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MAGRAM--A Computer Code for Quantitative Electron-microprobe Analysis of Radioactive Materials

R. Natesh, E. M. Butler,
and D. R. O'Boyle

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R. Natesh,* E. M. Butler,
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Materials Science Division

October 1971

*Now with EBR-II Project

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ABSTRACT

A FORTRAN-IV computer code, called MAGRAM, has been developed to correct and plot X-ray data collected with a shielded electron-microprobe analyzer. The measured X-ray intensities of up to three elements are corrected for system dead-time effects, beam-current drift, X-ray background, atomic number, X-ray absorption, fluorescence effects, and gamma-induced secondary radiation. The program allows a maximum of 300 separate analyses to be corrected in a single run and has printer and CALCOMP plotting options for 1 to 99 points. The application of the program to measurements of the radial redistribution of uranium and plutonium in irradiated mixed-oxide fuel is illustrated.

I. INTRODUCTION

Electron-microprobe analysis is a widely used experimental technique for determining the chemical composition of a small volume of material (approximately 1 μ^3) by excitation of the microvolume with a finely focused electron beam. The beam, usually $<1\mu$ in diameter, generates characteristic X rays in the microvolume, which are diffracted by a crystal X-ray spectrometer and counted by standard X-ray techniques. Because of the excellent resolution of the method, microprobe analysis has been useful in diversified metallurgical studies including phase equilibria, diffusion, and corrosion phenomena. In the field of nuclear materials, the electron-microprobe analyzer has been used to study compatibility reactions between fuel and cladding materials, solid-state diffusion kinetics, and metallic and ceramic multicomponent phase systems. Thus it seemed desirable to adapt microprobe techniques to investigate the complex fuel-cladding-fission-product reactions that occur in highly irradiated fuel elements.

Early microprobe analysis of irradiated fuel specimens[1-3] was conducted at several laboratories using commercial microprobe analyzers without special gamma shielding. To reduce the fluorescent background due to hard gamma radiation and to facilitate handling, the mass of the specimen being analyzed was kept small so that the gamma activity was sufficiently low to allow the specimen to be handled outside a hot cell

This technique was appropriate for some initial studies of irradiated fuel; however, an examination of an entire cross section of an irradiated fuel element would be more efficient if both the specimen chamber and X-ray detection system were shielded. In response to the need for analyzing reactor fuel specimens, a commercial microprobe[4] was developed that has the equivalent of 4.3 in. of tungsten shielding around the specimen chamber so that a highly irradiated specimen (gamma activity, 50 R at 9 in.) could be examined safely.[5]

Although the shielding greatly reduces the gamma-induced scattered fluorescent and secondary radiation detected by the proportional counters, in practice it is necessary to measure and correct for this background contribution before applying corrections for X-ray absorption, fluorescence, and atomic-number effects. This report describes a computer program for correcting the X-ray data obtained with a shielded microprobe analyzer and for plotting the corrected weight concentrations of the elements. The X-ray intensity measurements recorded on the radioactive specimen are corrected for irradiation-induced fluorescent radiation, and the corrected concentrations of each element are plotted using a plotting subroutine adapted by Fernow.[6] Corrections for detector dead time, beam-current drift, X-ray absorption, characteristic line fluorescence, and atomic-number effects are calculated using the MAGIC-II computer code developed by Gray.[7] The correction program developed by Gray was selected in preference to other published programs[8-14] because it performs a detailed calculation of each correction factor, has a comprehensive list of mass-absorption coefficients, and has an advanced method of calculating the background correction. For use in the MAGRAM code, Gray's table of mass-absorption coefficients was extended by Savage[15] to include elements with atomic numbers up to 94. The Microprobe Analysis General Correction for RadioActive Materials (MAGRAM) code was developed to quantitatively analyze radioactive samples and, in particular, to analyze X-ray data obtained from irradiated reactor fuels and cladding materials.

II. CORRECTION PROCEDURES

The physical basis for quantitative microprobe analysis is a measurement of the ratio of the number of X-ray photons emitted from the specimen being analyzed (unknown) to the number of photons emitted from a standard of known composition under identical instrument conditions. During both measurements, the accelerating voltage, beam current, spectrometer settings, and counting-time interval are held constant. For quantitative analysis of highly radioactive samples, the measured X-ray intensities must be corrected for both experimental errors (dead time, drift, and natural and gamma-induced background) and X-ray interaction effects (atomic-number effect, mass absorption, and fluorescence effects). The ratio of the characteristic X-ray intensity of element A from the unknown

to that of the standard is defined as the "k ratio" of element A. To establish the k ratio, the measured emergent X-ray intensities are corrected for errors due to system dead time and instrumental drift and for background radiation effects. After these corrections have been made, the k ratio for each element is calculated and used as the first approximation of the mass concentration C of each element n in the unknown. Finally, to obtain the true mass concentration, the k ratio is corrected for atomic-number effects, X-ray absorption effects, and secondary fluorescence excited by other characteristic lines. The usual form of the X-ray interaction correction is

$$C_n = k_n k_z k_a k_f, \tag{1}$$

where

C_n = true mass concentration of each element in the unknown,

k_n = relative intensity of emergent radiation for each element (after correction for dead time, drift, and background),

and

k_z, k_a, k_f = computed correction factors for atomic number, absorption, and fluorescence effects.

Since k_z, k_a, and k_f are dependent on the mass concentration, an iterative procedure to calculate C_n is used in the MAGRAM code.

A detailed treatment of the atomic number, absorption, and secondary fluorescence correction procedures that are incorporated in the MAGRAM code is given by Gray.[7] In addition, several excellent reviews[16-18] of the current theory of quantitative electron-microprobe analysis are available. The instrumental and X-ray corrections incorporated in the MAGRAM code are briefly discussed in the following sections.

A. Detector Dead Time, Instrument Drift, and Background Radiation

Because of coincidence losses, the microprobe X-ray detection system does not count every incident photon. The first operation performed on all measured data consists of a correction for dead-time losses using Heinrich's method[19] as programmed by Gray.[7] During an analysis, the incident electron-beam intensity may vary by as much as ±2%; thus a correction for instrument drift is required. The MAC-450 microprobe[4] has provisions for monitoring the incident electron-beam current on an aperture located above the objective lens. The correction for instrument drift is made by monitoring the electron-beam current and normalizing all intensity readings to the same beam current. When this correction is applied, it is assumed that the X-ray intensity is directly proportional to the beam

current. Experiments performed at ANL have shown that this is a valid assumption, provided the variation observed is $\lesssim 3\%$ for a properly aligned system.

The background observed during the analyses of nonradioactive samples is primarily due to the continuous X-ray spectrum. In the analyses of radioactive materials, an additional correction must be made for the background due to the scattered secondary and fluorescent radiation. Natesh et al.[5] found that the radiation-induced background intensity varied with specimen location relative to the X-ray detectors and have described a procedure to correct the raw data for this background. The background due to the gamma activity of the specimen is measured by turning the electron beam off and recording the background intensity at the characteristic wavelength of the element being analyzed. While these data are being collected, the spectrometer and pulse-height-analyzer settings are the same as those used when measuring the X-ray intensity on the sample.

In the MAGRAM code, the raw X-ray data are first corrected for dead time in the detection system. Following this correction, the background due to scattered radiation from the radioactive specimen is subtracted. The program then corrects for instrument drift and background due to the X-ray continuum. The intensity measurements from the standards are not corrected for radioactive background since the standards are remote from the sample and the background contribution from the radioactive specimen is negligible.

The background due to X-ray continuum is the sum of the background contributions from all elements present in the unknown sample. Thus, if n elements are present, the weighted background contributions from all n elements must be added to calculate the total continuum X-ray background. For example, consider the case in which elements A, B, C, and D are present in an unknown. To determine the total background due to the continuum, the spectrometer is tuned to the characteristic wavelength of element A, and readings are taken on the B, C, and D standards. Next, the element A standard is placed under the electron beam, and the spectrometer is detuned by moving 5/2 full-width-at-half-maximum off the peak on both sides of the characteristic line peak for element A, and readings are taken and averaged. The background due to the continuum for element A in the unknown is equal to the weighted background intensity obtained by detuning the spectrometer on the standard for element A plus the weighted contributions of the A peak intensities obtained on the B, C, and D standards. The advantage of this method of calculating background is that the spectrometer is never detuned while making measurements on the unknown. By subtracting the sum of the backgrounds due to the X-ray continuum and gamma activity from the observed line intensity, a corrected line intensity is obtained.

B. Atomic-number Correction

The atomic-number correction is applied to correct for the variation in efficiency of producing characteristic radiation from the elements in both the sample and the standard. The correction factor k_z depends on the relative stopping power and the backscattering efficiency of the sample and the standard and is calculated from

$$k_z = \frac{R_A \overline{(Z/A \ln 1.166E/J)}}{\overline{R}Z_A/A_A \ln (1.166E/J_A)}, \tag{2}$$

where

R = backscatter loss factor,

Z = atomic number,

A = atomic weight,

E = mean excitation potential $= \frac{E_o + E_C}{2} A$,

E_o = electron-beam accelerating voltage,

E_C = X-ray line-excitation voltage,

and

J = ionization potential of the elements

$$= 14.0\ Z\ [1.0 - \exp(-0.1\overline{Z})] + \frac{75.5Z}{\overline{Z}/7.5} - \frac{\overline{Z}Z}{100 - \overline{Z}}.$$

The overscored terms indicate a weighted average over the composition of the sample.

C. Absorption Correction

The absorption correction factor k_a compensates for the difference in absorption of the characteristic X radiation in the unknown and standard. In the absorption correction, both the X-ray absorbing power of the specimen and the depth below the specimen surface at which the X rays are produced are considered. The latter factor involves the depth of penetration of the electron beam, which depends on the electron-absorption process. The X-ray absorption factor given by Philibert[20] is

$$k_a = \frac{1 + \left(\frac{hR(O)}{R(\infty) + hR(O)}\right)\frac{\chi}{\sigma}}{\left(1 + \frac{\chi}{\sigma}\right)\left(1 + \frac{h}{1 + h}\frac{\chi}{\sigma}\right)} \times \frac{\left(1 + \frac{\overline{\chi}_A}{\sigma}\right)\left(1 + \frac{\overline{h}}{1 + \overline{h}}\frac{\overline{\chi}_A}{\sigma}\right)}{1 + \left(\frac{\overline{h}R(O)}{R(\infty) + \overline{h}R(O)}\right)\frac{\overline{\chi}_A}{\sigma}}, \tag{3}$$

$$\chi = \left(\frac{\mu}{\rho}\right) \operatorname{cosec} \theta,$$

$$\left(\frac{\mu}{\rho}\right)_i^A = \text{mass-absorption coefficient of the ith element for A radiation,}$$

$$\overline{\chi}_A = \sum \left(\frac{\mu}{\rho}\right)_n^A C_n, \text{ where } C_n \text{ is the weight fraction of the nth element in the unknown,}$$

$$\theta = \text{X-ray take-off angle (45° for the MAC probe),}$$

$$\sigma = \text{electron mass-absorption coefficient}$$

$$= 2.54(10^5)/(E_o^{1.5} - E_c^{1.5}),$$

$$h = 4.5A/Z^2,$$

and

$$R(\ ) = \text{electron backscatter factor. } R(O) \text{ is taken as 1.1, and } R(\infty) \text{ is taken as 4.0.}$$

The overscored terms indicate a weighted average over the composition of the specimen, and the subscripts refer to values for a given element.

D. Fluorescence Correction

The fluorescence correction factor k_f used in the MAGRAM code for fluorescence of element A by B radiation is given by $k_f = 1/1 + k_{fA}$, where

$$k_{fA} = 0.5PC_B \frac{r_A - 1}{r_A} \omega_B \frac{A_A}{A_B} \left(\frac{\frac{E_o}{E_{CB}} - 1}{\frac{E_o}{E_{CA}} - 1} \right)^{1.67} \frac{(\mu/\rho)_A^B}{\overline{\chi}_B} \left(\ln \frac{1 + \alpha}{\alpha} + \ln \frac{1 + \beta}{\beta} \right), \tag{4}$$

$$\alpha = \frac{(\mu/\rho)_A^A}{\overline{\chi}_B} \operatorname{cosec} \theta,$$

$$\beta = \frac{\sigma}{\overline{\chi}_B},$$

P = a constant, the value of which depends upon the X-ray series (K, L, M) to which the fluorescing and fluoresced spectral lines belong, e.g., for fluorescence of an L line by a K line P = 2.4,

r_A = absorption jump ratio, the ratio of the mass-absorption coefficients on either side of the relevant absorption edge,

and

ω_B = fluorescent yield for element B, i.e., the probability of ionized B atoms emitting an X-ray photon of characteristic wavelength λ_B.

III. PROGRAMMING CONSIDERATIONS

A. Main Program

The output data from the MAC microprobe are automatically punched on paper tape and are then corrected by the main MAGRAM program for the effects discussed in Sec. II. The main program has 860 statements and no subroutines, and is stored on magnetic tape. To run this program, the largest option on the IBM-FORTRAN H compiler is used. Core storage required is 250K bytes. A complete listing of the MAGRAM code, including the various plotting subroutines, is given in Appendix A. Throughout the program, comment statements have been liberally inserted to define the calculations in process and to explain the program logic. Typical running time on the IBM-360/75 required to correct data for three elements measured at 100 locations is less than 20 sec. The matrix of mass-absorption coefficients and other constants given at the end of the main program greatly reduces the number of data input cards. At ANL, the main program and plotting subroutines are stored on magnetic tape. This procedure reduces the number of input cards to a minimum.

The MAGRAM program has been designed to correct input data for one to three elements. Corrections for an additional element are calculated by difference. Up to 300 data points (three elements each) may be corrected by the main program. By suitable changes in format, raw data for eight elements may be corrected. A list of symbols used in the main program and their common designations are given in Appendix B.

B. Plotting Subroutines

To obtain concentration plots as a function of specimen position, several plotting subroutines were added to the main program. One subroutine creates a printer plot, which follows the tabular output of the main program. A second subroutine causes CALCOMP graphs of the corrected concentrations to be prepared off line. Both plotting options exist as library programs at ANL and would have to be modified for use at another installation. The present plotting subroutines allow 99 data points (three elements each) to be corrected and plotted.

he GRAPHS subroutine, the user indicates whether plots are to be generated and, if so, the types desired. GRAPHS also calculates weight ratios needed for the weight-ratio plots and stores these data and the position data (called RAD for radial position). Either or both of the two plotting routines are called by GRAPHS through the use of a test variable. Additional description of the two plotting routines and the test variables is given in Appendix C.

IV. MAGRAM INPUT AND OUTPUT

The input for MAGRAM consists of two parts. One is the internally stored data matrix listed at the end of the program (see Appendix A). The other part consists of initialization cards that identify the problem and contain the data obtained with the microprobe. This section describes the latter part of the input and the entire output.

