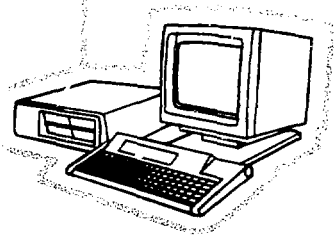
No.3

Nuclear Analysis Software

Part 2: Gamma Spectrum Analysis, Activity Calculations and Neutron Activation Analysis (GANAAS)



International Atomic Energy Agency, 1991

COMPUTER MANUAL SERIES No. 3

Nuclear Analysis Software

Part 2: Gamma Spectrum Analysis, Activity Calculations and Neutron Activation Analysis (GANAAS)

INTERNATIONAL ATOMIC ENERGY AGENCY, VIENNA, 1991

NUCLEAR ANALYSIS SOFTWARE
PART 2: GAMMA SPECTRUM ANALYSIS, ACTIVITY CALCULATIONS AND NEUTRON ACTIVATION ANALYSIS (GANAAS)
IAEA, VIENNA, 1991
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FOREWORD

During the period 1987-1991, the Physics Section of the IAEA has organized a number of actions leading to creation of a software library for nuclear analysis. Using such mechanisms as research and technical contracts, and by inviting some short-term experts, several software packages have been developed. The initial versions were tested in different laboratories, mainly in developing coutries. Based on the comments and recommendations received, numerous improvements were made, both in respect to the applied algorithms as well as in user-friedly presentation.

As a result of these efforts, the following software packages are available at present:

- *Spectrum reformatting and transfer programs (SPEDAC)*
- *Gamma spectrum analysis, activity calculations and neutron activation analysis system (GANAAS)*
- *Quantitative x-ray analysis system (QXAS)*
- *Positron annihilation fitting procedure (POSFIT)*
- *Moessbauer spectrum analysis program (MOSA).*

As frequently observed in development of software, good manuals are rather scarce, and appear as a rule later than the software itself. The same applies to the IAEA nuclear analytical software. The complete operation manuals for all available software packages will only be completed and published by the end of 1992.

The present volume is Part 1 of five publications, and covers the programs for transfer of spectrum from a stand-alone multichannel analyzer to a computer, and the spectrum reformatting.

The IAEA software packages for nuclear analysis belong to the category of open domain software. There is no limitation to them being copied and distributed, except for commercial purposes. The source codes of all programs are available on request.

EDITORIAL NOTE

In preparing this material for the press, staff of the International Atomic Energy Agency have mounted and paginated the original manuscripts and given some attention to presentation.

The views expressed do not necessarily reflect those of the governments of the Member States or organizations under whose auspices the manuscripts were produced.

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CONTENTS

Chapter 1

INTRODUCTION

A spectrum acquired with a multichannel analyzer is usually stored with a suitable device (tape, cassette tape, diskette, hard disk). Every manufacturer of multichannel analyzers uses his own method for storage, and records the spectra in his own format. Furthermore, the formats to save the spectra evolve in time: the same manufacturer can have several formats for different generations of multichannel analyzers. A similar situation prevails with the spectrum analysis programmes. They require spectra in a particular format as the input to the analysis. Again, these input formats are many and differ from each other considerably.

SPEDAC set of routines was developed to provide the spectroscopist with a tool for converting the spectral formats. They can read the spectra recorded in a number of formats used in different multichannel analyzers, to a number of analysis programmes. In fact, all the major formats are represented.

Another serious problem for the user of a stand-alone multichannel analyzer is the transfer of spectra from the MCA to the computer. For several well known types of MCAs, the Version 5.0 of SPEDAC offers a set of routines for spectrum transfer, using the most simple methods of interfacing. All the transfer programmes described in this manual have been carefully tested with the corresponding stand-alone multichannel analyzers.

