The SPECTRA program library:
A PC based system for gamma-ray spectra analysis and INAA data reduction

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U.S. Geological Survey

Open File Report 94-168

UNITED STATES DEPARTMENT OF THE INTERIOR

U.S. GEOLOGICAL SURVEY

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ABSTRACT

This manual describes a PC based system for the analysis of gamma-ray spectra and for the complete reduction of data from INAA experiments. The spectral data analysis software includes algorithms for iterative fitting and non-fitting methods for the integration of gamma-ray lines. Graphics algorithms may be called for the analysis of complex spectral features and to define the integration mode for selected "regions-of-interest" for the analysis of subsequent spectra. Corrections for gain and zero drift, pulse pile-up, and spectral interferences are incorporated in the program. Individual peaks and spectra may be selected for re-analysis after the completion of an initial INAA run, and a suspended INAA run may be restarted. The degree of user interaction with the spectral and analytical data during spectral data analysis and the averaging of multiple results is controlled by the user and can extend from essentially batch analysis (minimal interaction) to thorough review by the analyst at each stage of the data reduction process. Additional programs for the creation of input data files, and for report form generation of the analytical data are described. Graphics algorithms are available for use after spectral data analysis to compare the data from alternate photopeaks and to evaluate detector performance during a given counting cycle. During the preparation of the final report of analysis, plotting routines can be used to prepare plots of chondrite normalized rare earth element patterns and to compare the data from reference samples with accepted values. A database of data for control samples can be used to prepare quality control charts to evaluate long term precision and to search for systematic variations in data on reference samples as a function of time. The entire software library can be accessed through a user-friendly menu interface with internal help.

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Acknowledgments

The programs described in this document have evolved over a period of approximately 25 years. The initial development of the SPECTRA program was carried out while the first author was associated with the Nuclear Chemistry Center at the Massachusetts Institute of Technology, and the Institute of Geophysics and Planetary Physics at U.C.L.A. The authors have benefited from numerous discussions and suggestions made by colleagues during the development of these programs, particularly: W.V. Boynton, G.W. Kallemeyn, J. Kimberlin, R.J. Knight, F.T. Kyte, J.S. Mee, J.P. Op de Beeck, C.A. Palmer, K.L. Robinson, J.J. Rowe, L.J. Schwarz, G.A. Wandless, P.H. Warren and J.T. Wasson.

1. INTRODUCTION

The purpose of this manual is to document the implementation of the program SPECTRA and its associated utilities on 386 and higher personal computers running under the DOS operating system. The previous VAX implementation of the software library has been described in Baedecker and Grossman (1989). This report provides additional details on the installation of the program library under DOS, the application of the library to INAA data processing, and new features of the software. The report also provides additional recommendations regarding the use of SPECTRA for INAA data reduction.

The SPECTRA program is an integrated set of algorithms for both gamma-ray spectra analysis and the processing of the results of that analysis to yield concentration values in neutron activation analysis experiments. Procedures for the analysis of gamma-ray spectra include algorithms for smoothing, peak location, centroid and energy determination, and iterative and non-iterative methods for photopeak integration. Instrumental neutron activation analysis calculations are an integral part of the SPECTRA program because of the advantages in carrying out the INAA analysis while the spectral data are resident in memory. In particular, the determination of upper limits and corrections for spectral interferences are facilitated in an integrated system. Selected analytical lines may be designated for interactive graphical analysis. The graphics procedures may also be called automatically under special circumstances such as for the analysis of peaks having poor counting statistics or unexpected interferences. Interactive line/isotope identification algorithms are callable in conjunction with the algorithms for graphical presentation of the spectral data. A particularly useful feature of SPECTRA is the ability to reprocess selected peaks in selected spectra following the completion of an initial SPECTRA INAA run.

The original SPECTRA program was developed for batch processing on main-frame computer systems. The principal mode of photopeak integration within the program consisted of simple summation procedures, rather than iterative least squares fitting, because the latter approach engendered a much greater expense for computer time. However, procedures for iterative least squares fitting have been incorporated in SPECTRA for the analysis of poorly resolved spectral features, particularly during interactive graphical analysis when the user has the capability to carefully monitor the results of the fitting process.

The SPECTRA program is the first stage in a complete INAA data reduction system that incorporates spectral data analysis, averaging of the results from multiple lines and multiple countings, and report form generation. Data on control samples can be passed to a quality control data base for the preparation of control charts and for monitoring long term precision. The entire software library is extremely flexible in permitting as much or as little interactive analysis of the data as seems desirable. All of the programs in the library (with the exception of the spectral data file conversion utilities) can be called from a single, user-friendly, menu interface called SPECMENU. SPECMENU provides a convenient interface to the SPECTRA library as well as to MS-DOS.

2. PROGRAM INSTALLATION

2.1 Hardware requirements

SPECTRA needs 1.03 megabytes of memory to run. SPECTRA.EXE is bound to a loader that lets it make use of extended memory. The DOS "memory" command can be used to determine the amount of extended memory available on a given system. If it's too low, a virtual memory version of SPECTRA is available from the authors. This latter version makes use of virtual memory (i.e. swapping of memory to disk) to make up for shortfalls in physical memory.

SPECTRA will only run on IBM 80386 PCs equipped with a math co- processor, 80486 machines and their clones. The program will not run on 80286 machines. SPECTRA and associate utilities can be run as a DOS application from Windows via the SPECMENU interface; however, execution speed is somewhat degraded.

The executable program files currently require ~5 megabytes of disk storage. The data files required to run SPECTRA, the test data files included on the distribution diskettes, the documentation files, and the graphics print drivers require an additional 600 kilobytes of disk storage.

In interactive plotting mode, SPECTRA does graphics to the video monitor. If interactive plotting is to be used, then a mouse is required on the system.

2.2 Installing the program library.

The SPECTRA program library can be installed using the INSTALL program included on the first distribution diskette. Place the diskette in the appropriate floppy drive (e.g. disk B), type B: to make that drive the current drive, and type INSTALL. The program will create two new directories on the system's hard drive: (1) a program directory where the .EXE files and ancillary data files will reside (the SPPATH directory), and (2) a user work directory (the USERPATH directory). The default file names for these directories are C:\SP and C:\INAA, respectively. The user has the option of assigning different names to these directories during the INSTALL procedure. The USERPATH directory may contain several of the same data files as the C:\SP directory except that they can be tailored by an individual user as necessary and will be used preferentially during program execution. We recommend that separate working directories be created for each irradiation data set under the USERPATH directory (i.e. data for irradiation 899 would be kept in a directory C:\INAA\899). We also recommend the creation of two additional directories under the INAA directory: C:\INAA\TEST and C:\INAA\CNTL. The INSTALL program will automatically create the C:\INAA\TEST directory and install the test data set distributed with the SPECTRA library. The CNTL directory is only required if a quality control data base is to be created as described in section 3.6.

The library is distributed on two diskettes as six self-extracting archive .EXE files that are decompressed during the INSTALL procedure. SPECEXE1.EXE and SPECEXE2.EXE contain all of the executable programs in the SPECTRA library. SPECDATA.EXE contains miscellaneous data files required by programs in the library. SPECDOC.EXE contains several documentation files. The TESTDATA.EXE file contains test data files that the install program will place in the C:\INAA\TEST directory.

GPDRVR.EXE contains the graphic print drivers (and associated .EXE and .BAT files) required to dump graphics images that have been stored on disk to a printer. These GrafPrint™ drivers are distributed with the SPECTRA library with the permission of AnSoft, Inc. As noted below, the GPRINT.BAT and/or SPECMENU.DEF files will need to be modified with a text editor in order to specify the appropriate print driver for your system's printer.

A few modifications to the AUTOEXEC.BAT file (and possibly the CONFIG.SYS file) may be required. The user is given the option of allowing INSTALL to automatically revise the AUTOEXEC.BAT file. The SPPATH directory name (default = C:\SP;) needs to be added to the DOS PATH command in AUTOEXEC.BAT. Lines similar to the following will also need to be added to the AUTOEXEC.BAT file only if the default directory path names were <u>not</u> used in setting up the SPECTRA library on the hard disk:

```
SET SPPATH=C:\SP                (this is the default)
SET DRVRPATH=C:\SP              (this is the default)
SET USERPATH=C:\INAA            (this is the default)
SET CNTLPATH=C:\INAA\CNTL       (this is the default)
```

If the interactive graphics algorithms in the SPECTRA library are to be used, then your mouse driver must be loaded in memory by a command in either the AUTOEXEC.BAT or CONFIG.SYS file. At the moment, the SPECTRA mouse handling routines only work in 640x480 resolution. A test program, MOUSTEST, is included in the SPECTRA library to test the function of the mouse. If the mouse is not working at the default resolution of the monitor, try including the following command in the AUTOEXEC.BAT file:

```
SET LPLOT=HH,640,480,16
```

where HH is the hexadecimal number needed to initialize the BIOS video mode in 640 x 480 pixel resolution with 16 colors. The documentation for the system video card must be consulted to find the proper value for HH, since it is arbitrarily chosen by the card maker.

The graphics routines also require that the memory area between hexadecimal A000 and BFFF be excluded if a memory manager is available on the system. For many memory managers (such as QEMM, CEMM, 386MAX) this can be done by appending text such as the following to the memory manager's driver install command in the CONFIG.SYS file:

X=A000-BFFF or EXCLUDE=A000-BFFF

See the memory manager's documentation for specific information on how to exclude memory areas. CONFIG.SYS will not be modified by the SPECTRA INSTALL command. After altering the AUTOEXEC.BAT and CONFIG.SYS files it is necessary to re-boot the system.

Several programs in the library are designed to work with the system monitor set in 132 column mode (i.e. the programs VIEWFILE, REVIEW, and FSRWIND). Three .BAT files, included on the distribution diskettes, should be revised using a text editor (such as the DOS EDIT command) in order to insert the correct commands needed to place your monitor in 132 column mode and to change it back to 80 column mode: REVIEW.BAT, VIEW132.BAT, and FSRW.BAT. These batch files are not required if the corresponding programs are called from SPECMENU, however the commands to take the monitor in and out of 132 column mode will need to be inserted in the file SPECMENU.DEF. Consult the documentation for the system video card in order to determine the correct commands for your system.

3. INAA DATA PROCESSING

INAA data processing using the SPECTRA system is conducted in four stages using four main programs:

(1) Spectral data analysis and INAA calculations (program: SPECTRA)
(2) Averaging of INAA results from multiple lines to yield a single concentration value for each element determined in a single sample count (program: SUMMARY1).
(3) Averaging of the results from multiple sample countings to yield a single concentration value for each sample, final report form generation and the preparation of normalized multi-element plots (program: SUMMARY2).
(4) Incorporation of data on control samples into a quality control data base (program: CNTLEDIT).

This section describes the INAA data reduction process as carried out using the SPECTRA program library. Since the individual programs in the library can be activated from the SPECMENU interface, it is not necessary for the user to be familiar with the names of individual programs. However, the user should have a general understanding of the overall processing scheme in order to tailor the input data files to his own use. In the first three stages of the processing scheme, a preprocessor program must be run in order to create the input control file for the data reduction program that is used at that stage. The use of preprocessor programs saves having to input essential information multiple times if, for some reason, a processing step must be repeated. SPECEDIT is used to create the input control file for the SPECTRA program, ISRSETUP for the SUMMARY1 program, and FSRSETUP for the SUMMARY2 program. In order to provide the capability of allowing different laboratories to customize the programs for their own use, program defaults can be specified in a series of ASCII .DEF files, which can be modified with a text

editor. The default values of program variables for the SPECEDIT, ISRSETUP, and FSRSETUP programs are assigned in the files SPECEDIT.DEF, ISR.DEF, and FSR.DEF, respectively. Program defaults for the other programs in the library can also be modified by editing their .DEF files.

3.1 Preparing the input files for SPECRA/INAA processing

A flow chart depicting the first stage of the data reduction process is shown in Figure 1. Program names are circled, input/output data files are shown in rectangles. (In some cases, multiple programs/files are shown in single circles/rectangles for simplicity.)

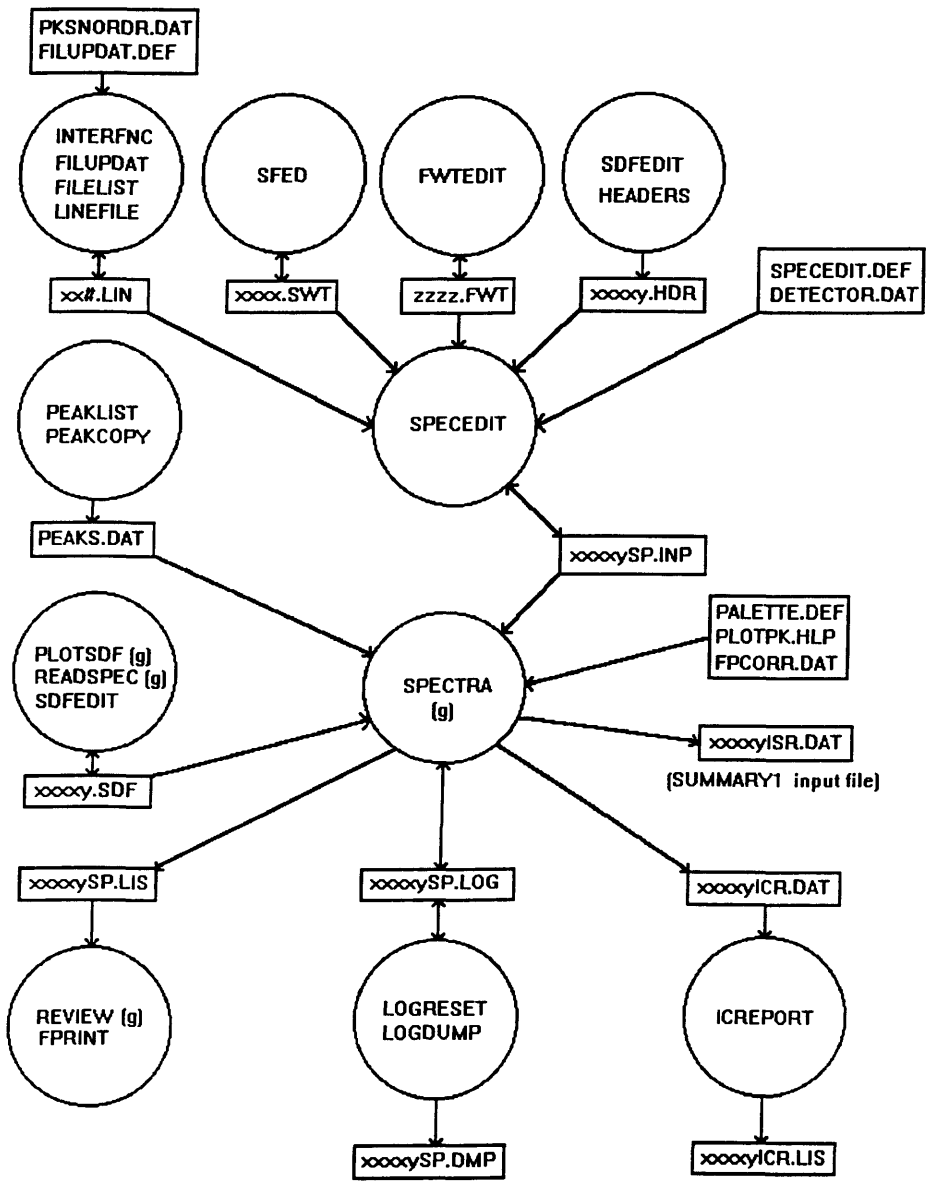

Figure 1. Flow chart of spectral data analysis.

The input and output file names of nearly all programs in the SPECTRA library are defined using the 4-5 character job identification string [xxxxy for SPECTRA and SUMMARY1 programs, and xxxx for SUMMARY2 programs; where xxxx is the name of the data set and y is a sequential count identifier (a,b,c,d,... etc.)]. (The job identification string is limited to 5 characters for INAA processing because of the input/output file naming conventions use by SPECTRA; see Figure 1.) Thus the SPECTRA input control file should be named xxxxySP.INP, where xxxxy corresponds to the name of the .SDF spectral data file. (In our laboratory, the file name P923CSP.INP would indicate the third (C) count of irradiation 923 processed by analyst P). The job identification string is passed automatically to the programs by SPECMENU. If the individual SPECTRA programs are called from DOS the program will request the job name at the first prompt, or the job i.d. string may be passed as in input argument on the command line (that is, the program can be started by typing "SPECEDIT xxxxy").