The first two cards identify the problem, identify the person submitting the problem, and describe the sample; this information appears on the printed output. The third card contains information regarding the instrument parameters used for the analysis. Included are items such as the accelerating potential, take-off angle, and detection-system dead time for each spectrometer. The fourth and fifth cards contain information regarding the elements analyzed and the types of standards used in the analysis. The remainder of the input data consists of cards listing the measurements obtained with the microprobe. If graphs are desired, an additional set of cards that lists the position of the analysis must be present. Before the plotting routines listed in Appendix A can be run at another computer installation, the computer center representative should be consulted. The following lists describe the input cards in detail.

Input Data Format

Column		Format
	First Card	
1-5	Problem number, or blank	A1, I4 (if blank, assigned by computer)
6-7	Blank	2X
8-22	Date of analysis	(3A4, A3)
23-24	Blank	2X
25-44	Name of person submitting problem	5A4
	Second Card	
1-71	Description of sample	71A1

Column		Format
	Third Card	
1-4	Accelerating voltage, keV	F4.1
5-6	Blank	2X
7-8	Number of compound standards (if blank, elemental standards assumed)	I2 (number is right justified)
9-10	Blank	2X
11-15	Counting interval, sec	F5.1 (if blank, 1.0 sec is assumed)
16-17	Blank	2X
18-22	Density of sample, g/cc	F5.2 (may be left blank)
23-24	Blank	2X
25-29	Film thickness, μ	F5.2 (may be left blank)
30-31	Blank	2X
32-35	X-ray emergence angle, deg	F4.1 (if blank, 52.5° is assumed)
36-37	Blank	2X
38-40	Dead time for element 1, μsec	F3.1 (if blank, 1.0 μsec is assumed)
41-43	Dead time for element 2, μsec	F3.1 (if blank, 1.0 μsec is assumed)
44-46	Dead time for element 3, μsec	F3.1 (if blank, 1.0 μsec is assumed)
	Fourth Card	
1-2	First element analyzed, chemical symbol	A2
3	Blank	1X
4-5	First element analytical line, KA, LA, MA	A2
6-7	Blank	2X
8-9	Second element analyzed, chemical symbol	A2
10	Blank	1X

		Format
	Fourth Card (Contd.)	
11-12	Second element analytical line	A2
13-14	Blank	2X
15	Repetition of above data for all elements	

If one more element is present in the sample than is analyzed (e.g., oxygen), and the concentration of that element is to be determined by difference, its chemical symbol is listed last without indicating an analytical line. Chemical symbols are right justified in their field. Analytical lines are indicated as KA, LA, MA, or MB for K alpha, L alpha, M alpha, or M beta. A typical sequence is given as: NB-LA--Zr-LA---N-KA---O, where the dashes indicate blanks.

Column		Format
	Fifth Card	
1-2	Number of the element in the list on the fourth card to which compound standard applies	I2 (right justified)
3-7	Standard name	A5 (left justified)
8-13	Weight fraction of element in binary-compound standard	F6.4
14-15	Chemical symbol of other element in compound standard	A2 (right justified)

A separate card is required for each element for which a binary-compound standard is used. The total number of cards required is equal to the "number of compound standards" listed on the second card.

Data from Standards

Column		Format
	First Card	
1-2	Number of observations on the standard	I2
	Other Cards	
1-2	Blank	2X
3-7	Beam current	F5.0
8-13	Blank	6X
14-18	Standard counts	F5.0

The above cycle is repeated for each element listed on the fourth card, in the order of listing. The total number of sets of standard data must equal the total number of elements analyzed.

Background Data from the First Standard

Column		Format
	First Card	
1-2	Number of background observations taken on first standard	I2 (right justified)
	Other Cards	
1-2	Blank	2X
3-7	Beam current	F5.0
8-13	Blank	6X
14-18	Background taken on first standard; spectrometer detuned	F5.0
19-24	Blank	6X
25-29	Background taken on first standard; spectrometer tuned to second analytical line	F5.0
30-35	Blank	6X
36-40	Background taken on first standard; spectrometer tuned to third analytical line	F5.0

The number of background data cards must equal the number of observations of background on the first standard.

Background Data from the Second Standard

Column		Format
	First Card	
1-2	Number of background observations taken on second standard	I2 (right justified)
	Other Cards	
1-2	Blank	2X
3-7	Beam current	F5.0
8-13	Blank	6X
14-18	Background taken on second standard; spectrometer tuned	F5.0

Other Cards (Contd.)

		Format
19-24	Blank	6X
25-29	Background taken on second standard; spectrometer detuned	F5.0
30-35	Blank	6X
36-40	Background taken on second standard; spectrometer tuned	F5.0

The number of background data cards must equal the number of observations of background on the second standard. The above sequence is repeated for data taken on each standard to determine contributions to other analytical lines. The total number of sets of background data must be equal to the total number of elements analyzed.

Radioactive-decay Data Format
(Electron beam turned off)

Column		Format
1-13	Blank	13X
14-18	Decays in counting time interval from first element analyzed	F5.0
19-24	Blank	6X
25-29	Decays in counting time interval from second element analyzed	F5.0
30-35	Blank	6X
36-40	Decays in counting time interval from third element analyzed	F5.0

Sample Data Format

1-2	Blank	2X
3-7	Beam current	F5.0
8-13	Blank	6X
14-18	Counts for first element	F5.0
19-24	Blank	6X
25-29	Counts for second element	F5.0
30-35	Blank	6X
36-40	Counts for third element	F5.0

This card is repeated for each observation. A maximum of 100 observations are permited.

Trailer Card

After the last analysis in a problem, a trailer card containing routing information is required.

Column		Format
3-7	99998 is inserted if data for a new problem follow	F5.0
	99999 is inserted if no new problem follows	

Graph-options Card

The first five columns of the card are used to designate the data to be plotted.

Column	Plot Requested
1	U versus radius, wt % (U, Pu, and (U + Pu) versus radius, wt %)*
2	Pu versus radius, wt %
3	(U + Pu) versus radius, wt %
4	Weight ratio Pu/U versus radius
5	Weight ratio Pu/(U + Pu) versus radius

The type of graph desired (printer plot or CALCOMP) is indicated by inserting code numbers 1-5 in columns 1-5.

Code Number	Graph Option
1	No graph
2	Printer plot only
3	CALCOMP graph only
4	Printer plot and CALCOMP graph
5	(Used only in column 1) A CALCOMP graph of U, Pu, and (U + Pu), wt % versus radius, and a CALCOMP and printer plot of U wt % versus radius

*A CALCOMP graph of the three functions on a single plot is produced only when 5 is used in column 1.

For example, a card with 52311 in the first five columns would request three separate CALCOMP graphs (the three weight percents versus radius, uranium versus radius, and (U + Pu) versus radius) and printer plots of uranium versus radius and plutonium versus radius.

The printer plot produces a maximum of two separate graphs. If the plots corresponding to columns 1, 2, and 3 are called, they will all appear on a single printer plot. If the plots corresponding to columns 4 and 5 are called, they will both be printed on a second graph.

The CALCOMP routine generates a maximum of six graphs. Each plot corresponding to columns 1-5 is prepared on a separate graph. A sixth CALCOMP graph containing three plots is obtained by using the number 5 in column 1 of the graph options card.

Radial-distance Card

One radial distance card (radii measured in mils) must be supplied for each observation if graphs are desired.

Column		Format
1-10	Radius	F10.0

Either right-justify the numbers to column 10, or code with a decimal point.

End Trailer Card

After the radial distance card for the last observation, a trailer card with 0.000 in the first five columns must be inserted in the deck.

A sample listing of the input and output cards for the MAGRAM code is given in Appendix D. Explanatory notes have been added to clarify possible points of confusion. The output contains a listing of the constants used in the correction process. These include the atomic numbers of the elements analyzed, absorption-edge wavelengths, mass-absorption coefficients, and backscatter factors. The standard intensities given are averages based on the input data and have been normalized to a constant incident-beam current, which is also listed. At ANL, the aperture current is monitored continuously and is assumed to be proportional to the beam current. The output listing also contains the continuum-background radiation matrix. In the example shown, the effect of interference from $UM\gamma$ on PuM_β is apparent. This interference, which is a function of the uranium concentration at the point being analyzed, is automatically corrected by the program. The X-ray intensity measurements, corrected for detector dead time and normalized to a constant beam current, appear in tabular form in the output. The K ratios for each element at each point are also listed. If compound standards are used, a note to that effect is

printed. The instrument data, the peak-to-background ratios for each element, and the computed minimum detectability limits are listed. The corrected concentrations, in terms of weight and atomic percents, are listed in the final output table. The depth of the region analyzed (in microns) is also included in the output. As the program is being run, a magnetic tape is generated containing all the data necessary to prepare CALCOMP plots, which are then prepared off line.

The printer plots, which are generated along with the computer output, give a good first approximation of concentration as a function of distance. Points are placed on the graph by means of a truncation method with a "resolution" of about 2 wt % on the ordinate and 1.25 mils on the abscissa. Weight percents of uranium, plutonium, and the sum of uranium and plutonium are plotted as a function of radial position. An additional printer graph contains plots of the weight ratios of plutonium-to-uranium, and plutonium-to-uranium-plus-plutonium. The CALCOMP graphs more accurately plot the same data, since the data points are positioned more accurately and the CALCOMP subroutine selects the scale range based upon the range of values plotted. Thus, if five separate CALCOMP graphs are prepared, each may have a different scale depending on the range of values plotted. Sample CALCOMP graphs of the uranium and plutonium distribution in a mixed-oxide fuel element are shown in Figs. 1 and 2.

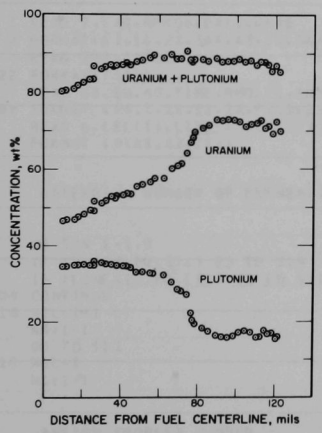

Fig. 1

Corrected Uranium, Plutonium, and Uranium-plus-Plutonium Concentrations as a Function of Radial Distance from the Fuel Centerline. Fuel is UO_2-20 wt % PuO_2 irradiated in EBR-II to 2.8 at. % burnup at a linear power rating of 17 kW/ft. Neg. No. MSD-53993.

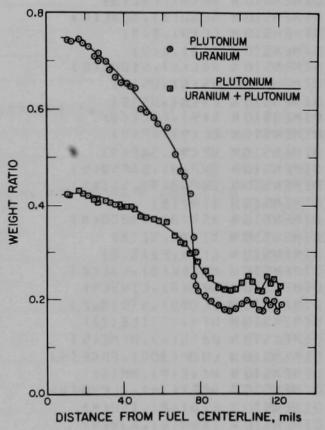

Fig. 2

Corrected Weight Ratios of Plutonium-to-Uranium and Plutonium-to-Uranium-plus-Plutonium as a Function of Radial Distance from the Fuel Centerline. Same mixed-oxide fuel element described in Fig. 1. Neg. No. MSD-53992.

