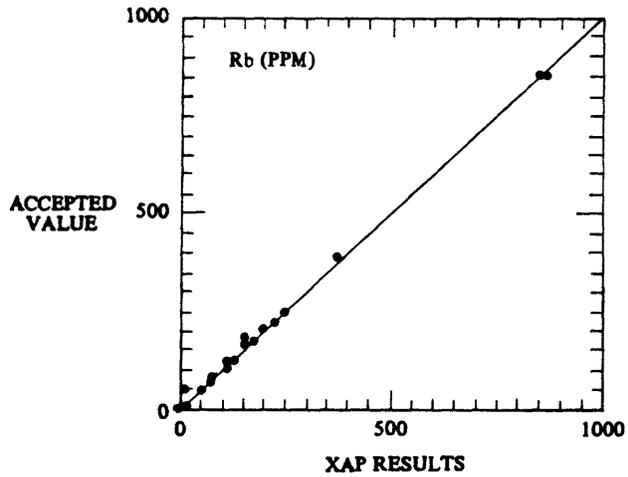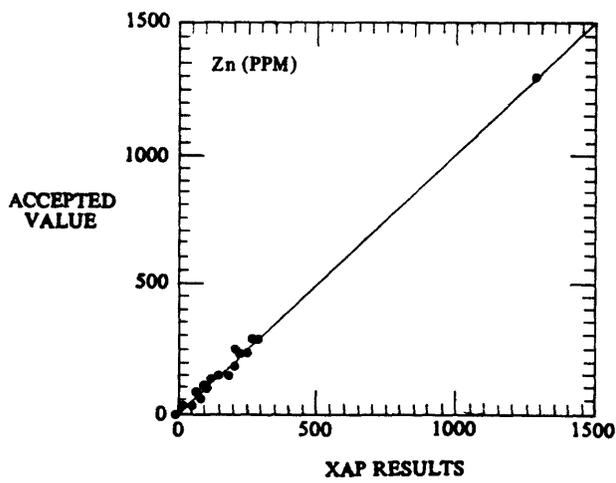
Figure 12.--XAP analytical results for Zn, Rb, Sr, Zr, Nb, and Y. All elements were measured using K-series peaks and counting times of 200 to 300 seconds. All values in parts per million. Accepted value corresponds to published values for standards or value determined in a proven laboratory.

19

CONCLUSIONS

XAP is capable of accurate deconvolution of complex X-ray spectra composed of overlapping X-ray peaks and background continuum. Successful analysis of standards and synthetic spectra reinforce the validity of least-squares analysis of filtered spectra. With minor modifications, XAP could be used to deconvolute a wide range of spectral types including those produced by (1) EDS attached to scanning electron microscopes and electron microprobes, (2) transmission optical spectrometers, and (3) ion microprobes. XAP could also be used to estimate mineral abundances from X-ray defractometer patterns of whole-rock powders.

DATA STORAGE

Data-file USGS-DF-06-3, consisting principally of a computer disk, was established in the archives of the United States Geological Survey Saudi Arabian Mission, Jeddah. No Mineral Occurrence Documentation System (MODS) localities were established in connection with work on this report.

This paper is based on work conducted by the authors under a work agreement with the Saudi Arabian Deputy Ministry for Mineral Resources.

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XAP Program Listing

```
10 SCREEN 0,0,0:WIDTH 80:COLOR 2,0:KEY OFF:CLS:CLOSE
20 DEFINT A-Z:DIM DAT$(100),CH!(1024),CHD!(1024),CHN!(1024),
     CURS(84),F!(20),R!(20,1
50),R$(20),RPTR%(20),RP%(20),M#(20,21),LROI%(20),UROI%(20),
     K#(20)
21 DIM CF!(20),U!(20),LIR%(20),UIR%(20),CTS!(20),SD!(20),
     DRFT!(20),MD#(20,21),A0!(20),A1!(20),A2!(20),KD#(20),
     FLG!(20),E1(15),PRO(60),NEU(60)
22 DEF SEG=64:POKE 23,&H40:IPTR=0:UMAX!=0:DC%=1:TL!=0:RES!=40:
     EA%=40:SFPTR%=0:ROICTR%=0:DRFT!(0)=1:FLPTR%=1
23 FPTR%=0:ROICTR%=0:ZERO!=0:GAIN!=0:FOR N%=1 TO 20:A0!(N%)=0:
     A1!(N%)=1:A2!(N%)=0:FLG!(N%)=1000^2:NEXT
24 FOR N%=0 TO 2:F!(N%)=-1/10:F!(N%+9)=-1/10:F!(N%+3)=1/10:
     F!(N%+6)=1/10:NEXT
25 FOR N%=0 TO 100:DAT$(N%)="":NEXT
26 XOFF$=CHR$(19):XON$=CHR$(17)
27 GOTO 60000
28 '
29 'Main menu
30 '
31 SCREEN 0,0,0:CLS:COLOR 2,0:LOCATE 1,33:PRINT "X A P   M E N U"
32 LOCATE 4,30:PRINT "  Initialization"
33 LOCATE 6,30:PRINT "  Transfer spectrum"
34 LOCATE 8,30:PRINT "  Recall spectrum"
35 LOCATE 10,30:PRINT "  Online data analysis"
36 LOCATE 12,30:PRINT "  Exit to DOS",
37 LOCATE 14,30:PRINT "  Logo",:LOCATE 1,1
38 LOCATE 25,24:PRINT USING "&";" J. E. Quick          July 27,
     1985",:LOCATE 1,1
40 LO%=14:LCTR%=4:GOSUB 65
42 IF LCTR%=4 GOTO 50 ELSE IF LCTR%=6 THEN CLS:GOTO 95 ELSE
     IF LCTR%=8 THEN CLS:GOTO 90 ELSE IF LCTR%=10 THEN CLS:GOTO 80
     ELSE IF LCTR%=12 THEN CLS:END ELSE IF LCTR%=14 GOTO 60000
     ELSE GOTO 40
45 '
46 '
48 ' Initialization submenu
