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**SAP3: A Computer Program for
X-Ray Fluorescence Data
Reduction for Environmental
Samples**

April 1977

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Battelle
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**SAP3: A Computer Program for
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Reduction for Environmental
Samples**

by
Kirk K. Nielson

April 1977

**Battelle
Pacific Northwest Laboratories
Richland, Washington 99352**

SAP3: A COMPUTER PROGRAM FOR X-RAY FLUORESCENCE DATA REDUCTION
FOR ENVIRONMENTAL SAMPLES

Kirk K. Nielson

ABSTRACT

A FORTRAN computer program is presented for quantitative multielement analysis of spectral data from both isotope- and x-ray tube-excited x-ray fluorescence systems. The program is designed for analysis of pelletized environmental samples (20-200 mg/cm²) using thin film spectrometer calibrations and subsequent mathematical matrix corrections for self absorption, particle size effects and enhancement. A background-independent direct peak analysis method permits rapid determination of net peak areas and peak overlap corrections. Matrix-corrected quantities of 24 elements can be determined from 1024 channels of raw spectral data in 20-40 sec with relative accuracies of a few percent. Options for applying the program to spectra from in-situ seabed analyses are also included.

SAP3: A COMPUTER PROGRAM FOR X-RAY FLUORESCENCE DATA REDUCTION
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Kirk K. Nielson

A computer program, SAP3, has been developed to automate spectral analysis and quantitative interpretation of x-ray fluorescence data from environmental samples. SAP3 was primarily developed for use with pelletized solid samples, but recent application has also been made to in-situ seabed analysis. SAP3 smooths spectral data, computes net peak areas, and computes elemental concentrations from a thin film spectrometer calibration. It then performs peak overlap corrections and three matrix corrections for (a) self absorption, (b) particle size and (c) enhancement. Spectral analysis and corrections require no operator attention beyond entry of sample parameters such as weight, analysis livetime, and if particle size corrections are desired, the estimated mean particle size and density.

SAP3 is unique among other x-ray data reduction programs in two major respects: its peak analysis method and its matrix correction method. Peak analysis uses a modification⁽¹⁾ of the Covell method⁽²⁾ which yields partial net peak areas which are independent of linear background and are proportional to the total net peak areas. The method is thus of particular advantage for x-ray fluorescence spectra, which are frequently too crowded for reliable background subtraction. The method has good precision and permits corrections for peak overlap using simple peak ratio (alpha) coefficients.

Matrix corrections rely on estimating an approximate light element ($Z \leq 13$) content of the sample from the incoherent and coherent scatter peaks after they have been corrected for absorption and for scattering from the heavy ($Z > 13$) elements, as illustrated in Figure 1. The total sample absorption due to both light and heavy elements is iteratively computed and used in self absorption, particle size and enhancement corrections. Since the corrections are based on the thin sample x-ray calibration, repeated calibrations for specific sample types are avoided. Samples having average atomic numbers ranging from

5 to 13 have been successfully analyzed by SAP3. Details of the theory and description of the peak analysis and matrix correction methods have been reported separately.^(1,3)

EXPERIMENTAL

Instrumentation. SAP3 was written to analyze data from three independent x-ray fluorescence systems: a Kevex Model 810 tube-excited system (Kevex, Inc., Burlingame, CA), a radioisotope-excited laboratory system, and a radioisotope-excited in-situ seabed analyzer.⁽⁴⁾ The Kevex system uses a tungsten anode x-ray tube to excite a secondary fluorescer of Ti, Cu, Zr, Mo, Ag, Sn, or Cs, which in turn excites the sample pellets. Samples are mounted in 35 mm slide frames and are held in an automated 16-position carousel in vacuum for sequential analysis. X-ray spectra are collected with an 80 mm² Si(Li) diode (Kevex, Inc.) having 200 eV resolution FWHM at 6.4 keV. Data are accumulated by a computer based analyzer system (Model 4410, Nuclear Data, Inc., Palatine, IL) which also operates a high speed paper tape punch (using ND41-1104 software) and the sample changer. Analysis to a preset livetime is controlled by a clock time base (Model ND-536CTB, Nuclear Data, Inc.) which corrects for dead time in the amplifiers and multichannel analyzer system.

The radioisotope-excited laboratory system uses Fe-55, Cd-109 or Am-241 sources for excitation and is equipped with an automated 11-position carousel in a vacuum chamber. The detector, multichannel analyzer and timing systems are similar to those used with the tube-excited system.

The in-situ seabed analyzer uses Cd-109 or Am-241 excitation and a down-looking 80 mm² Si(Li) detector. Resolution of 225 eV FWHM at 5.9 keV is achieved with the system under water and connected by 50 ft of cable to the amplifier and multichannel analyzer. The shipboard multichannel analyzer (Model NS 710A, Tracor Northern, Middleton, WI) is connected to a cassette tape system for storing data to be analyzed later by the PDP-15.

The PDP-15/20 computer used for data analysis has 24000 words memory and the input/output devices listed in Table I. The computer also has seventeen sense switches which permit operator interaction with the program during execution. Table II lists the options provided by the switches in SAP3.

Sample Preparation. Samples to be analyzed by either of the laboratory systems are usually pelletized directly from 180 to 1500 mg of dry sample in a 3.2 cm diameter, 27000 kg laboratory press. Geological and certain environmental samples such as flyash are similarly pelletized after first mixing with equal weights of cellulose (TLC reagent grade, J. T. Baker, Phillipsburg, NJ) in a tungsten carbide mixer mill (Model 5100, Spec, Inc., Metuchen, N. J.). Coarse solids requiring powdering are ground several minutes in the mixer mill before mixing with cellulose. No preparation is required for the seabed analyzer since it rests directly on the sediment surface under fresh or salt water.

Calibration. Calibration for SAP3 uses thin uniform deposits (50-120 $\mu\text{g}/\text{cm}^2$) of single metals or binary compounds evaporated onto 0.013 mm mylar backings (Micromatter, Inc., Seattle, WA). Sensitivities determined from the foils are plotted as a function of x-ray energy and the resulting curves are smoothed to establish the multielement thin-sample sensitivity curves shown in Figure 2. The thin standards are analyzed under identical conditions to those used for the samples except in the case of the seabed analyzer. Peak overlap coefficients are also determined from these standards. Calibration of the scatter peaks relies on analysis of a standard reference material. The spectrum from this analysis is then analyzed with various scatter peak calibration constants (using switch 13) until satisfactory results are obtained. The constants are then entered in the library for use in future analyses. The constants depend only on the instrumental geometry and excitation conditions.

PROGRAM DESCRIPTION

Main Program. The controlling routine, SAP3, is always resident in core and controls data analysis by calling various subroutines as illustrated by the flowchart in Figure 3. SAP3 also uses several sense switches (0, 1 and 15) to give the operator control over input/output options as indicated in Table II. The array EXT is also defined by SAP3 for use as hollerith sample numbers in accessing input data files stored on disk or DECTAPE.

BEG. Subroutine BEG is first called to read library data and initialize analysis parameters. The desired library name (FYLIB) is read from the computer terminal, after which the library is read from Disk 2. The various library parameters are listed in Table III. Figure 4 shows a typical library

for the zirconium secondary source on the Kevex 810 system. The computer terminal is next used to enter the following sample information: date analyzed, analysis livetime, particle size and density, sample series name, sample thickness (g/cm²) and beginning run number. The peak energy, calibration, peak overlap and blank data are then listed on the line printer as shown in Figure 5.

Parameters from log-log fits to x-ray cross sections as compiled by McMaster et al.⁽⁵⁾ are next used to compute mass absorption coefficients for all the heavy and light elements in the library. They are computed as the sum of the photoelectric, coherent and incoherent scattering cross sections, and are stored as cm²/μg in the arrays XE, XH, XEL and XL in the form

$$\begin{aligned} XE &= \mu_j(k) \csc\theta \\ XH &= \mu_j(k) \csc\theta + \mu_j(i) \csc\phi \\ XEL &= \mu_j'(k) \csc\theta \\ XL &= \mu_j'(k) \csc\theta + \mu_j'(i) \csc\phi, \end{aligned}$$

where $\mu_j(i)$ is the mass absorption coefficient of element j for x-rays from element i, $\mu_j(k)$ is the mass absorption coefficient for element j for the exciting radiation, $\mu_j'(k)$ and $\mu_j'(i)$ are the corresponding coefficients for the light element set, and θ and ϕ are the mean angles formed by the exciting and fluorescent radiation with the specimen surface. The summary data file, FYL, is then established with all zero values and control returns to SAP3.

RED/MR51. If switch 0 is off, data are to be read in from paper tape using subroutine RED. Actual reading of the tape is done in single 8-bit character increments using subroutine MR51. Each value returned by MR51 is examined by RED until a non-zero number is encountered. Successive groups of three characters are then read and combined for individual channel counts until the preset number of channels (NOCH) have been read. Sense switch 10 is checked by RED to halt the program until the operator has the paper tape ready.

REDDT. If spectra have been previously stored or transferred to DECTAPE or disk, they are read as a binary file using their series name, with the run number as the extension. Subroutine REDDT reads the binary files and provides three options if the requested file is not found: terminate immediately,

print a summary report of the analyses and terminate, or read a new series name and number and continue data analysis. Figure 3 illustrates these options.

LIST. Subroutine LIST prints the raw spectral data with the line printer as shown in Figure 6 and is called unless switch 1 is on.

SMOTH. Subroutine SMOTH is next called to smooth the spectral data using a 5-point least squares polynomial smoothing function.⁽⁶⁾ Smoothing is done on square root transformed data, after which the data are squared to restore their original form. The raw data remain unchanged in array RD, and the smoothed spectrum is located in array SM.

PKAR. Subroutine PKAR computes an energy scale for the spectrum using the coherent K_{α} scatter peak and the Fe K_{α} fluorescent peak. Centers of these peaks are located by searching over a 20 channel region of the expected location (assuming 25 ev/channel) and computing the peak centers by a least squares quadratic fit.⁽⁷⁾ If switch 4 is off, the energy scale from the previous spectrum is used. Peak locations in terms of channel number for all other peaks are then computed from the known energy, EN. From peak locations, integration windows are defined using a centered window of width

$$W = WM * (EN * WS + WI) ,$$

where WM is a width multiplier permitting selection of different window widths, and WS and WI are linear parameters to change the window width with peak energy. If WM equals unity, values of 0.3245 and 5.379 for WS and WI give a width which approximates the standard deviation (σ) of the K_{α} peak distributions, assuming a gaussian shape. The best value for WM has been discussed elsewhere⁽¹⁾ and may vary from about 1.2 to 1.7. Net peak areas (A) and backgrounds (B) are then computed by the modified Covell method, along with uncertainties (DA) based on counting statistics. Scatter peak areas are also computed here. A description of the formulas is given in Reference 1. If sample thickness and weight vary from sample to sample, the current values can be entered by using switch 8.