APPENDIX A

Listing of the MAGRAM Code

```
C                    ANL  MAGRAM  PROGRAM
C
C
C   MAGRAM: MICROPROBE ANALYSIS GENERAL INTENSITY CORRECTION FOR RADIO-
C   ACTIVE MATERIALS
C
C
C      PROGRAM CORRECTS RAW MICROPROBE X-RAY INTENSITY DATA FOR DEAD-
C      TIME LOSSES (FIXED-TIME OR FIXED-COUNT), BACKGROUND AS A
C      FUNCTION OF COMPOSITION, ABSORPTION (DUNCUMB-SHIELDS-PHILIBERT),
C      CHARACTERISTIC LINE FLUORESCENCE (REED), ATOMIC NUMBER EFFECTS
C      (DUNCUMB-DUNCUMB & DA CASA), AND INSTRUMENT DRIFT BASED ON BEAM
C      CURRENT. ALL PARAMETERS ARE STORED OR CALCULATED INTERNALLY.
C      AS MANY AS 3 ELEMENTS (AND ONE BY DIFFERENCE) MAY BE ANALYZED.
C
C      MAGRAM IS A MODIFICATION OF THE UNIVERSITY OF ILLINOIS MAGIC II PROGRAM
C      IT ALSO CORRECTS FOR RADIATION BACKGROUND OF HOT SAMPLES AND ADDS PRINTER
C      PLOT AND CALCOMP GRAPHING OPTIONS.
C
C
      COMMON WPC(9,300),MARY(5),AAA(102),PTITL(400),BBB(500),CNAM(40)
      REAL LIMIT(8)
      DIMENSION AVR(8),RDEV(8)
      DIMENSION AVWP(9),AVAP(9)
      DIMENSION WPDEV(9),APDEV(9)
      DIMENSION C1(8),ATOM(9)
      DIMENSION CO(8),C3(8)
      DIMENSION SR(8),FAL(8)
      DIMENSION SRSQ(8),ACAL(8)
      DIMENSION EC(9),E(8)
      DIMENSION Z(9),A(9)
      DIMENSION VAL(8),SIGMA(8)
      DIMENSION HS(8),US(8)
      DIMENSION FS(8),WS(9)
      DIMENSION R(9),FACT(8)
      DIMENSION EL(9),AP(9)
      DIMENSION WP(9),SAP(9)
      DIMENSION SWP(9),SAPSQ(9)
      DIMENSION SWPSQ(9),SSI(8)
      DIMENSION RINT(8)
      DIMENSION ASI(8) ,ABGD(8)
      DIMENSION XI(8),SI(8)
      DIMENSION C(9),PEAK(8)
      DIMENSION MPEAK(8),UAL(8)
      DIMENSION NAB(8),LINE(9)
      DIMENSION ELO(8),STD(8,2)
      DIMENSION U(9),TITLE(71)
      DIMENSION DATE(4),NAME(5)
      DIMENSION LOOP(300),EDGE(9)
      DIMENSION WAVE(9),MM(4)
      DIMENSION ABET(26),ALPHA(8)
      DIMENSION FIDI(8),TAU(8)
      DIMENSION TAUM(8),AJR(9)
      DIMENSION FYR(9),PF(8)
      DIMENSION BCSUM(8), STDSUM(8)
      DIMENSION BCAVG(8), BKGD(8)
      DIMENSION XXI(8), BEAM(300)
      DIMENSION BC(8,99), STDI(8,99)
      DIMENSION BKSUM(8,8), ABK(8,8)
      DIMENSION BK(8,99,8)
      DIMENSION AC(8,9),B(8,9)
```

```
      DIMENSION ROUT(8,300),P(100,36)
      DIMENSION NXI(8,300),NSI(8,300)
      DIMENSION APC(9,300),DECAY(300)
C
C
C       INITIALIZATION AND INPUT OF BASIC PARAMETERS
C
C
      READ(1,81) ((P(I,J),J=1,11),I=1,100)
   81 FORMAT (F7.3,A3,3F6.3,6F7.3)
      READ(1,82) ((P(I,J),J=12,22),I=1,100)
   82 FORMAT (7F7.3,4F5.3)
      READ(1,7) ((P(I,J),J=23,29),I=1,100)
    7 FORMAT (F5.3,4F7.3,F10.3,5X,E14.8)
      READ(1,8) ((P(I,J),J=30,34),I=1,100)
    8 FORMAT (5E14.8)
      READ(1,5) (MM(I),I=1,4)
    5 FORMAT (4A2)
      READ(1,530) ST2,LT2
  530 FORMAT (A3,A2)
      READ(1,500) (ABET(I),I=1,26)
  500 FORMAT (26A1)
      READ(1,501) PRFX,NMBR
  501 FORMAT (A1,I4)
      READ(1,280) (PTITL(K),K=1,400)
  280 FORMAT(80A1)
      READ(1,281) (CNAM(I),I=1,40)
  281 FORMAT(20A4)
C
C
C       INPUT PROBLEM DATA
C
C
    1 READ 2,TAG,NPROB,DATE,NAME
    2 FORMAT(A1,I4,2X,3A4,A3,2X,5A4)
      READ 222,TITLE
  222 FORMAT(71A1)
      READ 88,EQ,NB,TIME,RHO,T1,THETA,TAUM
   88 FORMAT (F4.1,2X,I2,2X,F5.1,2X,2(F5.2,2X),F4.1,2X,8F3.1)
      READ 6,(EL(I),LINE(I),I=1,9)
    6 FORMAT (9(A3,A2,2X))
C
C
C       DETERMINE NUMBER OF ELEMENTS IN SYSTEM, AND NUMBER ANALYZED
C
C
      DO 509 I=1,9
      IF (EL(I).EQ.ST2) GO TO 518
      IF (LINE(I).EQ.LT2) GO TO 510
  509 CONTINUE
  518 NEL=I-1
      NA=I-1
      GO TO 511
  510 NEL=I
      NA=I-1
C
C
C       ASSIGN PROBLEM NUMBER.
C
C
  511 IF (NPROB.NE.0) GO TO 502
      NMBR=NMBR+1
      IF (NMBR.LE.9999) GO TO 504
      DO 506 L=1,25
      IF (ABET(L).EQ.PRFX) GO TO 507
  506 CONTINUE
  507 PRFX=ABET(L+1)
```

```
      TAG=PRFK
  502 PRINT 615,TAG, NPROB, DATE
C
C
C      CHECK FOR X-RAY EMERGENCE ANGLE. IF NONE FURNISHED, ASSUME 52.5
C      DEGREES
C
C
      IF (THETA.EQ.0.) THETA = 52.5
      CSC=1./SIN(THETA*3.14159/180.)
C
C
C      DETERMINE OR CALCULATE, FOR EACH ELEMENT ANALYZED, ALL PARAMETERS
C      NECESSARY FOR CORRECTIONS
C
C
      PRINT 2000
 2000 FORMAT (//4X,7HELEMENT,3X,7HAT. NO.,5X,7HAT. WT.,4X,2HPF,7X,4HEDGE
     1,6X,2HEC,7X,4HWAVE,5X,1HU,8X,1HR/)
      DO 95 K=1,NA
      DO 102 I=1,100
      IF (P(I,2).EQ.EL(K)) GO TO 103
  102 CONTINUE
C
C
C      DETERMINE ATOMIC NUMBER AND ATOMIC WEIGHT, AND CALCULATE
C      FACTOR FOR ATOMIC NUMBER CORRECTION
C
C
  103 Z(K)=I
      A(K)=P(I,1)
      PF(K)=Z(K)*(14.*(1.-EXP(-.1*Z(K)))+75.5/(Z(K)**(Z(K)/7.5))-Z(K)/(
     1100.+Z(K)))
      NL=3
C
C
C      DETERMINE ANALYTICAL LINE ABSORPTION EDGE, CRITICAL EXCITATION
C      POTENTIAL AND WAVELENGTH, AND CALCULATE OVERVOLTAGE
C
C
      DO 4 M=1,2
      IF (LINE(K).EQ.MM(M)) GO TO 3
    4 NL=NL+1
      EDGE(K)=P(I,17)
      GO TO 96
    3 EDGE(K)=P(I,3*NL)
   96 EC(K)=P(I,NL)
      IF(LINE(K).EQ.MM(4)) GO TO 777
      WAVE(K)=P(I,NL+3)
      GO TO 778
  777 WAVE(K)=P(I,NL-2)
  778 U(K)=EO/EC(K)
      IF (U(K).GT.20.) U(K)=20.
      R(K)=0.
      KK=34
C
C
C      DETERMINE OVERVOLTAGE DEPENDENT BACKSCATTER LOSS FACTOR
C
C
      DO 107 J=1,6
      R(K)=U(K)*R(K)+P(I,KK)
  107 KK=KK-1
      PRINT 2001,EL(K),I    ,A(K),PF(K),EDGE(K),EC(K),WAVE(K),U(K),R(K)
 2001 FORMAT (6X,A3,7X,I2,6X,F8.3,2X,F8.3,2X,F7.3,3X,F6.3,3X,F7.3,3X,F5
     1.2,3X,F8.6)
```

```
   95 CONTINUE
      IF (NEL.EQ.NA) GO TO 98
C
C
C       IF AN ELEMENT IS TO BE DETERMINED BY DIFFERENCE, DETERMINE EXTRA
C       ELEMENT ATOMIC NUMBER, ATOMIC WEIGHT, CHARACTERISTIC LINE
C       ABSORPTION EDGE, CRITICAL EXCITATION POTENTIAL AND WAVELENGTH,
C       AND CALCULATE OVERVOLTAGE AND BACKSCATTER LOSS FACTOR
C
C
      DO 104 I=1,100
      IF (P(I,2).EQ.EL(NEL)) GO TO 105
  104 CONTINUE
  105 Z(NEL)=I
      A(NEL)=P(I,1)
      NL=3
      DO 100 J=1,2
      IF(Z(NEL).GE.81.AND.NL.EQ.3) GO TO 100
      IF (P(I,NL).LT.EO) GO TO 99
  100 NL=NL+1
      EDGE(NEL)=P(I,17)
      GO TO 101
   99 EDGE(NEL)=P(I,3+NL)
  101 EC(NEL)=P(I,NL)
      WAVE(NEL)=P(I,NL+3)
      LINE(NEL)=MM(NL-2)
      U(NEL)=EO/EC(NEL)
      IF (U(NEL).GT.20.) U(NEL)=20.
      R(NEL)=0.
      KK=34
      DO 108 J=1,6
      R(NEL)=U(NEL)*R(NEL)+P(I,KK)
  108 KK=KK-1
      PF(NEL)=0.
      PRINT 2001,EL(NEL),I      ,A(NEL),PF(NEL),EDGE(NEL),EC(NEL),WAVE(NE
     1L),U(NEL),R(NEL)
C
C
C       CALCULATE ABSORPTION COEFFICIENT MATRIX
C
C
   98 DO 200 I=1,NEL
      DO 200 J=1,NEL
      NZ=Z(J)
      F=1.0
      DO 202 M=9,18
      IF (WAVE(I).LT.P(NZ,M))GO TO 203
  202 CONTINUE
      CON=P(NZ,28)
      EX=P(NZ,23)
      GO TO 201
  203 INTER6M-8
      GO TO (204,205,206,207,208,209,210,211,212,213),INTER
  204 CON=P(NZ,24)
      EX=P(NZ,19)
      GO TO 201
  205 CON=P(NZ,25)
      EX=P(NZ,20)
      GO TO 201
  206 F=0.961
      GO TO 205
  207 F=0.917
      GO TO 205
  208 CON=P(NZ,26)
      EX=P(NZ,21)
      GO TO 201
  209 F=0.984
```

```
      GO TO 208
  211 F=0.946
      GO TO 208
  212 F=0.894
      GO TO 208
  213 CON=P(NZ,27)
      EX=P(NZ,22)
C
C
C       CALCULATE ABSORPTION COEFFICIENT OF ELEMENT J FOR I RADIATION
C
C
  201 AC(I,J)=(CON*WAVE(I)**EX)**F
  200 CONTINUE
      PRINT 52
      IF (NA.LE.3) GO TO 2060
      PRINT 648, (EL(I), LINE(I), I=1,NA)
      PRINT 646
      DO 2050 J=1,NEL
      PRINT 668, EL(J), (AC(I,J),I=1,NA)
 2050 CONTINUE
      GO TO 2065
 2060 PRINT 647, (EL(I), LINE(I),I=1,NA)
      PRINT 645
      DO 2065 J=1,NEL
      PRINT 667, EL(J), (AC(I,J),I=1,NA)
 2065 CONTINUE
C
C
C       CALCULATE COMMON EXPRESSIONS
C
C
      DO 30 I=1,NEL
   30 WS(I)=Z(I)/A(I)
      PRINT 2002
 2002 FORMAT ( //13X,2HWS,8X,1HE,8X,3HVAL,7X,5HSIGMA,6X,2HHS,8X,2HUS,8X,
     12HFS,7X,4HFACT/)
      DO 11 I=1,NA
      ALPHA(I)=1.
      E(I)=(EC(I)+EO)/2.
      VAL(I)=7.061+ALOG(E(I))
      SIGMA(I)=2.54E+05/(EO**1.5-EC(I)**1.5)
      HS(I)=4.5*A(I)/(Z(I)*Z(I))
      US(I)=1.+CSC*AC(I,I)/SIGMA(I)
      FS(I)=((1.+HS(I))*(1.+1.1*HS(I))/(4.+1.1*HS(I))*CSC*AC(I,I)/SIGMA(I
     1))/(US(I)*(1.+HS(I)*US(I)))
      FACT(I)=FS(I)*R(I)/(WS(I)*(VAL(I)-ALOG(PF(I))))
 2003 FORMAT ( 6X,A3,1X,F7.4,3X,F7.4,3X,F7.4,3X,F8.2,2X,F7.4,3X,F7.4,3X,
     1F7.4,3X,F8.5)
   11 PRINT 2003,EL(I),WS(I),E(I),VAL(I),SIGMA(I),HS(I),US(I),FS(I),FACT
     1(I)
      DO 900 I=1,9
      FYR(I)=0.
      AJR(I)=0.
      DO 900 J=1,8
  900 B(J,I)=0.
C
C
C       CALCULATE PHILIBERT-LENARD ELECTRON STOPPING POWER
C
C
      ESP=.25949E+05-EO*(.24640E+04-EO*(.10164E+03-EO*(.20072E+01-EO*
     1.15447E-01)))
      PRINT 2004,ESP
 2004 FORMAT (//4X,6HESP = ,E14.8//)
C
```

```
C
C       CHECK FOR FLUORESCENCE AND CALCULATE APPROPRIATE FLUORESCENCE
C       YIELDS AND ABSORPTION JUMP RATIOS
C
C
      DO 878 K=1,NEL
      N=Z(K)
      IF ((LINE(K).EQ.MM(3)).OR.(LINE(K).EQ.MM(4))) GO TO 878
      IF (LINE(K).EQ.MM(1)) GO TO 876
      AJR(K)=P(N,25)*P(N,10)**P(N,20)/(P(N,26)*P(N,12)**P(N,21))
      D=-.111065+Z(K)*(.013680-Z(K)*Z(K)*.217720E-06)
      GO TO 879
  876 AJR(K)=P(N,24)*P(N,9)**P(N,19)/(P(N,25)*P(N,9)**P(N,20))
      D=-.037948+Z(K)*(.034256-Z(K)*Z(K)*.116342E-05)
  879 D=D*D*D*D
      FYR(K)=D/(1.+D)
  878 CONTINUE
      DO 873 K=1,NA
      IF ((LINE(K).EQ.MM(3)).OR.(LINE(K).EQ.MM(4))) GO TO 873
      DO 852 I=1,NEL
      IF ((EDGE(K).LE.WAVE(I)).OR.(LINE(I).EQ.MM(3))) GO TO 852
      IF ((EDGE(K).LE.WAVE(I)).OR.(LINE(I).EQ.MM(4))) GO TO 852
      IF (LINE(I).EQ.LINE(K)) GO TO 855
      IF (LINE(I).EQ.MM(1)) GO TO 859
      GO TO 860
  855 FF=.5
      GO TO 856
  859 FF=.21
      GO TO 856
  860 FF=1.2
  856 FY=FYR(I)
      RJ=AJR(K)
C
C
C       CALCULATE FACTOR FOR FLUORESCENCE CORRECTION
C
C
      B(K,I)=FF*FY*(RJ-1.)*A(K)*AC(I,K)/(RJ*A(I))*((U(I)-1.)/(U(K)-1.))*
     1*1.67
      PRINT 2005,EL(I),EL(K),B(K,I)
 2005 FORMAT (  4X,24HFLUORESCENCE FACTOR FOR ,A3,13H FLUORESCING ,A3,3H
     1IS ,F9.6)
  852 CONTINUE
  873 CONTINUE
      DO 901 I=1,8
      SAP(I)=0.
      SWP(I)=0.
      SAPSQ(I)=0.
      SWPSQ(I)=0.
      SSI(I)=0.
      SR(I)=0.
  901 SRSQ(I)=0.
      SAP(9)=0.
      SAPSQ(9)=0.
      SWP(9)=0.
      SWPSQ(9)=0.
C
C
C       IF COMPOUND STANDARDS ARE USED INSTEAD OF PURE ELEMENTAL
C       STANDARDS, INPUT NECESSARY DATA AND CALCULATE APPROPRIATE
C       PARAMETERS TO CORRECT STANDARD DATA USING THE SAME GENERAL
C       METHODS OUTLINED
C
C
      IF (NB.EQ.0) GO TO 53
      DO 603 K=1,NB
      READ 13,IC,STD(K,1),STD(K,2),CS,EL2
```

```
                    6.4,A3)
      IF (P(I,2).EQ.EE2) GO TO 109
  106 CONTINUE
C
C
C      DETERMINE ATOMIC NUMBER AND ATOMIC WEIGHT OF SECOND ELEMENT IN
C      COMPOUND STANDARD
C
C
  109 Z2=I
      A2=P(I,1)
      NL=3
C

C
C
      DO 110 J=1,2
      IF (I.GE.81.AND.NL.GT.3) GO TO 110
      IF (P(I,NL).LT.EO) GO TO 94
  110 NL=NL+1
   94 EC2=P(I,NL)
      U2=EO/EC2
      IF (U2.GT.20.) U2=20.
      R2=0.
      KK=34
      DO 112 J=1,6
      R2=U2*R2+P(I,KK)
  112 KK=KK-1
C
C
C      CALCULATE SECOND ELEMENT ABSORPTION COEFFICIENT
C
C
      F=1.0
      DO 302 M=9,18
      IF (WAVE(ID).LT.P(I,M)) GO TO 303
      CON= P(I,28)
  302 CONTINUE
      EX= P(I,23)
      GO TO 301
  303 INTER=M-8
      GO TO (304,305,306,307,308,309,310,311,312,313),INTER
  304 CON= P(I,24)
      EX=P(I,19)
      GO TO 301
  305 CON=P(I,25)
      EX=P(I,20)
      GO TO 301
  306 F=0.961
      GO TO 305
  307 F=0.917
      GO TO 305
  308 CON=P(I,26)
      EX=P(I,21)
      GO TO 301
  309 F=0.984
      GO TO 308
  310 F=0.972
      GO TO 308
  311 F=0.946
      GO TO 308
  312 F=0.894