49 '
50 SCREEN 0,0,0:CLS:COLOR 2,0:LOCATE 1,29:
     PRINT "I N I T I A L I Z A T I O N"
52 LOCATE 4,30:PRINT "  Calibration check"
53 LOCATE 6,30:PRINT "  Recover calibration"
54 LOCATE 8,30:PRINT "  Recall standards"
55 LOCATE 10,30:PRINT "  Edit standards"
56 LOCATE 12,30:PRINT "  Flag abundances"
57 LOCATE 14,30:PRINT "  Prepare forms"
58 LOCATE 16,30:PRINT "  Set up DATASAVE file"
59 LOCATE 18,30:PRINT "  Return to Main Menu"
60 LO%=18:LCTR%=4:GOSUB 65
```

```
61 IF LCTR%=4 THEN CLS:GOTO 85 ELSE IF LCTR%=6 THEN GOSUB 20500:
    GOTO 50 ELSE IF LCTR%=8 THEN GOSUB 29000:GOSUB 29590:GOTO 50
    ELSE IF LCTR%=10 GOTO 29600
62 IF LCTR%=12 GOTO 52000 ELSE IF LCTR%=14 THEN GOSUB 50000:GOTO 50
    ELSE IF LCTR%=16 GOTO 75 ELSE IF LCTR%=18 GOTO 30 ELSE GOTO 60
64 LCTR%=4
65 LOCATE LCTR%,30:COLOR 4:PRINT USING "&";CHR$(16)+CHR$(16),:
    COLOR 2:LOCATE 1,1
66 X$=INKEY$:IF X$="" GOTO 66 ELSE IF X$=CHR$(0)+CHR$(72)
    GOTO 67 ELSE IF X$=CHR$(0)+CHR$(80) GOTO 68 ELSE
    IF X$=CHR$(13) GOTO 69 ELSE GOTO 66
67 LOCATE LCTR%,30:PRINT USING "&";" ",:IF LCTR%>4 THEN
    LCTR%=LCTR%-2:GOTO 65 ELSE LCTR%=LO%:GOTO 65
68 LOCATE LCTR%,30:PRINT USING "&";" ",:IF LCTR%<LO% THEN
    LCTR%=LCTR%+2:GOTO 65 ELSE LCTR%=4:GOTO 65
69 RETURN
74 '
75 'Prepare DATASAVE file
76 GOSUB 18000:CLS:GOSUB 18100:GOTO 50
79 '
80 'Analyze data
81 GOSUB 30900:GOSUB 100:GOSUB 1000:GOSUB 27000
82 FOR N%=0 TO 1024:CHD!(N%)=CH!(N%):NEXT
83 BPTR%=82:GOTO 30800
84 '
85 'Calibration check
86 GOSUB 100:GOSUB 1000:GOTO 20000
88 '
89 'Recall spectrum
90 LOCATE 10,24:PRINT "Use last transferred file (Y/N)?",
91 X$=INKEY$:IF X$="" GOTO 91 ELSE IF X$="Y" GOTO 92
    ELSE IF X$="N" GOTO 93 ELSE GOTO 91
92 FOR N%=0 TO 1024:CH!(N%)=CHD!(N%):NEXT:GOTO 94
93 CLS:GOSUB 33100
94 GOSUB 1400:GOSUB 30000:BPTR%=92:GOTO 30100

95 'Transfer data
96 GOSUB 100:GOSUB 1000:GOSUB 27000:GOSUB 30000:GOTO 30100
98 '
99 '
100 'Serial communication subroutine
101 '
160 OPEN "COM1:4800,O,7,1,RS,CS,DS" AS #1
170 LOCATE 24,28:PRINT "READY FOR DATA TRANSFER"
200 LOCATE ,,1
400 PAUSE= FALSE:ON ERROR GOTO 40000
510 B$=INKEY$: IF B$<>"" THEN IF B$=CHR$(27) THEN CLOSE #1:
    GOTO 30
530 IF EOF(1) THEN 510
570 IF LOC(1)>128 THEN PAUSE=TRUE:PRINT #1, XOFF$;
580 'READ CONTENTS OF COM. BUFFER
590 IF EOF(1) GOTO 592 ELSE GOTO 596
592 IF IPTR=0 GOTO 510 ELSE GOTO 900
596 A$=INPUT$(LOC(1),#1):IPTR=1
```

```
620 LFP=0
630 LFP=INSTR(LFP+1,A$,CHR$(10))     'LOOK FOR LF
640 IF LFP>0 THEN MID$(A$,LFP,1)=" ":GOTO 630
660 DAT$(DC%)=DAT$(DC%)+A$:TL!=TL!+LEN(A$):IF LEN(DAT$(DC%))>100
    THEN DC%=DC%+1:GOTO 570 ELSE IF EOF(1) GOTO 900
665 IF LOC(1)>0 GOTO 570
690 IF PAUSE THEN PAUSE=FALSE: PRINT #1,XON$;
710 GOTO 510
899 '
900 'check for eof
910 IF TL!<7737 GOTO 570 ELSE GOTO 950
950 RETURN
999 '
1000 'data reduction
1015 PRINT:LOCATE 24,29:PRINT "DATA TRANSFER COMPLETE":PRINT:
     LOCATE 24,33:PRINT "ANALYZING DATA"
1017 SNAM$=MID$(DAT$(1),71,20)
1020 K%=1:L%=1:Q%=0
1050 LNG%=LEN(DAT$(K%))