The first rudimentary version of SPEDAC was designed by Mr. S. Somwasdi (Thailand) at the time when he was a trainee in the IAEA Headquarters. Later, other programmers were involved in the improvement of the programmes, in particular P. Van Espen (Belgium), G. Bernasconi (Uruguay), and G. Espinosa (Colombia). They have shaped SPEDAC to its present form.

Notes:

Chapter 2

INSTALLATION

The SPEDAC core programme is recorded on one low density 5 1/4 inch diskette. This includes only the spectrum reformatting programmes. The additional spectrum transfer programmes can be obtained either on a separate 5 1/4 inch, double sided, high density diskette, or together with the spectrum reformatting programme, on a high density diskette.

The diskette with the Version 5.0 SPEDAC programme looks like shown below.

IAEA / RIPC / PHYSICS SECTION

SPEDAC
VERSION 5.1 / 1989

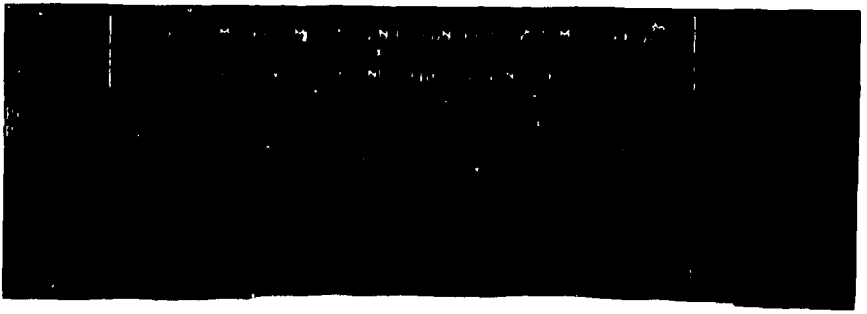
SPECTRUM REFORMATTING
SPECTRUM TRANSFER FROM MCAs

Although the SPEDAC programmes can be run from the floppy disk, it is advisable to copy SPEDAC to the hard disk, to speed up the operations.

Insert the diskette in Drive A:, select this drive as the active one, and type

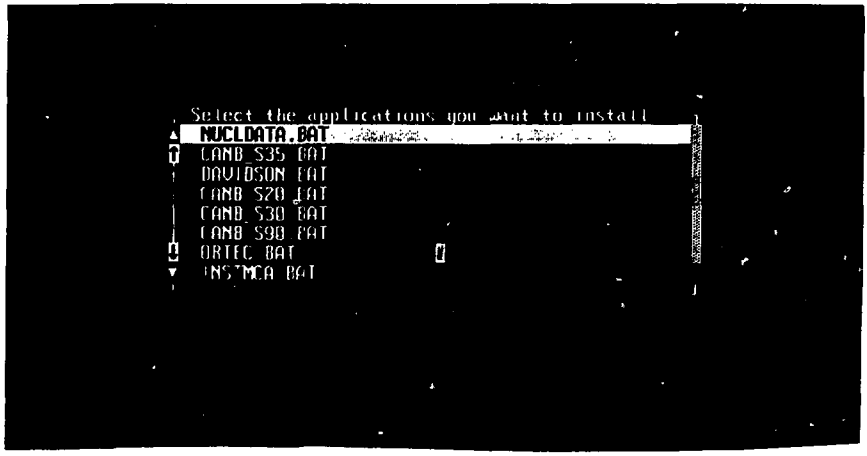
A: > INSTALL

The installation of the main programme will start immediately. The following display will be shown.



When the main SPEDAC programme has been installed, the programme will inform you that the next stage of installation can start, by the following display.

Press ENTER if you intend to install some of the spectrum transfer programmes. A selection scroll box will appear, as indicated below.



You can select as many transfer programmes as you wish. The selection is made by **ENTER**. An asterisk will appear in front of the selected programme. The selection is completed by **ESC**.

The transfer programmes will be installed one after another. An information frame will inform you which programme is to be copied to the hard disk; you have to confirm the selection by **ENTER**.