      GO TO 308
  313 CON=P(I,27)
      EX=P(I,22)
  301 AC2=(CON*WAVE(ID)**EX)**F
      C2=1.-CS
```

```
      WAB=CS*WS(ID)+C2*Z2/A2
C
C
C      CALCULATE OTHER PARAMETERS FOR COMPOUND STANDARD
C
C
      ZAB=CS*Z(ID)+C2*Z2
      PFAB=ZAB*(14.*(1.-EXP(-.1*ZAB))+75.5/(ZAB**(ZAB/7.5))-ZAB/(100.+
     1ZAB))
      RAB=CS*R(ID)+C2*R2
      ACAB=CS*AC(ID,ID)+C2*AC2
      UAB=1.+CSC*ACAB/SIGMA(ID)
      HAB=4.5/(ZAB*WAB)
      FAB=((1.+HAB)*(1.+1.1*HAB/(4.+1.1*HAB)*CSC*ACAB/SIGMA(ID)))/(UAB*(
     11.+HAB*UAB))
      ALPHA(ID)=CS*FAB*RAB/(FACT(ID)*WAB*(VAL(ID)-ALOG(PFAB)))
  603 EL0(K)=EL(ID)
C
C
C      CHECK FOR TYPE OF DATA (FIXED-TIME OR FIXED-COUNT) AND
C      ESTABLISH DEAD-TIME CORRECTION
C
C
   53 IF (TAG.EQ.ABET(26)) GO TO 331
      IF (TIME.EQ.0.) TIME=1.
      DO 10 J=1,NA
      IF (TAUM(J).EQ.0.) TAUM(J)=1.
   10 TAU(J)=1.0E-06*TAUM(J)
C
C
C       READ BEAM CURRENTS AND STANDARD INTENSITIES
C
C
      DO 5005 J=1,NA
      BCSUM(J)=0.
      STDSUM(J)=0.
      READ 5002,N
 5002 FORMAT (I2)
      NN=N
      DO 5003 K=1,N
      READ 5004,BC(J,K),STDI(J,K)
 5004 FORMAT(4(2X,F5.0,4X))
      IF (BC(J,K).EQ.0.) BC(J,K)=1.
      BCSUM(J)=BCSUM(J)+BC(J,K)
C
C
C      DEADTIME CORRECT STANDARD INTENSITIES AND AVERAGE DRIFT
C      CORRECTED INTENSITIES
C
C
      STDI(J,K)=STDI(J,K)*TIME/(TIME-TAU(J)*STDI(J,K))
 5003 STDSUM(J)=STDSUM(J)+STDI(J,K)
      BCAVG(J)=BCSUM(J)/NN
      IF (J.EQ.1) BCREF=BCAVG(1)
      SI(J)=STDSUM(J)/NN*BCREF/BCAVG(J)
 5005 ASI(J)=SI(J)
      PRINT 2008
 2008 FORMAT (//15X,53HSTANDARD INTENSITIES CORRECTED FOR DEADTIME AND C
     1RIFT)
      PRINT 2009,(EL(J),J=1,NA)
 2009 FORMAT (/4X,12HBEAM CURRENT,9(5X,A3,3X))
      PRINT 2010,BCREF,(SI(J),J=1,NA)
 2010 FORMAT (/7X,F8.1,3X,9(F9.2,2X))
      DO 5008 J=1,8
      DO 5008 K=1,8
 5008 BKSUM(J,K)=0.
C
```

```
                    TS AND BACKGROUNDS
C
C
      DO 5009 J=1,NA
      BCSUM(J)=C.
      READ 5002,N
      NN=N
      DO 5010 K=1,N
      READ 5011,BC(J,K),(BK(J,K,L),L=1,NA)
 5011 FORMAT(4(2X,F5.0,4X))
      IF (BC(J,K).EQ.0.) BC(J,K)=1.
      BCSUM(J)=BCSUM(J)+BC(J,K)
C
C
C       DEADTIME CORRECT BACKGROUNDS AND AVERAGE DRIFT-CORRECTED
C       BACKGROUNDS
C
C
      DO 5010 L=1,NA
      BK(J,K,L)=BK(J,K,L)*TIME/(TIME-TAU(L)*BK(J,K,L))
 5010 BKSUM(J,L)=BKSUM(J,L)+BK(J,K,L)
      BCAVG(J)=BCSUM(J)/NN
      DO 5014 L=1,NA
 5014 ABK(J,L)=BKSUM(J,L)/NN*BCREF/BCAVG(J)
      BKGD(J)=ABK(J,J)
 5009 NAB(J)=ABK(J,J)+.5
      PRINT 5100, TIME
      IF (NA.LE.3) GO TO 2080
      PRINT 5201, (EL(I), LINE(I), I=1,NA)
      PRINT 5202
      DO 2070 J=1,NA
      PRINT 5204, EL(J), (ABK(J,L), L=1,NA)
 2070 CONTINUE
      GO TO 331
 2080 PRINT 5101, (EL(I), LINE(I), I=1,NA)
      PRINT 5102
      DO 2085 J=1,NA
      PRINT 5104, EL(J), (ABK(J,L),L=1,NA)
 2085 CONTINUE
C
C
C       READ BEAM CURRENTS AND RAW INTENSITIES FROM UNKNOWN, AND
C       COMPUTE CONCENTRATIONS
C
C
  331 SWSAL=0.
      READ 2086,DUMMY,(DECAY(J),J=1,NA)
 2086 FORMAT(4(2X,F5.0,4X))
      DO 40 I=1,300
      ITER=0
      READ 5015, BEAM(I),(XI(J),J=1,NA)
 5015 FORMAT(4(2X,F5.0,4X))
      IF (BEAM(I).LE. 99997.) GO TO 5016
      KODE=BEAM(I)- 99997.
      GO TO 78
 5016 IF (TAG.NE.ABET(26)) GO TO 5017
      DO 5018 J=1,NA
 5018 SI(J)=1.
      GO TO 5019
 5017 IF (BEAM(I).EQ.0.) BEAM(I)=1.
 5019 DO 75 J=1,NA
      IF (TAG.NE.ABET(26)) GO TO 5020
      IF (ITER.NE.0) GO TO 22
      GO TO 333
 5020 IF (ITER.NE.0) GO TO 5023
      NSI(J,I)=ASI(J)
```

```
C
C
C       DEADTIME AND DRIFT CORRECT UNKNOWN INTENSITIES
C
C
      XXI(J)=XI(J)*TIME/(TIME-TAU(J)*XI(J))
      XXI(J)=XXI(J)-DECAY(J)
      XXI(J)=XXI(J)*BCREF/BEAM(I)
      NXI(J,I)=XXI(J)
C
C
C       CORRECT FOR STANDARD BACKGROUNDS
C
C
      XI(J)=XXI(J)-BKGD(J)
      IF (I.EQ.1) SI(J)=SI(J)-BKGD(J)
      SSI(J)=SSI(J)+SI(J)
      GO TO 333
 5023 ABGD(J)=0.
C
C
C       CORRECT FOR CONCENTRATION DEPENDENT BACKGROUNDS
C
C
      DO 5024 K=1,NA
 5024 ABGD(J)=ABGD(J)+C(K)*ABK(K,J)
      XI(J)=XXI(J)-ABGD(J)
C
C
C       FORM K-RATIOS
C
C
  333 RINT(J)=XI(J)/SI(J)
      IF (RINT(J).GT..9999) RINT(J)=.9999
      IF (RINT(J).LT.0.) RINT(J)=0.
      IF (ITER.EQ.2) ROUT(J,I)=RINT(J)+.0001
   75 CONTINUE
      IF (ITER.NE.2) GO TO 5030
      DO 41 J=1,NA
      SR(J)=SR(J)+RINT(J)
   41 SRSQ(J)=SRSQ(J)+RINT(J)*RINT(J)
 5030 DO 5040 J=1,NA
      RINT(J)=ALPHA(J)*RINT(J)
      IF (ITER.EQ.0) C(J)=RINT(J)
 5040 CONTINUE
   22 ITER=ITER+1
      IF (ITER.NE.1) GO TO 5060
      DO 5050 J=1,NA
      CO(J)=RINT(J)
 5050 CONTINUE
      GO TO 5070
 5060 IF (ITER.LE.2) GO TO 5070
      DO 5080 J=1,NA
 5080 CO(J)=C1(J)
 5070 IF (NEL.EQ.NA) GO TO 25
      C(NEL)=1.
      DO 24 J=1,NA
   24 C(NEL)=C(NEL)-C(J)
      IF (C(NEL).LT.0.) C(NEL)=0.0
   25 RAL=0.
      ZAL=0.
      WSAL=0.
      DO 902 J=1,8
      FIDI(J)=0.
  902 ACAL(J)=0.
C
C
```

```
                    ION COEFFICIENTS FOR UNKNOWN
C
      DO 26 K=1,NEL
      DO 26 J=1,NEL
      ACAL(K)=ACAL(K)+C(J)*AC(K,J)
      IF (ACAL(K).LE.0.) ACAL(K)=.0000001
      IF(ACAL(K).GT.100000.) ACAL(K)=100000.0
   26 CONTINUE
C
C
C      CALCULATE BACKSCATTER LOSS FACTOR, MEAN ATOMIC NUMBER AND MEAN
C      Z / A FOR UNKNOWN
C
C
      DO 27 J=1,NEL
      RAL=RAL+R(J)*C(J)
      ZAL=ZAL+Z(J)*C(J)
   27 WSAL=WSAL+WS(J)*C(J)
      HAL=4.5/(ZAL*WSAL)
      PAL=ZAL*(14.*(1.-EXP(-.1*ZAL))+75.5/(ZAL**(ZAL/7.5))-ZAL/(100.+ZAL
     1))
C
C
C      CALCULATE CONCENTRATIONS
C
C
      DO 28 K=1,NA
      UAL(K)=1.+CSC*ACAL(K)/SIGMA(K)
      YP=CSC*ACAL(K)
      DO 880 J=1,NEL
      Y=YP/ACAL(J)
      V=ESP/ACAL(J)
  880 FIDI(K)=FIDI(K)+C(J)*B(K,J)/ACAL(J)*(ALOG(1.+Y)/Y+ALOG(1.+V)/V)
      FAL(K)=((1.+HAL)*(1.+FIDI(K))*(1.+1.1*HAL/(4.+1.1*HAL)*CSC*ACAL(K)
     1/SIGMA(K)))/(UAL(K)*(1.+HAL*UAL(K)))
      C(K)=RINT(K)*WSAL*(VAL(K)-ALOG(PAL))*FACT(K)/(FAL(K)*RAL)
      IF (C(K).LT.0.) C(K)=0.0
      IF(C(K).GT..9999) C(K)=.9999
      IF (ITER.NE.1) GO TO 5090
      C1(K)=C(K)
      GO TO 28
 5090 IF (ITER.GT.2) C1(K)=C3(K)
      C3(K)=C(K)
      CDEN=CO(K)-2.*C1(K)+C3(K)
      IF (CDEN.LE.0.) CDEN=.0000001
      C(K)=(CO(K)*C3(K)-C1(K)*C1(K))/CDEN
      IF(C(K).GT..9999) C(K)=.9999
      IF (C(K).LE.0.) C(K)=C3(K)
   28 CONTINUE
C
C
C      TEST FOR CONVERGENCE AND CHECK NUMBER OF ITERATIONS
C
C
      IF (ITER.LT.3) GO TO 5019
      DO 85 M=1,NA
      DEL=ABS(C3(M)-C(M))
      IF (DEL.GE..0005) GO TO 86
   85 CONTINUE
      GO TO 87
   86 IF (ITER.LT.20) GO TO 5019
   87 LOOP(I)=ITER
C
C
C      SUM CONCENTRATIONS FOR AVERAGING
C
C
```

```
      SWSAL=SWSAL+WSAL
      DO 31 K=1,NA
      IF (SR(K).LT..0001) SR(K)=.0001
      IF(SRSQ(K).LT..00000001) SRSQ(K)=.00000001
      WP(K)=100.*C(K)
   31 WPC(K,I)=WP(K)
      IF (NEL.EQ.NA) GO TO 34
      WP(NEL)=100.
      DO 33 K=1,NA
   33 WP(NEL)=WP(NEL)-WP(K)
      IF (WP(NEL).LT.0.) WP(NEL)=0.
   34 WPC(NEL,I)=WP(NEL)
      DO 35 K=1,NEL
   35 ATOM(K)=WP(K)/A(K)
      DEN=0.
      DO 36 K=1,NEL
   36 DEN=DEN+ATOM(K)
      DO 40 K=1,NEL
      AP(K)=1000.*ATOM(K)/DEN
      APC(K,I)=AP(K)
      SAP(K)=SAP(K)+AP(K)
      SAPSQ(K)=SAPSQ(K)+AP(K)*AP(K)
      SWP(K)=SWP(K)+WP(K)
      SWPSQ(K)=SWPSQ(K)+WP(K)*WP(K)
   40 CONTINUE
   78 NS=I-1
      OBS=NS
      IF (NS.GT.1) GO TO 760
      DIV=1.
      GO TO 765
  760 DIV=OBS*OBS
C
C
C       CALCULATE AVERAGE K-RATIOS AND RMS DEVIATIONS
C
C
  765 DO 42 K=1,NA
      AVR(K)=SR(K)/OBS+.00005
   42 RDEV(K)=2.*SQRT((OBS*SRSQ(K)-SR(K)*SR(K))/DIV)+.00005
C
C
C       CALCULATE PEAK-TO-BACKGROUND RATIOS AND MINIMUM DETECTABILITY
C       LIMITS
C
C
      IF (TAG.EQ.ABET(26)) GO TO 334
      DO 730 K=1,NA
      PEAK(K)=SI(K)/(ALPHA(K)*BKGD(K))
      MPEAK(K)=PEAK(K)
      LIMIT (K)= 329./SQRT(SI(K)*PEAK(K))
  730 CONTINUE
C
C
C       CALCULATE AVERAGE CONCENTRATIONS
C
C
  334 DO 43 K=1,NEL
      AVWP(K)=SWP(K)/OBS+.005
      AVAP(K)=SAP(K)/OBS+.005
      WPDEV(K)=2.*SQRT((OBS*SWPSQ(K)-SWP(K)*SWP(K))/DIV)+.005
   43 APDEV(K)=2.*SQRT((OBS*SAPSQ(K)-SAP(K)*SAP(K))/DIV)+.005
      IF (NEL.EQ.NA) GO TO 76
      AVWP(NEL)=100.0
      AVAP(NEL)=100.0
      DO 77 K=1,NA
      AVWP(NEL)=AVWP(NEL)-AVWP(K)
   77 AVAP(NEL)=AVAP(NEL)-AVAP(K)
```

```
                                  ) GO TO 76
      AVAP(NEL)=0.
C
C
C      START OUTPUT OF ALL DATA INCLUDING CONSTANTS CALCULATED
C
C
   76 PRINT 615,TAG,NPROB,DATE
  615 FORMAT (1H1,//40X,15HPROBLEM NUMBER ,A1,I4//68X,3A4,A3//)
      PRINT 29
   29 FORMAT (/17X,6HATOMIC,5X,6HATOMIC,5X,11HBACKSCATTER,5X, 10HEXCITAT
     1ION,5X,10HABSORPTION,5X,11HFLUORESCENT/5X,7HELEMENT,5X,6HNUMBER,5X
     2,6HWEIGHT,7X,6HFACTOR,8X,9HPOTENTIAL,6X,10HJUMP RATIO,8X,5HYIELD//
     3)
      DO 39 I=1,NEL
      NZ=Z(I)
      AJR(I)=AJR(I)+.005
      FYR(I)=FYR(I)+.0005
      PRINT 38,EL(I),NZ,A(I),R(I),EC(I),AJR(I),FYR(I)
   38 FORMAT (7X,A3,8X,I3,5X,F8.3,7X,F5.3,10X,F7.3,8X,F6.2,11X,F5.3)
   39 CONTINUE
      PRINT 52
   52 FORMAT (///33X,28HMASS ABSORPTION COEFFICIENTS)
      IF (NA.LE.3) GO TO 637
      PRINT 648,(EL(I),LINE(I),I=1,NA)
  648 FORMAT (/3X,9HRADIATION,5X,8(A3,A2,6X))
      PRINT 646
  646 FORMAT (/,4X,8HABSORBER//)
      DO 658 J=1,NEL
      PRINT 668,EL(J),(AC(I,J),I=1,NA)
  668 FORMAT (9X,A3,3X,8(F8.0,4X))
  658 CONTINUE
      PRINT 5100, TIME
      PRINT 5201,(EL(I),LINE(I),I=1,NA)
 5201 FORMAT (/ 41X,11HBACKGROUNDS//1X,14HCONTRIBUTED TO,2X,8(A3,A2,6X))
      PRINT 5202
 5202 FORMAT (/2X,11HBY 100 % OF//)
      DO 5203 J=1,NA
 5204 FORMAT (9X,A3,3X,8(F6.1,4X))
 5203 PRINT 5204,EL(J),(ABK(J,L),L=1,NA)
      IF (NS.LE.1) GO TO 73
      PRINT 615,TAG,NPROB,DATE
      IF (TIME.EQ.1.) GO TO 626
      PRINT 617,(EL(I),I=1,NA)
  617 FORMAT (///33X,37HINTENSITIES (CPS X COUNTING INTERVAL)/35X,33HCOR
     1RECTED FOR DEAD-TIME AND DRIFT//6X,8(A3,10X)//)
      GO TO 610
  626 PRINT 627,(EL(I),I=1,NA)
  627 FORMAT (///43X,17HINTENSITIES (CPS)/35X,33HCORRECTED FOR DEAD-TIME
     1 AND DRIFT//6X,8(A3,10X)//)
  610 DO 688 I=1,NS
      PRINT 698,(NXI(J,I),NSI(J,I),J=1,NA)
  698 FORMAT (1X,8(I7,2H /,I7,1X))
  688 CONTINUE
      IF (TIME.EQ.1.) GO TO 619
      PRINT 620,(NAB(I),I=1,NA)
  620 FORMAT(//29X,46HSTANDARD BACKGROUNDS (CPS X COUNTING INTERVAL)//5X
     1,8(I4,9X))
      GO TO 621
  619 PRINT 622,(NAB(I),I=1,NA)
  622 FORMAT (//39X,26HSTANDARD BACKGROUNDS (CPS)//5X,8(I4,9X))
  621 PRINT 623,(TAUM(I),I=1,NA)
  623 FORMAT (//40X,24HDEAD-TIME (MICROSECONDS)//6X,8(F3.1,10X))
      IF (TIME.EQ.1.) GO TO 625
      PRINT 695,TIME
  695 FORMAT (//36X,18HCOUNTING INTERVAL,,F6.1,8H SECONDS)
  625 PRINT 15,TAG,NPROB,DATE
```

```
      PRINT 694,(EL(I),I=1,NA)
  694 FORMAT (18X,33HINDIVIDUAL K-RATIOS CORRECTED FOR/17X, 36HDEAD-TIME
     1, DRIFT AND BACKGROUND ONLY//5X,1HN,4X,8(A3,5X))
      DO 568 I=1,NS
      PRINT 578,LOOP(I),(ROUT(J,I),J=1,NA)
  578 FORMAT (3X,I3,2X,8(F6.4,2X))
  568 CONTINUE
      IF (NB.EQ.0) GO TO 1008
      PRINT 74
      PRINT 674,(ELO(K),STD(K,1),STD(K,2),K=1,NB)
  674 FORMAT (//17X,A3,37HDETERMINED RELATIVE TO A STANDARD OF ,A4,A1)
      GO TO 1008
  637 PRINT 647,(EL(I),LINE(I),I=1,NA)
  647 FORMAT (/25X,9HRADIATION,5X,3(A3,A2,8X))
      PRINT 645
  645 FORMAT (/,26X,8HABSORBER//)
      DO 657 J=1,NEL
      PRINT 667,EL(J),(AC(I,J),I=1,NA)
  667 FORMAT (31X,A3,3X,3(F8.0,6X))
  657 CONTINUE
      PRINT 5100, TIME
 5100 FORMAT (////36X,18HCOUNTING INTERVAL,,F6.1,10H SECOND(S))
      PRINT 5101,(EL(I),LINE(I),I=1,NA)
 5101 FORMAT ( /41X,11HBACKGROUNDS//19X,14HCONTRIBUTED TO,5X,3(A3,A2,8X
     1))
      PRINT 5102
 5102 FORMAT (/23X,11HBY 100 % OF//)
      DO 5103 J=1,NA