QUAN. Subroutine QUAN uses net peak areas and thin film calibration data to compute elemental concentrations in the sample. Since matrix effects are important in the relatively thick (20-200 mg/cm) samples considered here,

three types of corrections are also employed for self absorption, enhancement and particle size effects. Since the corrections and the resulting concentrations are interdependent, calculations are iterative to achieve self consistent results.

In the first iteration, uncorrected concentrations are arbitrarily increased to approximate self absorption and thereby reduce iterative calculation time. Self absorption (COR) and scattering (YC,YI) by the heavy elements are first computed, and the difference between the observed scatter and that from the measured elements is determined (VC,VI). This excess scatter (both coherent and incoherent, computed separately) is then attributed to two light elements whose incoherent/coherent scattering cross section ratios most nearly approximate that of the excess scatter (R). Simultaneous equations are then solved for the quantities of the two light elements, TH1 and TH2, which are proportional to the excess incoherent and coherent intensities illustrated in Figure 1.

Once the representative light element concentrations are estimated, their additional absorption is added and the total is stored in CORL. Sample absorption of only the exciting radiation is stored in UK for the heavy element contribution, and UN for the total (heavy plus light element contributions). Particle size correction factors (FPS) are next computed unless switch 14 is off, and all three matrix corrections are applied to compute new elemental concentrations. Self absorption corrections are also applied to the measured scatter (SMI,SMC), and peak overlap corrections are applied to the corrected concentrations. The entire process is then repeated until, after five iterations, enhancement corrections (SF) are also included. When the total absorption for element 2 of the analysis list changes by less than 0.01%, iteration terminates and uncertainties from peak overlap corrections are added to the statistical peak uncertainties computed by PKAR. Corrected elemental quantities are stored in QC.

Equations for enhancement corrections were derived from those of Clark,⁽⁷⁾ and equations for particle size corrections were derived from those of Berry et al.⁽⁸⁾ A more detailed explanation of this correction scheme is given in Reference 3.

PRNT. Subroutine PRNT prints the multielement analysis results on the line printer for each sample as shown in Figure 7 unless prevented by switch 11. It

also stores elemental concentrations on a disk file for the summary report. Sample analysis parameters are first printed, followed by a table including the integration window boundaries in channel numbers, the net peak area and uncertainty (including overlaps), the background area, the particle size correction factor, the self absorption correction factor, the enhancement correction factor, the magnitude of the peak overlap correction, the peak identification, the concentration and uncertainty after all corrections are applied, and the two-sigma detection limit for the element in the given sample matrix. In cases where the detection limit exceeds the concentration, the detection limit is also printed in the concentration column and is flagged with a < symbol. The uncertainty printed in such cases is replaced by the actual computed concentration to permit comparison of the computed concentration with the detection limit.

After the analysis printout, concentrations and uncertainties are stored in adjacent locations for each element in the disk file FYL. RD and SM are used as working arrays since the current spectral data have no further use. Concentrations below the detection limit are flagged in this file by zeroing the uncertainty and storing only the detection limit.

REP. Subroutine REP is called when no further data are to be analyzed, as signalled by turning on switch 15 for paper tape input or by typing an instruction for the file input mode. Subroutine REP reads the file FYL as generated by PRNT, and deletes FYL from the disk. Appropriate headings are then printed with six elements per page and concentrations and uncertainties are printed from each spectrum in the series as illustrated in Figure 8. If the uncertainty is zero, the number in the concentration position is appropriately flagged with the < symbol. The program terminates immediately after REP has been executed.

SPECIAL OPTIONS. Several additional options are available to the user through use of the sense switches indicated by Table II. Switch 2 may be used in cases of a very low average Z (atomic number) sample such as paraffin, for which oxygen may not be the best light element to hold fixed. Switch 8 makes attenuation corrections for mylar sample covers using factors stored in the array RAB. These are applied by subroutine QUAN. Switch 9 is used with data from the in-situ x-ray fluorescence system which stores livetime in channel 1 of the spectrum. Since sample weights are not known, they are estimated from the scatter and used to

normalize computed elemental masses. The self absorption function must also be modified for infinitely thick samples, as done by switch 9. Switch 12 causes all corrections to depend on the scatter determined sample thickness instead of normalizing to a known sample pellet thickness. This switch is usually used with switch 9. Switch 13 permits reading of new scatter peak calibration constants for an individual spectrum to permit rapid calibration of the scatter peaks when making up a new library. Switch 16 can be used to terminate iterations by QUAN before convergence is reached.

DISCUSSION

The SAP3 program as listed in the Appendix was fitted to a 24K, PDP-15 computer using the overlay structure described in the comments of the main program listing (Appendix). The time required for reducing 1024 channels of raw spectral data to matrix corrected quantities of 24 elements is approximately 20 sec for most homogeneous samples and 20-40 sec for particulate samples. Low-Z samples are analyzed fastest because of the smaller effect of varying correction factors on the bulk sample composition. The number of iterations in the correction loop in QUAN is usually 5-15.

The precision and accuracy of the peak analysis and matrix correction methods used by SAP3 has been discussed elsewhere in evaluations using standard reference materials.^(1,3) Concentrations with accuracies of 1-5 percent relative error have been routinely obtained in analyses of effluent, biological and geological materials having adequate peak counting statistics. Concentration precisions determined from repeated analyses are usually comparable to the appropriately combined precisions of the given peak, its overlapping peaks, and the scatter peaks used for the matrix corrections. The concentrations and correction factors for a typical geological sample, USGS-BCR-1 rock are illustrated in Figure 9 as they were determined by SAP3.

Direct analysis of relatively thick sample pellets avoids the potential contamination and chemical yield errors encountered in attempting to reduce environmental samples to a thin uniform geometry by precipitation. The avoidance of multiple standard requirements for thick sample analysis reduces the cost of X-ray fluorescence analyses and also avoids errors from trying to match unknown samples with standards of significantly different composition.

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Table I

List of Input/Output Devices and Their Unit Assignments

<u>Unit</u>	<u>Device</u>
1	Disk 3
3	Data Input: Disk 3 DECTAPE 3 Paper Tape Reader
4	Computer Terminal
6	Disk 2
7	Line Printer

Table II
Computer Sense Switch Options

<u>Switch</u>	<u>Option</u>
0	Read spectrum from (+) File (-) Paper Tape
1	Suppress raw data listing (+)
2	Read new fixed light element Z (+)
4	Compute new energy scale (+)
8	Read individual sample thickness and apply absorption correction for mylar pellet wrapper (+)
9	Time = RD(1); Infinite thickness self absorption function (+)
10	Suppress halts in paper tape reading (+)
11	Suppress individual sample analysis printout (+)
12	Use scatter peak determined sample thick- ness for absorption corrections.(+)
13	Read new scatter peak calibration constants (+)
14	Do particle size corrections (+)
15	Change input data set name/number (+)
16	Manual termination of iteration (+)

Table III

Identification of Constants Read From Library By SAP3, Subr. BEG

<u>Constant</u>	
UNIT	Units for elemental analysis results (ppm, $\mu\text{g}/\text{cm}^2$, etc.)
NOCH	Number of channels of input data.
SS	Source of exciting radiation, or secondary source.
PU	Percent uncertainty in calibration data.
NLE	Number of light elements ($Z \leq 13$) in the library.
NPKR	Number of heavy element peak regions.
WM	Width multiple (of σ) for peak analysis windows.
Y(1)	Normalization factor for data output (for units change).
B3	Incoherent scatter peak calibration.
B4	Coherent scatter peak calibration.
SIL(K)	Incoherent scattering cross sections (cm^2/g) for light elements (Reference 5).
SCL(K)	Coherent scattering cross sections (cm^2/g) for light elements (Reference 5).
UL(1-4,K)	LN-LN fit coefficients (zero to third order) for photoelectric cross sections (barns) for light elements (Reference 5).
UL(5,K)	Conversion factor (barns to cm^2/g) for light elements (Reference 5).
ELIT(K)	Light element symbol (H,He,Li, etc.)
EL(K)	Peak Region identification (ie., Fe $K\alpha$).
EN(K)	Peak energy (keV).
CAL(K)	Elemental sensitivity ($\text{counts} \cdot \text{cm}^2 / \mu\text{g} \cdot \text{min}$).
SIH(K)	Incoherent scattering cross sections (cm^2/g) for heavy elements (Reference 5).
SCH(K)	Coherent scattering cross sections (cm^2/g) for heavy elements (Reference 5).

Table III (cont'd)

UM(1-4,K)	LN-LN fit coefficients (zero to third order) for photoelectric cross section (barns) (Reference 5).
UM(5,K)	Energy (keV) of absorption edges.
UM(6,K)	Absorption function jump ratios.
UM(7,K)	Conversion factor (barns to cm^2/g) for heavy elements.
FY(K)	Fluorescent yields (Reference 9).
RAB(K)	Multielement attenuation factors for use with mylar-wrapped samples.
IEL(K,J)	Subscripts of interfering elements for peak overlap corrections.
OLP(K,J)	Peak overlap correction factors [$\times(-10000.)$ in library].
CA(J)	System blank ($\mu\text{g}/\text{cm}^2$).
SP(J)	Scatter peak energies (keV).

Figure 1. Schematic Diagram of the Light Element Contribution to X-ray Scattering from Which Absorption Corrections Are Computed

Figure 2. K α X-ray Fluorescence Sensitivities for Secondary Source and Isotope Excitation