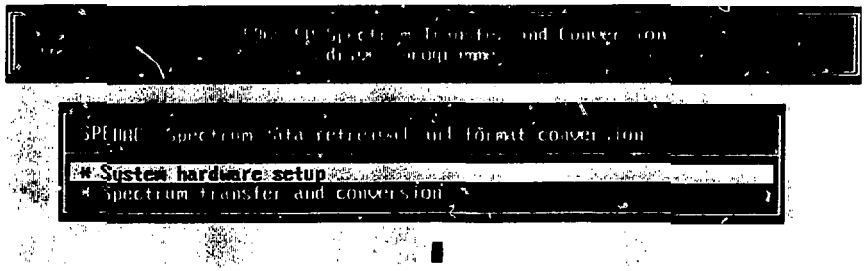
Chapter 3

HARDWARE SETUP

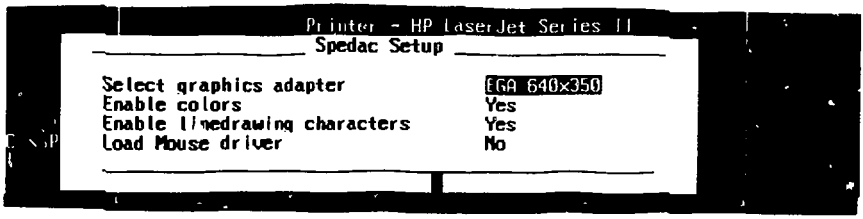
Assuming that you PATH includes the statement C:\SPEDAC\BIN, the programme can be started by typing

C:> SPEDAC

The first menu will appear as shown below.



The top line in the menu is used to set up the computer input and output features, according to the type of peripheral devices connected to the computer. Selecting this menu option, the following frame will be displayed.



The adjustments that can be made by entering the proper information, are described below.

SELECTION OF GRAPHIC ADAPTOR AND MONITOR

The first part of the hardware setup involves the selection of graphic adaptor and monitor. Two types of graphic cards are currently supported:

- CGA (640 x 200 (color adaptor with 640 pixels horizontally and 200 vertically), and
- EGA 640x350 (enhanced graphic adaptor with resolution of 640x350 pixels).

EGA is the default adaptor in GANAAS. In fact, the software will work also with VGA cards and monitors; it will, however, deliver only the EGA resolution.

Between the two options, the space bar acts as a toggle switch. The same applies for all the entries in this frame.

In the second line, you can enable or disable colors. If the colors are enabled in the EGA mode, both text and graphics will be in color. In CGA mode, only text will be in colors, graphics in black and white. The default position is with colors enabled.

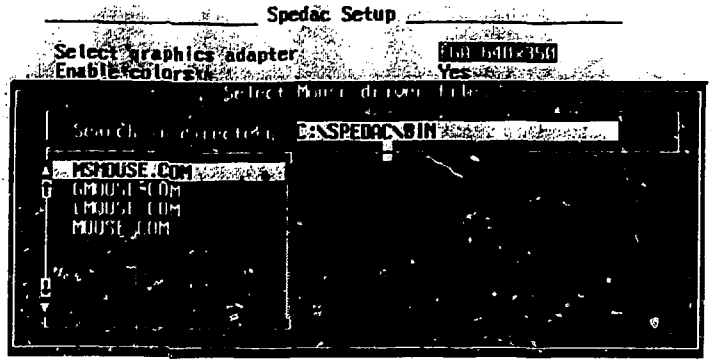
The next decision refers to line drawing characters. They are part of the IBM character set to draw lines around the text. Some (old) CGA cards do not support the extended character set. Most printers can be set to print these characters.. If strange characters appear on the screen, disable the line drawing characters. If the printer output contains strange characters, check the dip switches on the printer, or disable the line drawing characters.

MOUSE DRIVER

The GANAAS was developed in such a way that all the operations can be controlled by a mouse, in addition to the inputs from the keyboard.