In the following sections we describe the preparation of the various input files that should be created prior to running SPECEDIT. The default gamma-ray energy calibration data and detector parameters are stored in the SPECEDIT.DEF and DETECTOR.DAT files respectively. These files allow SPECTRA to be tailored for use by a given laboratory and will not have to be routinely edited. If SPECTRA is to be used for INAA data reduction, users will find it convenient to prepare 4 different types of data files prior to creating the SPECTRA input control file with SPECEDIT: .LIN, .SWT, .HDR and .FWT files. The analytical line data in the .LIN files will generally not have to be modified from one INAA run to the next. The .SWT files contain sample data that will need to be defined for each INAA sample set. The .FWT files contain concentration data for multi-element comparison standards (referred to as "flux monitors" hereafter). The .HDR files can be used to define the order of sample counting for different (replicate) counts of a given sample set.

Default calibration data: SPECEDIT.DEF

Default data values that tend to remain constant from one SPECTRA run to the next can be defined in the file SPECEDIT.DEF in the C:\SP directory. For example, in our laboratory, separate calibration sources are used to prepare calibration spectra for coaxial and for planar LEPD detector counts for every sample count. The default isotope list and energies of the calibration lines are stored in the SPECEDIT.DEF file and can be modified with a text editor to customize the SPECEDIT program for any laboratory. In addition to calibration data the file contains variables to define the default number of channels used for both detector types, the lines used for gain (and zero) shift correction, the character string used in the sample name for flux monitor identification, the numbers of flux monitors in a given sample count, etc. Additional documentation on the SPECEDIT.DEF file can be found in the file SPECEDIT.DOC.

Detector performance parameters: DETECTOR.DAT

In addition to the default calibration data contained in the file SPECEDIT.DEF, a second file, DETECTORS.DAT, is used to store efficiency, pulse pile-up, and peak shape data for individual detectors in

the laboratory. It must be in the SPPATH directory and can be edited with a text editor to make it useful for other laboratories. A three letter code is used to identify each detector. The DETECTOR.DAT file contains the parameters for defining the detector efficiency calibration, the coefficients for two different modes of pulse pile-up correction, and for a peak shape calibration of the detector (used for iterative least squares fitting of spectral features). The inclusion of peak shape data in this file is optional because SPECTRA normally defines the peak shape parameters from an analysis of energy/peak shape calibration spectra which are placed at the front of each spectral data file. However, the option of including peak shape data in the DETECTOR.DAT file is provided for laboratories that choose to use a separate calibration spectrum for peak shape.

The following parameters are defined in the DETECTOR.DAT file:

DETECTOR ID (3 characters)

DETECTOR TYPE CODE (2 characters, user selectable) that indicates whether the detector is a coaxial detector or a planar low energy photon detector.

SLOPE (slope of linear (> 200 keV) part of the log-log efficiency curve)

CURVE (curvature of the quadratic used to define the low energy portion of the log-log efficiency curve)

EJP (junction point (in keV) between the linear and quadratic parts of the log-log efficiency curve)

TPU(1) (pulse pile-up resolving time (in microseconds) of the detector-amplifier system)

alternatively TPU(1) and TPU(2) can be used to define a quadratic calibration of pulse pile-up correction factor as a function of dead time where

$$\text{corr. factor} = 1.0 + TPU(1) * D.T. + TPU(2) * (D.T.)^2$$

FFD(1,2) The intercept of *fwhm* vs. channel number calibration

FFD(1,1) The slope (x 10**3) of the *fwhm* vs. channel number calibration.

FFD(2,2) The intercept of the low energy tail junction point vs. channel number calibration.

FFD(2,1) The slope (x 10**3) of the low energy tail junction point vs. channel number calibration.

The efficiency calibration parameters can be determined using the EFFCALIB program as described in Baedecker and Grossman (1989). The determination of the pulse pile-up resolving time is treated in the same publication. Least squares fitting of spectral features in SPECTRA is also described in Baedecker and Grossman (1989). The model consists of a symmetrical Gaussian function in the central and higher energy portion of the peak and an exponential tail in the low energy side of the photopeak with a functional form identical to that used by SAMPO (Routti and Prussin, 1969). The peak shape parameters can be defined simply by analyzing a calibration spectrum with SPECTRA. The shape parameters will be reported on the first page of the SPECTRA xxxxySP.LIS output file.

INAA analytical line data: .LIN files

.LIN files contain the data on the analytical lines for the indicator radionuclides used during INAA processing. In our laboratory we use a three character convention as the prefix for the name of each .LIN file. The first two characters define the detector type, and the third character defines the number of the count in the counting sequence (i.e. 1 = 5-7 days decay; 2 = 14 days decay; 3 = 60 days decay). We use GE as a symbol for coaxial Ge detectors and IG as a symbol for intrinsic germanium planar low energy photon detectors. These may have been poor choices for acronyms, since most of our coaxial detectors are now intrinsic germanium and both detector types are fabricated from Ge crystals. However, old habits die hard, and we have continued to use that convention. The mnemonic symbols used to represent high energy and low energy detectors can be redefined to suit the preference of any analyst by editing the various .DEF files that are included on the distribution diskettes (SPECEDIT.DEF, FILUPDAT.DEF, and ISR.DEF).

.LIN files can be created and edited using the LINEFILE program. The .LIN files routinely used in our laboratory are included on the distribution diskette. These files may be placed either in the SPPATH or USERPATH directories. The .LIN files contain the element name, gamma-ray energy, half-life, and the data used for interference corrections. Up to four interference corrections can be defined for each analytical line. The interference correction data include the separation (in keV) of the interference from the analytical line, the energy of a reference line of the interfering radionuclide that is used for making the interference correction, and the intensity ratio of the interfering line to the reference line. The .LIN files may also include the flux monitor concentration data for the most commonly used multi-element standard used for analysis. This flux monitor is identified by the def_fname parameter in the SPECEDIT.DEF file. The element contents for all other flux monitors are defined by separate zzzz.FWT files as described below.

File listings of the data in the .LIN files that are suitable for printing can be created with LINEFILE or the FILELIST utilities. FILUPDAT is a utility that can be used to conveniently update a collection of .LIN files using the data in two master .LIN files: GEMASTER.LIN and IGMASTER.LIN. Thus if it becomes necessary to correct gamma-ray energy, half-life, flux monitor concentration or interference correction data in multiple .LIN files, this can be easily accomplished by simply revising the xxMASTER.LIN files and running the FILUPDAT utility.

The INTERFNC utility is a convenient tool for identifying potential spectral interferences that may be encountered during INAA processing. The program will search for all lines in the SPECTRA isotope library (PEAKS.DAT) that are within $\pm$ x keV from the analytical lines in any .LIN file where x is user definable. A half-life filter to screen out shorter-lived species can also be applied. Instead of the PEAKS.DAT (or PEAKSU.DAT) files, the INTERFNC program expects the isotope library to be in a file PKSNORDR.DAT, which is created from the PEAKS.DAT file by INTERFNC or by the PEAKLIST utility. INTERFNC creates a printable output file xxx.INT for each xxx.LIN file processed.

INAA Sample data: .SWT files

An xxxx.SWT file should be created for each irradiation. This file can be created with the SFED "Sample File EDitor". The .SWT file contains the name and weight data for each sample in the irradiation set. In the SPECTRA program library, 18 characters have been allocated for the INAA sample name. The first nine characters (or "lab number") have been allocated to the sample identification number assigned by our laboratory's central laboratory information management system (LIMS). The second nine characters (or "field number") are used for the identification number assigned by the submitter. The entire 18 characters can be used as a single identification number, but the 18 character field will be split into two nine character fields in the column headings of the tabular reports generated by the programs SUMMARY1 and SUMMARY2.

The .SWT file may also contain counting time and decay time information; although, these data are generally included in the .SDF spectral data file. If multiple analytical jobs are included in an INAA sample set, a four character job identification number is placed in columns 81-84 of the .SWT file. This information is subsequently used for breaking out the data for separate jobs in preparing the final reports of analyses.

Specifying the order of sample counting: .HDR files

Each sample is also assigned a two digit identification number in columns 85-86 of the .SWT file. This two digit number can be used to define the sample counting sequence for multiple countings of the sample set. In our laboratory, the counting sequence may not be the same from count to count for the early sample counts because the least active samples are counted first. In this case the SPECEDIT user must either create separate .SWT files for each count (with the samples in the proper sequence) or use .HDR files to define the counting sequence for each set of spectral data. .HDR files are ASCII files that contain one line of data for each spectrum in the corresponding spectral data file (named xxxxy.SDF). If any of the SPECTRA file conversion utilities are used to create the .SDF spectra data file the .HDR files are created automatically. They can be created using the SDFEDIT program which reads (and edits) .SDF files. The sample counting sequence for each count can be defined by entering the two digit code for each sample into the previously created xxxxy.HDR files using the HEADERS program. The HEADERS program permits the counting sequence to be entered by the user from the terminal, or one of several predetermined sequences can be selected as defined in the HEADERS.DEF file.

Flux Monitor data: .FWT files

.FWT files contain flux monitor concentration data for any of the flux monitors included in the irradiation sample set. They may be created with the FWTEDIT utility and can be placed in the SPPATH, USERPATH, or the irradiation directory. Each flux monitor is identified by its sample name in the xxxxySP.INP file. The first four characters of the 18 character sample name field is the string used to tell

SPECTRA that the sample is a flux monitor and is defined by the def_fmid parameter in the SPECEDIT.DEF file. Characters 10-17 define the flux monitor and should be identical to the name of its .FWT file.

3.2 Preparing the input file for SPECTRA (SPECEDIT)

The input file xxxxySP.INP contains the control information SPECTRA needs to run. The file APPENDX1.TXT describes the format of this file. The xxxxySP.INP file should be created with the program SPECEDIT. If default gamma-ray energy calibration data have been defined in the SPECEDIT.DEF file, the .LIN analytical line files have been prepared, and the .SWT sample name/weight and (optional) .HDR counting sequence files have been prepared for an irradiation sample set, then the creation of the SPECTRA input control file xxxxySP.INP is easy with the use of the SPECEDIT program.

The SPECEDIT user is provided with three screens to define the input variables for SPECTRA: screen 1 to define detector energy/efficiency calibration data; screen 2 to set spectra processing options; and screen 3 to set INAA processing options. Figure 2 shows a sequence of six screen menus produced by SPECEDIT. For INAA processing, screen number 1 asks the user for submitter, irradiation number, count number, detector ID, and count date. The user is given the option of entering calibration and gain/zero shift information from the terminal or of accepting the default values as read from the SPECEDIT.DEF file. Pulse pile-up, detector efficiency, and (optional) peak shape data are obtained for the detector specified from the DETECTOR.DAT file or may be entered manually from the terminal.

The "spectra processing options" screen asks for the number of spectra to be analyzed and gives the user the option of setting various spectral data processing control variables (or accepting the default values). The spectral data processing control options that can be defined within SPECEDIT are as follows:

Turn on/off INAA processing. (Def. = on)
# of channels in spectrum. (Def. = 4096) (maximum = 8192)
# of spectra to be processed.
Spectra skipping parameters. (used alternatively):
    (skip to tagword #, # of blocks, # of spectra) (Def. = 0,0,0)
Mode of peak integration:
    "Central Peak Area" (CPA or Wasson) Method. Peak integration over fixed channel limits of summation.
        (This is the default integration method using 5 channels.)
        (The integration width may be incremented by 2 at various specified channel numbers.)
        CPA areas may be corrected for peak broadening. (Def. = off)
    Peak integration by Total Peak Area summation.
        Turn off/on non-linear baseline for TPA/CPA peak integration. (Def. = on)

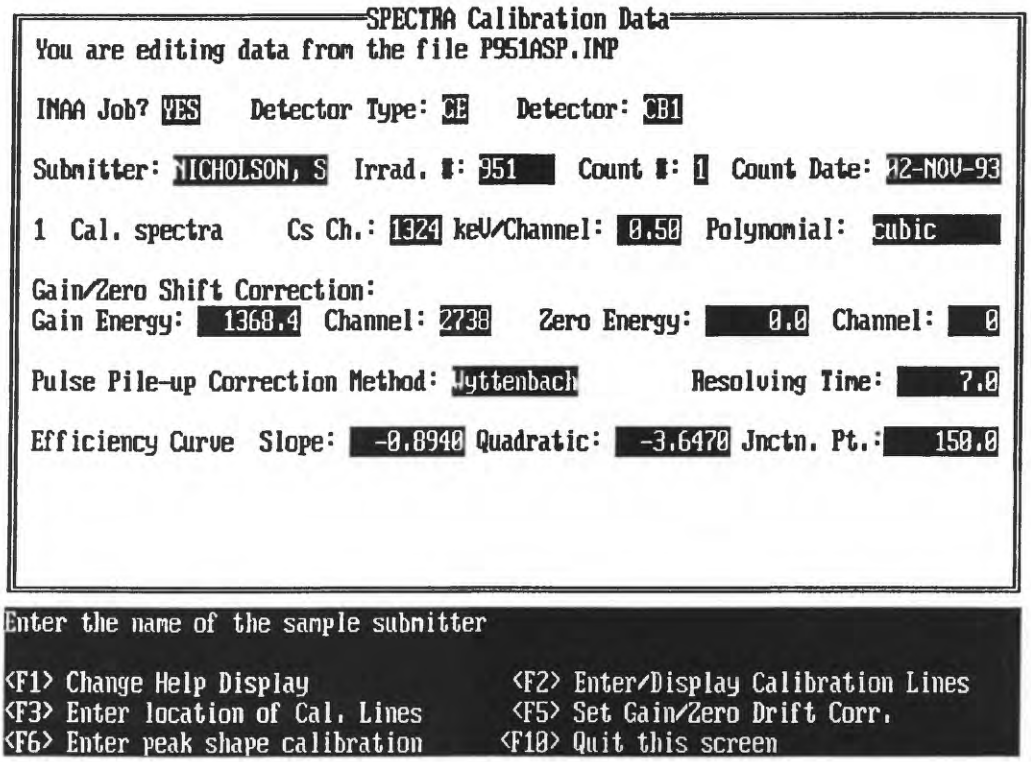

Figure 2a. SPECEDIT screen 1: Calibration Data.

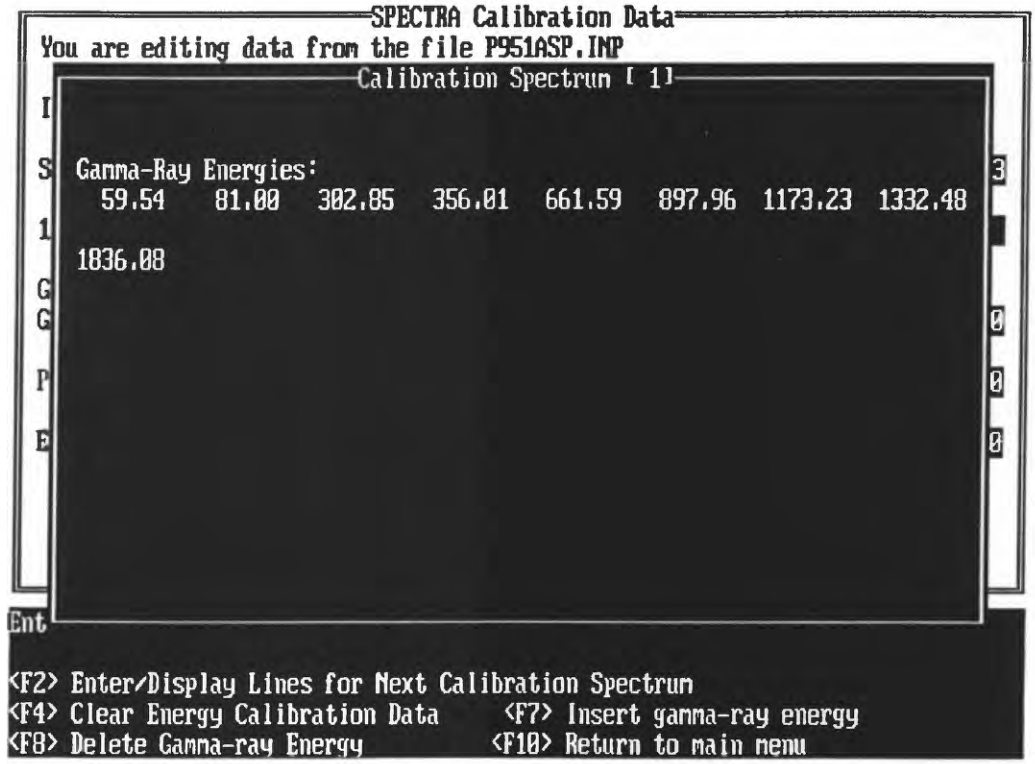

Figure 2b. SPECEDIT screen 1: Calibration lines.