Figure 3. Flowchart for SAP3


```

SAP3LP.P.M1024ZR 00.000030.000140024 1.7 32. 5300000. 3400000.
.387 .011 2.44964-3.34953-.047137.0070996 1.674 H
.183 .028 6.06488-3.29055-.107256.0144465 6.647 HE
.164 .038 7.75370-2.81801-.241738.0262542 11.52 LI
.162 .051 9.04511-2.83487-.210021.0229526 14.96 SE
.160 .067 9.95057-2.74173-.215138.0227845 17.95 S
.152 .091 10.6879-2.71400-.200530.0207248 19.94 C
.144 .118 11.2765-2.65400-.200445.0200765 23.26 N
.138 .148 11.7130-2.57229-.205893.0199244 26.57 O
.133 .180 12.0963-2.44148-.234461.0219537 31.55 F
.131 .225 12.4485-2.45819-.212591.0196489 33.51 NE
.129 .256 12.6777-2.24521-.274873.0250270 36.19 NA
.127 .292 12.8793-2.12574-.299392.0267643 40.38 MG
.125 .312 13.1738-2.18203-.258960.0222840 44.78 AL
.123 .347 13.2682-1.98174-.316950.0273928 46.63 SI
AL K 1.487 0.800 1244.311413.174-2.182-.2590.02228 1.56011.98844.78
SI K 1.739 1.49 1284.346813.268-1.982-.3169.02739 1.83910.44246.63
P K 2.014 2.7 1253.362313.374-1.863-.3394.02888 2.149 9.95451.43
S K 2.307 4.4 1299.401513.739-2.048-.2733.02300 2.47210.33353.24
CL K 2.622 6.6 1243.416213.619-1.719-.3542.02908 2.822 9.48758.87
K KA 3.312 15.3 1214.483213.798-1.540-.3945.03236 3.607 8.84464.93
CA KA 3.690 20.5 1228.523214.295-1.886-.2836.02263 4.038 9.11266.55
TI KA 4.508 37. 1100.548214.351-1.663-.3315.02621 4.965 8.53079.53
V KA 4.949 47. 1067.575914.760-1.889-.2719.02158 5.465 8.77084.59
CR KA 5.411 60. 1073.635714.802-1.824-.2791.02173 5.989 8.77986.34
MN KA 5.895 77. 1043.663514.897-1.799-.2837.02221 6.540 8.61291.22
FE KA 6.400 93. 1049.725414.346-1.235-.4180.03217 7.112 8.22192.74
CO KA 6.925 115. 1017.762514.705-1.389-.3866.03033 7.709 8.37697.85
NI KA 7.472 139. 1042.847414.239-.9677-.4781.03661 8.333 7.85597.45
CU KA 8.041 170. 0982.873214.581-1.184-.4138.03121 8.979 7.957105.5
ZN KA 8.631 205. 0966.925214.411-.9331-.4774.03628 9.659 7.602108.6
GA KA 9.243 240. 0927.941813.618-.3184-.6113.0458110.367 7.400115.8
HG LA 9.987 69. 06163.05517.186-2.085-.0853 12.284 3.926333.1
SE KA11.210 352. 08921.03413.076.18326-.6943.0502312.658 6.884131.1
PB LB12.611 122. 06073.12417.796-2.377-.0456 13.035 4.034344.11
AS KA10.532 305. 09101.01713.472-.0774-.6605.0492211.868 7.193124.4
BR KA11.907 388. 09061.09113.227.13713-.6832.0495413.474 6.974132.7
RB KA13.375 430. 08741.15713.020.38274-.7324.0529915.200 6.853141.9
SR KA14.142 95. 08671.19213.589.00220-.6389.0460116.105 7.058145.5
.0357 .047 .0604 .0761 .0942 .138 .163 .219 .250 .282 .314 .347 .381 .414 .445 .47
.510 .390 .596 .380 .567 .622 .669 .691
1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.
1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
1 -649 2 -500 3 -522 6 130 8 958 9 92410 824
11 45912 -6413 -41014 -60815 -43016 -27716 -211 19 156720 320021 -921
22 130423 -5
61600020-2405201307020-6809 7 -88 12 -35 11 -2112 -17
16 2012 -13 14 -9020 22427 -5421 -15 20 -32
20 -26
2430005 5 -720 6 -53 12 3
.24
.171 .026 -.944
15.26115.74617.09617.6871.41421.4451

```

Figure 4. Library for SAP3 as Read by Subroutine BEG

SAP3L WIDTH MULTIPLE = 1.700

NO.	PEAK	ENERGY	CALIB	BLANK	OVERLAP1	OVERLAP2	OVERLAP3
1	AL K	1.487	0.800	0.000	0	0.0000	0
2	SI K	1.739	1.450	0.000	1	0.3649	6
3	P K	2.014	2.700	0.000	2	0.0500	20
4	S K	2.307	4.400	0.000	3	0.0522	20
5	CL K	2.622	6.600	0.000	0	0.0000	20
6	K KA	3.312	15.300	0.000	0	0.0000	7
7	CA KA	3.690	20.500	0.000	6	-0.0130	0
8	TI KA	4.508	37.000	0.000	0	0.0000	12
9	V KA	4.949	47.000	0.000	8	-0.0958	0
10	CR KA	5.411	60.000	0.000	9	-0.0924	11
11	MN KA	5.895	77.000	0.000	10	-0.0824	12
12	FE KA	6.400	93.000	0.240	11	-0.0459	0
13	CO KA	6.925	115.000	0.000	12	0.0064	16
14	NI KA	7.472	139.000	0.000	13	0.0410	12
15	CU KA	8.041	170.000	0.171	14	0.0608	0
16	ZN KA	8.631	205.000	0.026	15	0.0430	14
17	GA KA	9.243	240.000	0.000	16	0.0277	20
18	HG LA	9.987	69.000	0.000	16	0.0211	20
19	SE KA	11.210	352.000	0.000	0	0.0000	21
20	PB LB	12.611	122.000	0.000	19	-0.1567	0
21	AS KA	10.532	305.000	0.000	20	-0.3280	0
22	BR KA	11.907	388.000	0.000	21	0.0921	20
23	RB KA	13.375	430.000	0.000	22	-0.1304	20
24	SR KA	14.142	95.000	-0.944	23	0.0005	0

PARTICLE SIZE = 0.0024667 CM., RHOH = 2.5000000 RHOL = 1.0000000 G/CM**2
ICAL= 5300000., CCAL= 3400000.

Figure 5. Calibration and Overlap Data Printout from Subroutine BEG

RAW DATA	LSTD1 2									
93590	0	0	0	0	0	0	0	0	0	/ 10
0	0	0	0	0	0	0	0	0	0	/ 20
0	0	0	0	0	0	0	0	0	0	/ 30
96	4229	971	0	0	0	10	193	226	190	/ 40
214	188	191	176	189	177	173	158	168	157	/ 50
185	171	209	217	241	265	286	294	283	306	/ 60
277	272	308	383	526	621	750	783	803	748	/ 70
617	528	399	334	291	258	248	221	239	180	/ 80
150	156	172	125	143	139	147	144	122	162	/ 90
131	148	140	136	116	131	158	133	128	133	/ 100
125	161	152	137	161	145	179	168	160	178	/ 110
150	165	157	147	156	145	173	144	128	164	/ 120
154	161	186	244	280	402	521	691	1008	1171	/ 130
1392	1387	1454	1287	1043	823	676	570	669	888	/ 140
1415	2271	3335	4683	6046	7016	7749	7340	6816	5529	/ 150
4084	2803	1798	1162	905	844	942	1071	1241	1264	/ 160
1356	1208	1005	728	568	401	260	214	164	170	/ 170
266	393	630	1050	1739	2498	3532	4600	5540	5702	/ 180
5860	5258	4592	3684	2853	2029	1399	1037	800	666	/ 190
612	715	814	968	1176	1316	1397	1367	1246	1089	/ 200
888	664	473	333	290	237	253	218	270	289	/ 210
267	298	312	310	346	314	336	308	281	310	/ 220
284	283	261	286	291	278	311	362	451	635	/ 230
888	1186	1526	1896	2100	2265	2207	2000	1783	1429	/ 240
1184	1020	1004	1222	1806	3369	6240	11391	21044	35546	/ 250
57477	85296	117991	149050	173914	186242	185044	168899	142021	109513	/ 260
77712	50899	31227	17319	9308	4762	2501	1344	954	865	/ 270
1015	1278	1763	2673	4191	6387	9710	13833	18743	23484	/ 280
27884	30743	31195	29193	25589	20489	15208	10464	6792	4032	/ 290
2326	1190	586	334	175	118	99	104	82	109	/ 300
92	83	87	73	67	58	74	61	44	61	/ 310
59	50	51	58	53	74	92	119	102	143	/ 320
150	136	154	127	150	118	96	79	90	83	/ 330
91	106	145	158	181	174	195	241	268	293	/ 340
400	476	564	637	743	694	728	666	585	454	/ 350
337	252	165	120	87	68	50	58	63	41	/ 360
58	67	75	76	96	110	148	132	195	229	/ 370
216	192	176	190	155	123	132	116	128	154	/ 380
194	222	239	306	280	269	256	237	256	206	/ 390
205	159	193	148	115	134	119	100	124	96	/ 400
116	115	91	83	69	83	88	70	87	69	/ 410
63	71	66	65	77	81	85	85	103	102	/ 420
131	111	107	127	129	116	83	99	87	75	/ 430
72	59	82	78	77	67	89	80	89	88	/ 440
96	89	89	81	94	96	120	113	118	123	/ 450
125	158	156	126	111	144	136	127	123	124	/ 460
123	125	143	115	125	137	147	116	128	154	/ 470
138	122	113	119	125	120	124	134	140	154	/ 480
123	143	132	123	161	155	161	155	145	139	/ 490
167	151	129	154	191	157	169	194	173	212	/ 500
208	232	233	260	291	297	303	336	369	340	/ 510
400	413	401	463	427	428	366	372	373	363	/ 520
347	368	327	329	337	337	396	434	500	619	/ 530
772	863	997	1153	1306	1419	1512	1489	1401	1276	/ 540

Figure 6. Listing of Raw Spectral Data from Subroutine PRNT

1287.	1068.	915.	841.	740.	707.	625.	625.	637.	621.	/ 550
628.	621.	683.	700.	744.	786.	848.	908.	988.	1119.	/ 560
1270.	1513.	1777.	2003.	2284.	2459.	2636.	2830.	2883.	2738.	/ 570
2673.	2501.	2384.	2156.	2159.	2005.	1977.	2044.	2085.	2188.	/ 580
2323.	2464.	2593.	2774.	2978.	3233.	3390.	3728.	4097.	4374.	/ 590
4713.	5224.	5758.	6455.	7341.	8270.	9424.	10817.	12664.	14473.	/ 600
16381.	18773.	21575.	24270.	27200.	30544.	33528.	36458.	38976.	41535.	/ 610
42718.	43633.	44285.	43530.	42355.	40109.	38233.	35524.	33032.	29877.	/ 620
27598.	25274.	24409.	24029.	25354.	27626.	30955.	35043.	40056.	44366.	/ 630
47870.	49441.	50083.	47726.	44447.	38941.	32810.	26607.	20376.	15055.	/ 640
11002.	7659.	5111.	3661.	2663.	2069.	1714.	1560.	1462.	1396.	/ 650
1367.	1376.	1424.	1468.	1529.	1668.	1668.	1672.	1834.	1927.	/ 660
1959.	2073.	2229.	2428.	2577.	2839.	3175.	3462.	3671.	4035.	/ 670
4668.	5132.	5795.	6470.	7278.	8109.	9063.	9837.	10670.	11525.	/ 680
12307.	12801.	13555.	13615.	13808.	13849.	13796.	13393.	12801.	12180.	/ 690
11754.	10749.	9958.	9077.	8372.	7755.	7042.	6489.	6049.	5877.	/ 700
6037.	6445.	7264.	8156.	9191.	10707.	12071.	12943.	13746.	13348.	/ 710
13301.	12048.	10506.	9055.	7452.	6039.	4873.	3864.	3322.	2819.	/ 720
2510.	2316.	1932.	1767.	1484.	1303.	1046.	756.	529.	385.	/ 730
261.	197.	111.	78.	57.	42.	32.	26.	25.	29.	/ 740
25.	27.	20.	33.	23.	27.	22.	22.	18.	30.	/ 750
28.	35.	29.	34.	20.	30.	30.	37.	23.	36.	/ 760
36.	43.	44.	35.	36.	52.	38.	35.	33.	40.	/ 770
49.	42.	30.	21.	51.	44.	37.	35.	42.	37.	/ 780
48.	50.	53.	43.	45.	49.	41.	46.	48.	46.	/ 790
46.	58.	58.	36.	53.	52.	59.	56.	47.	57.	/ 800
38.	58.	66.	52.	51.	54.	49.	64.	64.	44.	/ 810
68.	44.	65.	44.	66.	64.	57.	77.	66.	86.	/ 820
57.	76.	79.	77.	82.	78.	69.	69.	78.	59.	/ 830
88.	77.	74.	54.	75.	74.	67.	78.	73.	95.	/ 840
103.	82.	77.	86.	80.	90.	85.	81.	88.	87.	/ 850
74.	82.	100.	88.	102.	101.	127.	126.	124.	131.	/ 860
124.	123.	128.	141.	150.	157.	165.	160.	178.	163.	/ 870
174.	169.	175.	191.	151.	171.	168.	154.	153.	140.	/ 880
135.	141.	151.	149.	162.	170.	204.	169.	184.	191.	/ 890
164.	199.	175.	183.	171.	161.	162.	147.	144.	124.	/ 900
126.	129.	135.	134.	139.	125.	105.	125.	125.	136.	/ 910
150.	97.	132.	134.	161.	165.	146.	142.	162.	111.	/ 920
129.	130.	141.	137.	145.	144.	157.	156.	140.	155.	/ 930
134.	143.	144.	155.	162.	162.	163.	152.	154.	164.	/ 940
178.	173.	193.	168.	176.	187.	211.	189.	173.	164.	/ 950
172.	161.	172.	170.	154.	157.	168.	193.	162.	175.	/ 960
190.	185.	183.	193.	190.	190.	173.	205.	170.	175.	/ 970
194.	192.	207.	190.	191.	185.	202.	207.	196.	174.	/ 980
161.	177.	196.	194.	180.	182.	173.	190.	186.	166.	/ 990
190.	181.	193.	191.	194.	197.	212.	200.	177.	212.	/ 1000
191.	189.	198.	218.	213.	220.	187.	201.	190.	214.	/ 1010
204.	200.	216.	203.	185.	224.	221.	226.	199.	218.	/ 1020
207.	220.	205.	230.							