 5104 FORMAT (31X,A3,3X,3(F6.1,6X))
 5103 PRINT 5104,EL(J),(ABK(J,L),L=1,NA)
      IF (NS.LE.1) GO TO 73
      PRINT 15,TAG,NPROB,DATE
   15 FORMAT (1H1,24X,15HPROBLEM NUMBER ,A1,I4//52X,3A4,A3//)
      IF (TIME.EQ.1.) GO TO 643
      PRINT 655,(EL(I),I=1,NA)
  655 FORMAT (///16X,37HINTENSITIES (CPS X COUNTING INTERVAL)/18X,33HCOR
     1RECTED FOR DEAD-TIME AND DRIFT//14X,3(A3,16X)//)
      GO TO 642
  643 PRINT 654,(EL(I),I=1,NA)
  654 FORMAT (///26X,17HINTENSITIES (CPS)/18X,33HCORRECTED FOR DEAD-TIME
     1 AND DRIFT//14X,3(A3,16X)//)
  642 DO 687 I=1,NS
      PRINT 697,(NXI(J,I),NSI(J,I),J=1,NA)
  697 FORMAT (2X,3(7X,I7,2H /,I7))
  687 CONTINUE
      IF (TIME.EQ.1.) GO TO 652
      PRINT 651,(NAB(I),I=1,NA)
  651 FORMAT (//12X,46HSTANDARD BACKGROUNDS (CPS X COUNTING INTERVAL)//1
     13X,3(I4,15X))
      GO TO 665
  652 PRINT 537,(NAB(I),I=1,NA)
  537 FORMAT (//22X,26HSTANDARD BACKGROUNDS (CPS)//13X,3(I4,15X))
  665 PRINT 664,(TAUM(I),I=1,NA)
  664 FORMAT (//23X,24HDEAD-TIME (MICROSECONDS)//14X,3(F3.1,17X))
      IF (TIME.EQ.1.) GO TO 663
      PRINT 662,TIME
  662 FORMAT (//19X,18HCOUNTING INTERVAL,,F6.1,8H SECONDS)
  663 PRINT 15,TAG,NPROB,DATE
      PRINT 70,(EL(J),J=1,NA)
   70 FORMAT (18X,33HINDIVIDUAL K-RATIOS CORRECTED FOR/17X, 36HDEAD-TIME
     1, DRIFT AND BACKGROUND ONLY//9X,1HN,7X,3(A3,13X))
      DO 702 I=1,NS
      PRINT 71,LOOP(I),(ROUT(J,I),J=1,NA)
   71 FORMAT (7X,I3,5X,3(F6.4,10X))
  702 CONTINUE
      IF (NB.EQ.0) GO TO 1008
      PRINT 74
```

```
                    NOTE***)
                    (K,1),STD(K,2X,K=1,NB)
   51 FORMAT (//24X,A3,19HDETERMINED RELATIVE/24X,17HTO A STANDARD OF ,
     1A4,A1)
 1008 IF (NS.LE.1) GO TO 73
      DO 1270 L=1,2
      IF (NA.GT.3) GO TO 1200
      PRINT 15,TAG,NPROB,DATE
      GO TO 1110
 1200 PRINT 615,TAG,NPROB,DATE
 1110 PRINT 89,NAME,TITLE
      PRINT 66,EO,THETA
      IF (TAG.EQ.ABET(26)) GO TO 1130
      PRINT 67
      DO 1130 K=1,NA
      PRINT 68,EL(K),MPEAK(K),LIMIT(K)
 1130 CONTINUE
      IF (NA.GT.3) GO TO 1240
      PRINT 1150
 1150 FORMAT (//23X,20HCHEMICAL COMPOSITION/26X,14HWEIGHT PERCENT/26X,14
     1HATOMIC PERCENT/)
      IF (NEL.EQ.NA) GO TO 1152
      PRINT 1153,EL(NEL)
 1153 FORMAT (19X,A3,24HDETERMINED BY DIFFERENCE/)
 1152 PRINT 1154,(EL(K),K=1,NEL)
 1154 FORMAT (/3X,3HOBS,9X,4(A3,13X)/)
      DO 1170 I=1,NS
      PRINT 1160,I,(WPC(K,I),K=1,NEL)
 1160 FORMAT (/3X,I3,5X,4(F8.3,8X))
      PRINT 1165,(APC(K,I),K=1,NEL)
 1165 FORMAT (11X,4(F8.3,8X))
 1170 CONTINUE
      GO TO 1270
 1240 PRINT 1250
 1250 FORMAT (//46X,20HCHEMICAL COMPOSITION/49X,14HWEIGHT PERCENT/49X,14
     1HATOMIC PERCENT/)
      IF (NEL.EQ.NA) GO TO  1252
      PRINT 1253,EL(NEL)
 1253 FORMAT (42X,A3,24HDETERMINED BY DIFFERENCE/)
 1252 PRINT 1254,(EL(K),K=1,NEL)
 1254 FORMAT (13X,3HOBS,7X,9(A3,8X)/)
      DO 1270 I=1,NS
      PRINT 1260,I,(WPC(K,I),K=1,NEL)
 1260 FORMAT (/3X,I3,4X,9(F8.3,4X))
      PRINT 1265,(APC(K,I),K=1,NEL)
 1265 FORMAT (10X,9(F8.3,4X))
 1270 CONTINUE
   73 DO 69 L=1,2
      PRINT 15,TAG,NPROB,DATE
      PRINT 89,NAME,TITLE
   89 FORMAT(5X,13HSUBMITTED BY ,5A4//5X,14HDESCRIPTION - ,71A1//)
      PRINT 49,NS
   49 FORMAT (/18X,33HMEAN CHEMICAL COMPOSITION AND TWO/18X, 21HSIGMA LI
     1MITS BASED ON,I4,9H ANALYSES,///29X,6HWEIGHT,12X,6HATOMIC/16X,7HEL
     2EMENT,6X,7HPERCENT,11X,7HPERCENT//)
      DO 45 K=1,NA
      PRINT 44,EL(K),AVWP(K),WPDEV(K),AVAP(K),APDEV(K)
   44 FORMAT (18X,A3,2X,F8.3,2H -,F6.3,2X,F8.3,2H -,F6.3/)
   45 CONTINUE
      IF (NEL.EQ.NA) GO TO 47
      PRINT 48,EL(NEL),AVWP(NEL),WPDEV(NEL),AVAP(NEL),APDEV(NEL)
   48 FORMAT (18X,A3,1H*,1X,F8.3,2H -,F6.3,2X,F8.3,2H -,F6.3///21X, 26H*
     1 DETERMINED BY DIFFERENCE)
   47 PRINT 64
   64 FORMAT  (//5X,65H-----------------------------------------------
     1----------------///13X,42HMEAN INTENSITY RATIOS AND TWO SIGMA LIMI
     2TS//21X,7HELEMENT, 12X,1HK//)
```

```
      DO 63 K=1,NA
      PRINT 65,EL(K),AVR(K),RDEV(K)
   65 FORMAT (23X,A3,7X,F6.4,2H -,F7.4)
   63 CONTINUE
      PRINT 66,EO,THETA
   66 FORMAT (///13X,20HACCELERATING VOLTAGE,13X,F5.1,4H KEV//13X, 21HX-
     1RAY EMERGENCE ANGLE,12X,F5.1,8H DEGREES)
      IF (T1.EQ.0.) GO TO 83
      PRINT 84,T1
   84 FORMAT (/13X,14HFILM THICKNESS,19X,F6.2,8H MICRONS)
C
C
C      CALCULATE DEPTH OF ANALYZED REGION
C
C
   83 IF (RHO.EQ.0.) GO TO 92
      DM=.033*OBS/(SWSAL*RHO)*SQRT(EO*EO*EO)+.005
C
C
C      CONTINUE OUTPUTTING OF DATA
C
C
      PRINT 93,RHO,DM
   93 FORMAT (/13X,7HDENSITY,26X,F6.2//13X,24HDEPTH OF ANALYZED REGION,9
     1X,F6.2,8H MICRONS)
   92 IF (TAG.EQ.ABET(26)) GO TO 69
      IF (NA.GT.3) PRINT 15,TAG,NPROB,DATE
  747 PRINT 67
   67 FORMAT (//13X,44HSTANDARD PEAK-TO-BACKGROUND RATIOS (P/B) AND/17X,
     134HMINIMUM DETECTABILITY LIMITS (MDL)//16X,7HELEMENT,6X,3HP/B,13X,
     23HMDL//)
      DO 341 K=1,NA
      PRINT 68,EL(K),MPEAK(K),LIMIT(K)
   68 FORMAT (18X,A3,5X,I5,2H/1,8X,F7.4,5H WT %//)
  341 CONTINUE
   69 CONTINUE
C
C     DETERMINE IF GRAPHS ARE DESIRED
C
      READ 60,(MARY(I),I=1,5)
   60 FORMAT(5I1)
      DO 61 I=1,5
      IF(MARY(I)-1) 61,61,62
   62 CALL GRAPHS
      GO TO 320
   61 CONTINUE
C
C
C      CHECK FOR MORE DATA.
C
C
  320 GO TO (1,80), KODE
   80 PRINT 1002,TAG,NPROB
 1002 FORMAT (1H0,//10X,27HLAST PROBLEM NUMBER USED IS,1X,A1,I4)
      STOP
      END
      SUBROUTINE GRAPHS
C     THIS SUBROUTINE DETERMINES WHICH GRAPHING OPTIONS ARE DESIRED.
C     RADII, AND CORRECT WEIGHT PERCENTS AND WEIGHT PERCENT RATIOS ARE
C     CALCULATED AND STORED IN COMMON.
C     PROGRAMMED BY RICK FERNOW(JULY 1969)
      COMMON WPC(9,300),MARY(5),RAD(102),  AAA(400),Y(500)
      MU5=MARY(5)
      DO 35 J=1,100
      READ 5,RAD(J)
    5 FORMAT(F10.0)
      IF(RAD(J).LT.0.001) GO TO 12
   35 CONTINUE
```

```
      Y(I)=WPC(1,I)
      Y(NPTS+I)=WPC(2,I)
      Y(2*NPTS+I)=WPC(1,I)+WPC(2,I)
      Y(3*NPTS+I)=       WPC(2,I) /WPC(1,I)
    1 Y(4*NPTS+I)=       WPC(2,I) /(WPC(1,I)+WPC(2,I))
      JIM=1
      LET=1
      DO 31 K=1,5
      IF(MARY(K).NE.5) GO TO 10
      CALL CALPLT(NPTS,7,1)
      LET=2
   10 IF(K.NE.5)GO TO 2
      IF(MU5.EQ.3.OR.MU5.EQ.4)GO TO 2
      IF(LET.EQ.1)GO TO 2
      CALL CALPLT(NPTS,6,2)
    2 IF(MARY(K).EQ.0) MARY(K)=1
      IF(MARY(1).EQ.5) MARY(1)=4
      MU=MARY(K)
      GO TO(31,32,33,32),MU
   32 IF(JIM.EQ.2) GO TO 34
      CALL PPLOT(NPTS,JIM)
   34 IF(MARY(K).NE.4) GO TO 31
   33 CALL CALPLT(NPTS,K,LET)
      LET=2
      IF(K.NE.5)GO TO 31
      CALL CALPLT(NPTS,6,2)
   31 CONTINUE
      RETURN
      END


      SUBROUTINE CALPLT(NPTS,K,LET)
C     THIS SUBROUTINE PREPARES CALCOMP GRAPHS
C     PROGRAMMED BY RICK FERNOW (JULY 1969)
      COMMON AAA(9,300),BBB(5),RAD(102),  CCC(400),Y(500), NAME(40)
      DIMENSION BUFF(1000),ORD(102),ORD1(102),ORD2(102),ORD3(102)
      IF(K.EQ.6)GO TO 9
      IF(LET.EQ.2) GO TO 7
      CALL PLOTS(BUFF,4000,11)
    7 CALL PLOT(-.75,-.5,3)
      CALL PLOT(7.75,-.5,2)
      CALL PLOT(7.75,10.5,2)
      CALL PLOT(-.75,10.5,2)
      CALL PLOT(-.75,-.5,2)
      GO TO(1,2,3,4,5, 9,15),K
    1 JO=10
      KO=15
      DO 8 I=1,NPTS
    8 ORD(I)=Y(I)
      GO TO 6
    2 JO=14
      KO=16
      DO 58 I=1,NPTS
   58 ORD(I)=Y(I+NPTS)
      GO TO 6
    3 JO=18
      KO=18
      DO 60 I=1,NPTS
   60 ORD(I)=Y(2*NPTS+I)
      GO TO 6
    4 JO=23
      KO=22
      DO 64 I=1,NPTS
   64 ORD(I)=Y(3*NPTS+I)
```

```
      GO TO 6
    5 JO=29
      KO=27
      DO 73 I=1,NPTS
   73 ORD(I)=Y(4*NPTS+I)
      GO TO 6
   15 DO 17 I=1,NPTS
      ORD1(I)=Y(I)
      ORD2(I)=Y(NPTS+I)
   17 ORD3(I)=Y(2*NPTS+I)
      ORD1(NPTS+1)=0.00
      ORD1(NPTS+2)=10.00
      ORD2(NPTS+1)=0.00
      ORD2(NPTS+2)=10.00
      ORD3(NPTS+1)=0.00
      ORD3(NPTS+2)=10.00
      CALL SCALE(RAD,7.5,NPTS,1,10.)
      CALL AXIS(0.0,0.0,NAME(10),10,10.0,90.0,0.00,10.00,10.)
      CALL AXIS(0.0,0.0,NAME(1),-33,7.5,0.0,RAD(NPTS+1),RAD(NPTS+2),10.)
      CALL LINE(RAD,ORD1,NPTS,1,-1,78)                          U   :  +
      CALL LINE(RAD,ORD2,NPTS,1,-1,92)                          PU  :  *
      CALL LINE(RAD,ORD3,NPTS,1,-1,04)                          SUM :  X
      CALL PLOT(10.0,0.0,-3)
      RETURN
    6 IF(K.NE.3) GO TO 10
      ORD(NPTS+1)= 0.00
      ORD(NPTS+2)=10.00
      GO TO 11
   10 CALL SCALE(ORD,10.0,NPTS,1,10.)
   11 CALL SCALE(RAD,7.5,NPTS,1,10.)
      CALL AXIS(0.0,0.0,NAME(JO),KO,10.0,90.0,ORD(NPTS+1),ORD(NPTS+2),10
     1.)
      CALL AXIS(0.0,0.0,NAME(1),-33,7.5,0.0,RAD(NPTS+1),RAD(NPTS+2),10.)
      CALL LINE(RAD,ORD,NPTS,1,-1,78)
      CALL PLOT(10.0,0.0,-3)
      RETURN
    9 CALL PLOT(0.,0.,999)
      RETURN
      END
      SUBROUTINE PPLOT(NPTS,JIM)
C     THIS SUBROUTINE PLOTS WEIGHT PERCENTS AND WEIGHT PERCENT RATIOS VERSUS
C     RADIAL DISTANCE IN THE SAMPLE.  IT WILL GIVE A ROUGH GRAPH ON THE PRINTER.
C     PROGRAMMED BY RICK FERNOW(JULY 1969)
      COMMON AAA(9,300),MARY(5),RAD(102),TITLE(400) ,Y(500)
      DIMENSION ORD(100),GRAPH(55,130)
      INTEGER HORZ(100),VERT(100)
      MU1=MARY(1)
      MU2=MARY(2)
      MU3=MARY(3)
      MU4=MARY(4)
      MU5=MARY(5)
C     CALCULATE THE ARRAY OF HORIZONTAL VALUES
      DO 30 J=1,NPTS
   30 HORZ(J)=IFIX(0.80*RAD(J)+14.0)
      DO 61 L=1,5
      IF(L.EQ.1) GO TO 35
      IF(L.NE.4) GO TO 17
C     CLEAR THE GRAPH ARRAY
   35 DO 29 I=1,130
      DO 29 J=1,55
   29 GRAPH(J,I)=TITLE(7)
C     CONSTRUCT THE AXES
      DO 1 I=1,50
    1 GRAPH(I,13)=TITLE(30)
      DO 2 J=13,122
    2 GRAPH(50,J)=TITLE(34)
C     INSERT MARKERS AT THE PROPER PLACES
```

```
                                        !)
      DO 4 J=13,117,8
    4 GRAPH(50,J)=TITLE(82)
C     NUMBER THE AXES
      DO 5 I=1,46
      GRAPH(I,12)=TITLE(I+135)
    5 GRAPH(I,11)=TITLE(I+190)
      GRAPH(1,10)=TITLE(236)
      GO TO(50,50,50,51,51),L
   51 DO 52 I=6,46,5
   52 GRAPH(I,10)=TITLE(239)
      GRAPH(1,11)=TITLE(239)
   50 DO 6 J=12,120
    6 GRAPH(51,J)=TITLE(J+229)
C     LABEL THE AXES AND DETERMINE THE CORRECT SET OF Y VALUES
      DO 7 J=43,75
    7 GRAPH(53,J)=TITLE(J-42)
   17 IF(MARY(L).EQ.0) MARY(L)=1
      MU=MARY(L)
      GO TO(20,20,16,20,19),L
   16 IF(MU3.EQ.2) GO TO 20
      IF(MU3.EQ.4) GO TO 20
      GO TO(21,18,21,18),MU1
   21 GO TO(61,18,61,18),MU2
   19 IF(MU5.EQ.2) GO TO 20
      IF(MU5.EQ.4) GO TO 20
      GO TO(61,18,61,18),MU4
   20 GO TO(61,44,61,44),MU
   44 GO TO(45,46,47,48,49),L
   45 DO 15 I=1,NPTS
   15 ORD(I)=Y(I)
      IP=49
      GO TO 40
   46 DO 58 I=1,NPTS
   58 ORD(I)=Y(I+NPTS)
      IP=38
      GO TO 40
   47 DO 60 I=1,NPTS
   60 ORD(I)=Y(2*NPTS+I)
      IP=237
      GO TO 40
   48 DO 64 I=1,NPTS
   64 ORD(I)=Y(3*NPTS+I)*100.
      IP=351
      DO 54 J=82,89
   54 GRAPH(55,J)=TITLE(J+269)
      GO TO 9
   49 DO 73 I=1,NPTS
   73 ORD(I)=Y(4*NPTS+I)*100.
      IP=239
      DO 55 J=97,108
   55 GRAPH(55,J)=TITLE(J+262)
    9 DO 10 I=16,31
   10 GRAPH(I,5)=TITLE(I+70)
      GO TO 41
   40 DO 8 I=20,29
    8 GRAPH(I,5)=TITLE(I+15)
   41 DO 12 J=1,NPTS
      VERT(J)=IFIX(51.0-0.50*ORD(J))
      IF(VERT(J).EQ.0) VERT(J)=1
      IH=HORZ(J)
      IV=VERT(J)
      IF(GRAPH(IV,IH).NE.TITLE(7)) GO TO 53
      GRAPH(IV,IH)=TITLE(IP)
      GO TO 12
   53 GRAPH(IV,IH)=TITLE(238)
```

```
   12 CONTINUE
      IF(L.LT.3) GO TO 61
      IF(L.EQ.4) GO TO 61
C     PRINT OUT ALL THE CHARACTERS IN THE ARRAY
   18 PRINT 28
   28 FORMAT(1H1,'PRINTER PLOT')
      DO 26 I=1,55
   26 PRINT 27,(GRAPH(I,J),J=1,130)
   27 FORMAT(1H ,130A1)
   61 CONTINUE
      JIM=2
      RETURN
      END
```