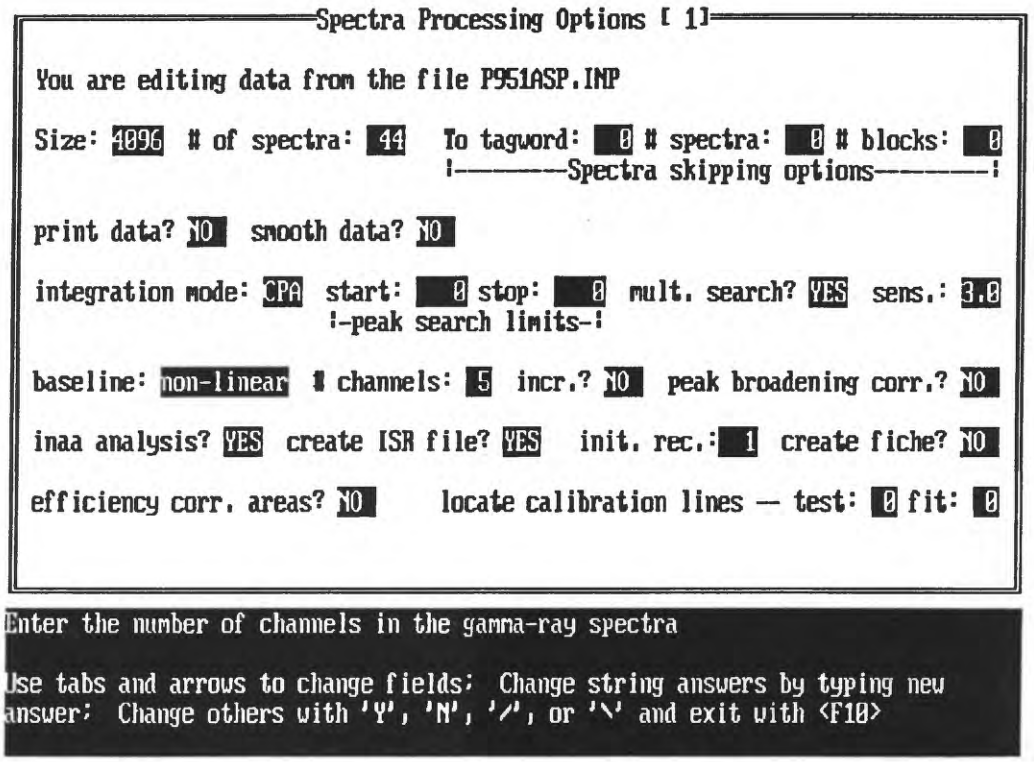

Figure 2c. SPECEDIT screen # 2: spectra processing options.

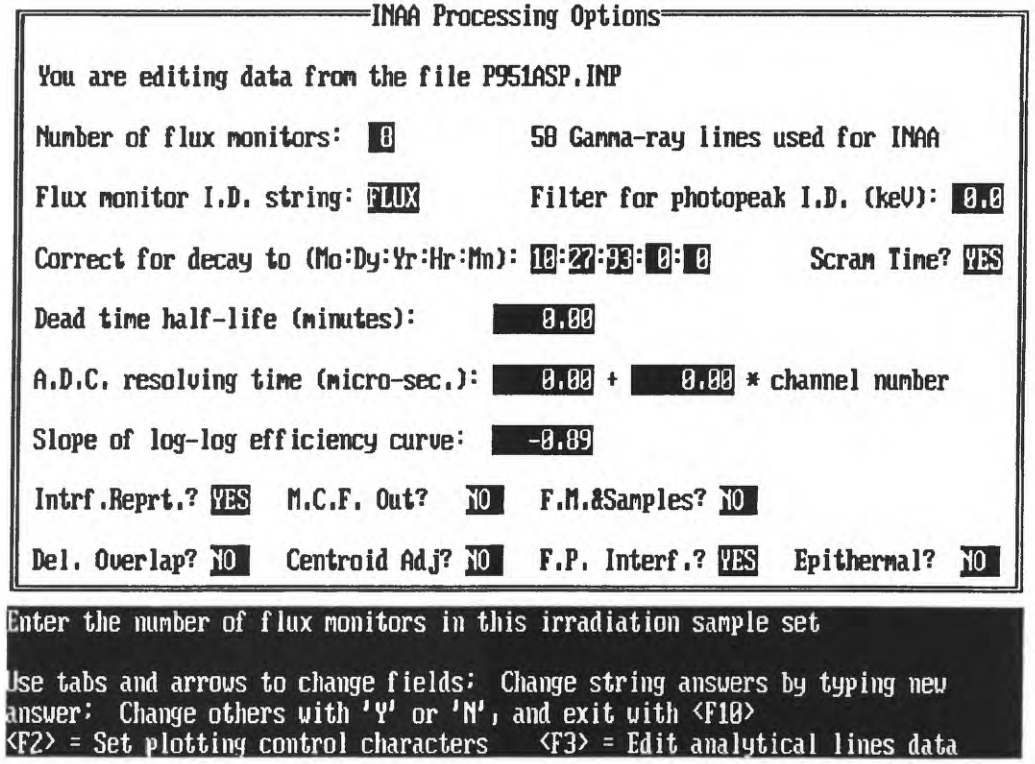

Figure 2d. SPECEDIT screen # 3: INAA processing options.

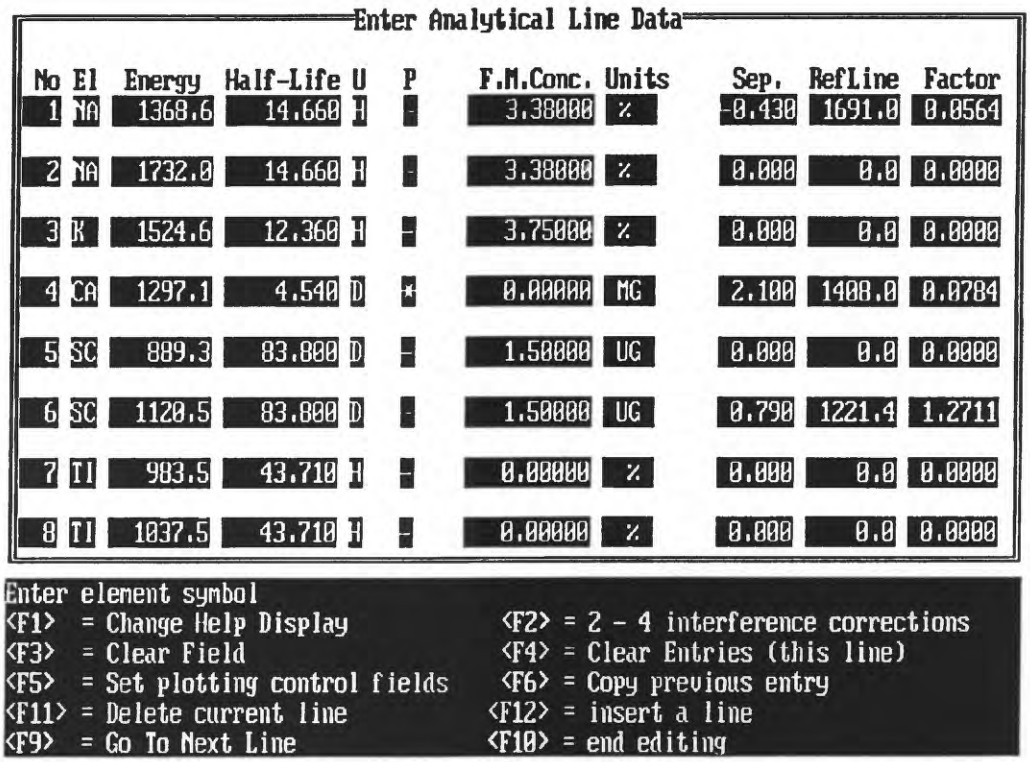

Figure 2e. SPECEDIT screen # 3: Editing INAA line data.

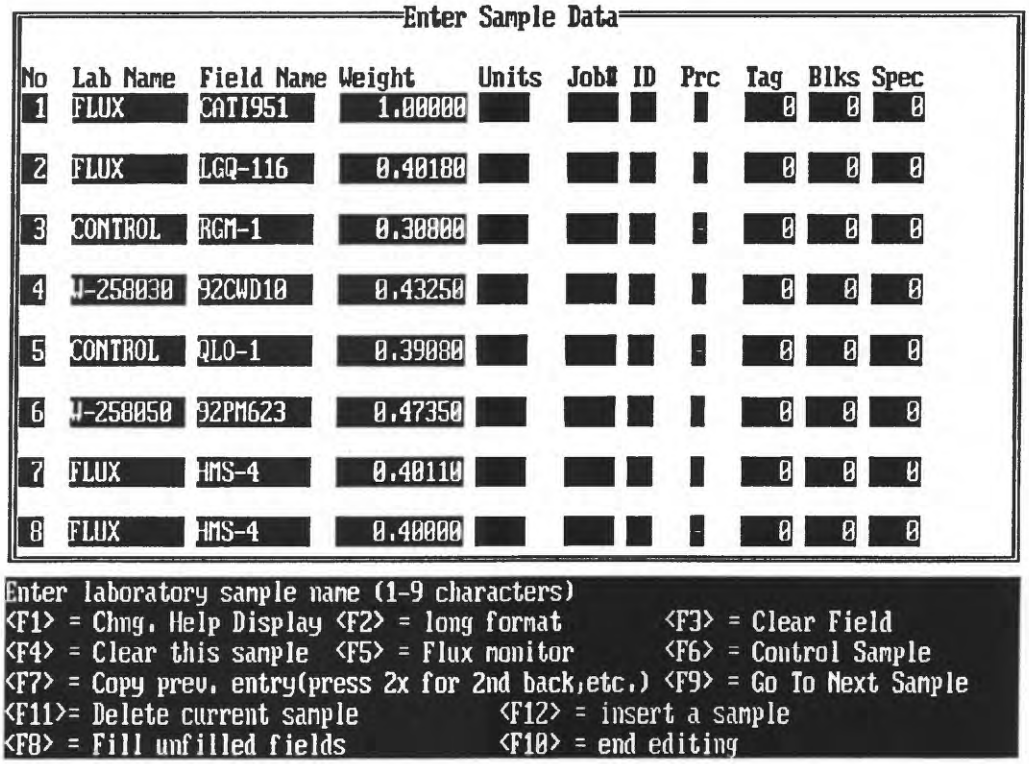

Figure 2f. SPECEDIT: Editing INAA sample data.

Peak integration by iterative least squares fitting.

Set chi-squared minimization procedure for fitting integration. (Marquardt/Gauss-Newton) (Def. = Marquardt)

Turn off/on search of residuals for additional components. (Def. = off)

Turn on/off smoothing of spectral data. (Def. = off)

Set lower and upper channel peak search limits. (Def. = 20: # of channels in the spectrum -- 4096/8192)

Print raw spectral data in line printer output. (Def. = off)

Print smoothed spectral data in line printer output. (Def. = off)

Create output file of peak search data (non INAA processing only). (Def. = off)

Create output file for Initial Summary Report (ISR). (INAA processing only) (Def. = on)

Set peak search sensitivity level. (Def. = 3 sigma)

Filter for location of energy calibration lines (+/- N channels). (Def. = 20)

Filter for location of energy calibration lines [difference from a polynomial. fit to the data (+/- N channels)] (Def. = 2)

Limit on number of spectral data read errors. (Def. = 10)

Turn off/on second derivative search for complex peaks. (Def. = on)

Turn micro-fiche output on/off. (Def. = off)

Correct peak areas for efficiency calibration. (Def. = off)

Enter revised label information.

After the spectra processing options have been set, the program asks the user to specify a .LIN file to define the analytical lines that will be used in the analysis, if SPECTRA is to be processing INAA data. The program accepts the data from the specified file and presents the user with screen # 3 to define the INAA processing options.

The INAA processing control options that can be defined within SPECEDIT are as follows:

Enter the number of INAA flux monitors (< = 20)

Enter a 4 character string used to identify flux monitors from characters 1:4 of the sample name (Def. = 'FLUX')

Alter the plotting control parameters for the analytical lines. (function key <F2>)

Edit the analytical line data. (<F3>)

Set the initial month/day/year/time-of-day for decay corrections.

(The date/time of the end of sample irradiation should be entered here for accurate fission product interference corrections on Ba and La.)

Set the filter for location of analytical lines (+/- N keV). (Def. = 1.0)

Write monitor comparator factors to a .STD data file. (Def. = off)

Process both samples and flux monitors for concentration output. (Def. = samples only)

Prepare interference correction report output file. (Def. = on)

Enter ADC resolving time to compute dead times.

Half life of dead time (for decay correction of short lived nuclides).
(The dead time decay is assumed to be exponential.)
Slope of log-log efficiency curve (for energies > approx. 150 keV)
Peak centroids may be shifted in INAA processing. (Def. = off)
Unexpected overlapping peaks deleted in INAA processing. (Def. = off)
Turn off/on the fission product interference correction for flux monitors. (Def. = on)
Epithermal/thermal neutron irradiation (Def. = thermal). This allows a separate set of fission product interference coefficients to be used for epithermal neutron irradiations.

After the INAA processing options have been set, the program then asks the user to specify a .SWT file to define the sample names and sample weights. SPECEDIT searches the current working directory for an xxxxy.HDR file. If one is found, the sample sequence is defined from the two digit sample numbers stored in the .HDR file. If the .HDR file is not found then the sample sequence remains unchanged as set in the .SWT file. After the .SWT data has been processed. the program can be terminated. However, SPECTRA has the ability to process multiple INAA sample sets in a single .SDF spectral data file. Therefore, the SPECEDIT user is also given the option to set up processing for additional samples before terminating the program.

The input xxxxySP.INP file created with SPECEDIT may be edited with SPECEDIT in order to change any of the spectra processing or INAA processing control variables, or to edit the analytical line or sample data. The lines selected for interactive plotting can be displayed and redefined by pressing the <F2> function key when the INAA processing menu is displayed.

3.3 SPECTRA processing.

Additional input files to SPECTRA

Once the xxxxySP.INP file has been created with SPECEDIT, SPECTRA processing can be initiated. The SPECTRA program processes data from an xxxxy.SDF spectral data file. The .SDF file contains records of length 774 written with a fortran statement like:

```
      WRITE (UNIT,10) ITAG, ISIZE, (IDATA(I),I=1,256)
10    FORMAT (258A3)
```

Where ITAG is the tagword of the spectrum, ISIZE is the number of channels in the spectrum, and IDATA contains the raw counts data. A 4096-channel spectrum would have 16 such records in the file. The maximum number of channels for SPECTRA processing is 8192. The maximum number of counts in a single channel is 16,777,215 (2^{24}-1).

SPECTRA looks for counting time information in the first six integer channels of the spectral data as follows:

channel 1: live time duration in seconds
channel 2: not used
channel 3: start of count date (YYMMDD)
channel 4: start of count time (HHMMSS)
channel 5: percent dead time
channel 6: clock time duration in seconds

(These data can also be passed to SPECTRA in the xxxxySP.INP input control file.) SPECTRA expects one or more spectra to be used for peak shape and energy calibration in front of each set of spectral data in the .SDF file. A few conversion utilities (e.g. SPETOSDF, CHNTOSDF) are included in the SPECTRA library to convert some commercial file formats into the SPECTRA .SDF format.