It is probable that the mouse driver has been activated at the beginning of the computer session. In this case, the last line on the setup menu can be ignored; the mouse will operate properly anyway. On the other hand, if no mouse driver was activated before GANAAS was called, the suitable mouse driver can be selected from the setup menu. Placing the highlight bar on the *Load mouse driver* line, and pressing the space bar will change the **No** to **Yes**. The **ENTER** key will confirm your choice. The **ECS** will display a scroll box, (see illustration on top of Page 115).

First, it will display the default directory where the mouse drivers are expected to be stored. This can be changed to any other directory, in case that your particular mouse driver file is stored someplace else. After the correct directory name is displayed, press **ENTER**. The list of available files with mouse drivers will be shown. In case of the default directory (C:\SPEDAC\BIN), four files are available. Select the correct type of mouse with the highlight bar, and press **ENTER**. Or click on the line with the left mouse button, and then click again in the field outside the scroll box.



The meaning of the four files is a follows:

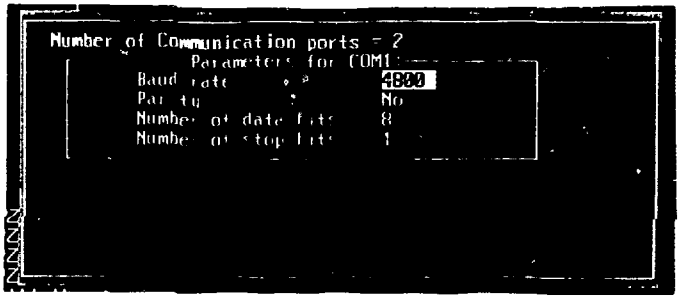
- MSMOUSE Microsoft serial mouse
- LMOUSE Logitech serial mouse
- GMOUSE Genius serial mouse
- MOUSE Bus mouse.

With these selection most of the available mice can be initiated, except for some rather exotic ones.

SELECTING COMMUNICATION PARAMETERS

The RS232 serial communication ports on the personal computer can be used to connect an external multichannel analyzer. Some parameters will have to be set properly: the baud rate, the parity, the number of data bits, and the number of stop bits. Obviously, a free serial communication port will have to be selected. *All these operations are made using the frame as shown below. With the up and* down arrow keys the individual entries are selected. The left and right arrow keys will change the value of the selected parameters.

After the correct values for the communication port number one (COM1) have been defined, it is possible (although probably very seldom needed) to set also the parameters for the second (COM2)serial port.



The spectrum transfer from an external, stand-alone multichannel analyzer will proceed correctly only if the communication parameters of the computer will be the same as those for the MCA output port. To set these parameters correctly, it is important to check, and possibly modify the settings in the MCA.

When all the parameters are set according to the required specifications (they depend on the type of the MCA and its output ports), press **ESC**. The newly defined data will be written to the SPEDAC.SET file.

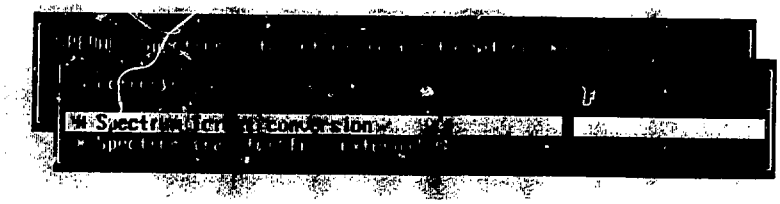
There is no need to run the hardware setup programme every time when GANAAS is started. The communication programme reads the data from the SPEDAC.SET file, and sets all the parameters accordingly. On the other hand, the hardware setup programme can be used any time when the need for some modification arises.

