Volume 08

Section 04

08-S-04-212

Revision 0

Date: 6/29/81

CHEMISTRY INSTRUCTION

GERMANIUM SPECTROSCOPY SOFTWARE

SAFETY RELATED

Prepared: _____

Reviewed: _____ / _____
Technical Review Independent Review

PSRC: NA PSRB 4/6/81

Approved: _____
Plant Chemist

Concurrence: _____
Chemistry/Radiation Control Superintendent

List of Effective Pages:

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1.0 PURPOSE

The Germanium Spectroscopy (GS) Software package supports all phases of counting and calibration. The software package can be broken into the following groups of programs:

1.1 System Initiation

1.2 Data Acquisition

1.3 Calibration

1.4 Spectrum Analysis

1.5 Utility Functions

The System Initiation program permanently stores parameters needed to perform calibrations and run the other GS programs. The GS EDAT program stores the calibration sources data. These data are required to run the calibration curves. The GS L1B program sets up the nuclide identification libraries. These libraries are used in spectrum analysis to identify and qualify nuclides.

The GSMCA programs are primary programs for Ge(Li) counting and calibration. The program can be used to control the acquisition of spectra and must be used to transfer spectra from the MCA to the computer memory. Once the spectrum is transferred, analysis is performed by other programs.

If the sample counted was a calibration standard, the spectrum can be analyzed by the GSEECL program. The program takes the data from the spectrum and performs a nonlinear least square fit to the data and determines an efficiency curve for that detector and geometry. The curves are stored permanently for use by other analysis programs. The GSEECL program must be run on spectra for each geometry and shelf for which samples will be run for quantitative analysis.

The GSRAP analysis spectra is for identification and quantification of unknown sources. During routine operation, spectra will be accumulated using the GSMCA program with the analysis performed by the GSRAP program.

There are several other utility programs that provide non-routine functions such as plotting, spectrum storage and retrieval and data file listing.

2.0 REFERENCES

2.1 Program Manual, Germanium Spectroscopy Package

3.0 DEFINITIONS

3.1 Program Variables

3.1.1 MSUSp$ - n mass storage unit specific for programs, normally : C12.

3.1.2 MSUSd$ - Mass storage unit specific for data, normally : D12.

3.1.3 N-Channels - Number of channels in MCA, normally 2048.

3.1.4 Crt - The select code for the HP9845 Crt, normally 16.

3.1.5 Prt - The select code for the system printer, normally 5 in the Counting Room and 0 in the Hot Lab.

3.1.6 Aux-prt - The select code for the system auxiliary printer, normally 0.

3.1.7 Plotter $ - The name of the system plotter, can be GRAPHICS or 7225A.

3.1.8 Plotter - sc $ - The select code for the system plotter, normally 7, 5.

3.1.9 Where $ - An internal counter for keeping track of where the program is in stage of completion.

3.1.10 Comments $ - The comment statement for the spectrum in memory.

3.1.11 Perf - Y, N - Determines if the paper used is perforated. Normally perforated paper will be used so perf will be Y.

3.1.12 Company $ - The company name and station (Mississippi Power and Light Company, Grand Gulf Nuclear Station).

3.1.13 Month, day, year - Determines if dates and time are entered as year, month, day, hour and minute or month, day, year, hour, and minute when 0, the former sequence is used, and when 1, the latter sequence is used. Month, day, year is normally 0.

3.1.14 Sc - The select code for the ND 66 MCA, normally 11.

3.1.15 Tlive - The number of seconds of live time the spectrum in memory was counted.

3.1.16 Tclock - The number of seconds of clock time the spectrum in memory was counted.

3.1.17 D - A 4096 register array in which the spectrum is stored. The subscript of D corresponds to the channel the data represents.

3.1.18 Begin - Determines the channel number that the peak search program begins; normally 1.

3.1.19 Nchan - Determines the channel number that the peak search program stops.

3.1.20 Units - The sample volume in unit determined by units.

3.1.21 Dtctrs - The name of the data file where the energy and efficiency calibration data is stored. The file name is GSDETn, where n is the cyrstal number.

3.1.22 En-coef - Determines the gain curve for each crystal.

3.1.23 Eff-coef - Determines the efficiency calibration curve.

3.1.24 Resolution - The $\pm$ range allowed when making energy comparisons to library values. Normally, 2 for sample spectra, and 5 for calibration spectra.