In addition to the .SDF and SP.INP files, SPECTRA expects to find three other input files in the C:\SP directory: PEAKSU.DAT (or PEAKS.DAT), PALETTE.DEF, and PLOTPK.HLP. These are included on the distribution diskettes and will probably not have to be modified. The PLOTPK.HLP file simply contains the menu of the commands used in conjunction with the mouse during interactive processing of spectral features. PALETTE.DEF defines the colors used in plotting to a color monitor and gives users the option of changing them to suit their own tastes. PEAKSU.DAT is the binary version of PEAKS.DAT and contains all of the isotope line intensity data that are used by SPECTRA for isotope and line identification during interactive processing. PEAKS.DAT is an ASCII file that contains data taken from the compilation by Browne, Firestone and Shirley (1986) and can be edited with a text editor. PEAKSU.DAT can be created from PEAKS.DAT using the PEAKCOPY utility. The PEAKLIST utility creates two data files of the PEAKS.DAT isotope data that are suitable for printing. The PEAKLIST output file PEAKS.PRN lists all of the energy and intensity data for each isotope and the file PKSNORDR.PRN provides a tabulation in order of increasing gamma-ray energy.

Running SPECTRA

SPECTRA first asks the user if interactive plotting is to be turned on. If interactive plotting is enabled and INAA processing has be specified, then the program will plot to the terminal screen the spectral region for each of the peaks selected in the .LIN data file (or those selected using SPECEDIT -- INAA option screen, <F2> function key). If plotting is not enabled, the program will operate nearly in batch mode except that it will pause to permit the user to review the flux monitor data prior to processing the sample data. [Note: If interactive plotting is enabled and the SPECTRA job does not include INAA processing of the data, then the user is given the option of plotting each spectrum after the peak search and photopeak integration for that spectrum is complete. Individual peaks may be selected in the plotted spectrum for interactive plotting and analysis.]

When the SPECTRA program is initiated, first it prints to the screen much of the processing control information defined in SPECEDIT to ensure that everything has been defined as expected. The program then processes the calibration spectra as defined by the SPECEDIT program (or in the SPECEDIT.DEF file). The calibration data are displayed on the screen and the program gives the user the option of displaying terminal plots of the calibration data: (1) gamma-ray energy vs. channel number, (2) *fwhm* vs. channel number, (3) low energy tailing parameter vs. channel number, and (4) the log-log efficiency curve based on the coefficients defined within SPECEDIT.

After processing the calibration data, the program will then process all of the flux monitor spectra pausing as it processes each peak designated for interactive analysis. Plotting an analytical line on the terminal screen is controlled by a single character code for each line listed in the input control file:

- ' ': Plot in all spectra under any of the following conditions:
  - o Peak is an upper limit.
  - o Peak is a weak line. (R.S.D. > 5 %)
  - o Peak is an overlapping peak, and interference corrections have not be specified (or if an overlapping peak is deleted when that option of the program is enabled).
  - o Centroid is greater than 2 channels from its expected location.
  - o The least squares fitting routine failed or the failed or the maximum residual value is greater than three standard deviations.
- '*': Plot in all spectra.
- '+': Plot in sample spectra only (not flux monitor spectra)
- '-': Never plot
- 'a': Plot if the slope of the baseline is positive
- 'b': Plot it the peak height:baseline ratio < 0.01

Figure 3 shows the help menu of the one letter commands used for interactive analysis. Note in particular the peak integration options (f/F to call up least squares fitting, and the space_bar to adjust the baseline in non-fitting modes); the options to modify the number of components in the region-of-interest (the D,I,S,T,<, and > options), and the isotope/line identification options (P and Y). Other particularly useful features are the ability to set the integration mode and region with the ! command for the analysis of subsequent spectra and the \ option to reprocess a previously processed peak.

```
          ***** PLOTPK : MENU OF CROSS-HAIR OPTIONS *****
            GRAPHICS DISPLAY                    PEAK INTEGRATION
A B C: Increase scaling factor        F    : Fit ROI (< 19 peaks)
1 2 3: Decrease scaling factor        M    : Move analytical line centroid
H    : Histogram toggle               N    : Move X-hair     line centroid
L    : Log/Linear toggle              U    : Upper limit (convert to)
R    : Residuals toggle (fitting)     +  - : Add/Subtract 2**20 (overflow)
X  x : Expand/contract region         SpBar: Change baseline (left & right)
[{]} : Shift plotting region l/r           MODIFY NO. COMPONENTS IN ROI
=  |  : Redraw/(original scale/width)  D I  : Delete/Insert Peak at X-hair
$    : Scale (ROI/full screen) toggle S    : Split multiplet (  2 groups)
*    : Header information toggle      T    : Split multiplet (> 2 groups)
%    : Header format (h/v) toggle     <  > : Include next peak/multiplet
V  ^ : Change plotting control list              MISCELLANEOUS
            DATA DISPLAY              G    : Plot region of spectrum
E    : Energy, Channel, Counts        W    : Baseline Parameters to Screen
O    : Peak Search Data to Screen     !    : Store ROI parameters
P    : Spectral lines for isotope     \    : Replot previous ROI
Y    : Isotopes for spectral line     K  & : K:Quit SPECTRA, or &:Spawn out
z  Z : Plot first/second derivatives  Q    : Accept all peak area values
       [ Mouse buttons:  left = SpBar  |  center = f(it)  |  right = Q(uit) ]
```

Figure 3. Menu of commands used for interactive processing of spectral features.

In addition to two digital methods of photopeak integration (the CPA and TPA methods -- integration modes 0 and 1 respectively), SPECTRA contains four models for least squares fitting of photopeaks:

model 2:	symmetrical Gaussian photopeak on a step function baseline *fwhm* fixed to a value based on the calibration data
model 3:	symmetrical Gaussian photopeak on a step function baseline *fwhm* is a variable during the fitting process.
model 4:	symmetrical Gaussian photopeak + a low energy tail; *fwhm* and tailing parameters are fixed based on the calibration data
model 5:	symmetrical Gaussian photopeak + a low energy tail; *fwhm* and tailing parameters are variable during the fitting process.

Model 4 is the default model (selected by the "f" cross-hair option). However, the other three models may be selected using the "F" cross-hair option.

The P and Y cross-hair options can be used for isotope identification. The P option puts lines on the screen at the locations where lines for a particular isotope are expected. The height of the line is defined by the expected intensity value using the most intense peak of the isotope of interest in the spectrum for scaling. The Y cross hair option will cause a listing of all isotopes that may have a peak with the gamma-ray energy at the cross-hair location. In addition to primary photopeaks, SPECTRA will search the spectrum and isotope data base to check for possible sum or escape peaks at the cross-hair location.

After all of the flux monitors have been processed, the program gives the user the opportunity to review the comparator factors relative to the mean. The program will make some decisions for the user with regard to the rejection of outliers, but it allows the user the opportunity to include or exclude individual results or to investigate apparent problems by interactively reanalyzing selected peaks in selected spectra. For example, the program presents the user with a screen that looks something like the following:

Flux Monitor:	HMS-4	HMS-4	HMS-4	CATI864	HMS-4	HMS-4	HMS-4	CATI864
NA (1368.6)	0.964	0.971	0.985	---	1.005	1.037	1.037	---
NA (1732.0)	0.969	0.968	0.986	---	0.986	1.053	1.037	---
K (1524.6)	1.064	0.890	1.046	---	* n.f.* *	n.f.* *	n.f.*	---
CA (1297.1)	---	---	---	1.006	---	---	---	0.994
SC (889.3)	1.002	1.004	0.984	---	1.015	1.004	0.990	---
SC (1120.5)	0.946	1.003	0.999	---	1.012	1.039	1.000	---
LU (208.4)	1.007p	0.982p	1.004p	---	1.016p	0.997p	0.994p	---
CR (320.1)	0.964	1.127*	1.011	---	1.001	0.938*	1.023	---
SB (1691.0)	1.089*	0.958	0.960	---	1.040	1.042	0.931*	---
U (228.2)	0.971	0.985	1.035	---	0.992	0.997	1.019	---
U (277.6)	0.927*	0.994	1.004	---	0.961	1.033	1.008	---

The six counts for Na and Sc agree within $\pm$ 4% of 1.000. There is poor agreement between the three results for K, and the 1525 keV peak was not found in the last three spectra of HMS-4. HMS-4 is not used as a standard for Ca, and the two counts of the Ca standard are in good agreement. All of the Lu peaks were plotted during processing as indicated by the p's. SPECTRA rejected the high and low results for Cr and Sb, and the low result for the U 278 keV peak. When this table is displayed on the terminal screen, the user has the option of toggling on/off averaging for any of the flux monitor results or checking any of the results by interactively replotting the analytical lines on the terminal screen. Once all of the flux monitor results have been reviewed and accepted, SPECTRA will then process all of the sample spectra.

SPECTRA output files

SPECTRA creates five different output files, as follows:

(A) Listing file xxxxySP.LIS. This ASCII file contains the primary output from SPECTRA including the results of the energy calibration, the peak search and integration data for all spectra, the results on flux monitors, and the elemental concentrations determined in samples. It can be printed on a line printer or selectively reviewed on the monitor screen with the REVIEW program. The FPRINT utility can be used to print the entire xxxxySP.LIS file or selected pages on an HP LaserJet or compatible printer.

The SPECTRA xxxxySP.LIS file lists peak area and location information for each peak found in each spectrum, the channels used for baseline definition, and the specific activity and concentration data for peaks used for INAA. If iterative least squares fitting was used to determine the peak area, a return code from the fitting algorithm is also printed:

kkmmn : where n is the integration mode (2,3,4,5)

mm is the number of iterations

kk if > 0 is an error code:

1) wont converge -- > 30 iterations
2) singular matrix -- inversion procedure failed
3) negative fitting parameter
4) junction point out of range -- exponential tail
5) large error (> 100%) in peak area
6) Marquardt search parameter exceeds limit
7) Error in Marquardt search (divide by zero trap)
8) Error in Gauss-Newton minimization (overflow trap)
9) chi-squared increases on 30 tries (G-N minimization)
10) greater than 18 peaks in fitting region
11) greater than 300 channels in fitting region
12) fitting region too small for least squares analysis

If the least squares fitting process fails (with the exception of error 1 -- non-convergence), the TP area is reported. (If CPA is the default integration mode, the CP area is reported. That is, even if the fit is successful, the reported area is for the specified width of the CP region.)

A single character code is often placed next to the peak area to provide additional information regarding the processing of a particular peak. The following codes are used:

+ : The peak is wider than expected based on the Energy/peak shape calibration -- possible unresolved doublet.

* x : The peak is one of x partially resolved peaks.

t : The CPA integration limits were outside of the peak boundary channels, the TPA area is reported.

u : The peak was converted to an upper limit during INAA processing because the interference correction was large (> 50%).

x : The peak centroid was > 1 channel from an expected location.

z : The peak centroid was redefined to the expected location during INAA processing.

Interactive plotting codes:

p : single peak, peak area not redetermined

P : multiplet peak, peak area not redetermined

s : single peak, reprocessed using CPA or TPA integration

M : multiplet peak, reprocessed using CPA or TPA integration

f : single peak, reprocessed using least squares fitting

F : multiplet peak, reprocessed using least squares fitting

The REVIEW program permits the user to look at selected portions of the large xxxxySP.LIS file (either selected energy ranges or data for selected elements) for selected spectra. The program also provides terminal and hard copy plots of FWHM vs. time, gain shift vs. time, dead-time vs. time, etc. in order to look for problems in detector performance during the counting cycle. The REVIEW program works best if the monitor is set to 132 column mode. Consult the documentation on the monitor utility programs to see how this can be accomplished. We have included a batch file REVIEW.BAT, which may have to be revised to call the appropriate utility for individual systems. The batch file puts the monitor in 132 column mode and then calls up the REVIEW program (called REVIEW80). (The REVIEW.BAT file is not needed if REVIEW is called from SPECMENU, however, as mentioned above, the correct commands to put the monitor in and out of 132 column mode must then be inserted in the SPECMENU.DEF file.)

(B) "Rerun" file xxxxySP.RRN. If SPECTRA is run two or more times on the same set of spectral data, the results from runs subsequent to the first are listed in this file instead of the xxxxySP.LIS file.

(C) "Log" file xxxxySP.LOG. This binary file contains data that are needed in order to go back and rerun a portion of a job using SPECTRA or to continue execution of a previously suspended SPECTRA run. (This file is created for INAA spectral data processing only and not for simple peak-search jobs.) The contents of this file can be viewed with the LOGDUMP program, which also can create a printable ASCII file xxxxySP.DMP. If SPECTRA is being re-run (for a 2nd, 3rd, ... or nth time) after an initial SPECTRA run has gone to completion, and a decision is made to terminate the re-run prematurely, then SPECTRA will continue where the user left off if SPECTRA is restarted. However, the LOGRESET program can be used to reset the LOG file to its status when the initial SPECTRA processing was completed.

(D) Summary data file xxxxyISR.DAT (optional). This binary file contains the analytical results from all of the analytical lines for all samples. The data for multiple lines can be averaged and tabulated using the SUMMARY1 program. The data in one or more xxxxyISR.DAT files can be reviewed on the monitor screen with the ISRDUMP program. The ISRPLOT program can be used to prepare scatter plots of the analytical data from one line against that of second or from one count against that of a second.

(E) Interference report file xxxxyICR.DAT (optional). This binary file contains data about spectral and fission product (flux monitors only) interference corrections that were made by SPECTRA. This data may be summarized and put into a printable ASCII output file using the ICREPORT program.

Additional programs for plotting/processing xxxxy.SDF files

In addition to SPECTRA there are three utilities that have been developed for processing spectral data in a .SDF spectral data file: READSPEC, SDFEDIT, and PLOTSDF. READSPEC is a utility to read and plot spectral data (either the entire spectrum or regions of interest) on the monitor screen and to create file dumps of the plots in a format compatible with the GPRINT utility for creating hard copy plots on the printer. READSPEC will also create plots in HPGL format. The same interactive isotope identification algorithms used in SPECTRA have also been incorporated in READSPEC and may be called if polynomial

energy calibration coefficients are provided by the user. The SDFEDIT program can be used to edit a .SDF file to (a) reorder or delete spectra in a .SDF file, (b) change spectra tagwords, (c) enter corrected date and time information, or (d) to create a .HDR file. The PLOTSDF program can be used to overlay plots of a given region in multiple spectra in order to check for changes in detector performance during a counting sequence (*fwhm* changes or gain/zero drift).

3.4 SUMMARY1 processing.

The next stage of INAA processing is to average the results from multiple lines in order to produce a single value for each element of interest in each sample and to store the resulting average values in an answer file for the final stage of analytical report form generation. The report created for a single counting of the sample set is called an "Initial Summary Report" (ISR), and the program SUMMARY1 processes the data in the xxxxyISR.DAT file created by SPECTRA as shown in the flow chart of Figure 4.