Figure 6 (continued)

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LSTD1 2 62.564 MG/CM**2 PCT. CALIB. UNCORT. = 0.0
MO DA YR= 2 18 77 0.464 N + 0.325 O NORM FACTOR = 32.0000
ITERATIONS = 15 KEV=CH+0.02485 + 0.031 P. SIZE (MICRON)= 37.00
MINUTES = 20.000 INCOH A = 643559
SEC. SOURCE = ZR X-RAY FLUORESCENCE ANALYSIS COH A = 609115.

NO	CHANNELS	NET AREA +/-	BKGND P.S.	ABSOR ENHAN	OVERLAP (P.P.M)	REGION	P.P.M +/-	2 SIG. DL. (P.P.M)
1	53.6	-92.	2843.	112.132	0.00	AL K	< 0.4335E+05	0.434E+05
	63.6	73.	1.528	0.854			-0.2706E+05	
2	63.7	2606.	3611.	74.039	-0.23E+05	SI K	0.2447E+06	0.285E+05
	73.8	148.	1.492	0.866			0.1518E+05	
3	74.7	-202.	2235.	77.847	0.13E+05	P K	< 0.1106E+05	0.111E+05
	84.9	68.	1.975	0.871			-2608.	
4	86.4	-71.	1503.	54.641	32.	S K	< 3441.	0.344E+04
	96.8	56.	1.776	0.868			-2130.	
5	99.0	34.	1562.	38.978	75.	CL K	< 1475.	0.148E+04
	109.6	57.	1.587	0.870			523.4	
6	126.6	5491.	5963.	20.892	0.45E+03	K KA	0.1423E+05	570.
	137.5	135.	1.322	0.869			340.1	
7	141.7	36508.	21912.	16.276	-0.18E+03	CA KA	0.5095E+05	601.
	152.9	287.	1.250	0.882			402.5	
8	174.4	27621.	19411.	11.234	0.33E+03	TI KA	0.1423E+05	213.
	186.0	269.	1.167	0.888			135.5	
9	192.0	5703.	6281.	8.770	-0.13E+04	V KA	368.7	98.9
	203.9	167.	1.133	0.881			49.83	
10	210.5	329.	3357.	7.273	-60.	CR KA	< 39.93	39.9
	222.6	107.	1.111	0.882			2.793	
11	229.8	9666.	10022.	5.839	0.16E+03	MN KA	1419.	42.6
	242.2	191.	1.093	0.983			24.85	
12	250.0	1072398.	465401.	4.756	-58.	FE KA	0.9457E+05	182.
	262.7	1463.	1.080	0.999			129.1	
13	271.0	-10589.	196882.	3.969	0.61E+03	CO KA	< 81.30	81.3
	283.9	682.	1.069	0.999			-19.46	
14	292.8	-3423.	5061.	4.702	0.12E+03	NI KA	< 14.09	14.1
	306.1	107.	1.071	0.999			-75.28	
15	315.6	583.	1013.	3.976	0.00	CU KA	17.69	3.93
	329.2	55.	1.063	0.999			2.186	
16	339.2	3968.	3045.	3.417	1.0	ZN KA	112.0	4.92
	353.1	108.	1.058	0.999			3.035	
17	363.6	791.	1418.	2.986	3.1	GA KA	19.70	2.62
	377.9	69.	1.053	0.999			1.438	
18	393.4	-248.	1792.	2.605	2.4	HG LA	< 8.872	8.87
	408.0	68.	1.048	0.999			-13.34	
19	442.2	115.	1707.	2.191	0.75E-02	SE KA	< 1.394	1.39
	457.6	68.	1.042	0.999			1.204	
20	490.2	-103.	5012.	1.907	-0.19	PB LB	< 6.276	6.28
	514.3	121.	1.037	0.999			-2.845	
21	415.1	302.	1136.	2.095	0.12E-05	AS KA	5.007	1.42
	430.1	58.	1.045	0.999			0.7568	
22	470.1	-310.	2393.	2.032	0.45	BR KA	< 1.441	1.44
	485.8	81.	1.041	0.999			-2.235	
23	528.8	7751.	10145.	1.802	0.95E-06	SB KA	53.78	2.34
	545.3	190.	1.035	1.000			1.320	
24	559.4	11303.	25927.	1.719	0.27E-01	SR KA	367.9	16.3
	576.4	292.	1.032	1.000			8.734	

Figure 7. Individual Sample Analysis Report Printed by Subroutine PRNT

X-RAY FLUORESCENCE SERIES LSTD1, MO-DA-YR = 2-18-77 20.00 MIN.
 ZR SECONDARY SOURCE, CONCENTRATIONS AND UNCERTAINTIES IN P.P.M

NO	CA	TI	V	CR	MN	FE
1	0.5081E+05 486.0	0.1412E+05 136.2	379.3 50.38	< 43.72 0.0000	1429 25.45	0.9416E+05 131.2
2	0.5168E+05 488.3	0.1441E+05 137.3	372.8 50.45	< 40.42 0.0000	1435. 25.14	0.9558E+05 130.5
3	3673. 114.7	< 77.20 0.0000	< 28.28 0.0000	2380. 26.63	793.5 17.69	0.5209E+05 79.34
4	3711. 115.5	< 77.93 0.0000	< 28.69 0.0000	2272. 26.49	826.5 17.73	0.5294E+05 79.52
5	0.3882E+05 373.1	6648. 96.67	183.1 37.67	< 31.19 0.0000	749.9 17.85	0.4679E+05 87.44
6	0.3934E+05 372.5	6868. 96.93	85.40 37.72	< 31.94 0.0000	753.0 17.92	0.4731E+05 87.94
7	0.1567E+05 281.3	3579. 71.52	< 62.06 0.0000	< 23.96 0.0000	222.7 10.93	0.1795E+05 52.53
8	0.1666E+05 283.6	3365. 71.24	81.03 32.32	< 28.12 0.0000	239.3 10.94	0.1775E+05 52.61
9	0.1595E+05 300.3	4500. 82.15	< 66.45 0.0000	< 33.54 0.0000	236.9 13.29	0.2868E+05 68.31
10	0.1538E+05 301.0	4392. 81.57	< 66.72 0.0000	< 28.97 0.0000	241.4 13.08	0.2794E+05 67.90
11	0.7999E+05 492.7	6476. 105.2	185.7 39.21	146.7 19.41	1253. 24.42	0.7647E+05 119.8
12	0.7819E+05 483.7	6449. 102.3	181.0 38.22	121.7 18.81	1158. 23.34	0.7349E+05 115.2
13	0.4991E+05 480.0	0.1401E+05 135.0	239.4 49.69	< 39.99 0.0000	1323. 24.84	0.8959E+05 126.3
14	0.4956E+05 481.2	0.1420E+05 135.0	376.9 49.53	46.39 20.17	1372. 24.65	0.9091E+05 127.0
15	0.4995E+05 332.7	90.40 13.83	< 14.83 0.0000	< 7.639 0.0000	215.5 6.240	728.7 9.116
16	0.4880E+05 326.5	94.75 13.20	< 14.48 0.0000	< 7.634 0.0000	214.3 6.209	650.8 8.684

Figure 8. One of Four Pages of a Summary Report for a Series of Sixteen Samples, as Printed by Subroutine REP

Figure 9. Correction Factors and Analytical Results for USGS BCR-1 as Computed by SAP3

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APPENDIX

SAP3: SPECTRAL ANALYSIS PROGRAM WITH 3 MATRIX CORRECTIONS
(SELF ABSORPTION, ENHANCEMENT AND PARTICLE SIZE).

WRITTEN BY KIRK K NIELSON
PHYSICAL SCIENCES DEPARTMENT
BATTELLE PACIFIC NORTHWEST LABORATORIES
RICHLAND, WASHINGTON 99352
02-11-77-REV.

OVERLAY DESCRIPTION FOR 'CHAIN':
NAME XCT FILE: SAP3J
LIST OPTIONS AND PARAMETERS: BKR, 24K, SZJ
DEFINE RESIDENT CODE: SAP3J
DESCRIBE LINKS & STRUCTURE:
L1=BEGJ
L2=RED, MR51, REDDTJ
L3=LIST, SMOTH, PKARJ
L4=QUANJ
L5=PRNTJ
L6=REPJ
L1:L2:L3:L4:L5:L6J
J

SENSE SWITCH OPTIONS:

0 READ RAW DATA FROM FILE (+); PAPER TAPE (-).
1 SUPPRESS RAW DATA LISTING (+).
2 READ IN FIXED LIGHT ELEMENT Z (+).
4 FLOAT ENERGY SCALE (+).
8 ABS. CORR. FOR MYLAR PELLET PACKAGE & THICKNESS READ-IN(+).
9 TIME = RD(1); DIVIDE RESULTS BY CALC'D WT.; INF. THICK. ABS. CORR.
10 SUPPRESS HALTS IN PAPER TAPE READING (+).
11 SUPPRESS SPECTRUM ANALYSIS PRINTOUT (+).
12 DETERMINE THICKNESS FROM SCATTER (NO NORMALIZATION) (+).
13 READ NEW SCATTER PEAK CALIBRATION CONSTANTS (+).
14 DO PARTICLE SIZE CORRECTIONS (+).
15 CHANGE INPUT DATA/SET NUMBER (+).
16 MANUAL TERMINATION OF ITERATION LOOP (+).