3.1.25 Max-chnls - The maximum number of channels allowed in a peak, normally 15.

3.1.26 Sensitivity - Determines the sensitivity of the peak search program to peaks, normally 3.5. Higher values result in less sensitivity.

3.1.27 Term-Fretn - Determines the factor that terminates the peaks in spectra, normally 1.01.

3.1.28 Geom $ - The geometry code for the spectrum in memory, XXXX-N where XXXX is a four letter name and N is the shelf number.

3.1.29 Cnt-strt - The date and time the spectrum in memory was counted, e.g., March 11, 1981 at 1246 would be 81 3 11 12 46.

3.1.30 Yield - The fraction yield of a chemical separation. If not done the value should be 1.

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3.1.31 Cllct-strt - The date and time the sample collection was started for the spectrum in memory.

3.1.32 Cllct-stp - The date and time the sample collection was stopped for the spectrum in memory.

3.1.33 Libname $ - The library name (Data File) used to analyze the spectrum in memory.

3.1.34 Prog 1 $ - A default program name that will be loaded when restarting certain programs.

3.1.35 Prog 2 $ - A default program name that will be loaded when restarting certain programs.

3.1.36 Id$ - The spectrum data file identification, normally RAP _ __.

3.1.37 Oper-init $ - The initials of the person running the program.

3.1.38 Dummy - An array for storing miscellaneous constants.

3.1.39 Dummy $ - Stores miscellaneous alpha-numeric values.

3.1.40 Unit$ - The units of the sample volume.

3.1.41 Reactor - The number of the reactor from which the sample was taken.

3.1.42 Current-date - The date and time the spectrum was analyzed.

4.0 PREREQUISITES

4.1 Program Files on : C12

4.1.1 GSMCA

4.1.2 GSRAP

4.1.3 GSPKSR

4.1.4 GS2LLD

4.1.5 GSRPRT

4.1.6 GSDRA

4.1.7 GSRSTR

4.1.8 GSBDRA

4.1.9 GSKEYS

4.1.10 GSHPKY

4.1.11 GSRCNC

4.1.12 GSSSTR

4.1.13 GSNXTL

4.1.14 GSPROG

4.1.15 GSEDAT

4.1.16 GSLIB

4.1.17 GSEECL

4.1.18 GSRES

4.1.19 GSCLCK

4.1.20 GSSPLT

4.1.21 GSREVU

4.1.22 GSPUTM

4.1.23 GSGETM

4.1.24 GSDETL

4.1.25 GSCOPY

4.2 Data Files on : C12

4.2.1 GSDET1 (Counting Room only)

4.2.2 GSDET2 (Counting Room only)

4.2.3 GSDET3 (Hot Lab only)

4.2.4 YEAR

4.2.5 GSSSDN

4.2.6 LENVL

4.2.7 LRWIOD

4.2.8 LOFGAS

4.2.9 LPARTI

4.2.10 LISOTP

4.3 Data Files on : D12

4.3.1 Spectrum Data (RAPnnS) where nn can be 00 to 99

4.3.2 Spectrum Results (RAPnnR) where nn can be 00 to 99

5.0 PRECAUTIONS

5.1 The following change to the master operating disk need to be made to prepare the Hot Lab Master Operating Disk:

5.1.1 Change line 690 of GSMCA from N-adcs=3 to N-adcs=1.

6.0 INSTRUCTIONS

6.1 Normal System Parameters

6.1.1 Printer Select Code - 5 or 0

6.1.2 Auxiliary Printer Select Code - 0

6.1.3 MCA Select Code - 11

6.1.4 Plotter - GRAPHICS

6.1.5 Plotter Select Code - 13

6.1.6 Msus for programs - : C12

6.1.7 Msus for data - : D12

6.2 Initialize Data Files

6.2.1 Calibration Sources Data File

a. The GSEDAT program is used to store calibration source data in data file GSSSDN on Msusp.

b. The following information is required by the GSEDAT program:

(1) Source number (assigned sequentially)

(2) Source essay date

(3) Gamma peak data

(a) Peak energy in KeV

(b) Gamma transitions per disintegrations

(c) Half-life of nuclide in days

(d) Total activity in disintegrations per second

c. The calibration source data can be edited with the GSEDAT program

d. Additional information can be found in Section 2.0 of the Program Manual, Germanium Spectroscopy Package.