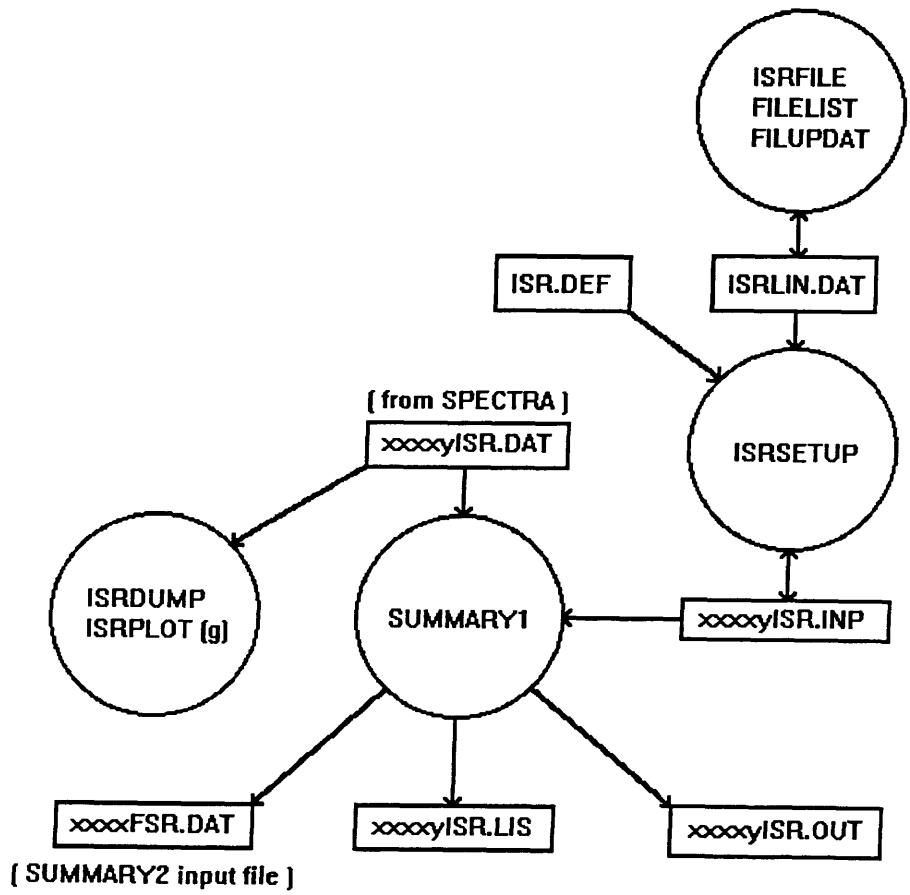

Figure 4. Flow chart of Intermediate Summary Report generation

The input control file, xxxxyISR.INP, is required by SUMMARY1. This file is created by the ISRSETUP program, which can create and edit the xxxxISR.INP file. The ISRSETUP program can be customized for various applications and sample matrices by editing the ASCII ISR.DEF file with a text editor. The ISR.DEF file permits the definition of default lists of elements that are to be determined in different high energy and low energy counts of the samples. Different element lists for up to 10 sample types can be defined in the ISR.DEF file.

The lines to be averaged for the determination of each element are defined by the ISRLIN.DAT data file. Each record in ISRLIN.DAT defines the gamma-ray lines used for an element for a particular detector type or detector/count number combination. If no count number is specified then the record is assumed to be valid for all counts. If no detector type is specified, then the record is assumed to be valid for both detector types. Fields on each record can be used to define the units and number of decimal places reported in the xxxxyISR.LIS file. If it is necessary to override the units passed from SPECTRA or to report more than two places past the decimal point, these fields may be edited. The ISRLIN.DAT file can be edited with a text editor or with the ISRFILE program. A printable listing of the file can be prepared by the FILELIST program, and the gamma-ray energy data can be updated from the GEMASTER.LIN and IGMASTER.LIN files using the FILUPDAT utility.

The averaging of results in the SUMMARY1 program is based on a priority value for each analytical line for a given element as assigned in the ISRLIN.DAT file. Thus, all number one priority lines are automatically included in the average value reported and are weighted by their estimated variances based on counting statistics. If the results from two number one priority lines do not overlap within two standard deviations then the data values are flagged (with a "#" symbol) in the .LIS line printer output of both the SUMMARY1 and SUMMARY2 programs. The results from lower priority peaks are included in the mean only if they fall within two standard deviations of the mean of the higher priority lines.

We have found that in some applications it may be desirable to use different analytical lines or averaging priorities for different sample types. Therefore, we have incorporated the option in ISRSETUP of reading different ISRLIN.DAT files for different sample types. For example the program searches the USERPATH and SPPATH directories for ISRXXXX.DAT files, where XXXX is the four letter code for a given sample type (e.g. ISRROCK.DAT for rock samples; ISRCOAL.DAT for coal samples, etc.).

A previously created xxxxyISR.INP file can also be edited with ISRSETUP to add or delete elements, add or delete lines for a given element, change the priority scheme for line averaging, etc. SUMMARY1 can be run in either a batch or interactive mode. In batch mode the program processes the data in the xxxxyISR.DAT file, averages the results from multiple lines, stores the results in the xxxxFSR.DAT file, and creates the printable ASCII summary report xxxxyISR.LIS. In interactive mode, the user has the option of reviewing the averaging process for all elements having multiple lines and overriding the default averaging if desired. It is also possible to create separate sample data sheets for each sample

that show the individual results for each line along with the average concentration values. The data sheets are stored in a third SUMMARY1 output file xxxxyISR.OUT. A sample data sheet is shown in Figure 5.

Instrumental Neutron Activation Analysis Report 06/04/93 16:17:07.08

SAMPLE DATA SHEET

Irradiation Number: P835C

Sample : M-198067 1665M
Weight : 0.41220
Tag Word : 25
FSR Record: 79

Element	lines:			results:			average	(%sigma)
CA (%)	1297			7.84			7.84	(2.49)
SC (PPM)	889			24.55			24.55	(0.20)
CR (PPM)	320			142.8			142.8	(0.65)
FE (%)	1099	1291		5.36	5.38		5.37	(0.31)
CO (PPM)	1173	1332		27.8	28.1		28.0	(0.47)
NI (PPM)	810			48.4			48.4	(19.53)
SE (PPM)	264			0.35			0.35	(97.13)
ZN (PPM)	1115			65.			65.	(7.70)
RB (PPM)	1076			8.7			8.7	(11.54)
SR (PPM)	514			588.0			588.0	(5.17)
ZR (PPM)	756	765	724	71.	<172.*	<163.*	71.	(40.12)
SB (PPM)	1691			<0.18			<0.18	(0.00)
CS (PPM)	795			0.43			0.43	(14.18)
BA (PPM)	496			305.			305.	(3.25)
CE (PPM)	145			15.			15.	(1.81)
ND (PPM)	91			11.			11.	(7.69)
EU (PPM)	778	1408	244	0.84	0.94	0.84	0.90	(2.12)
TB (PPM)	298	1177	879	0.42	0.40	0.48	0.43	(3.73)
YB (PPM)	396	282		1.8	2.2		1.9	(3.83)
LU (PPM)	208			0.24			0.24	(0.26)
HF (PPM)	482	133		1.7	1.7		1.7	(2.35)
TA (PPM)	1221	1189	1231	0.20	0.20	0.30*	0.20	(10.30)
TH (PPM)	312			1.3			1.3	(2.70)

Error limits are estimates of one standard deviation based on counting errors
*: result excluded from mean

Figure 5. Sample data sheet prepared by SUMMARY1

After SUMMARY1 has been run once for a set of data and has stored the average concentration values in the xxxxFSR.DAT file, it may be necessary to rerun the program for several reasons: (1) if the xxxxISR.DAT file has been changed by rerunning SPECTRA for selected elements, (2) if a decision is made to add additional elements to the ISR element set for a given count, (3) if a decision is made to change the priority scheme for line averaging, etc. When SUMMARY1 is run again, it can operate in one of three modes selected interactively by the user: (1) all of the data previously entered are replaced with the new

values defined in the current SUMMARY1 run; (2) only data for selected elements are replaced; or (3) or data values that have changed by re-running SPECTRA are replaced.

As mentioned above, two utilities are available to interactively review the data in xxxxyISR.DAT files: ISRDUMP and ISRPLOT. The ISRDUMP program lists the data for selected elements and selected samples to the terminal screen. ISRPLOT also permits the preparation of scatter plots of the results from one analytical line against that of a second for comparison. ISRPLOT can also process multiple xxxxyISR.DAT files, thus permitting the comparison of the results from one count of the samples to that from a second.

3.5 SUMMARY2 processing.

After ISR processing is complete for all counts, and the xxxxFSR.DAT file is complete, SUMMARY can be run to average the results from multiple counts and complete the "Final Summary Report" (FSR) c analysis. A flow chart of this stage of the data processing procedure is shown in Figure 6.

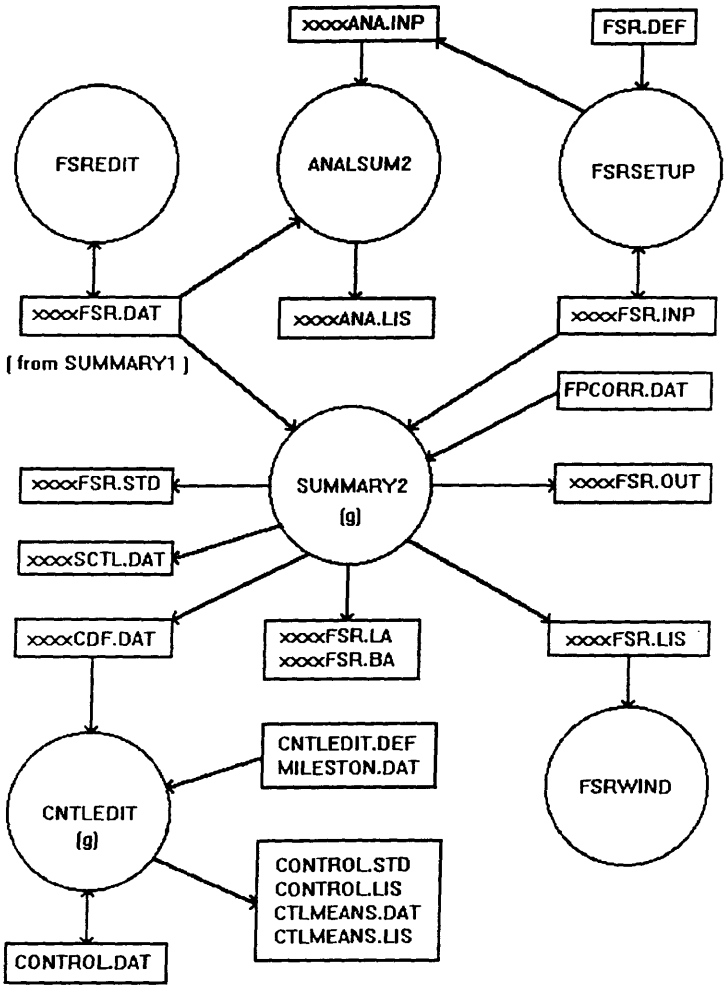

Figure 6. Flow chart of Final Summary Report generation

As in the previous stages, a preprocessor program FSRSETUP is used to prepare the input control file for SUMMARY2. FSRSETUP can be tailored for use in different laboratories by editing the FSR.DEF file. It permits the definition of different default element lists for different sample types and a list of the analysts in the laboratory. FSRSETUP is used to create the input files for both the SUMMARY2 and the ANALSUM2 programs. The first time that FSRSETUP is run, it examines all xxxxyISR.DAT files to check the precision of the best data for each element for each sample. A new data file STATS.DAT is created that is also used by FSRSETUP in order to suggest to the user additional elements that might be included in the final summary report beyond the list of default elements (or elements that could be deleted if only upper limits have been calculated by SPECTRA).

The ANALSUM2 program can be used to assist in the detection of systematic errors during a series of multiple counts and should be run before SUMMARY2. This program searches a final summary data file to find the names of all counts present. (These correspond to the xxxxY designations of the original input files used to run SPECTRA.) The analyst chooses one of these counts to use for normalization. The program then finds all records belonging to a given sample and divides the elemental concentrations for the elements specified in the xxxxANA.INP file by those in the normalizing record if present in that record. The default elements used for comparison can be defined in the FSR.DEF control file. For rock samples, we generally use the elements Fe, Co, Sc, Ce and Eu. In each record, all data with relative precisions below 10% are averaged. An average of 1.0 indicates complete agreement between that count and the normalizing count. Deviations from 1.0 indicate systematic errors (such as improper counting geometry, poor dead time corrections, etc.); such errors can be corrected using the FSREDIT program. The output is placed in a file xxxxANA.LIS that can be printed or viewed with a text editor.

The output for each sample looks like the following:

```
Sample: W-123456 BOZO-1
rec:     27      57      67      92
 ff: 1.000   1.000   1.000   1.000
 ct: P835A   P835B   P835C   P835D
det:   PG5     NIG     PG5     CB1
tag:    34      32      13       6
cor:   yes      no     yes     yes
SC    0.99       -   =1.00    1.05
FE    0.98       -   =1.00    1.05
CO    0.97       -   =1.00    1.06
CE    0.82    1.01   =1.00    1.02
EU      ~        -   =1.00    1.05
      ----    ----    ----    ----
avg:  0.94    1.01    0.00    1.04
```

There is clear evidence here that the last count has a systematic bias of about 5%. The ~ symbol for Eu in the first count means that Eu had poor precision (> 10% error) and the ratio was not calculated. The - symbols for count B mean that those elements were not determined in that sample count. A correction can be made for the apparent bias using the MULT option of FSREDIT.

ANALSUM2 next calculates the agreement between counts for specific elements in order to search for problems with the determination of specific elements. First, a correction is made internally for the systematic errors between records as calculated above. Then the average ratio of each element between all possible pairs of counts is calculated and presented in a report. Here, deviations from a value of 1.0 may indicate poor flux monitor calibration in a specific count, improper interference corrections in a specific count, etc. These errors may be corrected by rerunning SPECTRA or by using FSREDIT.

FSREDIT can be used to edit the xxxxFSR.DAT file in order to correct errors that are discovered during the last data processing stage, which can be corrected without repeating SPECTRA or SUMMARY1 processing. The FSREDIT options are as follows:

NAME	:	Change the entire sample name for a given record. (18 char: LABNumber + FLDNumber)
LABN	:	Change the sample lab number for a given record. (9 characters)
FLDN	:	Change the sample field number for a given record. (9 characters)
JUSTFY	:	Left-justify the field names.
CHANGE	:	Change a single character in the sample names for multiple records.
REPL	:	Replace multiple characters in the sample names in multiple records.
INCHAR	:	Insert a character in the sample names in multiple records.
DLCHAR	:	Delete a character in the sample names in multiple records.
DLFLDN	:	Delete the entire field name in multiple records.
LOCATE	:	Search for a given lab or field name.
MASS	:	Change the sample weight and renormalize the data for a given record.
CHNGWT	:	Change the sample weight and do not renormalize the data.
UNMIX	:	Change the sample name and the sample weight (and adjust the data) for multiple records.
SKPMIX	:	Enter record numbers to be ignored in using the UNMIX option.
MULT	:	Multiply all data in a given record by a specified factor.
FUDGE	:	Multiply data for a given element (in one or more records) by a specified factor.
UNITS	:	Change the designated units. [The data are not renormalized. (Use the FUDGE option if needed.)]
LIMIT	:	Express the results as upper limits for selected elements.
NSF	:	Change the number of places past the decimal point in the report.
LSTDAT	:	List the data on the terminal screen for a specified record.
LIST	:	List the sample names and weights to the terminal screen.
VALUE	:	Change specific values in specified records.

BLANK	:	Make blank or background corrections.
RECS	:	Check for valid records in the data file.
FAKE	:	Fake a flux monitor for selected elements. (Where no flux monitor was included in the irradiation set, but specific activities were calculated and stored in the xxxxFSR.DAT file.)
SETFLG	:	Change the character flags that control SUMMARY2 (FSR) averaging.
COUNTS	:	List the record numbers of the first occurrences of SPECTRA counts.
QUIT	:	End the edit procedure for the current file.

Producing the final report of averages of the different counts for each sample is an iterative procedure. This involves running the SUMMARY2 program, checking the output for errors or discrepancies, and resolving problems with inconsistent results either by re-running SPECTRA and SUMMARY1 for specific elements in specific spectra or by using the FSREDIT program.

The SUMMARY2 program produces two line printer output data files: xxxxxFSR.LIS and xxxxFSR.OUT. xxxxFSR.LIS is a listing of all data in the XXXXFSR.DAT data file with the concentration values from multiple counts for a given sample in adjacent columns for easy comparison. This file may be reviewed using the FSRWIND(ow) program. xxxxFSR.OUT is in two sections: (1) average results from multiple countings for each sample with the data for replicate samples in adjacent columns to facilitate comparisons and (2) average results from the analysis of replicate samples. The .LIS and .OUT files can be printed on an HP LaserJet printer using the FPRINT utility.

The SUMMARY2 program tests for and rejects outliers when the averages of multiple counts (for the .OUT report) are calculated based on the following criteria:

(1) All data with counting errors greater than 30% (relative standard deviation) are treated as upper limits.

(2) When only upper limits are available, the lowest value is reported.

(3) All data listed as upper limits are ignored in the computation of a mean value.

(4) All values are weighted by their variance in the computation of the mean.

(5) In the calculation of the weighting factors, the standard deviation values are all arbitrarily increased by 2% in order to avoid over-weighting results with very small (<1%) Poisson counting error.