1055 X$=MID$(DAT$(K%),L%,1):IF X$=CHR$(7) GOTO 1100
1060 L%=L%+1:IF L%>LNG% THEN L%=1:K%=K%+1:GOTO 1050 ELSE
     GOTO 1055
1099 '
1100 'Interpret strings
1105 PTR%=0
1110 GOSUB 9000
1120 GOSUB 9100:X%=ASC(X$)
1122 IF PTR%=0 GOTO 1124 ELSE GOTO 1130
1124 IF X%=75 THEN PTR%=1:GOTO 1190 ELSE GOTO 1160
1125 IF X%=13 THEN GOSUB 9000:GOTO 1290
1130 IF PTR%=1 GOTO 1132 ELSE GOTO 1140
1132 IF X%=69 THEN PTR%=2:GOTO 1190 ELSE GOTO 1160
1140 IF PTR%=2 GOTO 1142 ELSE GOTO 1150
1142 IF X%=86 THEN PTR%=3:GOTO 1190 ELSE GOTO 1160
1150 IF PTR%=3 GOTO 1152 ELSE GOTO 1160
1152 IF X$=CHR$(13) THEN GOSUB 9000:GOTO 1200
1160 PTR%=0
1190 GOSUB 9000:GOTO 1120
1199 '
1200 'Calculate channel contents
1210 GOSUB 9000:NCTR%=0:ACTR%=0:NUM$=""
1220 GOSUB 9100:X%=ASC(X$)
1225 IF X%=13 THEN GOSUB 9000:GOTO 1290
1230 IF X%<>32 GOTO 1240 ELSE NCTR%=NCTR%+1
1235 IF NCTR%=7 GOTO 1260 ELSE GOTO 1290
1240 IF X%>47 THEN IF X%<58 GOTO 1250
1245 GOTO 1290
1250 NCTR%=NCTR%+1
1252 NUM$=NUM$+X$:IF NCTR%=7 GOTO 1260 ELSE GOTO 1290
1260 ACTR%=ACTR%+1:Q%=Q%+1:NCTR%=0
1264 CH!(Q%)=VAL(NUM$):NUM$="":IF Q%<13 GOTO 1270
1265 IF CH!(Q%)>UMAX! THEN UMAX!=CH!(Q%)
1266 IF Q%=1025 GOTO 1300
1270 IF ACTR%<100 GOTO 1290
```

```
1280 GOTO 1100
1290 GOSUB 9000:GOTO 1220
1300 TIM!=CH!(1):RETURN
1399 '
1400 'find maximum channel
1410 UMAX!=0:FOR N%=13 TO 1024:IF CH!(N%)>UMAX! THEN UMAX!=CH!(N%)
1415 NEXT
1420 RETURN
2000 END
8999 '
9000 'Advance string counter, L%
9010 L%=L%+1:IF L%>LNG% THEN L%=1:K%=K%+1:LNG%=LEN(DAT$(K%))
9020 RETURN
9099 '
9100 'Read character from string
9110 X$=MID$(DAT$(K%),L%,1):RETURN
9999 END
10000 '
14999 '
15000 'Calculate matrix core
15001 '
15010 FOR N%=0 TO 21:FOR M%=0 TO 20:MD#(M%,N%)=0:NEXT:NEXT
15020 FOR I%=STRT% TO STP%:PTR%=0
15030 YUZ%=0
15040 FOR Q%=1 TO ROICTR%:J%=RPTR%(Q%)
15050 IF I%>LROI%(J%)/RES! THEN IF I%<UROI%(J%)/RES!
      THEN K%=I%-LROI%(J%)/RES!:CH!(J%)=R!(J%,K%):YUZ%=1:
      GOTO 15070
15060 CH!(J%)=0
15070 NEXT
15080 IF YUZ%=0 GOTO 15130
15100 FOR M%=1 TO ROICTR%:J%=RPTR%(M%):MD#(M%,0)=MD#(M%,0)+CH!(J%):
      MD#(0,M%)=MD#(0,M%)+CH!(J%)
15110 FOR N%=1 TO ROICTR%:K%=RPTR%(N%):
      MD#(M%,N%)=MD#(M%,N%)+CH!(J%)*CH!(K%):NEXT
15120 NEXT
15130 NEXT
15140 RETURN
15199 '
15200 'calculate total channels
15210 FOR N%=1 TO 1024:CH!(N%)=0:NEXT
15220 FOR N%=1 TO ROICTR%:X%=(LROI%(N%)/RES!)+1:
      Y%=(UROI%(N%)/RES!)-1
15230 FOR J%=X% TO Y%:CH!(J%)=1:NEXT:NEXT
15240 CHIN%=0:FOR N%=1 TO 1024:CHIN%=CHIN%+CH!(N%):CH!(N%)=0:NEXT
15299 RETURN
15999 '
16000 'hardcopy on Epson Printer
16040 WIDTH "LPT1:",255
16050 LPRINT CHR$(27) "@"
16055 LPRINT: LPRINT: LPRINT
16060 LPRINT CHR$(27) "3" CHR$(24)
16100 FOR I=0 TO 79
16102 LPRINT:LPRINT TAB(6);
```

```
16105 LPRINT CHR$(27)"*"CHR$(5)CHR$(144)CHR$(1);
16110 FOR J=0 TO 99
16140 DEF SEG=&HB800:M=PEEK(80*(99-J)+I):N=PEEK(8192+80*(99-J)+I)
16150 LPRINT CHR$(N);CHR$(N);CHR$(M);CHR$(M);
16190 NEXT
16210 NEXT
16220 LPRINT CHR$(27) "@"
16300 RETURN
16998 '
16999 '
17000 'Least-squares spectral analysis
17001 '
17020 ICTR%=0
17029 '