1.008 H	.014					999.	999.	999.		
4.003HE	.025					499.	999.	999.		
6.939LI	.055			228.		226.5	999.	999.		
9.012BE	.111			114.		111.	999.	999.		
10.811 B	.188	.005		67.6		65.6	999.	999.		
12.011 C	.284	.006		44.7		43.68	999.	999.		
14.007 N	.400	.009		31.60		30.99	999.	999.		
15.999 O	.532	.007		23.62		23.32	524.	999.		
18.998 F	.685	.009		18.32		18.09	398.	999.		
20.183NE	.867	.018		14.610		14.30	2275.	677.		
22.990NA	1.072	.031		11.910		11.56	9247.3	398.8		
24.312MG	1.303	.049		9.890		9.51	2197.3	249.3		
26.982AL	1.560	.073		8.339		7.94	8142.5	169.49		
28.086SI	1.840	.101		7.125		6.73	8105.0	123.		
30.974 P	2.144	.132		6.157		5.784	81.0	93.7		
32.064 S	2.470	.165		5.372		5.019	64.1	75.2		
35.453CL	2.820	.200		4.728		4.397	52.1	61.8		
39.948AR	3.203	.245		4.192		3.871	43.2	50.2		
39.102 K	3.608	.295		3.741		3.437	36.4	41.8		
40.080CA	4.038	.346		3.358	36.33	3.070	30.7	35.13		
44.956SC	4.489	.402	.007	3.031	31.35	2.762	26.8	30.6		
47.900TI	4.965	.455	.004	2.749	27.42	2.497	23.4	26.94		
50.942 V	5.464	.513	.002	2.504	24.25	2.269	19.72	23.8		
51.996CR	5.989	.575	.002	2.290	21.64	2.070	17.84	21.24		
54.938MN	6.538	.640	.003	2.102	19.45	1.896	16.15	19.05		
55.847FE	7.111	.707	.004	1.936	17.59	1.743	14.65	17.202		
58.933CO	7.710	.779	.003	1.789	15.972	1.608	13.38	15.618		
58.710NI	8.332	.854	.004	1.658	14.561	1.488	12.3	14.242		
63.540CU	8.980	.933	.002	1.541	13.336	1.381	11.27	13.014		
65.370ZN	9.661	1.022	.008	1.435	12.254	1.283	10.06	11.862		
69.720GA	10.368	1.117	.017	1.340	11.292	1.196	9.517	10.828		
72.590GE	11.104	1.217	.029	1.254	10.436	1.117	8.773	9.924		
74.922AS	11.865	1.323	.041	1.176	9.671	1.045	8.107	9.125		
78.960SE	12.655	1.434	.054	1.105	8.990	.980	7.503	8.407		
79.909BR	13.470	1.553	.069	1.040	8.375	.920	6.959	7.753		
83.800KR	14.324	1.677	.089	.980	7.817	.866	6.47	7.168		
85.470RB	15.202	1.807	.110	.926	7.318	.816	6.008	6.644		
87.620SR	16.107	1.941	.133	.875	6.863	.770	5.592	6.173		
88.905 Y	17.038	2.079	.157	.829	6.449	.728	5.217	5.756		
91.220ZR	17.999	2.223	.180	.786	6.071	.689	4.879	5.378		
92.906NB	18.987	2.371	.205	.746	5.724	.653	4.575	5.031		
95.940MO	20.004	2.523	.227	.709	5.407	.620	4.304	4.719		
99.000TC	21.047	2.678	.253	.675	5.115	.589	4.058	4.436		
101.070RU	22.119	2.838	.279	.643	4.846	.561	3.835	4.180		
102.905RH	23.220	3.002	.307	.613	4.597	.534	3.629	3.943		
106.400PD	24.348	3.173	.335	.585	4.368	.509	3.437	3.723		
107.870AG	25.517	3.351	.398	.559	4.154	.486	3.256	3.516		
112.400CD	26.716	3.538	.440	.535	3.956	.464	3.085	3.326		
114.82 IN	27.942	3.730	.443	.512	3.772	.444	2.926	3.147		
118.690SN	29.195	3.929	.511	.491	3.600	.425	2.777	2.982		
121.750SB	30.486	4.132	.528	.470	3.439	.407	2.639	2.830		
127.600TE	31.811	4.342	.572	.451	3.289	.309	2.510	2.688		