Chapter 4

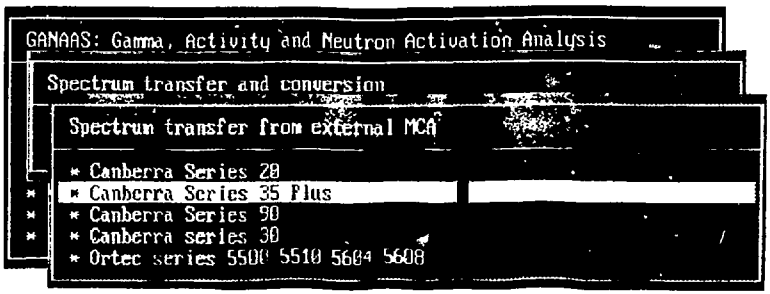
SPECTRUM TRANSFER

To perform spectrum analysis, the file with the spectrum, in a suitable format, should be available to the computer. It is rather usual that such spectrum files are stored on the hard disk. For stand-alone multichannel analyzers, the spectra have to be transfered to the computer. This is done using a serial interface port on the computer side, and the TTY or EIA connector port on theMCA side. In addition to a suitable cable, a computer programme must be available.

To initiate the spectrum transfer, select **Spectrum transfer and conversion* from the main SPEDAC menu. The submenu as shown below will appear.



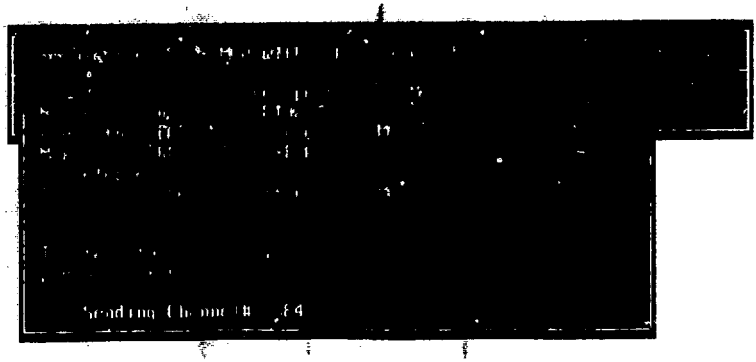
Select **Spectrum transfer from external MCA*, and a list of installed transfer programmes will be displayed, as shown below.



Chose the appropriate MCA by placing the lightbar on this line, and **ENTER**. Or use the mouse. In the example below, the Canberra Series 35 Plus is selected.

Note that some of the transfer programmes have been designed to work in both directions, i.e. the spectrum can be transferred from MCA to the computer, or from the computer to the MCA. Others work in one direction only, from MCA to the computer.

In the Series 35 Plus example,. select the option **Tranfer spectrum from MCA to disk*, and the next frame will be displayed.



The display informs you how to operated the keys on the multichannel analyzer and on the computer to start the transfer. The bottom line will inform you about the progress of spectrum transfer.

By setting the parameters on the MCA as advised in the frame, the transfer will be initiated. At the end of successful transfer, as appropriate message will be displayed, and the operator will be asked to name the spectrum to be saved on the hard disk, or in another storage media.

It should be noted that the transfer programmes, simultaneously with moving the spectral data from MCA to the computer, perform the reformatting, so that the spectrum stored in the file in the selected directory is in the GANAAS format.

The communication with other MCAs is performed in a similar manner.