17030 'load matrix
17035 ICTR%=ICTR%+1:PRINT:PRINT:
      PRINT USING "Iteration number ##";ICTR%:PRINT
17040 M#(0,0)=0:X%=0:FOR N%=0 TO ROICTR%:M#(N%,STDS%+1)=0:NEXT
17042 FOR M%=1 TO ROICTR%:IF RP%(M%)=0 GOTO 17049 ELSE X%=X%+1
17044 Y%=0:FOR N%=1 TO ROICTR%:IF RP%(N%)=0 GOTO 17047
      ELSE Y%=Y%+1
17045 M#(X%,Y%)=MD#(M%,N%)
17047 NEXT
17049 NEXT
17050 FOR I%=STRT% TO STP%:PTR%=0
17060 YUZ%=0
17070 FOR Q%=1 TO STDS%:J%=RPTR%(Q%)
17080 IF I%>LROI%(J%)/RES! THEN IF I%<UROI%(J%)/RES!
      THEN K%=I%-LROI%(J%)/RES!:CH!(J%)=R!(J%,K%):YUZ%=1:
      GOTO 17100
17090 CH!(J%)=0
17100 NEXT
17110 IF YUZ%=0 GOTO 17160
17120 M#(0,0)=M#(0,0)+1:M#(0,STDS%+1)=M#(0,STDS%+1)+CHN!(I%)
17130 FOR M%=1 TO STDS%:J%=RPTR%(M%):
      M#(M%,STDS%+1)=M#(M%,STDS%+1)+CHN!(I%)*CH!(J%)
17150 NEXT
17160 NEXT
17170 GOSUB 17430
17179 '
17180 'Solve matrix by Gauss method
17189 '
17190 GOSUB 17430
17200 FOR I%=0 TO STDS%-1
17210 ROW%=I%:COL%=I%:GOSUB 17370:GOSUB 17430
17220 X#=M#(I%,I%):IF X#=0 THEN CLS:PRINT "Singular":END
17230 FOR N%=0 TO STDS%+1:M#(I%,N%)=M#(I%,N%)/X#:NEXT
17240 FOR J%=I%+1 TO STDS%:X#=M#(J%,I%)
17250 FOR N%=I% TO STDS%+1:M#(J%,N%)=M#(J%,N%)-X#*M#(I%,N%):NEXT
17260 NEXT
17270 NEXT
17280 IF M#(STDS%,STDS%)<>0 THEN
      M#(STDS%,STDS%+1)=M#(STDS%,STDS%+1)/M#(STDS%,STDS%)
      ELSE CLS:PRINT "singlular":INPUT "CONTINUE";X$:GOTO 17360
```

25

```
17290 FOR I%=1 TO STDS%:J%=STDS%-I%
17300 FOR K%=J%+1 TO STDS%:
      M#(J%,STDS%+1)=M#(J%,STDS%+1)-M#(J%,K%)*M#(K%,STDS%+1):NEXT
17310 NEXT
17320 GOSUB 17430
17330 X%=STDS%:PTR%=0:FOR M%=1 TO STDS%:IF M#(M%,STDS%+1)<=0
      GOTO 17332 ELSE GOTO 17340
17332 RP%(RPTR%(M%))=0:X%=X%-1:PTR%=1:K#(RPTR%(M%))=0:
      X$=R$(RPTR%(M%))
17333 IF LEFT$(X$,1)="*" THEN X$=MID$(X$,2,LEN(X$)-1) ELSE
      IF LEFT$(X$,1)="#" THEN X$=MID$(X$,2,LEN(X$)-1)
17334 PRINT USING "&";X$+" is below the limit of detection!":BEEP
17340 NEXT:STDS%=X%
17350 IF PTR%=1 THEN GOSUB 17600:GOTO 17030 ELSE
      PRINT "Solution complete!":GOSUB 17700:GOSUB 17900:
      GOSUB 17750:GOSUB 17500:IF FLPTR%=1 GOTO 17355 ELSE
      GOSUB 18500:GOSUB 18300
17355 CLOSE:IF BPTR%=82 GOTO 80
17356 LOCATE 24,28:BEEP:PRINT USING "&";"Hit any key to continue!",:
      LOCATE 1,1
17357 X$=INKEY$:IF X$="" GOTO 17357 ELSE GOTO 30
17360 END
17369 '
17370 'reorder matrix
17380 X#=(M#(ROW%,COL%)):FOR M%=ROW%+1 TO STDS%:
      IF ABS(M#(M%,COL%))>ABS(X#) THEN X#=M#(M%,COL%):HI%=M%
17390 NEXT
17400 IF X#=M#(ROW%,COL%) GOTO 17420
17410 FOR N%=0 TO STDS%+1:X#=M#(HI%,N%):M#(HI%,N%)=M#(ROW%,N%):
      M#(ROW%,N%)=X#:NEXT
17420 RETURN
17429 '
17430 'report matrix solution
17435 'FOR M%=0 TO STDS%:FOR N%=0 TO STDS%+1:
      PRINT USING "###.#### ";M#(M%,N%),:NEXT:PRINT:NEXT:PRINT
17440 RETURN
17499 '
17500 'Print solution
17501 RPTR=-1:FPTR%=FPTR%+1
17502 IF FPTR%=4 THEN FPTR%=1:LPRINT CHR$(12);:GOSUB 51000
17505 LPRINT:LPRINT CHR$(27);"!";CHR$(24);:LPRINT USING "&";
      "        Sample: "+SNAM$,:LPRINT CHR$(27);"!";
      CHR$(0);:LPRINT USING "  Counting time #### sec";TIM!:
      LPRINT
17506 PRINT:PRINT:LOCATE 24,23:PRINT USING "&";
      "    Sample: "+SNAM$:LOCATE 24,28:PRINT USING
      "Counting time #### sec";TIM!:PRINT
17508 LPRINT USING "&";"         Ele      Conc     % s.d.
           Ele      Conc     % s.d."