SAP3 MAIN PROGRAM.....

LOGICAL ISENSEW

DIMENSION FIL(2), EXT(40), FYLIB(2)
COMMON RD(1024), SM(1024), EN(30), CAL(30), EL(30), A(30), CA(30)
COMMON DA(30), S(30), SP(4), IEL(3, 30), OLP(3, 30), Q(30), DQ(30)
COMMON QC(30), DL(30), UM(7, 30), UL(5, 14), STH(30), SCH(30), SIL(14)
COMMON SCL(14), ENLIT(14), ELIT(14), COR(30), CORL(30), IDAT(4)
COMMON X(4), Y(4), XE(30), XEL(15), ABC3, ABC4, THETA, PHI
COMMON UNIT, NPKR, NRUN, SERIES, NOCH, AX, BX, TIME, SS, PU, WM
COMMON XH(30, 30), XL(30, 15), SF(30), FY(30), RAB(30), FYL(2), SB1, SB2
DATA EXT/4H 001, 4H 002, 4H 003, 4H 004, 4H 005, 4H 006, 4H 007,
4H 008, 4H 009, 4H 010, 4H 011, 4H 012, 4H 013, 4H 014, 4H 015,
4H 016, 4H 017, 4H 018, 4H 019, 4H 020, 4H 021, 4H 022, 4H 023,
4H 024, 4H 025, 4H 026, 4H 027, 4H 028, 4H 029, 4H 030, 4H 031,
4H 032, 4H 033, 4H 034, 4H 035, 4H 036, 4H 037, 4H 038, 4H 039,
4H 040/
CALL BEC(P8, RHO, RHOL)
FIL(1)=SERIES
CONTINUE
IF(.NOT. ISENSEW(0)) CALL RED(RD, NOCH)


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IF(.NOT. ISENSW(0)) J=3
FIL(2)=EXT(NRUN)
7 IF(ISENSW(0)) CALL REDDT(RD, NOCH, FIL, J)
  IF(J.EQ.3) GO TO 6
  IF(J.EQ.0) GO TO 4
  IF(J.EQ.2) GO TO 3
  IF(J.EQ.1) GO TO 5
6 CONTINUE
  IF(ISENSW(1)) GO TO 2
  CALL LIST(RD, NOCH, SERIES, NRUN)
2 CALL SMOTH
  CALL PKAR
  CALL QUAN(TH1, TH2, L, LEM, ITER, PS, RHO, RHOL)
  CALL PRNT(TH1, TH2, L, LEM, ITER, PS, RHO, RHOL)
  NRUN=NRUN+1
  IF(.NOT. ISENSW(15)) GO TO 1
  IF(.NOT. ISENSW(0)) GO TO 3
  GO TO 5
3 NRUN=NRUN-1
  CALL REP
4 STOP 1
5 WRITE(4, 15)
15 FORMAT(1X, 'SERIES & NUMBER (A5, I4)')
  READ(4, 10) SERIES, NRUN
10 FORMAT(A5, I4)
  RNR=EXT(NRUN)
  FIL(1)=SERIES
  FIL(2)=RNR
  GO TO 7
END
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C THIS ROUTINE READS IN LIBRARY DATA & INITIALIZES PARAMETERS.
C
      SUBROUTINE BEG(RS,RHO,RHOL)
      DIMENSION FYLIB(2)
      COMMON RD(1024),SM(1024),EN(30),CAL(30),EL(30),A(30),CA(30)
      COMMON DA(30),B(30),SP(4),IEL(3,30),OLP(3,30),Q(30),DQ(30)
      COMMON QC(30),DL(30),UM(7,30),UL(5,14),SIH(30),SCH(30),SIL(14)
      COMMON SCL(14),ENLIT(14),ELIT(14),COR(30),CORL(30),IDAT(4)
      COMMON X(4),Y(4),XE(30),XEL(15),B3,B4,THETA,PHI
      COMMON UNIT,NPKR,NRUN,SERIES,NCOH,AX,BX,TIME,SS,PU,WM
      COMMON XH(30,30),XL(30,15),SF(30),FY(30),RAB(30),FYL(2)
      DATA ZR/5HZR /,AG/5HAG /,CD/5HCD109/
      DATA FYLL/5HSUMRY/,FYL/4H 001/
      DATA FYLIB(2)/4H 001/

C
C READ IN LIBRARY
C
      WRITE(4,322)
322  FORMAT(' ','LIBRARY NAME = ? (AAAAA)')
      READ(4,306) FYLIB(1)
      CALL SEEK(6,FYLIB)
      READ(6,100) UNIT,NCOH,SS,PU,NLE,NPKR,WM,Y(1),B3,B4
100  FORMAT(5X,A5,I4,A5,F7.2,6X,I2,I4,F7.2,F8.0,2F9.0)
10  READ(6,101) (SIL(K),SCL(K),(UL(J,K),J=1,5),ELIT(K),K=1,NLE)
101  FORMAT(2F6.0,5F8.0,2X,A5)
      READ(6,2) (EL(K),EN(K),CAL(K),SIH(K),SCH(K),(UM(J,K),J=1,7),
C K=1,NPKR)
2  FORMAT(A5,2F6.0,2F5.0,6F6.0,F5.0)
      READ(6,4) (FY(K),K=1,NPKR)
4  FORMAT(16F5.0)
      READ(6,4) (RAB(K),K=1,NPKR)
      DO 1 K=1,3
1  READ(6,102) (IEL(K,J),OLP(K,J),J=1,NPKR)
102  FORMAT(11(I2,F5.0))
      READ(6,103) (CA(J),J=1,NPKR)
103  FORMAT(13F6.0)
      READ(6,103) (SP(J),J=1,4),THETA,PHI
      CALL CLOSE(6)
      DO 5 K=1,3
      DO 6 L=1,NPKR
6  OLP(K,L)=OLP(K,L)*(-0.0001)
5  CONTINUE
      IDAT(4)=NLE
      Y(3)=1.
      Y(4)=1.

C
C READ IN SAMPLE PARAMETERS.
C
      WRITE(4,200)
200  FORMAT(' DATE (MO DA YR)')
      READ(4,201) (IDAT(I),I=1,3)
201  FORMAT(3(I2,1X))
      WRITE(4,202)
202  FORMAT(' TIME IN MIN. (F7.2) = ?')
      READ(4,203) TIME
203  FORMAT(F7.2)
      IF(.NOT.ISENSW(14)) GO TO 30
      WRITE(4,320)
320  FORMAT(' ','PARTICLE SIZE(MICRONS),RHOH,RHOL',/,/,/,
C 'NNNNNN NNNN NNNN')

```



```

      READ(4,321) PS,RHO,RHOL
321  FORMAT(E6.2,1X,E4.1,1X,E4.1)
      PS=PS*0.66667/10000.
30  CONTINUE
      WRITE(4,303)
305  FORMAT(' ','SERIES = ? '(A5)')
      READ(4,306) SERIES
306  FORMAT(A5)
      WRITE(4,207)
207  FORMAT(' ','SAMPLE THICKNESS (GM/CM**2) = ? '(F7.2)')
      READ(4,203) Y(2)
      WRITE(4,205)
205  FORMAT(' ','BEGINNING RUN NUMBER = ? (I4)')
      READ(4,206) NRUN
206  FORMAT(I4)
C
C  WRITE CALIBRATION DATA ON LINE PRINTER.
C
      WRITE(7,210) FYLIB(1),WM
210  FORMAT(' ',' ',A5,' WIDTH MULTIPLE = ',F7.3,/)
      WRITE(7,211)
211  FORMAT(' ','NO. PEAK ENERGY CALIB BLANK OVERLAP1',
C  ' OVERLAP2 OVERLAP3',/)
      DO 7 I=1,NPKR
      WRITE(7,212) I,EL(I),EN(I),CAL(I),CA(I),(IEL(J,I),OLP(J,I),
C  J=1,3)
212  FORMAT(' ',I2,1X,A5,2F9.3,F8.3,3(1X,I2,F8.4))
7  CONTINUE
      WRITE(7,215) PS,RHO,RHOL
215  FORMAT(' ','PARTICLE SIZE = ',F10.7,' CM., RHOH = ',F11.7,
C  ' RHOL = ',F11.7,' G/CM**2')
      WRITE(7,216) B3,B4
216  FORMAT(' ','ICAL=',F10.0,' COAL=',F10.0)
C
C  INITIALIZE MASS ABSORPTION COEFFS. FROM PARAMETERS OF MCMASTER ET AL.,
C  UCRL-50174, SEC II, REV. I, (1969).
C
      ENSS=SP(2)
      EP=ALOG(ENSS)
      NPP=NPKR+4
      DO 43 J=1,NPKR
      XE(J)=EXP(UM(1,J)+UM(2,J)*EP+UM(3,J)*EP*EP+UM(4,J)*EP**3)
43  XE(J)=(XE(J)/UM(7,J)+SIH(J)+SCH(J))*THETA/1000000.
      DO 40 K=1,NPP
      IF(K.LE.NPKR) E=ALOG(EN(K))
      L=K-NPKR
      IF(K.GT.NPKR) E=ALOG(SP(L))
      DO 39 J=1,NPKR
      C=PHI/1000000./UM(7,J)
      XH(K,J)=C*(EXP(UM(1,J)+UM(2,J)*E+UM(3,J)*E*E+UM(4,J)*E**3)+
C  (SIH(J)+SCH(J))*UM(7,J))
      IF(EN(K).LT.UM(5,J)) XH(K,J)=XH(K,J)/UM(5,J)
39  XH(K,J)=XH(K,J)+XE(J)
40  CONTINUE
      DO 44 J=1,NLE
      XEL(J)=EXP(UL(1,J)+UL(2,J)*EP+UL(3,J)*EP*EP+UL(4,J)*EP**3)
44  XEL(J)=(XEL(J)/UL(5,J)+SIL(J)+SOL(J))*THETA/1000000.
      DO 42 K=1,NPP
      IF(K.LE.NPKR) E=ALOG(EN(K))
      L=K-NPKR

```



```
      IF(K.GT.NPKR) E=ALOG(SP(L))
      DO 41 J=1,NLE
      C=PHI/10000000./UL(5,J)
41      XL(K,J)=C*(EXP(UL(1,J)+UL(2,J)*E+UL(3,J)*E+E+UL(4,J)*E**3)+
      1      (SIL(J)+SCL(J))*UL(5,J))+XEL(J)
42      CONTINUE
C
C  ZERO THE SUMMARY DATA FILE, FYL.
C
      FYL(1)=FYLL
      FYL(2)=FYLM
      CALL ENTER(1,FYL)
      WRITE(1) RD
      WRITE(1) SM
      CALL CLOSE(1)
      RETURN
      END
```