Constants and mass absorption coefficients stored internally

126.904	I	33.167	4.559	.631	.433	3.149		.374	2.388	2.554
131.300	XE	34.590	4.782	.672	.416	3.017		.358	2.274	2.429
132.905	CS	35.987	5.011	.726	.400	2.892		.345	2.167	2.314
137.340	BA	37.452	5.247	.780	.385	2.776		.331	2.068	2.205
138.910	LA	38.934	5.484	.832	.371	2.666	14.88	.318	1.978	2.105
140.120	CE	40.453	5.723	.883	.357	2.562	14.04	.306	1.893	2.012
140.907	PR	42.002	5.963	.926	.344	2.463	13.343	.295	1.814	1.926
144.240	ND	43.574	6.209	.973	.332	2.370	12.68	.285	1.739	1.844
147.	PM	45.198	6.461	1.027	.320	2.282	12.	.274	1.667	1.768
150.35	SM	46.849	6.717	1.073	.309	2.200	11.47	.265	1.600	1.695
151.96	EU	48.519	6.981	1.126	.298	2.121	10.96	.256	1.538	1.627
157.250	GD	50.233	7.243	1.185	.288	2.047	10.46	.247	1.478	1.563
158.924	TB	52.002	7.515	1.241	.279	1.977	10.00	.238	1.422	1.502
162.500	DY	53.793	7.790	1.295	.270	1.909	9.59	.230	1.369	1.445
164.93	HO	55.619	8.068	1.351	.261	1.845	9.20	.223	1.319	1.391
167.26	ER	57.487	8.358	1.401	.252	1.784	8.82	.216	1.271	1.339
168.934	TM	59.380	8.650	1.461	.244	1.727	8.48	.209	1.225	1.289
173.04	YB	61.300	8.944	1.528	.237	1.672	8.149	.202	1.182	1.243
174.97	LU	63.310	9.249	1.589	.229	1.620	7.840	.196	1.140	1.199
178.49	HF	65.310	9.558	1.662	.222	1.570	7.539	.190	1.100	1.155
180.948	TA	67.403	9.877	1.743	.215	1.522	7.252	.184	1.061	1.114
183.85	W	69.508	10.200	1.814	.209	1.476	6.983	.178	1.025	1.075
186.20	RE	71.658	10.531	1.890	.203	1.433	6.729	.173	.989	1.037
190.2	OS	73.856	10.868	1.967	.197	1.391	6.490	.168	.956	1.001
192.2	IR	76.101	11.212	2.048	.191	1.351	6.262	.163	.924	.967
195.09	PT	78.381	11.562	2.133	.186	1.313	6.047	.158	.893	.934
196.967	AU	80.720	11.921	2.220	.180	1.276	5.840	.154	.864	.903
200.590	HG	83.109	12.286	2.313	.175	1.241	5.648	.149	.835	.872
204.37	TL	5.249	12.660	2.406	.170	1.207	5.460	.145	.808	.843
207.19	PB	5.076	13.041	2.502	.165	1.175	5.286	.141	.782	.815
208.980	BI	4.909	13.426	2.603	.161	1.144	5.118	.137	.757	.789
210.	PO		13.814	2.683	.156	1.114		.133	.732	.763
210.	AT		14.214	2.787	.152	1.085		.129	.709	.739
222.	RN		14.619	2.892	.148	1.057		.126	.687	.715
223.	FR		15.031	3.000	.144	1.030		.123	.665	.692
226.	RA		15.444	3.105	.140	1.005		.119	.645	.671
227.	AC		15.871	3.219	.136	.980		.116	.625	.650
232.038	TH	3.941	16.300	3.325	.133	.956	4.138	.115	.606	.630
231.	PA	3.827	16.733	3.436	.129	.933	4.022	.110	.587	.610
238.030	U	3.716	17.165	3.545	.126	.911	3.910	.107	.570	.592
237.	NP	3.611	17.610	3.666		.889		.104	.553	.574
239.	PU	3.505	18.054	3.778		.868	3.696	.102	.537	.557
243.	AM		18.504	3.887		.848		.099	.521	.540
247.	CM		18.930	3.971				.097	.507	.521
247.	BK		19.452	4.132				.091		
251.	CF		19.930	4.253				.091	.475	.491
254.	ES		20.410	4.374				.089	.461	.476
253.	FM		20.900	4.498				.087	.448	.462

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677.491999.
405. 999.
250.700999.
170.490999.
124.960999.
94.000999.
75.800999.
61.990708.462999.
50.563490.043999.846999.846

2.335
2.786
2.652
2.852
2.661
2.9212.365
2.8892.370
2.8502.346
2.8132.390
2.8032.452
2.7842.59
2.8512.870
2.7802.7701.309
2.7802.68 1.34
2.7732.61 1.38
2.7482.5921.42
2.8472.6521.46
2.7962.5811.520

42.2	783	65.5	72	696.5	22	696.5	229	99.	2.80	22.54	1.522
35.4	912	83.7	09	488.1	14	488.1	149	99.	2.81	02.52	1.524
30.8	26	23	0.44	73	83.8	42	38	3.842	99.	2.79	52.49	51.526
27.2	90	20	5.6	06	358.	32	63	58.32	699	2.82	12.47	81.529
24.1	72	18	6.4	37	327.	99	23	27.992	99.	2.84	72.30	82.453
21.5	81	16	7.3	15	291.	72	02	91.720	99.	2.84	72.38	91.926
19.3	80	14	7.7	72	255.	10	42	55.104	999.	2.86	42.66	01.94
17.5	25	13	3.4	56	229.	59	42	30.000	99.	2.83	62.64	41.965
15.9	15	12	3.1	19	202.	00	02	08.371	999.	2.84	12.68	81.98
14.5	25	11	0.8	95	182.	05	71	88.400	999.	2.73	42.69	31.991
13.2	88	10	6.0	00	159.	50	0	166.000	99.	2.73	42.74	91.820
12.1	31	9.2	30	137.	000	143.	900	99.		2.77	12.65	61.85
11.1	00	78.4	19	116.	087	120.	487	712.	534	712.534	999.	2.56	02.63	61.88
10.1	87	68.8	78	96.	936	102.	633	431.	989	431.989	999.	2.76	92.47	11.915
9.3	67	60.9	24	84.6	86	88.2	433	00.	924	300.924	999.	2.58	92.65	01.97
8.6	46	53.5	56	73.7	10	76.5	79	21	8.66	122	7.800	999.	2.78	22.67	22.05
7.9	84	48.3	36	65.4	94	68.3	09	176.	863	179.	682	399.	002	2.77	12.64	72.14
7.3	92	43.0	7	55.6	72	57.9	89	129.	500	139.	461	421.	002	2.62	62.63	32.242
6.8	62	38.4	91	50.1	14	51.9	84	110.	89	512	1.403	388.	002	2.59	32.60	62.34
6.3	87	34.6	80	44.3	10	46.0	72	91.8	38	93.1	49	317.	002	2.66	82.79	12.44
5.9	62	31.4	99	39.6	87	41.2	86	77.6	82	78.7	68	275.	600	2.57	82.59	42.53
5.5	79	28.4	75	35.5	65	36.9	72	66.1	37	67.1	85	240.	002	2.75	22.72	82.583	.40
5.2	30	26.4	69	32.7	09	34.1	54	59.7	79	60.5	97	214.	100	2.66	12.73	41.923	.48
4.9	13	24.4	13	30.0	84	31.4	02	53.2	78	54.2	01	186.	900	2.75	12.71	21.99	.70
4.6	30	22.5		27.5	78	28.8	53	47.5	08	48.1	40	162.		2.70	2.67	52.19	1.2
4.3	69	20.9	45	25.4	61	26.5	11	42.6	60	43.0	39	145.	500	2.61	32.65	72.46	1.46
4.1	30	19.4	54	23.3	42	24.4	92	38.5	61	39.2	86	136.	800	2.42	62.68	22.55	1.56
3.9	07	18.1	09	21.6	03	22.6	99	34.9	41	35.4	94	122.	600	2.67	42.70	12.60	41.59
3.7	00	16.8	78	20.1	19	21.0	61	30.8	2	31.1	4	110.	500	2.42	72.70	02.393	.385
3.5	05	15.8	74	18.6	03	19.6	14	28.1	3	29.5	0	101.	000	2.46	92.70	32.57	41.60
3.3	24	14.7	64	17.3	14	18.2	85	26.7	18	27.1	66	91.	100	2.39	62.70	12.55	1.60
3.1	56	13.8	67	16.0	50	17.2	00	24.2	8	24.9	0	85.	800	2.56	2.70	22.50	01.593
3.0	00	13.0	20	15.0	72	16.0	14	22.6	99	23.1	14	76.	600	2.47	52.61	82.37	1.48
2.8	56	12.2	75	14.1	86	15.0	80	21.1	24	21.5	28	72.	000	2.52	62.64	42.16	1.26
2.7	20	11.5	75	13.3	45	14.1	93	19.6	60	20.0	50	66.	900	2.45	32.64	81.94	.92
2.5	93	10.8		12.4	10	13.2	32	17.8		18.4	41	60.1	2.44	2.61	61.88	0	.757
2.4	74	10.1	86	11.6	41	12.4	28	16.7	66	17.0	89	53.	718	2.43	52.60	91.92	.83
2.3	63	9.5	90	10.9	07	11.6	72	15.5	60	15.8	90	49.	004	2.41	52.65	71.96	.90
2.2	61	9.1	08	10.2	94	11.0	36	14.6	12	14.9	07	45.	851	2.37	52.60	62.04	1.24
2.1	66	8.6	42	9.7	41	10.4	59	13.7	56	14.0	36	42.	811	2.32	62.61	52.13	1.44
2.0	79	8.2	05	9.2	70	9.9	75	13.1	22	13.3	94	40.	716		2.61	72.28	1.72
1.9	97	7.8	70	8.8	38	9.5	56	12.4	59	12.7	37	39.	334		2.61	12.43	1.95
1.9	19	7.5	5	8.4	26	9.1	37	11.7	91	12.0	73	37.	6		2.61	2.58	2.12
1.8	46	7.1	96	8.0	47	8.7	32	11.2	88	11.5	52	35.	864		2.62	32.72	22.26
1.7	76	6.8	88	7.6	82	8.3	74	10.7	11	11.0	13	34.	420		2.67	42.74	62.36
1.7	12	6.5	92	7.3	44	8.0	30	10.1	86	10.4	61	32.	991		2.71	12.75	52.4
1.6	50	6.3	01	7.0	14	7.6	94	9.7	24	9.9	89	31.	159		2.74	02.68	52.39
1.5	92	6.0	57	6.7	32	7.3	99	9.3	04	9.5	74	29.	782		2.75	52.66	42.38
1.5	37	5.8	25	6.4	48	7.1	20	8.9	10	9.1	74	28.	456		2.76	02.63	22.37
1.4	84	5.6	19	6.1	81	6.8	43	8.6	01	8.8	47	27.	606		2.76	82.60	12.36
1.4	33	5.3	74	5.9	33	6.5	79	8.1	86	8.4	87	26.	284		2.76	92.60	02.35
1.3	86	5.1	70	5.7	06	6.3	59	7.8	65	8.1	15	25.	448		2.76	32.56	82.34
1.3	41	4.9	77	5.4	77	6.1	27	7.5	62	7.8	05	24.	492		2.76	42.55	82.32
1.2	97	4.7	67	5.2	41	5.8	82	7.2	23	7.4	61	23.	040		2.74	42.53	32.31
1.2	55	4.5	85	5.0	20	5.6	50	6.8	70	7.1	10	21.	924	2.5	172.61	32.58	92.30
1.2	16	4.4	07	4.8	15	5.4	35	6.5	90	6.8	30	20.	837	2.0	432.66	82.54	12.28
1.1	77	4.2	36	4.6	20	5.2	34	6.3	30	6.5	60	19.	837		2.72	52.51	2.25
1.1	41	4.0	71	4.4	33	5.0	43	6.0	73	6.3	00	18.	949		2.76	22.49	22.22
1.1	06	3.9	15	4.2	60	4.8	61	5.8	30	6.0	90	17.	966		2.70	32.46	82.17
1.0	72	3.7	62	4.0	93	4.6	86	5.5	90	5.8	10	17.	172		2.65	32.52	02.06
1.0	40	3.6	16	3.9	36	4.5	18	5.3	74	5.5	84	16.	339		2.51	12.52	82.068
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.9	79	3.3	46	3.6	34	4.1	98	4.9	52	5.1	53	14.	664		2.69	92.33	32.19
.9	51	3.2	17	3.4	92	4.0	47	4.7	57	4.9	55	13.	874		2.60	12.45	62.280
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.825	2.665	2.865	3.385	3.953	4.133	10.753	2.68	52.15	1.82	
.803	2.571	2.762	3.270	3.817	3.993	10.260	2.72	72.15	41.76	
.781	2.479	2.663	3.172	3.679	3.852	9.770	2.71	52.28	1.73	
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.687	2.090	2.237	2.721	3.121	3.282	7.955		2.81	92.03	
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.622	1.836	1.950	2.427	2.757	2.915	6.892		2.85	2.22	
.607	1.777	1.886	2.361	2.678	2.834	6.637		2.86	2.25	
.593	1.721	1.825	2.297	2.601	2.756	6.401		2.87	2.27	