17510 FOR N%=1 TO ROICTR%:X$=R$(N%):IF LEFT$(X$,1)="(" GOTO 17550
17515 APTR%=0:IF LEFT$(X$,1)="*" THEN APTR%=1:
      X$=MID$(X$,2,LEN(X$)-1) ELSE IF LEFT$(X$,1)="#" THEN
      APTR%=2:X$=MID$(X$,2,LEN(X$)-1) ELSE X$=X$+" %"
17520 IF LEN(X$)<5 THEN X$=X$+" ":GOTO 17520
```

26

```
17525 RPTR=-RPTR:IF RPTR>0 THEN LPRINT:
      LPRINT USING "&";"          ",
17527 IF K#(N%)<FLG!(N%) THEN X%=0 ELSE X%=24
17528 LPRINT CHR$(27);"!";CHR$(X%);
17530 LPRINT USING "&";"    "+X$,
17535 LOCATE 24,23:PRINT USING "&";"    "+X$,
17540 IF RP%(N%)<>0 THEN LPRINT USING "######.#    ";K#(N%),:
      LPRINT USING "####.## ";2*SD!(N%), ELSE
      LPRINT USING "&";"    BDL        ",
17545 IF RP%(N%)<>0 THEN PRINT USING "######.#    ";K#(N%),:
      PRINT USING "####.##";2*SD!(N%) ELSE
      PRINT USING "&";"    BDL"
17550 NEXT
17560 LPRINT:LPRINT CHR$(27);"!";CHR$(0):
      LPRINT USING "            Chi squared  ###.###";CHI!
17565 PRINT:LOCATE 24,23:
      PRINT USING "   Chi squared  ###.###";CHI!:PRINT
17570 LPRINT:LPRINT
17580 RETURN
17599 '
17600 'Eliminate negative solutions from calculation
17610 CTR%=0:FOR N%=1 TO ROICTR%
17620 IF RP%(N%)=0 GOTO 17630
17625 CTR%=CTR%+1:RPTR%(CTR%)=N%
17630 NEXT
17640 RETURN
17699 '
17700 'calculate k-values
17710 FOR N%=1 TO ROICTR%:K#(N%)=0:NEXT
17720 FOR N%=1 TO STDS%:X#=M#(N%,STDS%+1):KD#(RPTR%(N%))=X#:
      K#(RPTR%(N%))=X#*CF!(RPTR%(N%))
17725 K#(RPTR%(N%))=K#(RPTR%(N%))*U!(RPTR%(N%))/U!(0)
17727 GOSUB 17800
17728 NEXT
17729 RETURN
17749 '
17750 'Calculate abundances
17760 FOR N%=1 TO STDS%:J%=RPTR%(N%):X#=K#(J%):
      K#(J%)=A0!(J%)+A1!(J%)*X#+A2!(J%)*X#*X#
17765 IF K#(J%)<0 THEN K#(J%)=0
17770 NEXT
17780 RETURN
17799 '
17800 'Estimate precision
17810 IF X#>0 GOTO 17815 ELSE GOTO 17850
17815 IF A0!(RPTR%(N%))<0 GOTO 17816 ELSE GOTO 17820
17816 IF A2!(RPTR%(N%))=0 THEN XD#=-A0!(RPTR%(N%))/A1!(RPTR%(N%)):
      GOTO 17819
17817 XD#=SQR(A1!(RPTR%(N%))^2-4*A2!(RPTR%(N%))*A0!(RPTR%(N%)))
17818 IF A2!(RPTR%(N%))>0 THEN
      XD#=(-A1!(RPTR%(N%))+XD#)/(2*A2!(RPTR%(N%))) ELSE
      XD#=(-A1!(RPTR%(N%))+XD#)/(2*A2!(RPTR%(N%)))
17819 X#=X#*(K#(RPTR%(N%))-XD#)/K#(RPTR%(N%)):IF X#<0 GOTO 17850
17820 SD!(RPTR%(N%))=100*SQR(SD!(RPTR%(N%)))/(CTS!(RPTR%(N%))*X#)
```

```basic
17830 GOTO 17899
17850 SD!(RPTR%(N%))=999.99
17860 RETURN
17899 '
17900 'Calculate Chi-squared
17905 CHI!=0:PRINT:BEEP:PRINT "Calculating Chi-squared!"
17910 FOR I%=STRT% TO STP%:PTR%=0
17920 YUZ%=0
17930 FOR Q%=1 TO STDS%:J%=RPTR%(Q%)
17940 IF I%>LROI%(J%)/RES! THEN IF I%<UROI%(J%)/RES! THEN
      K%=I%-LROI%(J%)/RES!:CH!(J%)=R!(J%,K%):YUZ%=1:GOTO 17960
17950 CH!(J%)=0
17960 NEXT
17970 IF YUZ%=0 GOTO 17996
17990 TOT#=0:FOR M%=1 TO STDS%:J%=RPTR%(M%):
      TOT#=TOT#+KD#(J%)*CH!(J%):NEXT
17995 TOT#=((CHN!(I%)-TOT#)^2)/ABS(CHN!(I%)):CHI!=CHI!+TOT#
17996 NEXT
17997 CHI!=CHI!/(CHIN%-ROICTR%)
17998 RETURN
17999 '
18000 'Open disk file for storage
18002 CLS:LOCATE 10,20:
      PRINT "Do you wish to store data on disk (Y/N)?",
18004 X$=INKEY$:IF X$="" GOTO 18004 ELSE IF X$="Y" THEN
      FLPTR%=0:GOTO 18010 ELSE FLPTR%=1:GOTO 18030
18010 CLS:LOCATE 10,18:INPUT;"Target file";DUMP$:LOCATE 10,48:
      INPUT;"Target Drive";X$
18020 DUMP$=X$+":"+DUMP$
18030 RETURN
18100 IF FLPTR%=1 GOTO 18210
18110 FLPTR%=0
18120 CLOSE #3:OPEN DUMP$ AS 3 LEN=167:
      FIELD #3,3 AS D0$,12 AS D1$,102 AS D2$,50 AS D3$
18130 NA%=1
18140 GET #3,NA%:ST$=D0$:IF ST$="zzz" GOTO 18160 ELSE
      IF ASC(ST$)=0 THEN ST$="zzz":GOTO 18160
18150 NA%=NA%+1:GOTO 18140
18160 LOCATE 11,25:
      PRINT USING "Number of entries in file = ###";(NA%-1)
18170 IF NA%>100 THEN FLPTR%=1:LOCATE 13,22:
      PRINT "File is full!  Hit any key to continue!":BEEP:
      GOTO 18180 ELSE GOTO 18190
18180 X$=INKEY$:IF X$="" GOTO 18180 ELSE CLS:GOTO 18210
18190 LOCATE 13,28:PRINT "Hit any key to continue!"
18200 X$=INKEY$:IF X$="" GOTO 18200 ELSE CLS
18210 CLOSE #3:RETURN
18298 '
18299 '
18300 'Store Data on disk
18305 OPEN DUMP$ AS 3 LEN=167:
      FIELD #3,3 AS D0$,12 AS D1$,102 AS D2$,50 AS D3$
```

```
18310 SC$="":NE%=0:SD$="":FOR N%=1 TO ROICTR%:
      IF LEFT$(R$(N%),1)="(" GOTO 18315 ELSE
      X!=K#(N%):SC$=SC$+MKS$(X!):X#=2*100*SD!(N%):
      IF X#>29999 THEN X#=29999
18312 SD%=X#:SD$=SD$+MKI$(SD%):NE%=NE%+1
18315 NEXT
18317 SC$=MKI$(NE%)+SC$
18320 FOR N%=1 TO ROICTR%:IF SD!(N%)>299 THEN SD!(N%)=299
18330 NEXT
18335 IF LEN(SNAM$)>12 THEN X$=LEFT$(SNAM$,12) ELSE X$=SNAM$
18337 ST$=MID$(STDF$,3,3)
18340 LSET D0$=ST$:LSET D1$=X$:LSET D2$=SC$:LSET D3$=SD$:
      PUT #3,NA%:LSET D0$="zzz":LSET D1$="zzz":LSET D2$=SC$:
      LSET D3$=SD$:PUT #3,(NA%+1)
18350 NA%=NA%+1:IF NA%<101 GOTO 18380 ELSE CLOSE #3:CLS:
      X%=LEN(DUMP$)+13:X%=(80-X%)/2:LOCATE 10,X%:
      PRINT "File "+DUMP$+" is full!"
18360 LOCATE 12,X%:BEEP:PRINT "Hit any key to continue!"
18370 X$=INKEY$:IF X$="" GOTO 18370 ELSE CLS:FLPTR%=1:GOTO 18390
18380 CLOSE #3:OPEN DUMP$ AS 3 LEN=167:
      FIELD #3,3 AS D0$,12 AS D1$,102 AS D2$,50 AS D3$
18390 RETURN
18499 '
18500 'Report current data file name
18505 IF FLPTR%=1 GOTO 18520
18510 X%=LEN(DUMP$):X%=(80-X%-23)/2:COLOR 0,2:LOCATE 25,X%:
      PRINT USING "&";" Storing data in file "+DUMP$+" ",:
      COLOR 2,0:LOCATE 1,1
18520 RETURN
19998 '
19999 '
20000 'Calibration check
20001 '
20002 VMAX!=1:UMAX!=1:FOR N%=130 TO 192:IF CH!(N%)>UMAX! THEN
      UMAX!=CH!(N%):VMAX!=CH!(N%):CHM%=N%:FEMAX!=VMAX!
20003 NEXT
20004 GOSUB 25000:GOSUB 25100:FECTR!=CENTER!-40
20006 VMAX!=1:FOR N%=324 TO 387:
      IF CH!(N%)>UMAX! THEN UMAX!=CH!(N%)
20007 IF CH!(N%)>VMAX! THEN CHM%=N%:VMAX!=CH!(N%):SRMAX!=VMAX!
20008 NEXT
20009 GOSUB 25000:GOSUB 25200:SRCTR!=CENTER!-40
20010 GOSUB 30500:GOSUB 30600
20020 FOR N%=130 TO 192:X%=10*(N%-130):GOSUB 30280:NEXT
20025 XD%=310:YD%=1:GOSUB 30320
20030 FOR N%=324 TO 387:X%=10*(N%-324)+5:GOSUB 30300:NEXT
20035 XD%=310:YD%=91:GOSUB 30320
20100 LOCATE 2,1:PRINT USING "Center #####.## ev";FECTR!,:
      LOCATE 4,1:PRINT USING "Offset #####.## ev";FECTR!-6400,:
      LOCATE 2,62:PRINT USING "Peak max  #######";FEMAX!,
20110 LOCATE 16,1:PRINT USING "Center #####.## ev";SRCTR!,:
      LOCATE 18,1:PRINT USING "Offset #####.## ev";SRCTR!-14142,:
      LOCATE 16,62:PRINT USING "Peak max #######";SRMAX!