(6) When the 2 sigma error for any datum does not overlap the 2 sigma error on the mean, the datum flagged (with a "!"). (If any datum has an error greater than 15%, then the criterion for flagging is 1.5 sigma. This is to prevent low precision data from being retained in the mean when higher precision data may be omitted.)

(7) If less than 50% of the data are flagged, then the flagged data are omitted (and the "!" flags converted to "D") in a recalculation of the mean. After recalculation of the mean, the criteria of step 6 are reapplied. If more than 50% of the remaining data are now flagged, the "!" flags (second pass) are converted to "?", and the mean calculated in step six is retained.

All flags (including the "#" flags from SUMMARY1) are reported along with the individual analytical results in the first section of the SUMMARY2 output file xxxxFSR.LIS. The analyst then has the option of reviewing the flagged data and editing (either inserting or deleting) the "X" or "D" flags (that specify data deletion in computing sample means) by using the SETFLG of the FSREDIT program. ("D" flags are set automatically by SUMMARY2, "X" flags are set by the user using FSREDIT.) FSREDIT can also be used to correct incorrect sample names and sample weights (with appropriate renormalization of the data), to re-normalize sample data to correct for apparent systematic errors (e.g. due to variations in counting geometry between samples and standards), or to re-normalize data for a given element (based on an alternate standard).

The SUMMARY2 program makes corrections for fission product interferences in the determination of zirconium, molybdenum, lanthanum, cerium, and neodymium if uranium has been determined. Where the magnitude of the correction exceeds 20% of the uncorrected value, the value is flagged with an "x" and if the correction exceeds 50%, the value is flagged with a "*" in the report of analysis. Because fission product ^{140}La grows through decay of fission product ^{140}Ba, the magnitude of the fission product interference is dependent on the time between the end of irradiation and the time of counting. The correction for the interference is as follows:

$$[La]_{corr.} = [La]_{meas.} - [U] * x_{La} * (e^{0.01497 * t} - 0.9489)$$

where x_{La} for thermal neutron irradiations has a value of 2.7e-3 and is defined by the formula:

$$\frac{\sigma_f * a(U) * aw(La) * (1 - e^{(-\lambda_1 * t_1)}) * \lambda_2 * Y}{\sigma_l * a(La) * aw(U) * (1 - e^{(-\lambda_2 * t_1)}) * (\lambda_2 - \lambda_1)}$$

where:
- σ_f = fission cross section for U-235 (583.54 barns)
- σ_l = (n,γ) cross section for La-139 (8.94 barns)
- a(U) = isotopic abundance of U-235 (0.0072)
- a(La) = isotopic abundance of La-129 (0.999)
- aw(U) = atomic wt of U (238.03)
- aw(La) = atomic wt of La (138.91)
- λ_1 = decay constant for Ba-140 (0.00226/h)
- λ_2 = decay constant for La-140 (0.01723/h)
- Y = fission yield of Ba-140 (0.0623)
- t_1 = time of irradiation (6.5 hours assumed)

The value of the second constant (0.015) is $\lambda_2 - \lambda_1$ where t is in hours.

The value of the third constant (0.9489) is

$$\frac{\lambda_1 * (1.0 - e^{(-\lambda_2 * t_1)})}{\lambda_2 * (1.0 - e^{(-\lambda_1 * t_1)})}$$

Another uranium fission product, ^{103}Ru, has a gamma-ray line at 497.1 keV that interferes with the best line from ^{131}Ba at 496.2 keV. Because ^{103}Ru does not have a second line that is strong enough to use to make a correction, this interference is treated like a direct fission product correction. SUMMARY2 calculates a mean uranium content for each sample in the file based on all counts. It next locates those records that contain barium data derived solely from the 496.2 keV line (identified by a hidden, internal flag) and makes the correction as follows:

$$[Ba]_{corr.} = [Ba]_{meas\ @\ 496.4} - [U] * x_{Ba} * e^{0.04098 * t}$$

where t is the time in days from the end of the irradiation to the start of the count, and x_{Ba} has a value of 2.8, and is defined by:

$$\frac{\sigma_f * a(U) * aw(Ba) * B.R.(Ru) * Y * (1 - e^{(-\lambda_1 * t_1)})}{\sigma_b * a(Ba) * aw(U) * B.R.(Ba) * (1 - e^{(-\lambda_2 * t_1)})}$$

where: σ_f = fission cross section for U-235 (583.54 barns)
σ_b = (n,γ) cross section for Ba-130 (13.5 barns)
a(U) = isotopic abundance of U-235 (0.0072)
a(Ba) = isotopic abundance of Ba-130 (0.001062)
aw(U) = atomic wt. of U (238.03)
aw(Ba) = atomic wt. of Ba (137.3)
λ_1 = decay constant for Ru-103 (0.0007357/h)
λ_2 = decay constant for Ba-131 (0.002443/h)
B.R.(Ru) = branching ratio for Ru 496 keV peak (0.89)
B.R.(Ba) = branching ratio for Ba 496 keV peak (0.51)
Y = fission yield of Ru-103 (0.031)
t_1 = time of irradiation (6.5 hours assumed)

The value of the second constant (0.04098) is $(lam_2\text{-}lam_1) * 24.0$ where t is the decay time in days.

Since the fission product corrections for both La and Ba depend on the decay time since the end of irradiation, this value is automatically stored in the xxxxFSR.DAT file if the time of the end of the irradiation is specified in the "INAA options" window when the xxxxySP.INP file is created with SPECEDIT. (If no decay time is stored in the xxxxFSR.DAT file, the fission product corrections for La and Ba are bypassed.) SUMMARY2 creates two ASCII output files, xxxxFSR.LA and xxxxFSR.BA, that report the magnitude of the fission product interference corrections made for La and Ba respectively.

The fission product correction coefficients are stored in a data file FPCORR.DAT that may reside in either the SPPATH program directory or the user's USERPATH directory. The coefficients x_{La} and x_{Ba} for the La and Ba corrections, respectively, are stored in the file. However, since both of these coefficients are a function of irradiation time, the irradiation time for which the coefficients were determined and the true irradiation time should be store on the first line of the FPCORR.DAT file.

In some INAA laboratories, Gd is determined by a late LEPD count. However, we have found that the precision of the Gd measurement is frequently poor; and when Gd is not determined directly, we estimate the Gd content by interpolation by fitting the other REE data to a quadratic equation (excluding Eu because of the frequent presence of high or low Eu anomalies). SUMMARY2 also checks the Gd data and will warn the user if the Gd content is sufficiently high that there is a danger of a significant (> 2%) self shielding problem for the sample.

The analyst has the option of creating plots of chondrite (or shale) normalized REE data to the terminal screen or of creating separate plot files of the chondrite normalized data with each plot corresponding to one page of printed output (10 samples per plot). A typical plot is shown in Figure 7. The plot files xxxxFSR.PG1, ..PG2, ..PG3 etc. can be plotted on the system printer using the GPRINT command.

SUMMARY2 creates a binary output file xxxxCDF.DAT that contains all of the data for the reference samples included in a given irradiation set. In addition, the program creates a quality control plot of the data on control samples normalized to the mean values stored in the data file CTLMEANS.DAT. A typical control chart is shown in Figure 8.

After the first run of SUMMARY2, the analyst should use the program FSRWIND(ow) to view the xxxxFSR.LIS file in order to look at the side by side comparison of the data for individual counts. The FSRWIND program requires that the PC screen be set in 132 column mode. The FSRW.BAT file is designed to perform this function, but it may need to be modified (like REVIEW.BAT) to call the appropriate monitor utility program for a particular system. (FSRW.BAT is not needed if FSRWIND is called from SPECMENU, but the SPECMENU.DEF file must be edited to contain appropriate monitor utilities to place the screen in 132 and 80 column modes.) The xxxxFSR.LIS file shows when two or more priority-one lines did not agree during SUMMARY1 averaging (flagged with a "#"), when the data were deleted as outliers by SUMMARY2 (flagged by a "D"), when the data were considered questionable but not deleted (flagged by a "!"), and when the analyst used FSREDIT to delete data (flagged by an "X"). The analyst should carefully

review both the FSRWIND presentation of the data to check for discrepancies, and the plots of chondrite normalized REE data to look for anomalous patterns (other than for Ce and Eu). Any problems that need to be resolved should be handled either by interactive analysis of the spectral data, or simply the rejection of questionable data using the SETFLG option FSREDIT. Once the data has been carefully reviewed, SUMMARY2 can be rerun in order to produce the final report of analysis if any of the editing options provided by the FSREDIT program have been exercised.

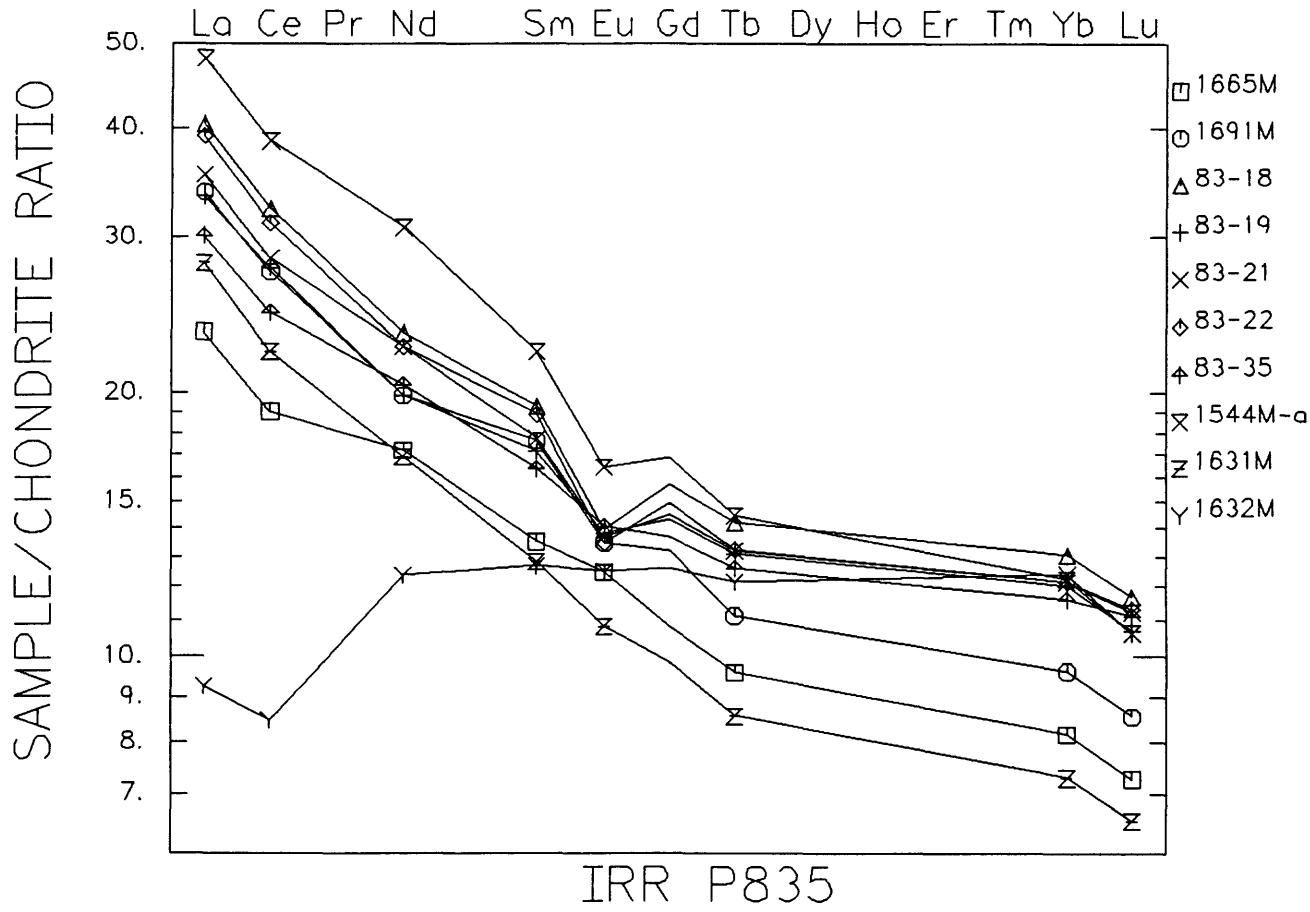

Figure 7. Plot of chondrite normalized REE data prepared by SUMMARY2

Two additional output data files can be produced by the SUMMARY2 program: (1) An ASCII data file (XXXXSCTL.DAT) in a format that is compatible with the USGS centralized analytical laboratory information management system and (2) An ASCII file (XXXX.STD) that is compatible with all of our software for graphic presentation and statistical analysis (e.g. regression, factor, and cluster analysis). These data files can also be used to produce high quality chondrite normalized rare earth plots. .STD files can be converted to Lotus 1-2-3 .WK1 format using the STDEDIT utility.

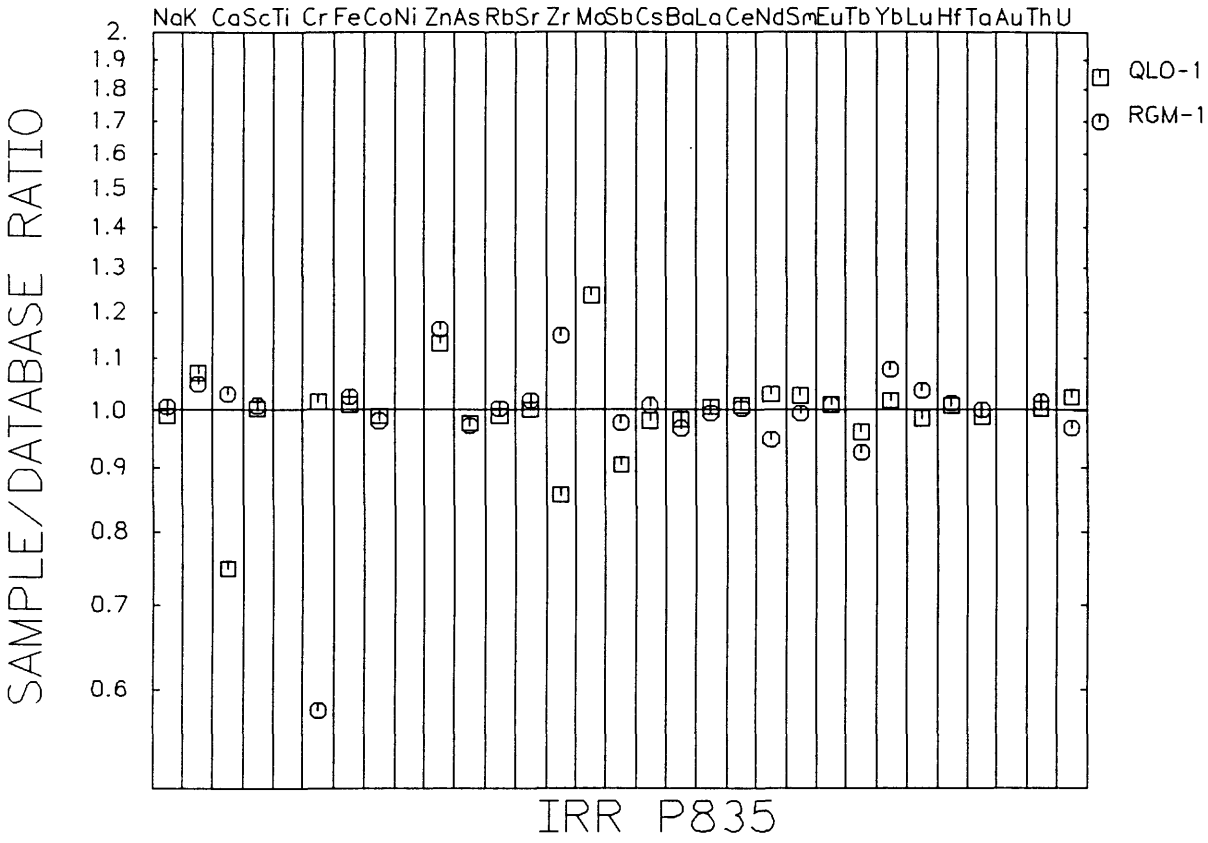

Figure 8. Plot of element data for an analysis of reference sample QLO-1 and RGM-1 relative to the mean values for the same sample as contained in the database

Since a given irradiation may contain data from multiple analytical jobs or data from a single job may be divided between multiple irradiations, the FSRCOPY program can be used to merge XXXXFSR.DAT files or to break them apart into multiple LLNNFSR.DAT files, where LLNN signifies the job names. The FSRCOPY programs matches the sample names in the irradiation xxxxFSR.DAT data set with the LLNN job name using the xxxx.SWT files, where the job LLNN job name is stored in columns 81-84. SUMMARY2 can then be used to process the data in the LLNNFSR.DAT files to prepare analytical reports and chondrite normalized plots for a particular job.