6.2.2 Nuclide Identification Library

a. The GSLIB program is used to create or edit nuclide identification libraries and store the libraries in data files starting with the letter L on Msusp.

b. The following information is required by the GSLIB program:

(1) Isotope name

(2) Isotope peak energy in KeV

(3) Peak classification

(a) Background - A peak observed in ambient background that is not used for calculating concentration.

(b) ID - A peak that is only used for identification and is not used for calculating concentration.

(c) Quantify - A peak that is identified and used for calculating concentration.

(d) Selected - A peak that is identified, quantified, and a Lower Limit of Detection (LLD) is calculated.

(4) Nuclide half-life in hours

(5) Gamma transitions per disintegrations per second

(6) Any secondary peaks that should be present when the primary peak is present

c. Libraries may be changed using GSL1B program.

d. The following precautions apply when changing a library:

(1) The library name must be changed whenever the order or number of selected nuclides is changed.

(2) Each library must have at least 1selected peak.

e. Additional information can be found in Section 3.0 of the Program Manual, Germanium Spectroscopy Package.

6.3 MCA Data Acquisition

6.3.1 The GSMCA program is used to control the ND 66 MCA functions and to transfer data between the ND 66 and the HP 9845.

6.3.2 The GSMCA program configures the ADC's with the following data:

a. Number of channels in spectra - 2048

b. Number of groups per Adc - 2

c. Digital offset - 0

d. Acquisition mode - PH - pulse height analysis

6.3.3 The GSMCA program uses the following 2 letter commands to control and manipulate the data between the ND 66 MCA and the HP 9845.

a. On - Starts data acquisition in the selected ADC group for the selected number of seconds live time. A spectrum identification label (up to 31 characters) may be entered.

b. OF - Stops data acquisition in the selected ADC.

c. WS - Transfers the data in the selected ADC group from the ND 66 MCA to the HP 9845.

d. EX - Exits from MCA manipulative mode, returns the ND 66 MCA keyboard to the interactive mode and returns the HP 9845 keyboard to the interactive mode. The next program to run can be loaded and executed.

e. EN - Exits from MCA manipulative mode, returns the ND 66 MCA and HP 9845 keyboards to the interactive mode and stops program execution.

f. HE - Prints a summary of 2 letter commands on the CRT.

g. LI - Lists spectrum data in memory to selected printer.

h. ER - Erases the contents of the selected ADC group.

i. SP - Displays the selected ADC group on the ND 66 MCA CRT.

j. RS - Transfers the spectrum data from the HP 9845 memory to the selected ADC group.

k. ST - Provides the current status of the MCA.

l. SE - Configures the selected ADC with the following data:

(1) Number of channels in spectra

(2) Number of groups per ADC

(3) Digital offset

(4) Sets acquisition mode to pulse height (PH)

m. KE - Sets the ND 66 MCA cursor to the selected channel.

n. PA - Displays the selected page (1-6) on the ND 66 MCA.

o. TI - Sets the MCA clock for hour, minutes, and seconds.

p. D - Sets the MCA clock for year, month, and date.

q. CO - Allows messages to be displayed on the ND 66 CRT.

6.3.4 Additional information can be found in Section 6.0 of the Program Manual, Germanium Spectroscopy Package.

6.4 Crystal Calibration

6.4.1 The GSEECL program is used to analyze spectra from calibration sources to set the gain (KeV/channel) and the efficiency for each detector. The program does a non-linear least squares fit to the data and stores the curves in GSDETn, where n is the number of the cyrstal.

6.4.2 The following information is required by the GSEECL program:

a. The calibration source number and mass of the source.

(1) The calibration source numbers are assigned sequentially by the GSEDAT program and the source data is found in data file GSSSbN.