20120 GAIN!=(10^5)*((SRCTR!-14142)-(FECTR!-6400))/(14142-6400)
```

```
20130 ZERO!=(14142*(FECTR!-6400)-6400*(SRCTR!-14142))/(14142-6400)
20140 LOCATE 25,1:PRINT USING "Gain ######";GAIN!,:
      LOCATE 25,15:PRINT USING "Zero #####";ZERO!,:LOCATE 1,70
20150 IF GAIN!=0 THEN IF ZERO!=0 GOTO 20190
20155 IF ABS(ZERO!)>ABS(GAIN!) GOTO 20180
20160 IF GAIN!=0 THEN LOCATE 25,32:
      PRINT USING "&";"No gain adjustment!",:GOTO 20200
20165 IF GAIN!>0 THEN LOCATE 25,32:
      PRINT USING "&";"Adjust gain CCW!",:GOTO 20200
20170 LOCATE 25,32:PRINT USING "&";"Adjust gain CW!",:GOTO 20200
20180 IF ZERO!=0 THEN LOCATE 25,32:
      PRINT USING "&";"No zero adjustment!",:GOTO 20200
20184 IF ZERO!>0 THEN LOCATE 25,32:
      PRINT USING "&";"Adjust zero CCW!",:GOTO 20200
20186 LOCATE 25,32:PRINT USING "&";"Adjust zero CW!",:GOTO 20200
20190 LOCATE 25,32:PRINT USING "&";"No Adjustments necessay!",
20200 LOCATE 25,67:PRINT USING "&";"ESC -- Exit",:LOCATE 1,70
20205 LOCATE 24,34:PRINT USING "#### Seconds";CH!(1),:LOCATE 1,70
20207 GOSUB 27000:GOSUB 20300:GOSUB 20400:LOCATE 24,1:
      PRINT USING "Drift ######";DRFT!(0),:LOCATE 1,1
20210 X$=INKEY$:IF X$="" GOTO 20210 ELSE IF X$=CHR$(27)
      GOTO 20220 ELSE IF X$="P" THEN GOSUB 16000:GOTO 20210
      ELSE GOTO 20210
20220 GOSUB 30900:GOTO 50
20250 GOSUB 27000:GOTO 20000
20299 '
20300 'Calculate drift
20310 DRFT!(0)=0
20320 FOR N%=505 TO 519:DRFT!(0)=DRFT!(0)+CH!(N%):NEXT
20330 DRFT!(0)=DRFT!(0)/CH!(1):CH!(2)=DRFT!(0)
20340 RETURN
20399 '
20400 'Store drift, gain, zero
20410 CLOSE #2:OPEN "specs" FOR OUTPUT AS #2
20420 X$=STR$(DRFT!(0)):Y$=STR$(GAIN!):Z$=STR$(ZERO!):
      WRITE #2,X$,Y$,Z$
20430 CLOSE #2
20499 RETURN
20500 'recover specs
20510 CLOSE #2:OPEN "specs" FOR INPUT AS #2
20520 INPUT #2,X$,Y$,Z$:DRFT!(0)=VAL(X$):GAIN!=VAL(Y$):
      ZERO!=VAL(Z$)
20530 CLOSE #2:BEEP
20599 RETURN
24999 '
25000 'calculate background for calibration
25002 M!=0:B!=0:GOTO 25040
25005 XY#=0:XX#=0:Z#=0:X#=0
25010 BOT%=CHM%-11:TOP%=CHM%-8:
      FOR K%=BOT% TO TOP%:GOSUB 25090:NEXT
25020 BOT%=CHM%+8:TOP%=CHM%+11:
      FOR K%=BOT% TO TOP%:GOSUB 25090:NEXT
25030 M!=(8*XY#-X#*Y#)/(8*XX#-X#*X#):
      B!=(XX#*Y#-XY#*X#)/(8*XX#-X#*X#)
```

30

```
25040 RETURN
25089 '
25090 'fit background
25095 XY#=XY#+K%*CH!(K%):XX#=XX#+K%*K%:Y#=Y#+CH!(K%):
     X#=X#+K%:RETURN
25099 '
25100 'Find center of peak with center near channel
25110 BOT%=CHM%-5:TOP%=CHM%+5:XY#=0:Y#=0
25120 FOR K%=BOT% TO TOP%
25130 CH!(0)=CH!(K%)-(M!*K%+B!):Y#=Y#+CH!(0):
     XY#=XY#+CH!(0)*K%:NEXT
25140 CENTER!=(XY#/Y#)*RES!
25150 RETURN
25199 '
25200 'Find center of peak with center between channels
25205 XY#=0:Y#=0
25208 IF CH!(CHM%+1)=CH!(CHM%-1) THEN
     BOT%=CHM%-5:TOP%=CHM%+5:GOTO 25220
25210 IF CH!(CHM%+1)>CH!(CHM%-1) THEN
     BOT%=CHM%-4:TOP%=CHM%+5 ELSE BOT%=CHM%-5:TOP%=CHM%+4
25220 FOR K%=BOT% TO TOP%
25230 CH!(0)=CH!(K%)-(M!*K%+B!):Y#=Y#+CH!(0):
     XY#=XY#+CH!(0)*K%:NEXT
25240 CENTER!=(XY#/Y#)*RES!
25250 RETURN
25998 '
25999 '
26000 'Digital linear filter
26030 FOR N%=BOT% TO TOP%
26040 CHN!(N%)=0:FOR K%=-10 TO 10:
     CHN!(N%)=CHN!(N%)+F!(K%+10)*CH!(N%+K%):NEXT
26050 NEXT
26070 RETURN
26099 '
26100 'normalize spectrum to live time
26110 FOR N%=BOT% TO TOP%:CHN!(N%)=CHN!(N%)/CH!(1):NEXT
26120 RETURN
26199 '
26200 'Measure Compton peak
26210 U!(CP%)=0:FOR N%=505 TO 519:U!(CP%)=U!(CP%)+CH!(N%):NEXT
26215 U!(CP%)=U!(CP%)/CH!(1)
26220 RETURN
26299 '
26300 'Meausre counts in iroi+bkg
26310 FOR N%=1 TO ROICTR%:
     I%=(LIR%(N%)/RES!)+1:J%=(UIR%(N%)/RES!)+1:SD!(N%)=0
26320 FOR K%=I% TO J%:SD!(N%)=SD!(N%)+CH!(K%):NEXT
26330 NEXT:RETURN
26998 '
26999 '
27000 'Correct spectrum for zero and gain
27002 '
27010 GN#=1+GAIN!/(10^5):ZN#=ZERO!/EA%
27020 FOR N%=14 TO 1023