```
C      THIS ROUTINE READS SPECTRUM FROM PAPER TAPE TO ARRAY VIS.
C      HIGH-SPEED PUNCHED TAPE IS FROM NUCLEAR DATA PROGRAM ND41-1104.
C
      SUBROUTINE RED (VIS,NOCH)
      LOGICAL ISENSW
      DIMENSION VIS(1024),IS1(3)
      IF(ISENSW(10)) GO TO 30
      WRITE(4,10)
10     FORMAT(31H TYPE OR AFTER PAPER TAPE READY)
      READ(4,20) C1
20     FORMAT (A1)
30     CALL MR51(I)
C      SEARCH FOR BEGINNING CHANNEL
      IF(I.EQ.0)GO TO 30
      CALL MR51 (I)
      CALL MR51 (I)
      DO 200 J=1,NOCH
      DO 210 K=1,3
      CALL MR51(IS1(K))
210     CONTINUE
      VIS(J)=0.
      VIS(J)=VIS(J)+FLOAT(IS1(2))*256+IS1(3))+FLOAT(IS1(1))*65536.
200     CONTINUE
      DO 220 K=1,3
      CALL MR51(IS1(K))
220     CONTINUE
      RETURN
      END
```

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```
.TITLE  MR51
/ WRITTEN BY J.R.KOSOROK 04-11-74 1144
/ USE KM15 SYSTEM TO READ A SINGLE 8 BIT
/ CHARACTER FROM PAPERTAPE
  .GLOBL  MR51, .DA
  .IODEV  3
/
/ TO CALL:
/      CALL MR51(I)
/
MR51      0
          JMS*   .DA
          JMP     STRT
I         .DSA    0      /ADDR. OF LOC. TO STORE TAPE CHAR.
STRT      .INIT   3, 0, EXT
          .READ   3, 3, BUFF, 3
          .WAIT   3
EXT       .CLOSE  3
          LAC     BUFF+2
          DAC*    1
          JMP*    MR51
BUFF      .BLOCK  4
          .END
```



```
C      SUBROUTINE REDDT READS SPECTRA FROM DECTAPE.  
      SUBROUTINE REDDT(VIS,NOCH,FIL,J)  
      LOGICAL ISENSM  
      DIMENSION VIS(1024),FIL(2),EXT(16)  
      DATA Y/1HY/  
      CALL FSTAT(3,FIL,1)  
      CALL CLOSE(3)  
      IF(I.EQ.0) GO TO 15  
      J=3  
      CALL SEEK(3,FIL)  
      READ(3) SIZE  
      READ(3) VIS  
      CALL CLOSE(3)  
      GO TO 25  
15     WRITE(4,20) FIL  
20     FORMAT(1X,A5,A4,' NOT ON DT3...TYPE:0(STOP),1(CONT),2(REP)')  
      READ(4,21)J  
21     FORMAT(I1)  
25     RETURN  
      END
```



```
C      THIS ROUTINE PRINTS RAW SPECTRAL DATA FROM ARRAY VIS.
C
      SUBROUTINE LIST (VIS, NOCH, SERIES, NRUN)
      DIMENSION VIS(1024)
      WRITE(7,100) SERIES, NRUN
100    FORMAT('RAW DATA', 5X, A5, I3)
      NN=NOCH/10
      DO 10 J=1, NN
      K=10*J
      KK=K-9
      WRITE(7,200) (VIS(L), L=KK, K), K
200    FORMAT(' ', 10(F7.0), ' / ', I4)
      IF(J/10*10.EQ.J) WRITE(7,300)
300    FORMAT(' ')
10    CONTINUE
      K=K+1
      KK=NOCH
      WRITE(7,200) (VIS(L), L=K, KK)
      RETURN
      END
```



```

C      THIS ROUTINE SMOOTHS RAW SPECTRAL DATA FROM ARRAY RD AND STORES
C      THE RESULTING SMOOTHED DATA IN ARRAY SM.
C
C      SMOOTHING IS 5-POINT LEAST SQUARES POLYNOMIAL SMOOTHING
C      BY THE METHOD OF SAVITZKY & GOLAY, ANAL. CHEM. 36,1627 (1964).
C      SMOOTHING IS DONE ON SQUARE ROOT TRANSFORMED SPECTRA.
C
      SUBROUTINE SMOTH
      COMMON RD(1024), SM(1024), EN(30), CAL(30), EL(30), A(30), CA(30)
      COMMON DA(30), B(30), SP(4), IEL(3,30), OLP(3,30), Q(30), DQ(30)
      COMMON QC(30), DL(30), UM(7,30), UL(5,14), SIH(30), SCH(30), SIL(14)
      COMMON SCL(14), ENLIT(14), ELIT(14), COR(30), CORL(30), IDAT(4)
      COMMON X(4), Y(4), XE(30), XEL(15), ABC3, ABC4, THETA, PHI
      COMMON UNIT, NPKR, NRUN, SERIES, NOCH, AX, BX, TIME, SS, PU, WM
      COMMON XH(30,30), XL(30,15), SF(30), FY(30)
      DO 1 I=1, NOCH
1      RD(I)=SQRT(RD(I))
      NNO=NOCH-4
      SM(1)=RD(1)
      SM(2)=RD(2)
      SM(NOCH)=RD(NOCH)
      SM(NOCH-1)=RD(NOCH-1)
      DO 2 I=3, NNO
2      SM(I)=(17*RD(I)+12*(RD(I+1)+RD(I-1))-3*(RD(I-2)+RD(I+2)))/35
      DO 3 I=1, NOCH
3      RD(I)=RD(I)*RD(I)
      SM(I)=SM(I)*SM(I)
      RETURN
      END

```



```

C   THIS ROUTINE COMPUTES PEAK AREAS BY A MODIFICATION OF THE
C   COVELL METHOD AS DESCRIBED BY K K NIELSON IN BNWL-SA-6063.
C
      SUBROUTINE PKAR
      LOGICAL ISENSM
      COMMON RD(1024), SM(1024), EN(30), CAL(30), EL(30), A(30), CA(30)
      COMMON DA(30), B(30), SP(4), IEL(3,30), OLP(3,30), Q(30), DQ(30)
      COMMON QC(30), DL(30), UM(7,30), UL(5,14), SIH(30), SCH(30), SIL(14)
      COMMON SOL(14), ENLIT(14), ELIT(14), COR(30), CORL(30), IDAT(4)
      COMMON X(4), Y(4), XE(30), XEL(15), ABC3, ABC4, THETA, PHI
      COMMON UNIT, NPKR, NRUN, SERIES, NOCH, AX, BX, TIME, SS, PU, WM
      COMMON XH(30,30), XL(30,15), SF(30), FY(30), RAB(30)
      COMMON FYL(2), SB1, SB2
      WS=0.32448
      WI=5.379
C   FIRST FIND ENERGY SCALE FROM SCATTER PEAKS...
C   SWITCH 4 CAUSES CALC. OF NEW ENERGY SCALE.
      IF(.NOT.ISENSM(4)) GO TO 12
      SPX=SP(2)
11     ICTR=IFIX(SFX/0.02485)
      IC=ICTR
C   ENERGY CALIBRATION PEAKS ARE LOCATED WITHIN 10 CHANNELS OF EXPECTED
C   POSITION. COHERENT K-ALPHA AND FE K-ALPHA PEAKS ARE USED.
      DO 7 J=1,10
        IF(SM(ICTR-1).GT.SM(ICTR).OR.SM(ICTR-2).GT.SM(ICTR))ICTR=
1       ICTR-1
        IF(SM(ICTR+1).GT.SM(ICTR).OR.SM(ICTR+2).GT.SM(ICTR))ICTR=
1       ICTR+1
7       CONTINUE
      ID=IABS(ICTR-IC)
      K=ICTR
C   CENTERS OF ENERGY CALIB. PEAKS ARE CALC'D BY METHOD OF
C   SAVITZKY & GOLAY, ANAL. CHEM. 36:1627 (1964).
      A21=(4.*(SM(K+4)-SM(K-4))+3.*(SM(K+3)-SM(K-3))+2.*(SM(K+2)-
C   SM(K-2))+SM(K+1)-SM(K-1))/60.
      A22=(28.*(SM(K+4)+SM(K-4))+7.*(SM(K+3)+SM(K-3))-8.*(SM(K+2)+
C   SM(K-2))-17.*(SM(K+1)+SM(K-1))-20.*SM(K))/924.
      C1=FLOAT(K)-A21/(2.*A22)
      IF(SPX.EQ.6.4) GO TO 8
      SPX=6.4
      ID1=ID
      C0=C1
      GO TO 11
8       BX=(6.4-SP(2))/(C1-C0)
      AX=SP(2)-BX*C0
      IF(ID1.LT.9.AND.ID.LT.9) GO TO 12
C   IF ENERGY CALIB. PEAKS ARE NOT FOUND, PRINT WARNING.
      WRITE(7,20)
20     FORMAT(' ','CHECK ENERGY SCALE.')
      CALL LIST (RD,NOCH,SERIES,NRUN)
12     CONTINUE
C   CALC. OF PHOTOPEAK AREAS, BKGR, AND UNCERT.
      DO 50 K=1,NPKR
      AR=0.0
      BK=0.0
      W=WM*(EN(K)*WS+WI)
      CH1=(EN(K)-AX)/BX-W/2.
      CH2=CH1+W
      I1=IFIX(CH1)
      I2=IFIX(CH2)

```



```

DO 1 I=I1,I2
1  AR=AR+RD(I)
  AR=AR-((CH1-FLOAT(I1)+0.5)*RD(I1)+(CH2-FLOAT(I2)-0.5)*RD(I2)
  BK=((CH1-FLOAT(I1))*(SM(I1+1)-SM(I1))+SM(I1))*W/2.
  B(K)=BK+((CH2-FLOAT(I2))*(SM(I2+1)-SM(I2))+SM(I2))*W/2.
  A(K)=AR-B(K)
  DA(K)=SQRT(A(K)+B(K)*(2.*W+9.)/15.)
50  CONTINUE
C   CALC. OF SCATTER PEAK AREAS NEXT...
DO 5 K=1,4
  AR=0.0
  W=WM*(SP(K)*WS+WI)
  CH1=(SP(K)-AX)/BX-W/2.
  CH2=CH1+W
  I1=IFIX(CH1)
  I2=IFIX(CH2)
DO 4 I=I1,I2
4  AR=AR+RD(I)
  AR=AR-((CH1-FLOAT(I1)+0.5)*RD(I1)+(CH2-FLOAT(I2)-0.5)*RD(I2)
  X(K)=AR
5  CONTINUE
C   SWITCH (8) OPTION; LIQUID SAMPLE WTS. & PELLET THICKNESS ARE READ IN.
  IF(.NOT.ISENSW(8)) GO TO 10
  WRITE(4,100) SERIES,NRUN
100  FORMAT(' ','ENTER SAMPLE THICKNESS (GM/CM**2) FOR ',A5,I3,
1    ' (7 SPACES)')
  READ(4,101) Y(2)
101  FORMAT(E7.2)
  WRITE(4,102) SERIES,NRUN
102  FORMAT(' ','ENTER SAMPLE WT. (GM) FOR ',A5,I3,' (7 SPACES)')
  READ(4,101) SAMWT
  Y(1)=7.92/SAMWT
10  RETURN
  END

```


C FILE=QUAN, KKN 92-11-77 VERSION
 C THIS ROUTINE COMPUTES ELEMENTAL QUANTITIES AND ABSORPTION CORRECTIONS,
 C ENHANCEMENT CORRECTIONS AND PARTICLE SIZE CORRECTIONS.
 C SAMPLE ABSORPTION IS COMPUTED BY ITERATIVE NORMALIZATION TO SCATTER PEAKS
 C AS DESCRIBED BY K K NIELSON, ANAL. CHEM. 49:641 (1977).