(2) The mass of the source is determined when the source is prepared from the calibration source. The mass of the source is the fractional amount of the calibration source used to prepare the source. The source number and the mass of the source should be attached to the source.

b. The detector that the source was counted on. The number entered determines the name of the data file where calibration data is stored, e.g., where detector number is 2, the calibration file would be GSDET2.

c. The geometry code for the source counted must be entered. The code consists of up to 4 alphanumeric characters followed by a dash and a shelf number.

d. The sample identification entered in the GSMCA can be modified or extended up to 80 characters.

e. The calibration source assay date and time is the time at which the calibration source strength was determined. The assay date and time should be present on each source.

f. The date and time the source was counted.

g. The decay corrected disintegration rates for each peak can be displayed on the CRT and any peaks that are low in activity can be deleted from the calibration source data.

h. The peak search parameters may be changed. The program sets the parameters to the following values:

(1) Peak sensitivity - 15

(2) Peak termination fraction - 1.01

(3) Maximum channels per peak - 15 for 2048 channels and 30 for 4096 channels

(4) Library tolerance - 5

i. The crystal gain or energy calibration is determined by performing a linear approximation between two widely separated peaks and then the current gain is calculated by a least squares method using all the peaks in the standard source. The gain is represented by the following formula:

$$G = X + Y(C) + Z(C)^2 + W(C)^3$$

Where:

G = Gain (KeV/channel)
X = Offset
Y = Linear Fit Coefficient
Z = Quadratic Fit Coefficient
W = Cubic Fit Coefficient
C = Channel

The Z and W coefficients will normally be zero.

6.4.3 Log plots of the efficiency curves should be dumped to the system printer.

6.4.4 Printouts of the efficiency curves in mass storage may be obtained by running the GSDETL program.

6.4.5 Additional information can be found in Section 4.0 of the Program Manual, Germanium Spectroscopy Package.

6.5 Spectrum Analysis

6.5.1 The GSRAP program is used to analyze spectra for the energy and number of counts in each peak, peak identification, activity concentration, estimation of errors, and lower limit of detection.

6.5.2 The following information is required by the GSRAP program:

a. The spectrum ID should be RAPss where ss can be a number from 00 to 99.

b. The reactor number should be the reactor from which the sample was taken. If the sample was from a system common to both reactors, the reactor number should be 0.

c. Operator's initials (up to 6 characters allowed).

d. The sample identification can be changed or additional information can be added up to 80 characters.

e. The sample volume and units must be entered in the format volume, unit (e.g., 1000 ml). The units specified will be the units recorded on the spectrum report.

f. The fractional yield is entered for those samples that were chemically separated and the fractional yield is the chemical yield obtained in the separation. The fractional yield for other samples should be 1. The default value for fractional yield is 1.

g. The computer will normally use perforated paper.

h. The activity calculations will normally be performed in uCi.

i. The clock time should be verified to be correct to within $\pm$ 5 minutes.

j. The collection start date and time is the date and time the sample flow to the collection device was started.

k. The collection stop date and time is the date and time the sample flow to the collection device was stopped. The period of time from the collection start to stop is used to calculate the decay during collection for identified nuclides.

l. The counting start date and time is the time that the spectrum collection started. The decay during counting is calculated from the clock time or real time needed to count the sample. The sample is also decay corrected from the end of the collection period to the start of the count.

m. The number of the detector is used to define which file (GSDETn) to use for gain and efficiency curves.

n. The geometry code must be a four letter code followed by a dash, followed by a simple digit (0-4).

o. The peak search parameters may be changed. The normal values are:

(1) Peak sensitivity - 3.5

(2) Peak termination fraction - 1.01

(3) Maximum channels per peak - 15 for 2048 channels and 30 for 4096 channels

(4) Library resolution - 2

p. The library to be used to identify the nuclide must be entered. The libraries will be six letter files, starting with L. Care must be exercised when choosing the library to match the sample being analyzed.

q. The program has an option to do manual detailed analysis for any questionable peaks.

r. Additional isotopes can be added or peaks deleted.

s. The spectrum and results can be stored on the Msusd (: D12). Normally, only spectra for release analysis will be stored.

6.5.3 Additional information can be found in Section 5.0 of the Program Manual, Germanium Spectroscopy Package.

6.6 Utility Programs

6.6.1 The GSRES program is used to measure the resolution of the Ge(Li) crystals by fitting Gaussian curves to the peaks.

a. The following information is required by the GSRES program:

(1) The computer normally uses perforated paper.

(2) Operator's initials (up to 6 characters allowed).

(3) The detector number is used to define the file (GSDETn).

(4) The program will perform resolution measurements on two peaks. The normal peaks used are 122 and 1332 KeV.