3.6 A data base management system for Quality Control (CNTLEDIT).

As described above, the SUMMARY2 program creates an xxxxCDF.DAT data file of data on control samples. The CNTLEDIT program is used to process the control data files from each irradiation to build and edit a data base (CONTROL.DAT) for laboratory quality control. (For the PC version of CNTLEDIT, the

control data for each reference sample is stored in a separate file.) The CNTLEDIT program is used interactively to (1) enter data into the data base, (2) prepare a tabulation of control data for a given irradiation with comparison to mean values on the same reference samples, (3) produce tabulations of data on reference samples (either individual determinations or tabulations of mean values), (4) produce data files (CONTROL.STD) compatible with our statistics package, and (5) prepare plots of the data in order to visually check for consistency in the reference sample data base. Two forms of data presentation are used routinely to evaluate the results on control samples. The first form is identical to the control plot (Figure 8) created by SUMMARY2. The second form is to present a plot of data for a particular element (relative to the mean) in a single reference sample as a function of time in order to check for temporal variations in the database. Figure 9 shows a plot of Ta data for AGV-1 for several years of data. An input data file, MILESTON.DAT, can be used to define dates when significant changes were made in the analytical protocol, which will cause CNTLEDIT to change plotting symbols in the preparation of the time series charts, as that show in Figure 9.

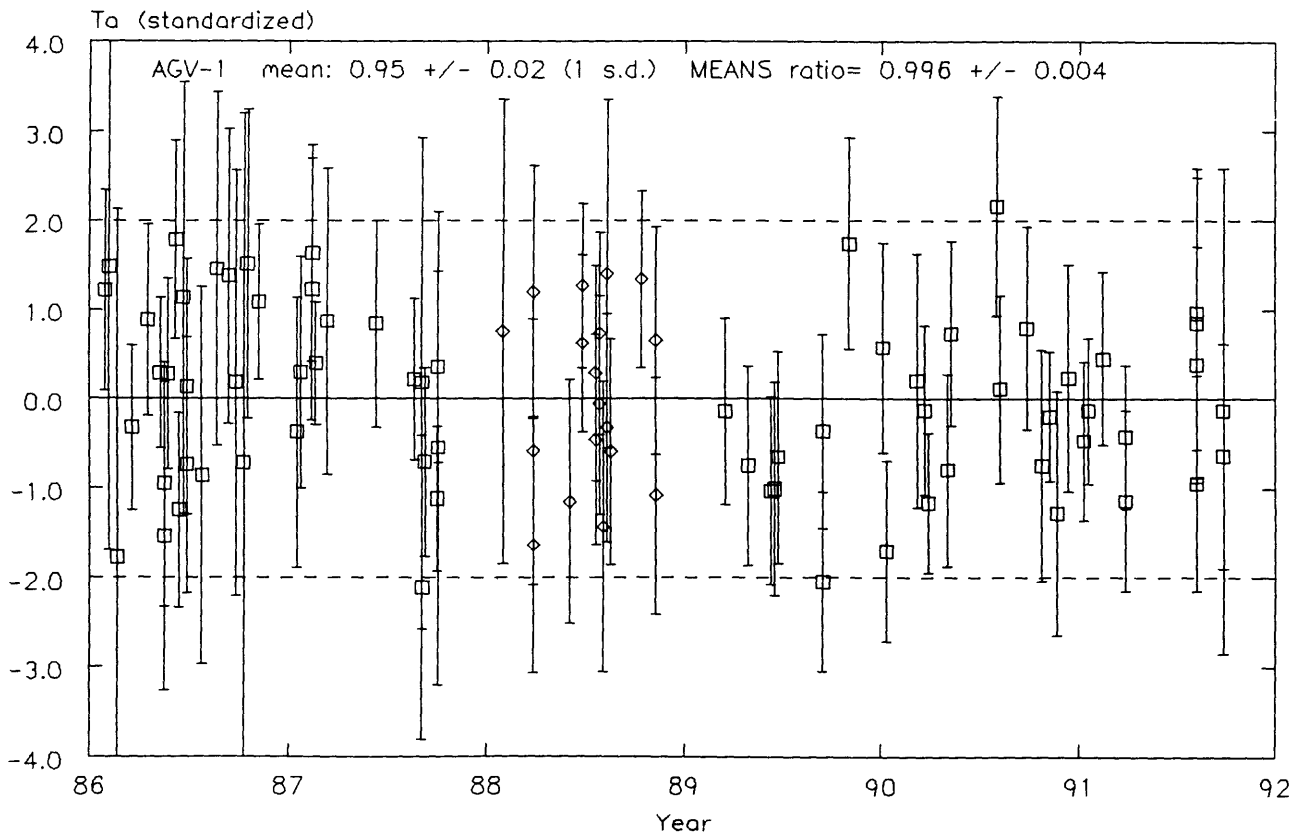

Figure 9. Plot of data for Ta relative to the mean in reference samples AGV-1 as a function of time

The option list for the CNTLEDIT program is as follows:

INDEX : Show a listing of the current contents of the CONTROL data file on the terminal screen and create a printable listing. (optional)

COPY : Enter the CONTROL data for a given irradiation into the data base.
(i.e. Copy data from an xxxxCDF.DAT file into the data base.)

ENTER : Enter data for a given sample from the terminal.

PRINT : Print listings of the data from the data base; the user may:
(1) Create a listing of data for all samples or selected samples,
(2) Create a listing of data for USGS standards only,
(3) Create a listing of average values only for all samples or selected samples,
(4) Limit the data listing and averaging by inclusive dates or by irradiation numbers,
(5) Create a new CONTROL data file with average values for all samples.

PLOT : Create quality control charts for selected standards/elements. [As in Figure 9]

MEANS : Create a new CTLMEANS.DAT file
and/or create a listing of the new or old CTLMEANS data
and create a comparison file of new:old CTLMEANS data.

STDD : Create a .STD data file of the CONTROL data.

EDIT : Edit the data file. (See EDIT options listed below)

HELP : Display the program options.

QUIT : Terminate the processing of the CONTROL data file.

The follow options are available under the EDIT command:

VALUE : Change data for one or more elements or mark data with flags.

IRRNO : Change an irradiation number.

DATE : Change an FSR date.

MULT : Multiply all data in a given record by a constant.

WEIGHT : Change sample weight and renormalize data for a given record.

RENORM: Renormalize data for selected elements in multiple records.

FLAG : Flag data for all elements in one or more records to delete from averaging.

UNFLAG : Remove all "delete" flags in one or more records.

FLGSET : Flag individual data values for selected elements in individual records.

RESEQ : Reorder records for a standard by date.

LIST : Show a comparison of data values and average values for the standard.

PLOT : Plot a comparison of data values and average values for the standard.
[This is identical to the SUMMARY2 control chart -- as in Figure 8]

RENAME : Rename all of the records for a standard.

HELP : Display the EDIT options.

QUIT : Terminate EDITing.

4. A menu interface to the SPECTRA library (SPECMENU)

All of the programs in the SPECTRA program library that are used for routine data processing are callable though a user-friendly menu interface called SPECMENU. [However, the spectral data file conversion utilities, the spectral data file editor (SDFEDIT), and the efficiency calibration program (EFFCALIB) have not been included in SPECMENU.] The various programs in the SPECTRA program library are callable from 1 of 5 menus:

Menu 1: Create SPECTRA input files -- Programs:
SPECEDIT, SFED, FWTEDIT, HEADERS, LINEFILE, INTERFNC, FILUPDAT, FILELIST, PEAKLIST

Menu 2: SPECTRA processing:
SPECTRA, READSPEC, PLOTSDF, REVIEW80, ICREPORT, LOGRESET, LOGDUMP

Menu 3: Initial Summary Report Processing:
ISRSETUP, SUMMARY1, ISRDUMP, ISRPLOT, ISRFILE, FILUPDAT, FILELIST

Menu 4: Final Summary Report Processing:
FSRSETUP, ANALSUM2, SUMMARY2, FSRWIND, FSREDIT, FSRCOPY, CNTLEDIT

Menu 5: General Utilities

SPECMENU locates all of the xxxxy.SDF files in the current working directory in order to construct a list of xxxxy spectral data job names. In menus 1 - 3 the job name is selected by using the space_bar or backspace keys. In menu 4 the .FSR data set selected for processing is chosen in a similar manner because the SPECMENU program has checked the current working directory to identify all xxxxFSR.DAT files.

The general utilities menu provides an interface to DOS and the following DOS commands: CD (change directory), MD (make a directory), RD (remove a directory), COPY (copy a file), REN (rename a file), DEL (delete a file). A file viewing utility is callable in order to view any ASCII input or output file on the terminal screen in either 80 or 132 column mode. Utilities are also included to print a file on an HP LaserJet or Inkjet printer (FPRINT) or to plot a graphics file to the printer or the screen (GP). A utility to obtain a directory listing is also accessible (DS).

SPECMENU has been designed to chain to the next program that would normally be called in the data processing sequence. For example, the program automatically chains to the SPECTRA program item in Menu 2 after execution of the SPECEDIT program under menu 1. Chaining may be turned off with the press of a function key (<F6>).

The SPECMENU program contains a built in HELP screen to provide some documentation of the functions performed by the various programs and utilities. Some of the general utilities accessible from menu 5 can be accessed more directly using function keys from any menu. <F1> changes the help screen to provide program documentation; <F2> shows a listing of files in the current working directory;

<F3> provides access to the file viewer to display the most recently created ASCII input/output file; <F5> prints an output file on an HP LaserJet or Inkjet printer; <F7> plots an output GrafPrint file on the system printer; <F8> calls up a word processing program of the users choice; and <F10> or the <Esc> key returns to the main menu.

An input data file SPECMENU.DEF can be edited with a text editor to tailor the SPECMENU program to individual systems. The command strings required to put the terminal screen in 132 column mode and return it to 80 column mode must be defined in SPECMENU.DEF in order to make the file viewing utility work. An optional word processor can be specified in SPECMENU.DEF in order to provide the capability to call up that work processor from within SPECMENU. The appropriate GrafPrint driver for the system printer must also be specified in SPECMENU.DEF in order plot GrafPrint files from within SPECMENU.

5. REFERENCES

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APPENDIX 1

An Annotated Summary of the Programs in the SPECTRA program library

The following programs create and edit the input files required to run SPECTRA, process the INAA output data from SPECTRA to prepare a complete report of analysis, and maintain a database for quality control:

SPECMENU: Provides a user-friendly menu interface, with internal documentation, to the programs in the SPECTRA program library.

A) SPECTRA and the programs used prior to running SPECTRA:

SPECEDIT: An editor for creating and editing the xxxxySP.INP input file for SPECTRA.

SFED: An editor for creating the INAA sample data in the format required by SPECTRA. The program creates and edits data in xxxx.SWT files.

FWTEDIT: An editor for creating the flux monitor weight files required by SPECEDIT when multiple flux monitors of differing composition are used for INAA. The program creates and edits data in xxxx.FWT files.

HEADERS: Edits an xxxxy.HDR file to define the sample counting sequence in a .SDF spectral data file from an INAA experiment. Sample numbers are entered from the keyboard to match the sample data in a .SWT file with the order of spectra in a .SDF file. [a pre-defined counting sequence can also be specified].

LINEFILE: An editor for creating and editing the yyy.LIN files used as input to SPECTRA. The .LIN files contain data pertaining to the analytical lines used for INAA calculations. This program will also produce a printable listing of the contents of any .LIN file, as will the FILELIST utility.

INTERFNC: A program to prepare a tabulation of potential spectral interferences of all lines in a designated yyy.LIN file. The program uses gamma-ray energy data in the SPECTRA isotope library to identify lines within a given energy interval of the lines in the .LIN file.

FILUPDAT: This utility will revise the gamma-ray energy, half-life, and spectral interference information in any .LIN file to be consistent with the data in the files GEMASTER.LIN and IGMASTER.LIN. The latter two files should be located in the SPPATH directory. It can also be used to revise the gamma-ray energy data in the file ISRLIN.DAT.

EFFCALIB: Program for calculating the efficiency curve coefficients for SPECTRA. The program processes calibration data in a .STD input file. For more documentation on this program see the file: EFFCALIB.DOC.

STDEDIT: This is an editor for .STD data files (such as the ones created by various SPECTRA utilities or used as an input data file by the EFFCALIB program). .STD data files can be created from or translated to .WK1 Lotus 1-2-3 spreadsheet files using the STDEDIT utility.

READSPEC: A program to print and make terminal and hardcopy plots of gamma-ray spectral data. Interactive isotope identification algorithms (using data in the isotope library PEAKS.DAT) may be called in conjunction with terminal plots when polynomial energy calibration coefficients are provided.

PEAKLIST: Creates a printable file listing all of the gamma-ray data in the SPECTRA isotope library. This program creates a listing for each isotope and an ordered listing of all of the gamma-rays in the library.

PEAKCOPY: This program converts the ASCII PEAKS.DAT file to the binary version read by SPECTRA. The data in this file is used by the interactive isotope identification algorithms that can be called from the routines used for graphics display of the spectral data in the programs SPECTRA and READSPEC.

SDFEDIT: A program to edit .SDF spectral data files. The order of spectra in the .SDF file can be modified or selected spectra deleted from the file. A .HDR file can be created, and subsequently edited with the HEADERS program, to define the order of sample counting in an INAA experiment. Counting date, time, duration, and dead time data can be listed to the terminal screen.

SPECTRA: The program includes algorithms for smoothing the spectral data, peak location, centroid and energy determination, and iterative and non-iterative methods for photopeak integration. Instrumental neutron activation analysis calculations can be made, including corrections for fission product and spectral interferences. Corrections for gain and zero drift and pulse pile-up are also incorporated in the program. Selected analytical lines may be designated for interactive graphical analysis, or the graphics procedures may be called automatically under special circumstances such as for the analysis of peaks having poor counting statistics or unexpected interferences. "Regions-of-interest" may be defined to control the analysis of spectral features in subsequent spectra. Interactive line/isotope identification algorithms are callable in conjunction with the algorithms for graphical presentation of the spectral data. Selected peaks in selected spectra may be selected for re-analysis after the completion of an initial SPECTRA INAA run, and a suspended INAA run may be restarted.

PLOTSDF: A program to overlay plots of a given region of spectral data in multiple spectra from a single .SDF file in order to check for changes in detector performance during a counting sequence (*fwhm* changes or gain/zero drift).

MOUSTEST: A program to test the function of the system mouse for compatibility with the programs in the SPECTRA library.

DS: A program to list the attributes of files in the current working directory.

B) Programs used for reviewing and processing output from SPECTRA:

ICREPORT: A program to prepare a report of spectral and fission product interference corrections made during a given SPECTRA run. The program processes data in the SPECTRA output file xxxxyICR.DAT.

REVIEW: This utility permits easy review of the SPECTRA output file xxxxSP.LIS on the terminal screen. In addition to other output options the user can review the energy calibration data, the flux monitor comparison summary, or the line location and intensity data for selected spectra. The spectra output can be limited to lines for selected isotopes. In addition the program will prepare scatter plots (terminal screen or hard copy) of 1) %DT vs. Time; 2) Gain-corr. vs. Time; 3) Gain-corr vs. %DT; 4) FWHM-change vs. Time; 5) FWHM-change vs. %DT.

ISRSETUP: A program to create and edit the input control file for the SUMMARY1 program. The program requires two input data files that may reside in either the SPPATH or the USERPATH directories: ISR.DEF and ISRLIN.DAT. The ISR.DEF lists the default element lists for given sample types, high energy or low energy detector counts, and count numbers. (In the USGS counting protocol the count numbers are defined as: 1 = 7 days decay; 2 = 2 weeks decay; and 3 = 2 months decay). ISRLIN.DAT defines the gamma-ray lines (and their priorities) the INAA results from which are to be averaged to yield element concentration values.