000.144					.10040335 E+01
.084					.10059716 E+01
.250					.10085924 E+01
.404					.10119003 E+01
.889					.10153530 E+01
1.350	.295				.10194915 E+01
2.311	.471				.10240062 E+01
3.529	.818				.10284504 E+01
4.943	.904				.10335616 E+01
7.322	1.098				.10390856 E+01
9.322	.80				.10442539 E+01
11.601	.700				.10499690 E+01
14.87	1.110	7.338			.10555707 E+01
18.122	1.88	8.5			.10614998 E+01
22.020	2.6	10.0			.10669828 E+01
27.626	3.330	11.2			.10730918 E+01
27.864	3.548	12.5			.10785874 E+01
35.312	4.567	13.715			.10843181 E+01
42.038	5.8	15.			.10905935 E+01
48.678	7.3	16.8			.10957055 E+01
54.052	8.8	18.1			.11017059 E+01
60.083	10.927	19.593			.11071056 E+01
64.977	12.056	.742			.11122901 E+01
77.899	12.661	6.095			.11173825 E+01
83.305	10.979	6.4			.11228172 E+01
97.144	12.734	6.8			.11276960 E+01
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117.098	15.520	7.839			.11371081 E+01
123.080	15.783	18.830			.11413858 E+01
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142.035	20.238	17.0			.11499011 E+01
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156.083	24.434	14.6			.11573735 E+01
188.918	26.852	13.5			.11614852 E+01
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277.847	41.921	7.356	6.		.11796616 E+01
291.277	44.976	22.304	8.		.11822350 E+01
325.568	49.133	20.0	14.		.11845544 E+01
332.	53.	18.4	18.		.11865519 E+01
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278.270	66.473	18.157	1478.	19	.11947537 E+01
325.561	70.806	14.947	108.		.11963426 E+01
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429.243	79.510	20.595	34.465		.11993455 E+01
360.505	87.573	30.1	51.8		.12009454 E+01
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	393.	102.108	83.443	403.675		.12043491E+01
	396.	107.580	76.	340.		.12050691E+01
	400.642	108.976	64.	259.		.12067255E+01
	406.	117.488	52.	210.		.12073447E+01
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		133.322	36.	120.		.12092015E+01
		138.475	31.8	81.		.12099530E+01
		143.5	30.8	57.		.12105282E+01
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		164.053	31.414	19.5		.12120670E+01
		171.439	32.195	9.0		.12127263E+01
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		239.732	50.412	14.5		.12156483E+01
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.088		311.716	81.287	20.128	6500.	.12165291E+01
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			122.	47.0		.12132737E+01
			144.388	48.		.12129561E+01
			155.	51.		.12121884E+01
			164.	56.		.12120564E+01
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-.51088316E-02	.11210435E-02	-.11886647E-03	.58783242E-05	-.10814593E-06
-.72186773E-02	.14225237E-02	-.14111194E-03	.66914334E-05	-.11980721E-06
-.10267103E-01	.19859984E-02	-.19498321E-03	.91950066E-05	-.16415866E-06
-.14245915E-01	.28139927E-02	-.28115056E-03	.13437614E-04	-.24230877E-06
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-.26131735E+00	.64271190E-01	-.72754737E-02	.37467921E-03	-.70793358E-05
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-.36629296E+00	.90982954E-01	-.10269137E-01	.52570012E-03	-.98751434E-05
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-.37232571E+00	.92206793E-01	-.10369838E-01	.52916608E-03	-.99150840E-05
-.37385404E+00	.92521425E-01	-.10396121E-01	.53009035E-03	-.99261452E-05
-.37506964E+00	.92727292E-01	-.10407283E-01	.53013042E-03	-.99190754E-05
-.37668731E+00	.93074957E-01	-.10438065E-01	.53130967E-03	-.99352238E-05
-.37738192E+00	.93098117E-01	-.10423582E-01	.52983961E-03	-.98970312E-05
-.37879579E+00	.93375409E-01	-.10444441E-01	.53043021E-03	-.99009704E-05
-.37972521E+00	.93481251E-01	-.10441243E-01	.52960782E-03	-.98758739E-05
-.38078480E+00	.93635483E-01	-.10444841E-01	.52918176E-03	-.98588646E-05
-.38159628E+00	.93703760E-01	-.10435839E-01	.52801171E-03	-.98265157E-05
-.38245741E+00	.93781724E-01	-.10428664E-01	.52693158E-03	-.97957581E-05

```
-.38317627E+00 .93812360E-01-.10414347E-01 .52542786E-03-.97562349E-05
-.38389147E+00 .93841810E-01-.10399708E-01 .52389703E-03-.97160336E-05
-.38422579E+00 .93736706E-01-.10366139E-01 .52125106E-03-.96528487E-05
-.38470337E+00 .93676237E-01-.10338166E-01 .51890823E-03-.95955598E-05
-.38518653E+00 .93618256E-01-.10310387E-01 .51656750E-03-.95381665E-05
-.38523503E+00 .93400300E-01-.10259642E-01 .51286035E-03-.94524679E-05
-.38541494E+00 .93224969E-01-.10214321E-01 .50944720E-03-.93724564E-05
-.38554613E+00 .93025953E-01-.10165031E-01 .50577736E-03-.92868621E-05
-.38503845E+00 .92596007E-01-.10082920E-01 .50016376E-03-.91610925E-05
-.38515389E+00 .92377917E-01-.10029531E-01 .49619830E-03-.90686893E-05
-.38516918E+00 .92113527E-01-.99686511E-02 .49175586E-03-.89659814E-05
-.38481991E+00 .91711352E-01-.98877062E-02 .48610989E-03-.88382291E-05
-.38416494E+00 .91188823E-01-.97887816E-02 .47936677E-03-.86873630E-05
-.38363713E+00 .90693381E-01-.96920228E-02 .47269105E-03-.85370969E-05
KALAMAMB

ABCDEFGHIJKLMNOPQRSTUVWXYZ
A0 001
```

Graph titles

```
RADIAL DISTANCE FROM CENTER(MILS)-WT PERCENT OF U WT PERCENT OF PU WT PERCENT OF
U+PU WT PERCENT RATIO  PU/U WT PERCENT RATIO  PU/(U+PU)0     0     0     0     0
0     0     0     0     0     0     9     8     7     6     5     4     3     2     1SX.
0         10        20        30        40        50        60        70        80        90        1
00        110       120       130     * :PU/U . :PU/(U+PU)
RADIAL DISTANCE FROM CENTER(MILS)   WT PERCENT OF U WT PERCENT OF PUWT PERCENT O
F U+PU  WT PERCENT RATIO  PU/U  WT PERCENT RATIO  PU/(U+PU)
/*
```

APPENDIX B

List of Symbols

Common Designation	Program Designation
Atomic number	AT.NO.
Atomic weight	AT.WT.
Analytical-line wavelength	WAVE
Analytical-line excitation	EC
Absorption edge of analytical line	EDGE
Fluorescent yield	W
Mean ionization potential, J	PF
Overvoltage ratio	U
Backscatter factor	R
Z/A	WS
$\lvert E_o + E_c \rvert / 2$	E
$\ln 1.166\bar{E}$	VAL
Electron-energy coefficient, σ	SIGMA
h in Philibert's equation	HS
$1 + \chi/\sigma$	US
$f(\chi)$	FS
$f(\chi)\ R/S$	FACT
Mean backscatter factor	RAL
Mean atomic number, $\bar{Z}$	ZAL
Mean $(\bar{Z}/\bar{A})$	WSAL
Mean h value, $\bar{h}$	HAL
Mean ionization potential, $\bar{J}$	PAL
Chi for an alloy, χ	YP
Mean overvoltage ratio	UAL
$f(\chi)$ for an alloy	FAL

APPENDIX C

Programming Notes for Plotting Subroutines

1. Subroutine GRAPHS

Subroutine GRAPHS calls plotting subroutines depending on the value of a variable MARY, which is read from the graph options card. This routine also calculates the plutonium-to-uranium and plutonium-to-uranium-plus-plutonium ratios, which are then plotted. The ratios to be plotted and the graph axis labels were determined when the program was written. For other ratios or axis labels, minor changes in the program would be necessary. The axis labels in use at ANL appear at the end of the listing. A test variable JIM ensures that the printer-plot subroutine PPLOT is called only once. Another test variable LET prevents calling the CALPLT and PPLOT subroutines more than once.

2. Subroutine CALPLT

All graphs generated by this subroutine are automatically scaled based on the range of values to be plotted, except the graphs of uranium-plus-plutonium wt % versus distance and of uranium, plutonium, and uranium-plus-plutonium versus distance. For these plots, the ordinate limits are always 0 and 100 wt %.

3. Printer Subroutine PPLOT

This subroutine is more restrictive with regard to scaling of the printer graph axes. All scaling is preset, and the maximum distance that can be plotted is 134 mils. Because the routine determines the location of a point by truncation, the points on the graph are located to within 2 wt % on the y axis and 1.25 mils on the x axis.

APPENDIX D

Listing of MAGRAM Input and Output

1. MAGRAM Input

A0120	Problem Number and Identification
HOV15 45-82 RADIAL DISTN. OF U & PU	
25.0 2 10.0 9.13 45.0 3.03.0	Microprobe analysis conditions (K.V., No. of standards, counting time, etc.)
U MA PU MB C	
1UO2 .8810 0	Identification of characteristic x-ray lines and compound standards
2PUO2 .8835 0	
1	
43000 22500	X-ray intensities measured on the standards (beam current and total counts in 10 sec.)
1	
43000 84000	
1	
43000 310 2550	Background matrix $\begin{array}{c} \text{on } UO_2 \\ \text{on } PuO_2 \end{array} \begin{array}{c} \begin{array}{cc} UMa & PuMB \end{array} \\ \begin{bmatrix} D & T \\ T & D \end{bmatrix} \end{array}$ D = Spectrometer Detuned to obtain background; T = Spectrometer tuned to analytical line
1	
43000 310 1550	
1000 500	Radioactive background, beam turned off
42950 19500 18380	
43100 19640 18270	X-ray intensities measured on the sample and beam current
43200 19600 18730	
43450 19290 19050	
43500 19470 18700	
99999	Card indicating end of data set
54444	Graph Options Card
92.0	
95.0	
98.0	Radial position cards
104.0	
107.0	
0.000	Card indicating end of problem

2. MAGRAM Output

PROBLEM NUMBER A 120

ELEMENT	AT. NO.	AT. WT.	PF	EDGE	EC	WAVE	U	R
U	92	238.030	1243.786	3.497	3.545	3.910	7.05	0.647279
PU	94	239.000	1270.345	3.282	3.778	3.505	6.62	0.641683
O	8	15.999	0.0	23.320	0.532	23.620	20.00	0.952346

MASS ABSORPTION COEFFICIENTS

RADIATION ABSORBER	U MA	PU MB
U	606.	493.
PU	764.	612.
O	172.	126.

	WS	E	VAL	SIGMA	HS	US	FS	FACT
U	0.3865	14.2725	9.7193	2146.62	0.1266	1.3992	0.6932	0.44765
PU	0.3933	14.3890	9.7275	2158.82	0.1217	1.4011	0.6928	0.43806

ESP = 0.25455039E 04

STANDARD INTENSITIES CORRECTED FOR DEADTIME AND DRIFT

BEAM CURRENT	U	PU
43C00.0	23058.41	861 71.44

COUNTING INTERVAL. 10.0 SECOND(S)

BACKGROUNDS

CONTRIBUTED TO BY 100 % OF	U MA	PU MB
U	31C.C	2552.0
PU	31C.C	1550.7

PROBLEM NUMBER A 120

ELEMENT	ATOMIC NUMBER	ATOMIC WEIGHT	BACKSCATTER FACTOR	EXCITATION POTENTIAL	ABSORPTION JUMP RATIO	FLUORESCENT YIELD
U	92	238.030	0.647	3.545	0.00	0.000
PU	94	239.000	0.642	3.778	0.00	0.000
O	8	15.999	0.952	0.532	21.10	0.004

MASS ABSORPTION COEFFICIENTS

RADIATION ABSORBER	U MA	PU MB
U	606.	493.
PU	764.	612.
O	172.	126.

COUNTING INTERVAL. 10.0 SECOND(S)

BACKGROUNDS

CONTRIBUTED TO BY 100 % OF	U MA	PU MB
U	310.0	2552.0
PU	310.0	1550.7

MBER A 120

INTENSITIES (CPS X COUNTING INTERVAL)
CORRECTED FOR DEAD-TIME AND DRIFT

U	PU
18636 / 23058	18002 / 86171
18712 / 23058	17829 / 86171
18629 / 23058	18250 / 86171
18211 / 23058	18466 / 86171
18370 / 23058	18095 / 86171

STANDARD BACKGROUNDS (CPS X COUNTING INTERVAL)

310 1551

DEAD-TIME (MICROSECONDS)

3.0 3.0

COUNTING INTERVAL, 10.0 SECONDS

PROBLEM NUMBER A 120

INDIVIDUAL K-RATIOS CORRECTED FOR
DEAD-TIME, DRIFT AND BACKGROUND ONLY

N	U	PU
3	0.8074	0.1883
3	0.8108	0.1862
3	0.8071	0.1912
3	0.7889	0.1941
3	0.7959	0.1896

NOTE

U DETERMINED RELATIVE
TO A STANDARD OF U02

PU DETERMINED RELATIVE
TO A STANDARD OF PU02

PROBLEM NUMBER A 120

SUBMITTED BY

DESCRIPTION - HOV15 45-82 RADIAL DISTN. OF U & PU

ACCELERATING VOLTAGE 25.0 KEV

X-RAY EMERGENCE ANGLE 45.0 DEGREES

STANDARD PEAK-TO-BACKGROUND RATIOS (P/B) AND
MINIMUM DETECTABILITY LIMITS (MDL)

ELEMENT	P/B	MDL
U	83/1	0.2393 WT %
PU	61/1	0.1446 WT %

CHEMICAL COMPOSITION
WEIGHT PERCENT
ATOMIC PERCENT

O DETERMINED BY DIFFERENCE

OBS	U	PU	O
1	72.206	15.681	12.114
	26.538	5.826	67.236
2	72.491	15.503	12.006
	27.195	5.792	67.013
3	72.193	15.924	11.884
	27.258	5.988	66.754
4	70.592	16.180	13.228
	24.899	5.684	69.417
5	71.185	15.800	13.015
	25.373	5.609	69.018

SUBMITTED BY

DESCRIPTION - HOV15 45-B2 RADIAL DISTN. OF U & PU

MEAN CHEMICAL COMPOSITION AND TWO
SIGMA LIMITS BASED ON 5 ANALYSES

ELEMENT	WEIGHT PERCENT	ATOMIC PERCENT
U	71.738 - 1.451	26.337 - 1.993
PU	15.822 - 0.462	5.785 - 0.265
O *	12.439 - 1.121	67.878 - 2.216

* DETERMINED BY DIFFERENCE

MEAN INTENSITY RATIOS AND TWO SIGMA LIMITS

ELEMENT	K
U	0.8020 - 0.0166
PU	0.1898 - 0.0054

ACCELERATING VOLTAGE 25.0 KEV

X-RAY EMERGENCE ANGLE 45.0 DEGREES

DENSITY 9.13

DEPTH OF ANALYZED REGION 1.13 MICRONS

STANDARD PEAK-TO-BACKGROUND RATIOS (P/B) AND
MINIMUM DETECTABILITY LIMITS (MDL)

ELEMENT	P/B	MDL
U	83/1	0.2393 WT %
PU	61/1	0.1446 WT %

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