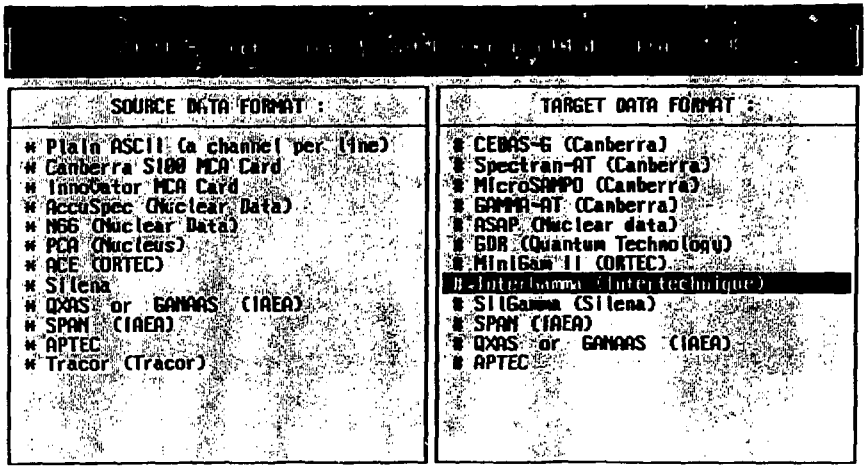
Chapter 5

SPECTRUM REFORMATTING

For operation of the spectrum conversion programme, select the **Spectrum format data conversion* form the *Spectrum transfer and conversion* menu.

The first frame of the programme will appear on the screen.

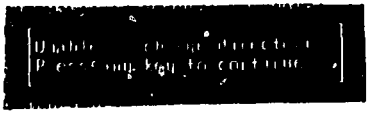
Let us look at the main display.



In the left column, the formats used by the MCAs are listed. The input spectrum file format can be selected by the lightbar; it is moved by the up and down arrow keys. The selection is confirmed by pressing **ENTEH.** An alternate way to select the input spectrum is with the mouse. Place the mouse cursor on the appropriate line and click the left button on the mouse.

The right windows on the display offers a number of spectrum analysis programmes. These are mostly commercial programmes of major manufacturers of nuclear equipment. It is usual that the manufacturers of MCA recommend the names of the directories where the spectrum files are stored. These name are taken as default by the SPEDAC. For example: if the spectrum file was created

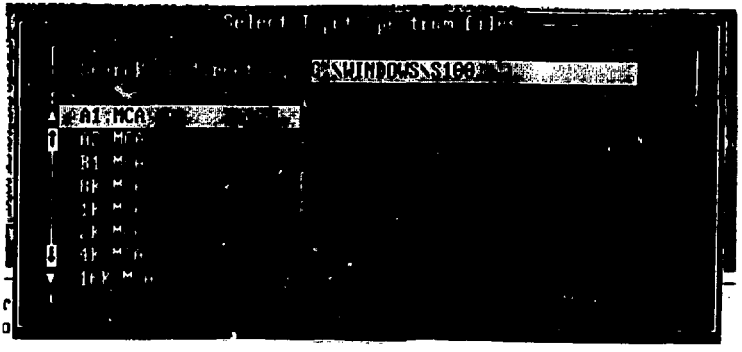
by the Canberra S100 card, it will be found in the directory C:\WINDOWS\S100. It can happen that this directory is not installed on your storage device, and your spectrum files are in a directory with a different name. In this case, the following message will appear on the screen.



Press any key. In the next frame you will have the opportunity to define the directory with the original spectrum files.

If the displayed name of the directory is satisfactory, press **ENTER**, or click with the mouse button at any point inside the small frame displaying the directory name. If not satisfied with the offered default directory, change it to the correct name.

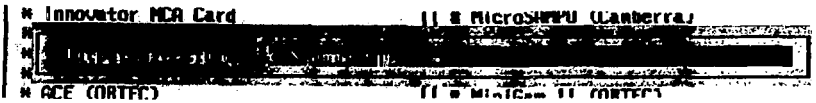
The display that appears now is a scrolling box containing all the spectrum files with the correct extension. For the example of the S100 card, the normal extension for the spectrum file is .MCA. All *.MCA files are shown.



The spectra are selected by placing the lightbar (either with arrow keys or with mouse) on the corresponding entry and pressing **ENTER**, or by the left mouse button. Any number of files can be selected. The chosen files are marked with an asterisk. The list of the available files can be longer than the size of the window. The remaining files can be made visible by scrolling. This is done by up or down arrow keys, or by mouse. Placing the mouse cursor on the arrow on the left side of the window will scroll up or down.