(5) The sample identification can be changed or additional information can be added up to 80 characters.

(6) The counting start date and time is the time that the spectrum collection started.

(7) The peak search parameters may be changed. The normal values used are:

(a) Peak sensitivity - 15

(b) Peak termination fraction - 1.01

(c) Maximum channels per peak - 15 for 2048 channels and 30 for 4096 channels

(d) Library resolution - 5

(8) The correct peaks for the resolution check should be identified from the spectrum.

b. Additional information can be found in Section 13.0 of the Program Manual, Germanium Spectroscopy Package.

6.6.2 The GSPUTM program is used to transfer spectrum data from the HP 9845 to the selected mass storage medium. Spectra are normally stored on the fixed disk (: D12).

a. If not available from a GSRAP program, the GSPUTM program will require the initial information to identify the spectrum and geometry counted to be entered.

b. The program stores the spectrum in a file that is compatible with the other Germanium Spectroscopy programs.

c. Additional information can be found in Section 7.0 of the Program Manual, Germanium Spectroscopy Package.

6.6.3 The GSGETM program is used to transfer spectrum data from the selected mass storage medium to the HP 9845 memory.

a. The spectrum identification and information is transferred to the HP 9845 memory.

b. The first five letters of the file name of the stored spectrum must be entered. The spectrum name usually will be in the form RAPnn.

c. Additional information can be found in Section 8.0 of the Program Manual, Germanium Spectroscopy Package.

6.6.4 The GSSPLT program is used to provide a plot of spectra on the HP 9845 CRT, the HP 9845 printer or the HP 7225A X-Y plotter.

a. The options available are:

(1) Digital listing of spectrum

(2) Changing spectrum comment

(3) Any region of the spectrum may be plotted

(4) Plot may be linear or log

(a) Vertical scales may be changed

(5) Plot may be individual data points or line drawing of the spectra

(6) A hard copy of spectra may be obtained on either:

(a) HP 9845 printer

(b) HP 7225A X-Y plotter

b. Additional information can be found in Section 9.0 of the Program Manual, Germanium Spectroscopy Package.

6.6.5 The GSCLCK program is used to set the data and time on the HP-98035A real time clock. The clock is battery powered so that

time will remain accurate even for short periods when the system power is turned off.

a. The options available are:

(1) Display the present date and time

(2) Change the date and time to the current date and time

NOTE

Loading and executing this program will destroy the spectrum stored in the HP 9845 memory. Some of the device select codes are also altered by the GSCLCK program. To eliminate select code problems, it is recommended that [SCRATCH C], [EXECUTE] be performed to clear any incorrect select codes. The net result being that the next program will put in its default values for the device select codes.

b. Additional information can be found in Section 10.0 of the Program Manual, Germanium Spectroscopy Package.

6.6.6 The GSDETL program will print out on the system printer the current values that determine the gain and the constants that determine the efficiency curves for all the geometries.

a. The values are obtained from data file GSDETn where n is the number of the crystal for which the data was requested.

NOTE

Loading and executing this program will destroy the spectrum stored in the HP 9845 memory.

b. Additional information can be found in Section 11.0 of the Program Manual, Germanium Spectroscopy Package.

6.6.7 The GSREVU program provides a listing of all data files on Msusd that contain Ge(Li) spectrum.

a. The program provides the following options:

(1) Lists all spectrum data file names, date and time counted, spectrum comment, operator's initials on either the CRT or system printer.

(2) The spectra can be reviewed and purged from the mass storage device.

NOTE

Loading and executing the program will destroy the spectrum stored in the HP 9845 memory.

b. Additional information can be found in Section 10.0 of the Program Manual, Germanium Spectroscopy Package.

6.6.8 The GSCOPY program provides a convenient method of copying or purging files or programs.

a. Because of the extreme ease with which files can be destroyed using this program, the following precautions should be followed:

(1) Double check all entries before execution.

(2) Use the write-protect switch on the disk drive being copied from to eliminate purging files.

(3) Use system commands such as [COPY TO] for copying single or small number of files or programs rather than the GSCOPY program.

b. Additional information can be found in Section 14.0 of the Program Manual, Germanium Spectroscopy Package.

7.0 DOCUMENTATION/CORRECTIVE ACTION

None