C
 SUBROUTINE QUAN(TH1,TH2,L,LEM,ITER,PS,RHO,RHOL)
 LOGICAL ISENSW
 COMMON RD(1024),SM(1024),EN(30),CAL(30),EL(30),A(30)
 COMMON CA(30)
 COMMON DA(30),B(30),SP(4),IEL(3,30),OLP(3,30),Q(30),DQ(30)
 COMMON QC(30),DL(30),UM(7,30),UL(5,14),SIH(30),SCH(30),SIL(14)
 COMMON SCL(14),ENLIT(14),ELIT(14),COR(30),CORL(30),IDAT(4)
 COMMON X(4),Y(4),XE(30),XEL(15),ABC3,ABC4,THETA,PHI
 COMMON UNIT,NPKR,NRUN,SERIES,NOCH,AX,BX,TIME,SS,PU,WM
 COMMON XH(30,30),XL(30,15),SF(30),FY(30),RAB(30),FYL(2)
 DATA FL1/SHC /,FL0/SH /,CD/SHCD109/

C
 ITER=0
 LEL=0
 LEM=LEL
 ABC1=ABC3
 ABC2=ABC4
 IF(.NOT.ISENSW(13)) GO TO 767

C SCATTER PEAK CALIBRATION CONSTANTS MAY BE READ IN TO OVERRIDE THE
 C LIBRARY VALUES TO AID IN RAPID CALIB. OF SCATTERED RADIATION (SW.13).
 READ(4,765) ABC1,ABC2

765 FORMAT(2F10.0)
 767 IFG=0

C SWITCH 2 PERMITS CHOICE OF ALTERNATE FIXED LIGHT ELEMENTS.
 IF(.NOT.ISENSW(2)) GO TO 768

766 WRITE(4,150)
 150 FORMAT(' ','Z OF FIXED LIGHT ELEMENT = ? (12)')
 READ(4,151) LEM
 LER=LEM

151 FORMAT(I2)
 IF(ITER.GT.0) GO TO 8

768 ITER=0
 NPP=NPKR+4
 CPR=0.
 TH1=0.
 NLE=IDAT(4)
 CORL(2)=1.
 CORL(NPKR+1)=0.000001
 CORL(NPKR+2)=0.000001

C SWITCH 9 TAKES LIVETIME FROM CHANNEL 1 & CONV. TO MINUTES.
 IF(ISENSW(9)) TIME=RD(1)/60.
 TINT=TIME
 IF(SS.EQ.CD) TIME=TIME*EXP(-0.00153*
 C (FLOAT(365*(IDAT(3)-76)+IDAT(1)*30+IDAT(2))-110.-30.))

C
 C QUANTITIES ARE CALC'D. HERE
 DO 5 I=1,NPKR
 Q(I)=A(I)/TIME/CAL(I)
 IF(ISENSW(8)) Q(I)=Q(I)/RAB(I)
 SF(I)=1.

5 QC(I)=Q(I)
 C QC AND SMI & SMC ARE ARBITRARILY INCREASED IN FIRST ITERATION
 C TO EXPEDITE CONVERGANCE.
 DO 79 I=1,12


```

79      QC(I)=QC(I)*6 *FLOAT(14-I)
      SMI=X(1)/ABC1/TIME*1.5
      SMC=X(2)/ABC2/TIME*1.5
C
C BEGINNING OF MAIN ITERATION LOOP.
C
43      CONTINUE
      LEM=LEL
C
C ENHANCEMENT CORRECTION EQUATIONS FROM B.C.CLARK.
C ADVAN. X-RAY ANAL. 17:258-260 (1974).
      IF(IFG.EQ.0) GO TO 11
      TK=Y(2)*1000000.
      DO 29 I=1,NPKR
      TM=0.0
      DO 28 J=1,NPKR
      IF(EN(J).LE.EN(I)) GO TO 28
      IF(QC(J)/TK.LE.0.00005) GO TO 28
      XJI=(XH(J,I)-XE(I))/PHI
      TM=TM+QC(J)*FY(J)*(1.-1./UM(6,J))*XE(J)/2./XE(I)*XJI*
1      (ALOG(1.+UN*PHI/(CORL(J)-UN))/UN+ALOG(1.+(CORL(I)-UN)*
2      PHI/(CORL(J)-UN))/(CORL(I)-UN)
28      CONTINUE
      SF(I)=1./(TM+1.)
29      CONTINUE
C
C OBSERVED ELEMENT EFFECTS ARE CALC'D. NEXT
C FIRST, CALCULATION OF ABSORPTION CORRECTIONS (COR)
11      CONTINUE
      YC=0.
      YI=0.
      UN=0.0
      DO 24 I=1,NPKR
      IF(QC(I).LE.0.) GO TO 24
      UN=UN+QC(I)*XE(I)
24      CONTINUE
      DO 15 K=1,NPP
      U=0.0
      DO 12 I=1,NPKR
      IF(QC(I).LE.0.) GO TO 12
      U=U+QC(I)*XH(K,I)
12      CONTINUE
      IF(K.GT.NPKR) GO TO 15
      YC=YC+SCH(K)*QC(K)*0.000001
      YI=YI+SIH(K)*QC(K)*0.000001
15      COR(K)=U
C
C FIND X-RAY SCATTER DUE TO LIGHT ELEMENTS.
68      VC=SMC-YC
      VI=SMI-YI
      TH=0.
      DO 4 I=1,NPKR
      IF(QC(I).GT.0.0) TH=TH+QC(I)
4      CONTINUE
      TH=TH/1000000.
C IF HEAVY ELEMENT SCATTER OVERESTIMATED, NORMALIZE DOWNWARD...
      IF(VC.GT.0..AND.VI.GT.0.) GO TO 70
      RQ=VC/SNC
      IF(VI/SMI.LT.RQ) RQ=VI/SMI
      RQ=(1.-ABS(RQ))*0.95

```



```

DO 72 I=1,NPKR
72  QC(I)=QC(I)*RQ
    GO TO 11
C
C  CHOOSE 2 REPRESENTATIVE LIGHT ELEMENTS & ESTIMATE THEIR MASSES.
70  Z=VI/VC
    IF(ISENSW(2)) GO TO 13
8    ITRE=0
6    CONTINUE
    ITRE=ITRE+1
    IF(R.GT.SIL(LEM)/SCL(LEM)) GO TO 32
    J=LEM+1
    DO 33 I=J,NLE
    IF(R.GT.SIL(I)/SCL(I)) GO TO 39
33   CONTINUE
    I=NLE
    GO TO 39
32  DO 34 I=1,LEM
    IF(R.GT.SIL(I)/SCL(I)) GO TO 36
34   CONTINUE
36   I=I-1
39   L=I
    IF(L.LE.0) L=1
    GO TO 38
13   L=8
    LEM=LER
38   TH2=(SIL(L)*VC-SCL(L)*VI)/(SIL(L)*SCL(LEM)-SCL(L)*SIL(LEM))
    TH1=(VI-TH2*SIL(LEM))/SIL(L)
    IF(TH1.GT.0.0.AND.TH2.GT.0.0) GO TO 71
C  IF A NEGATIVE MASS RESULTS, CHOOSE NEW REP. LIGHT ELEMENTS.
    IF(ITER.LT.5) GO TO 71
    IF(L.LT.LEM) GO TO 14
    IF(ISENSW(2)) GO TO 71
    IF(TH1.LT.0.) L=L-1
    IF(TH2.LT.0.) L=L+1
    GO TO 18
14   CONTINUE
    IF(TH1.LT.0.) L=L+1
    IF(TH2.LT.0.) L=L-1
18   CONTINUE
    IF(L.GT.0.AND.L.LE.NLE) GO TO 38
    IF(ITRE.GT.6) GO TO 756
    IF(ISENSW(15)) GO TO 71
C  IF NEGATIVE MASS STILL RESULTS, CHOOSE HEAVIER FIXED LIGHT ELEM.(LEM)
    LEM=LEM+1
    GO TO 6
71   CONTINUE
    RTH=(TH1+TH2+TH)/Y(2)
    IF(ISENSW(12)) RTH=1.
C
C  COMPUTE CORRECTION FACTORS FOR LIGHT ELEMENTS & HEAVY ONES
    GH=1000000.*Y(4)
    CP=CORL(2)
    DO 9 K=1,NPP
9    CORL(K)=(XL(K,LEM)*TH2+XL(K,L)*TH1)*GH+COR(K)
    UK=UN
    UN=UN+GH*(TH2*XEL(LEM)+TH1*XEL(L))
C
C  ELEMENTAL CONCENTRATIONS ARE CORRECTED NEXT.
    ITER=ITER+1