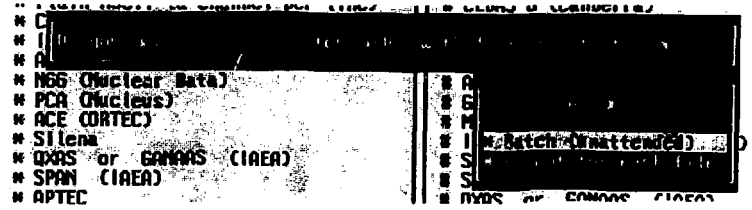
When all the files have been selected, press **ESC**.

A superimposed window will appear as shown below, and will ask you for the name of the directory where the reformatted files should be stored. The default directory is C:\GANAAS\SPECT. You can replace it by typing the name of another director where the new files should be stored. Press **ENTER,** or click the left mouse button, with the cursor inside the small window.



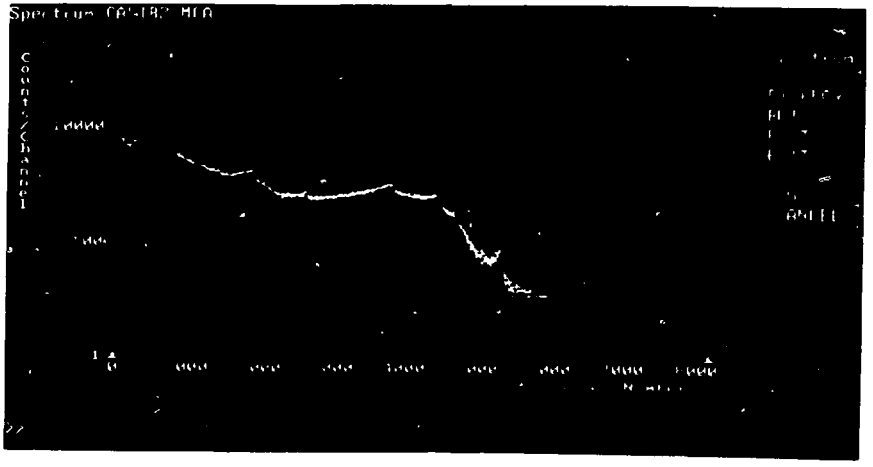
The next windows to be displayed depends on the number of selected files. If only one file was chosen, the window looks almost the same as the one before. However, here you have now the opportunity to specify the name of the reformatted output file. The default name is offered: it is identical with the name of the input file but has the extension, characteristic to the selected analysis programme input files.

If more than one file have been selected, the following display will appear.



The files can be reformatted in an automatic, unattended batch mode. In this case, all the new files will have the names of the original files but with the new extension. If you are more careful, you will select the second option: each spectrum, before being reformatted, will be displayed, and you can specify how it will be reshaped.

By selecting the second option, the graph of the spectrum will appear on the screen as shown below.



There are a number of operations that can be made using the facilities included in this spectrum handling tool. They are described later. For now, let us assume that the whole spectrum, exactly as it is seen, should be reformatted. Select **EXIT** in the right hand box, either by clicking on it by mouse, or by typing **E** or **EX** or **EXI** or **EXIT** (this is a general rule: the first letter will be sufficient if it uniquely defines the function; if two lines start with the same letter, the second letter must be added when making the selection). Press **ENTER**.

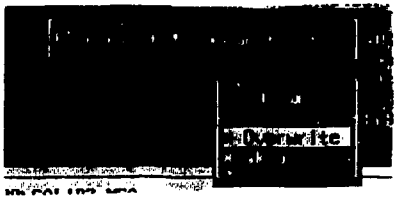
In the next frame (see bottom of Page 122) the opportunity is given to define the size of the reformatted spectrum. If the original input spectrum had 8192 channels, there are a number of choices that can be made. The selection is made with the highlight bar or with the mouse, followed by **ENTER**.

In the case that the number of channels in the original spectrum should be reduced, SPEDAC will give you the options to either compress the spectrum, or cut it at the specified channel number. Two decisions are required:

- The starting channel can be set in the windows as displayed below. The default value is 00001; it can be changed as desired.