SUMMARY1: A program to average analytical results from multiple lines and create an "Initial Summary Report" (ISR) of INAA data for a single counting of an INAA sample set. The program processes data in the SPECTRA output file xxxxyISR.DAT. The program creates a printable output file, xxxxyISR.LIS, an optional file of "Sample data sheets" that summarizes the data for individual lines, and stores the analytical data in the file xxxxFSR.DAT. The user has the option of interactively reviewing the averaging of data from multiple lines and selectively including or excluding lines from the averaging process.

ISRFILE: This is an editor to create and edit the ISRSETUP input file ISRLIN.DAT.

FILELIST: This program can be used to prepare a printable listing of the data in any .LIN data file, or the ISRLIN.DAT file.

ISRPLOT: This program interactively reads the analytical results in one or more xxxxyISR.DAT files for plotting on the terminal screen. For example, this program is useful for making scatter plots of results from a pair of analytical lines for a given element. The program also has the capability of creating an ASCII standard data file (an .STD file) for subsequent statistical analysis.

ISRDUMP: This file dumps the contents of an xxxxyISR.DAT file to the terminal screen for quick review.

ISRCOMP: This program compares two xxxxyISR.DAT files that were created using different parameters while running SPECTRA. The ratios of each line in each sample in one file are calculated relative to those in the other file.

DUMPMCF: This program makes an ASCII standard data file (.STD file) of flux monitor comparator factors from the binary .LOG file created by SPECTRA. This is useful for looking for systematic differences in count rate between standards.

LOGDUMP: Program to display the contents of a binary xxxxySP.LOG file on the terminal screen or to create a printable ASCII file xxxxySP.DMP.

LOGRESET: If SPECTRA is being re-run after an initial SPECTRA run has gone to completion, and a decision is made to terminate the re-run prematurely, then SPECTRA will continue where the user left off if SPECTRA is restarted. However, the LOGRESET program can be used to reset the LOG file to its status when the initial SPECTRA processing was completed.

C) Programs to do the final averaging of data from SPECTRA:

FSRSETUP: A program to create the input control file for the SUMMARY2 and ASUM programs.

SUMMARY2: A program to process the element concentration data from the SUMMARY1 program and create a "Final Summary Report" (FSR) of analysis. The program processes the data in the xxxxFSR.DAT data file. Fission product interference corrections on samples are made by the SUMMARY2 program. The decay time-dependent fission product interference corrections for Ba and La are reported in separate output files. The program produces a side by side listing of the results from replicate counts of the same sample for ease of comparison, and a side by side listing of results from replicate samples. The program also prepares a printable file xxxxFSR.LIS, and an output data file of the results from the analysis of control samples for subsequent entry into a quality control data base. The program will also prepare screen and hard copy plots of rare-earth distribution patterns and data on control samples relative to average values for the control samples in the quality control data base.

ANALSUM2: Analyzes the xxxxFSR.DAT file to look for systematic errors between successive counts of the samples. The program calculates the concentration ratios for selected elements (by default Fe, Co, Sc, Ce and Eu in rock samples) in each count to a reference count selected by the user. Systematic differences in the element ratios from one can be used as a guide to identify systematic counting errors (e.g. variations in counting geometry between counts). The program creates a printable file xxxxANA.LIS.

FSRWIND: Permits easy review of the xxxxFSR.LIS file on the terminal screen. This is particularly useful in reviewing the side by side listing of the results from individual sample counts for systematic errors. The program only works with the screen set in 132 column mode.

FSREDIT: A program to edit the results of an xxxxFSR.DAT file of analytical data.

FSRCOPY: The SUMMARY2 input file xxxxFSR.DAT normally contains data for a single irradiation. However, a single irradiation may contain data for multiple analytical sample sets, or, conversely, a single analytical sample set may be divided across more than one irradiation. The FSRCOPY utility is useful for sorting an xxxxFSR.DAT file, or merging multiple files into a single data set. The irradiation xxxx.SWT file will be used for the sorting operation if the job name is stored in columns 81-84 of the record for each sample in the irradiation sample set.

FPRINT: A utility to control the printing of any ASCII output file to a HP Laser printer in either landscape or portrait mode. The program adjusts line spacing for the maximum lines/page found in the file up to 80 lines per page (landscape) or 105 lines per page (portrait). The program looks at both parts of an xxxxFSR.OUT file to define a different line spacing for each part.

VIEWFILE: This utility permits the display of any ASCII output file to the terminal screen for ease of review. The program works in either 80 or 132 column mode. The screen width must be set by a call to the appropriate utility that is used to control the computer's graphics card prior to starting the VIEWFILE program.

D) A program to build and process a database for quality control:

CNTLEDIT: A program to transfer data for control samples to a quality control data base and produce reports of the data on the analysis of control samples. The program copies the data from the xxxxCDF.DAT files created by the SUMMARY2 program into the database. Concentration data can also be entered manually into the database with CNTLEDIT, and the data can be edited. The program also creates reports such as (1) a listing of data for all samples or selected samples; (2) a listing of data for USGS standards only; (3) a listing of average values only for all samples or selected samples; and (4) a .STD data file of the CONTROL data for subsequent statistical analysis. The reported data can be limited to a listing and averaging by inclusive dates or by irradiation numbers. The program prepares QA/QC time series plots of elemental data for given control samples to the screen and for plotting on the printer. Multi-element control plots for individual analyses of control samples (identical to those made routinely by SUMMARY2) can also be made by CNTLEDIT. Files of average values on controls samples (CTLMEANS.DAT files) are also created and printed by CNTLEDIT.

CNTLPLOT: A program to read .STD files created by CNTLEDIT and to produce time-series charts of the analytical data on control samples. [Identical charts can also be created by CNTLEDIT]

SPLOADER: This program is used by all programs in the SPECTRA program library in order to allow them to make use of extended memory.

E) Spectral data file conversion utilities:

CHNTOSDF: Converts ORTEC ADCAM MCA .CHN files to U.S.G.S. Radiochemistry .SDF Spectral Data Files. Creates corresponding .HDR file.

SPETOSDF: Converts Nuclear Data .SPE files to U.S.G.S. Radiochemistry .SDF Spectral Data Files. Creates corresponding .HDR file.

SPMTOSDF: Converts Oxford MCA .SPM files to U.S.G.S. Radiochemistry .SDF Spectral Data Files. Creates corresponding .HDR file.

APPENDIX 2

FILE SUMMARY -- SPECTRA distribution diskettes

A) Executable Program Files:

SPECMENU.EXE	(menu system for the SPECTRA program library)
SPECTRA.EXE	(process gamma-ray spectra -- calculates INAA results)
SUMMARY1.EXE	(average INAA results from multiple lines)
SUMMARY2.EXE	(create final summary report for multiple counts)
READSPEC.EXE	(creates listings and plots of spectral data)
PLOTSDF.EXE	(overlay a spectral region in multiple spectra to check detector performance, i.e. fwhm changes and gain/zero drift)
ICREPORT.EXE	(creates a summary report of interference corrections made during a given SPECTRA run.
SPECEDIT.EXE	(create/edit the SPECTRA input file)
ISRSETUP.EXE	(create/edit the SUMMARY1 input file)
FSRSETUP.EXE	(create/edit the SUMMARY2 input file)
SFED.EXE	(create/edit an INAA sample id/weight .SWT file for the SPECEDIT program)
LINEFILE.EXE	(create/edit a .LIN data file for SPECEDIT)
FWTEDIT.EXE	(create/edit a .FWT file for SPECEDIT)
ISRFILE.EXE	(create/edit the file ISRLIN.DAT for ISRSETUP)
HEADERS.EXE	(modify the sample numbers in a .HDR file for ISRSETUP)
FSREDIT.EXE	(edit a final summary report data file)
EFFCALIB.EXE	(calculates the efficiency calibration coefficients for the SPECEDIT program)
STDEDIT.EXE	(.STD file editor. creates the input file for EFFCALIB, converts .STD files to Lotus 1-2-3 .WK1 files).
REVIEW80.EXE	(aids in examining xxxxySP.LIS files from SPECTRA)
DUMPMCF.EXE	(creates an .STD file of monitor comparitor factors from a xxxxySP.LOG file)
ISRDUMP.EXE	(dumps the data from an xxxxyISR.DAT file to the terminal screen for review)
ISRPLOT.EXE	(plots data from one or more xxxxyISR.DAT files and creates .STD files for statistical analysis)
ISRCOMP.EXE	(compares the analytical results from two xxxxyISR.DAT files)
FILELIST.EXE	(create a printable listing of .LIN or ISRLIN.DAT files)
FILUPDAT.EXE	(update gamma-ray energy, half-life, and interference data in .LIN and ISRLIN.DAT files)
FSRCOPY.EXE	(merges multiple xxxxFSR.DAT files into a single file, or copies data from one file into multiple files)
PEAKCOPY.EXE	(creates an unformatted file PEAKSU.DAT from the ASCII file PEAKS.DAT)
PEAKLIST.EXE	(creates a printable listing (PEAKS.LIS) of the isotope data in PEAKS.DAT or PEAKSU.DAT)
INTERFNC.EXE	(creates a printable listing of spectral interferences for lines listed in any .LIN file)
LOGDUMP.EXE	(displays the contents of an xxxxSP.LOG file)
LOGRESET.EXE	(restores a SPECTRA xxxxSP.LOG file)
ANALSUM2.EXE	(looks for systematic changes in element concentration between replicate sample counts.
FSRWIND.EXE	(a program for reviewing the xxxxFSR.LIS output file on the terminal screen.)
CNTLEDIT.EXE	(builds the quality control data base and produces reports of data on control samples.)
CNTLPLOT.EXE	(plots time-series charts of data on control samples from .STD files created by CNTLEDIT)
VIEWFILE.EXE	(Lists files in 80 or 132 column mode to screen)
FPRINT.EXE	(Prints .LIS and .OUT files on an HP Laser printer)
MOUSTEST.EXE	(Tests mouse operation in graphics mode)

Executable Program Files (Continued):

CHNTOSDF.EXE	(Converts .CHN to .SDF spectral data files)
SPETOSDF.EXE	(Converts .SPE to .SDF spectral data files)
SPMTOSDF.EXE	(Converts .SPM to .SDF spectral data files)
SDFEDIT.EXE	(Edits .SDF spectral data files)
SPLOADER.EXE	(This file contains the loader that permits all other programs in the SPECTRA program library to execute in extended memory)
DS.EXE	(A directory listing utility for DOS)
VIEW80.BAT	(Puts VIEWFILE in 80 column mode)
VIEW132.BAT	(Permits VIEWFILE to work in 132 column mode)
FSRW.BAT	(Permits FSRWIND to work in 132 column mode)
REVIEW.BAT	(Permits REVIEW80 to work in 132 column mode)

(These last three .BAT files will need to be modified to be compatible with individual VGA utilities/drivers on individual systems)

B) Data Files

The following files must be in the SPPATH directory:

PLOTPK.HLP	(a SPECTRA data file -- menu of cross-hair commands)
PEAKS.DAT	(a SPECTRA data file -- gamma-energy data)
PEAKSU.DAT	(an unformatted version of PEAKS.DAT)
PALETTE.DEF	(a SPECTRA data file -- defines the colors used by the graphics algorithms)
SPECEDIT.DEF	(defines default calibration variables for SPECEDIT)
CNTLEDIT.DEF	(defines default element lists on control samples)
SPECMENU.DEF	(sets screen control, wordprocessor and plotter options used by the SPECMENU program.)
DETECTOR.DAT	(optional file for the SPECEDIT program)
GEMASTER.LIN	(a master file of gamma-ray energy, half-life and interference correction data for coax. detectors)
IGMASTER.LIN	(a master file of gamma-ray energy, half-life and interference correction data for LEP detectors)
CTLMEANS.DAT	(a file of mean values for control samples)

The following files may either be in the SPPATH or in the USERPATH directories:

ISRLIN.DAT	used as an input file for ISRSETUP
ISR.DEF	used as an input file for ISRSETUP
FSR.DEF	used as an input file for FSRSETUP
HEADERS.DEF	used as an input file for HEADERS
FILUPDAT.DEF	used as an input file for FILUPDAT
FPCORR.DAT	used as an input file to SPECTRA and SUMMARY2

The following files may either be in the SPPATH, the USERPATH, or in the current working directory:

All .LIN files used as input to SPECEDIT
All .FWT files used as input to SPECEDIT

The following file should be in the CNTLPATH directory:

MILESTON.DAT

C) Test Data Files

The following files should be in the DOS directory created for the test data set:

TESTD.SDF	(Test spectral data file	-- input to SPECTRA)
TESTDSP.INP	(Test control file	-- input to SPECTRA)
TESTDISR.INP	(Test control file	-- input to SUMMARY1)
TEST.SWT	(Test sample id/weight file	-- input to SPECEDIT)
TESTD.HDR	(Test 'header' file	-- input to SPECEDIT)
EFFCAL.STD	(Test efficiency data	-- input to EFFCALIB)

The following files may either be in the SPPATH or in the USERPATH directories:

GE1.LIN	(gamma-ray line file	-- input to SPECEDIT)
GE2.LIN	(gamma-ray line file	-- input to SPECEDIT)
GE3.LIN	(gamma-ray line file	-- input to SPECEDIT)
IG1.LIN	(gamma-ray line file	-- input to SPECEDIT)
IG2.LIN	(gamma-ray line file	-- input to SPECEDIT)
HMS4.FWT	(Test F.M. weight file	-- input to SPECEDIT)

D) Documentation Files

README.TXT	(This file)
APPENDX1.TXT	(Describes the SPECTRA input file)
SPECEDIT.DOC	(Documents the editors used to create the SPECTRA input file)
PALLETTE.DOC	(Documents the default graphics colors defined by PALLETTE.DEF)
EFFCALIB.DOC	(Documents the EFFCALIB program)

E) Printer drivers for hard copy plots of graphics output:

GPRINT3.BIN	(GrafPrint™ Driver called by graphics programs -- this should be placed in your DRVRPATH directory as defined in your AUTOEXEC.BAT file)
GP.EXE	(Program to send graphics files to your printer)
GPRINT.BAT	(A DOS batch file to run GP.EXE)

Printer drivers used by GP.EXE:

citgsx14.drv	Citizen GSX 140 24 pin printer
citmsp10.drv	Citizen MSP-10 9 pin printer
citmsp15.drv	Citizen MSP-15 9 pin printer - wide carriage
ega.drv	EGA 16 Color screen driver
egamono.drv	EGA 2 Color screen driver
epfx.drv	Epson FX series printers
epfxwc.drv	Epson FX series printers - wide carriage
eplq.drv	Epson LQ series printers
eplqlo.drv	
eplqlowc.drv	
eplqwc.drv	Epson LQ series printers - wide carrage
eps.drv	
herc.drv	Hercules 2 color screen driver
hpdjet.drv	HP DeskJet and DeskJet Plus printers
hpljet.drv	HP LaserJet, LaserJet II, LaserJet IID printers
hpljet2p.drv	HP LaserJet IIP printers
hpljet3.drv	HP LaserJet IIIP printers
hppjet.drv	HP PaintJet and PaintJetXL printers
hptjet.drv	HP ThinkJet printer
mcga.drv	MCGA 2 color screen driver
pcx.drv	Create PC Paintbrush .PCX files
vga.drv	Redisplay to a VGA color monitor
vgamono.drv	Redisplay to a VGA mono monitor

GP switches:

Flag	Description	Default	Alternate settings
/Q	Quiet	Off	display info on screen
/O:#	Output	PRN	file.dat
/F:#	Form	P (portrait)	L (landscape)
/R:#	Resolution	0 (low)	1, 2, 3 (high)
/D:#	Device_Name	HPLJET	(other devices listed above)
/P:#	Page Size	0 (half page)	1 (full) 2 (quarter)
/I:#	Invert Flag	0	1 (white on black)
/E:#	EMM Usage	1	0 (exp. mem. not used)
/l:#	Left margin	50	100 units per inch
/r:#	Right margin	50	(i.e. 1.5 inches = 150)
/t:#	Top margin	50	
/b:#	Bottom margin	50	
/c:#	Copies	1	
/T:#	Device Path	None	path to Device_Name.DRV

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