```



```

      UN=UN/THETA
      UK=UK/THETA
      DO 16 K=1,NPKR
C   EQUATIONS FOR PARTICLE SIZE CORRECTIONS...
      IF(.NOT.ISENSW(14)) GO TO 35
      COR(K)=COR(K)/PHI
      CORL(K)=CORL(K)/PHI
      CS=0.000001
      U1=(COR(K)/TH+(CORL(K)-COR(K))/(TH1+TH2))*RHO/2.
      U2=(UK/TH+(UN-UK)/(TH1+TH2))*RHO/2.
      U3=((COR(K)-UK)/TH+(CORL(K)-COR(K)-UN+UK)/(TH1+TH2))*RHO/2.
      U4=(UN-UK)*RHOL/(TH1+TH2)
      U5=(CORL(K)-COR(K)-UN+UK)*RHOL/(TH1+TH2)
      CC=(1./RHOL)/(1./RHOL+1./RHO)
      CR=1.-CC
      FPS=(1.-(CR*EXP(-U2*CS)+CC*EXP(-U4*CS))*(CR*EXP(-U3*CS)+CC*
C   EXP(-U5*CS)))/(1.-EXP(-U1*CS))
      FPS=FPS*(1.-EXP(-U1*PS))/(1.-(CR*EXP(-U3*PS)+CC*EXP(-U4*PS))*
C   (CR*EXP(-U3*PS)+CC*EXP(-U5*PS)))
      FPS=1./FPS
      COR(K)=COR(K)*PHI
      CORL(K)=CORL(K)*PHI
      GO TO 37
35  FPS=1.0
37  DQ(K)=FPS
      CORL(K)=CORL(K)/RTH
      IF(CORL(K).LE.50.) QC(K)=Q(K)*CORL(K)/(1.-EXP(-CORL(K)))*FPS*
C   SF(K)
      IF(CORL(K).GT.50.) QC(K)=Q(K)*CORL(K)*FPS*SF(K)
16  IF(ISENSW(9)) QC(K)=Q(K)*CORL(K)*FPS*SF(K)
      UN=UN*THETA
      UK=UK*THETA
C
C   ABS. CORR. OF SCATTER PEAK AREAS AND PEAK OVERLAP CORRECTIONS.
      CORL(K+1)=CORL(K+1)/RTH
      CORL(K+2)=CORL(K+2)/RTH
      SMI=X(1)/ABC1/TIME*CORL(NPKR+1)/(1.-EXP(-CORL(NPKR+1)))
      SMC=X(2)/ABC2/TIME*CORL(NPKR+2)/(1.-EXP(-CORL(NPKR+2)))
      J=0
2   J=J+1
      DO 1 I=1,NPKR
      K=IEL(J,I)
      IF(K.LE.0) GO TO 1
      IF(QC(K).LE.0.0) GO TO 1
      QC(I)=QC(I)+OLP(J,I)*QC(K)
1   CONTINUE
      IF(J.LE.2) GO TO 2
      IF(ISENSW(16)) GO TO 27
      IF(ABS(CORL(2)-CP)/CP.LE.0.0001.AND.IMG.EQ.1)GO TO 27
      IF(ABS(CORL(2)-CP)/CP.LE.0.005) GO TO 30
      IF(ITER.GE.6) GO TO 30
      GO TO 43
30  CONTINUE
      IFG=1
      IF(ITER.GE.35) GO TO 27
      GO TO 43
C
C   END OF MAIN ITERATION LOOP.
C
27  CONTINUE

```



```
C  CALC. OF Q WITHOUT OVERLAP CORRECTIONS TO PERMIT OVERLAP PRINTOUT
DO 49 I=1,NPKR
  IF(CORL(K).LE.50..AND..NOT.ISENSW(9))Q(I)=Q(I)*CORL(I)*DQ(I)*
C  SF(I)/(1.-EXP(-CORL(I)))
  IF(CORL(K).GT.50..OR.ISENSW(9))Q(I)=Q(I)*CORL(I)*DQ(I)*SF(I)
49  CONTINUE
C  UNCERTAINTIES FROM OVERLAPPING PEAKS ARE INCLUDED HERE.
  J=0
3    J=J+1
  DO 7 I=1,NPKR
    K=IEL(J,I)
    IF(K.LE.0) GO TO 7
    IF(QC(K).LE.0.) GO TO 7
    DA(I)=SQRT(DA(I)**2+DA(K)**2*ABS(OLP(J,I))*CORL(K)/CORL(I))
7    CONTINUE
    IF(J.LE.2) GO TO 3
C
  IF(SS.EQ.CD) TIME=TIMT
  TH1=TH1/RTH
  TH2=TH2/RTH
  RETURN
END
```


C THIS ROUTINE PRINTS OUT ANALYSIS RESULTS.

```

C
      SUBROUTINE PRNT(TH1,TH2,L,LEM,ITER,PS,RHO,RHOL)
      LOGICAL ISEN9W
      COMMON RD(1024),SM(1024),EN(30),CAL(30),EL(30),A(30),CA(30)
      COMMON DA(30),B(30),SP(4),IEL(3,30),OLP(3,30),O(30),DQ(30)
      COMMON QC(30),DL(30),UM(7,30),UL(5,14),SIH(30),SCH(30),SIL(14)
      COMMON SCL(14),ENLIT(14),ELIT(14),COR(30),CORL(30),IDAT(4)
      COMMON X(4),Y(4),XE(30),XEL(15),ABO3,ABO4,THETA,PHI
      COMMON UNIT,NPKR,NRUN,SERIES,NOCH,AX,BX,TIME,SS,PU,WM
      COMMON XH(30,30),XL(30,15),SF(30),FY(30),RAB(30),FYL(2)
      DATA FL1/5H /, FL0/5H /

```

C PAGE HEADING IS FIRST PRINTED...

```

C
      TH=0.
      WS=0.32448
      WI=5.379
      DO 48 I=1,NPKR
      IF(QC(I).GT.0.0) TH=TH+QC(I)
48      CONTINUE
      TH=TH/1000000.
      TH=TH+TH1+TH2
      F1=TH1/TH
      F2=TH2/TH
      TH=TH*1000.
      E1=ELIT(L)
      E2=ELIT(LEM)
      FL=FL0
      PARSIZ=PS*15000.
      IF(ISEN9W(11)) GO TO 86
      WRITE(7,100) SERIES,NRUN,TH,PU
100      FORMAT('1',A5,I5,10X,F9.3,' MG/CM**2',10X,
C      'PCT.CALIB.UNCRT.=',F4.1)
      WRITE(7,101) (IDAT(I),I=1,3),F1,E1,F2,E2,Y(1)
101      FORMAT(' ',3MO DA YR=',3I3,10X,F6.3,1X,A2,'+',F6.3,1X,
C      A2,6X,'NORM.FACTOR =',F10.4)
      WRITE(7,108) ITER,BX,AX,PARSIZ
108      FORMAT(' ',ITERATIONS=',I4,11X,'KEV=CH*',F7.5,'+',
C      F6.3,5X,'P. SIZE(MICRON)=',F8.2)
      WRITE(7,102) TIME,X(1)
102      FORMAT(' ',MINUTES=',F8.3,39X,'INCOH A =',F12.0)
      WRITE(7,103) SS,X(2)
103      FORMAT(' ',SEC.SOURCE =',A5,7X,
C      'X-RAY FLUORESCENCE ANALYSIS',6X,'COH A =',F12.0,/)
      WRITE(7,104) UNIT,UNIT,UNIT
104      FORMAT(' ',NO CHANNELS NET AREA   BKGND   ABSOR   ',
C      'OVERLAP REGION',4X,A5,4X,'2 SIG.DL.',/,/,',14X,'+/-',
C      7X,'P.S.   ENHAN   (',A5,')',13X,'+/-   (',A5,')',/,)

```

C LOOP FOR PEAK ANALYSIS PRINTOUT.....

```

C
86      CONTINUE
      DO 35 I=1,NPKR
      PSIZE=DQ(I)
      W=WM*(EN(I)*WS+WI)
      C1=(EN(I)-AX)/BX-W/2.
      C2=C1+W
      IF(CORL(I).LE.50.)CF=CORL(I)/(1.-EXP(-CORL(I)))
      IF(CORL(I).GT.50.)OR(ISEN9W(9)) CF=CORL(I)

```



```

      O1=(QC(I)-Q(I))*Y(1)
      IF(ISENSW(9)) O1=O1/TH*1000.
C   BLANK (CA) IS IN CALIBRATION UNITS (UG/CM**2).
      QC(I)=QC(I)-CA(I)
      QC(I)=QC(I)*Y(1)
      IF(ISENSW(9)) QC(I)=QC(I)/TH*1000.
      DQ(I)=SQRT((DA(I)/A(I))**2+(0.01+PU)**2)*Q(I)*Y(1)
      IF(ISENSW(9)) DQ(I)=DQ(I)/TH*1000.
      DL(I)=2.*SQRT(DA(I)*DA(I)-A(I))/A(I)*Q(I)*Y(1)
      IF(ISENSW(9)) DL(I)=DL(I)/TH*1000.
      IF(QC(I).GT.DL(I)) GO TO 50
      FL=FL1
      DQ(I)=QC(I)
      QC(I)=DL(I)
50    CONTINUE
      IF(ISENSW(11)) GO TO 88
      WRITE(7,105) I,C1,A(I),B(I),CF,O1,FL(I),FL,QC(I),DL(I)
105   FORMAT(' ',I2,F7.1,F11.0,F9.0,F7.3,G11.2,2X,A5,1X,A1,
C      G11.4,G10.3)
      WRITE(7,106) C2,DA(I),PSIZE,SF(I),DQ(I)
106   FORMAT(' ',F9.1,F11.0,F9.3,F7.3,11X,9X,G11.4)
88    CONTINUE
      IF(FL.EQ.FL1) DQ(I)=0.0
1     FL=FL0
35    CONTINUE
C
C   CONCENTRATIONS ARE STORED IN FYL FOR SUMMARY REPORT.
C   RD AND SM ARE USED HERE AS WORKING ARRAYS.
C
      IF(NRUN.GT.39) GO TO 37
      CALL SEEK(1,FYL)
      READ(1) RD
      READ(1) SM
      CALL CLOSE(1)
      DO 36 I=1,NPKR
      N1=NPKR*(NRUN-1)*2+2*(I-1)+1
      N2=N1+1
      RD(N1)=QC(I)
36    RD(N2)=DQ(I)
      CALL ENTER(1,FYL)
      WRITE(1) RD
      WRITE(1) SM
      CALL CLOSE(1)
37    RETURN
      END

```



```
SUBROUTINE REP
COMMON RP(2048), DM(60), EL(30), IDM1(30), DUM(820), IDAT(4)
COMMON X(53), ABC3, ABC4, THETA, PHI
COMMON UNIT, NPKR, NRUN, SERIES, NOCH, AX, BX, TIME, SS, PU, WM
COMMON DUMM(1440), FYL(2)
DATA BL/5H /, DL/5H/ /
CALL SEEK(1, FYL)
READ(1) RP
CALL CLOSE(1)
CALL DLETE(1, FYL, I)
K1=1
3 K2=K1+5
IF(K2.GT.NPKR)K2=NPKR
WRITE(7,10) SERIES, (IDAT(I), I=1,3), TIME
10 FORMAT('1', 'X-RAY FLUORESCENCE SERIES ', A5, ' ', MO-DA-YR',
C ' ', I3, ' ', I2, ' ', I2, 3X, F7.2, ' MIN. ')
WRITE(7,11) SS, UNIT
11 FORMAT(' ', A2, ' SECONDARY SOURCE, CONCENTRATIONS AND',
C ' UNCERTAINTIES IN ', A5, '/')
WRITE(7,12) (EL(K), K=K1, K2)
12 FORMAT(' ', 'NO', 6(5X, A2, 5X), /)
DO 2 J=1, NRUN
DO 1 K=K1, K2
N=NPKR+(J-1)*2
N2=N+K*2
N1=N2-1
DM(K)=RP(N1)
DUM(K)=RP(N2)
DUMM(K)=BL
IF(DUM(K).EQ.0.)DUMM(K)=DL
1 CONTINUE
WRITE(7,13) J, (DUMM(K), DM(K), K=K1, K2)
13 FORMAT(' ', /, ' ', I2, 1X, 6(A1, G11.4))
WRITE(7,14) (DUM(K), K=K1, K2)
14 FORMAT(' ', 2X, 1X, 6(1X, G11.4))
2 CONTINUE
K1=K1+6
IF(K1.GT.NPKR) GO TO 90
GO TO 3
90 RETURN
END
```


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