```

```
27030 X#=GN#*N%+ZN#:F#=X#-CINT(X#)
27040 CHN!(N%)=CH!(N%)+F#*(CH!(N%+1)-CH!(N%-1)+F#*(CH!(N%-1)
      -2*CH!(N%)+CH!(N%+1)))/2
27050 NEXT
27060 FOR N%=14 TO 1023:CH!(N%)=CHN!(N%)*GN#:NEXT
27070 RETURN
27998 '
27999 '
28000 'Set up region of interest
28002 '
28005 ROIPTR%=1
28010 GOSUB 28900:LOCATE 23,11:PRINT USING "&";"Define ROI:
          L--lower limit   U--upper limit    D--Done",
28020 LROI%(0)=-1:UROI%(0)=-1:GOTO 30110
28100 'set lroi
28110 LROI%(0)=E!-RES!:LX%=XD%:BEEP:GOSUB 30320:GOTO 30110
28200 'Set uroi
28210 UROI%(0)=E!+RES!:UX%=XD%:BEEP:GOSUB 30320:GOTO 30110
28300 IF LROI%(0)<0 GOTO 28310 ELSE IF UROI%(0)<0 GOTO 28310
28301 PUT (LX%,YD%),CURS,OR:PUT (UX%,YD%),CURS,OR:XD%=(UX%+LX%)/2:
      IF XD%>0 THEN X%=XD%:GOSUB 30320
28302 X!=(UROI%(0)-LROI%(0)-2*RES!)/RES!:IF X!<1 GOTO 28304 ELSE
      IF X!>150 GOTO 28306
28303 IF ROIPTR%=1 GOTO 28320 ELSE IF ROIPTR%=2 GOTO 28740
28304 GOSUB 28900:LOCATE 23,12:BEEP:PRINT USING "&";
      "Region is improperly defined -- hit any key to continue!",
28305 X$=INKEY$:IF X$="" GOTO 28305 ELSE GOSUB 28950:GOTO 28010
28306 GOSUB 28900:LOCATE 23,8:BEEP:PRINT USING "&";
      "Region exceeds 150 channel maximum --
      Hit any key to continue!",:GOTO 28305
28310 GOSUB 28900:GOSUB 28950:ROIPTR%=0:GOTO 30109
28320 ROICTR%=ROICTR%+1:LROI%(ROICTR%)=LROI%(0):
      UROI%(ROICTR%)=UROI%(0)
28330 GOSUB 28900:LOCATE 23,1:PRINT USING "Reference ##";ROICTR%,:
      PRINT USING "  Low: ##### ev";LROI%(0),:
      PRINT USING "  High: ##### ev";UROI%(0),:
      PRINT USING "&";"  ESC--abort  Any key--continue",:
      LOCATE 1,78
28340 X$=INKEY$:IF X$="" GOTO 28340 ELSE IF X$=CHR$(27) GOTO 28310
28345 IF ROIPTR%=1 THEN GOSUB 28700
28350 GOSUB 28900:LOCATE 23,10:
      INPUT;"Name of reference";R$(ROICTR%):LOCATE 23,50:
      INPUT;"Concentration";CF!(ROICTR%):DRFT!(ROICTR%)=DRFT!(0)
28352 IF LEN(R$(ROICTR%))<2 THEN R$(ROICTR%)=R$(ROICTR%)+" ":
      GOTO 28352
28354 CP%=ROICTR%:GOSUB 26200
28355 BOT%=(LROI%(ROICTR%)/RES!):TOP%=(UROI%(ROICTR%)/RES!):
      GOSUB 26000:GOSUB 28600
28360 GOSUB 28900:LOCATE 23,27:PRINT "Save standards (Y/N)?",:
      LOCATE 1,70
28365 X$=INKEY$:IF X$="" GOTO 28365 ELSE IF X$="N" GOTO 28370 ELSE
      IF X$="Y" THEN GOSUB 28500:GOTO 28370 ELSE GOTO 28365
28370 GOTO 28310
28499 '
```

```
28500 'Save standards
28505 GOSUB 28800
28510 CLOSE #2:OPEN STDF$ FOR OUTPUT AS #2
28511 X$=STR$(ROICTR%):WRITE #2,X$
28512 FOR N%=1 TO ROICTR%
28515 X$=R$(N%):WRITE #2,X$:X$=STR$(CF!(N%)):WRITE #2,X$:
      X$=STR$(CTS!(N%)):WRITE #2,X$:X$=STR$(U!(N%)):
      WRITE #2,X$:X$=STR$(DRFT!(N%)):WRITE #2,X$
28517 J%=((UROI%(N%)-LROI%(N%))/RES!)-2:X$=STR$(J%):WRITE #2,X$
28518 X$=STR$(A0!(N%)):WRITE #2,X$:X$=STR$(A1!(N%)):WRITE #2,X$:
      X$=STR$(A2!(N%)):WRITE #2,X$
28530 X$=STR$(LROI%(N%)+RES!):WRITE #2,X$:X$=STR$(UROI%(N%)-RES!):
      WRITE #2,X$
28535 X$=STR$(LIR%(N%)):WRITE #2,X$:X$=STR$(UIR%(N%)):WRITE #2,X$
28540 BOT%=(LROI%(N%)/RES!)+1
28550 FOR K%=1 TO J%:X$=STR$(R!(N%,K%)):WRITE #2,X$:NEXT
28560 NEXT
28570 CLOSE #2
28580 RETURN
28599 '
28600 'region of interest
28610 J%=(UROI%(ROICTR%)-LROI%(ROICTR%))/RES!:J%=J%-2
28620 FOR K%=1 TO J%:R!(ROICTR%,K%)=(CHN!(BOT%+K%)/CH!(1)):NEXT
28630 RETURN
28699 '
28700 'internal roi
28710 GOSUB 28900:LOCATE 23,13:PRINT "Internal region of interest!
      Hit any key to proceed!";:LOCATE 1,1
28720 X$=INKEY$:IF X$="" GOTO 28720
28730 ROIPTR%=2:GOTO 28010
28740 LIR%(ROICTR%)=LROI%(0)+40:UIR%(ROICTR%)=UROI%(0)-40:
      I%=(LIR%(ROICTR%)/RES!)+1:J%=(UIR%(ROICTR%)/RES!)+1:
      X!=(CH!(I%)+CH!(J%))/2:CTS!(ROICTR%)=0
28750 FOR K%=I% TO J%:CTS!(ROICTR%)=CTS!(ROICTR%)+CH!(K%)-X!
```

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33