- The following frame will offer the option to compress or cut the spectrum. Selection is made in the usual way.If the spectrum is to be compressed, the contents of two (or more) channnels will be added.

It might happen that the file with the name as selected in the preceding procedure, already exists in the defined directory. In such a case, SPEDAC will call your attention by displaying the following window.



Select ***Overwrite** option, the existing file will be erased and replaced with the new one. Selecting ***Skip** implies that no reformatting will be made, and the programme will return to the starting point, or to the processing of another file.

If operating in a batch mode, the other files will be displayed for your inspection, and will be reformatted.

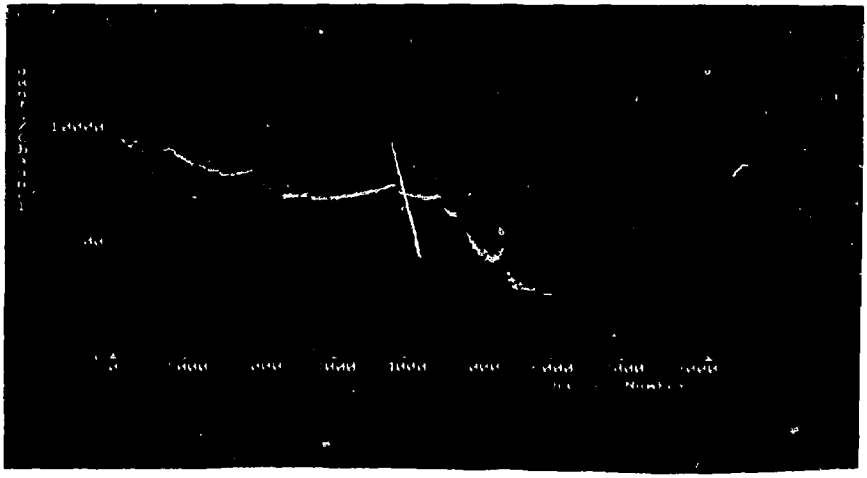
Notes:

Chapter 6

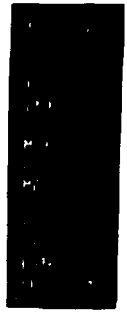
MANIPULATING SPECTRUM DISPLAY WITH SPEDAC

The graphic option of SPEDAC permits the operator to display the spectrum, and to manipulate it to a certain extent. The available functions are described below.

When a spectrum stored in a file and in a specific directory is called (see descriptions above), SPEDAC will switch to the graphics mode. The selected spectrum will be displayed, together with its name on the top, and a command box on the right, as shown in the figure below. The bottom line is reserved for commands.



The instructions for operation can be given by typing the command, as seen in the command box. It is not necessary to type the complete command; the first leter will be sufficient, if the command is defined unambiguously. Occasionally, you will have to type two or three letters. A more elegant and faster method is to use the mouse. Just place the mouse cursot to the desired command, and push the left mouse button.



DISPLAY

The first line on the command menu is selected by typing the letter **D**. The selected command appears on the bottom line, and pressing **ENTER** will implement it. The operation with the mouse is even faster.

Selecting the **DISPLAY** command will change the command box as shown on theleft. A number of options are given.

BEG and **END** commands can select a Region of Interest (ROI). They can be used by typing to the bottom line BEG=1800 END=4400 if you wish to display by the ROI between from 1800 to 4400 channels. The result will be as shown below.

The **MIN** and **MAX** function do to the vertical scale what ROI does to the horizontal. This can be useful if you wish to observe some of the peaks in greater detail Specifying Min=500 MAX=6000 will give you a good idea about a small peak in the middle of the spectrum.

The command **ROI** displays the selected region of interest. SPECTR displays the full, original spectrum.

Selecting **LIN** or **LOG** permits you to observe the spectra in linear or logarithmic scale

ROI

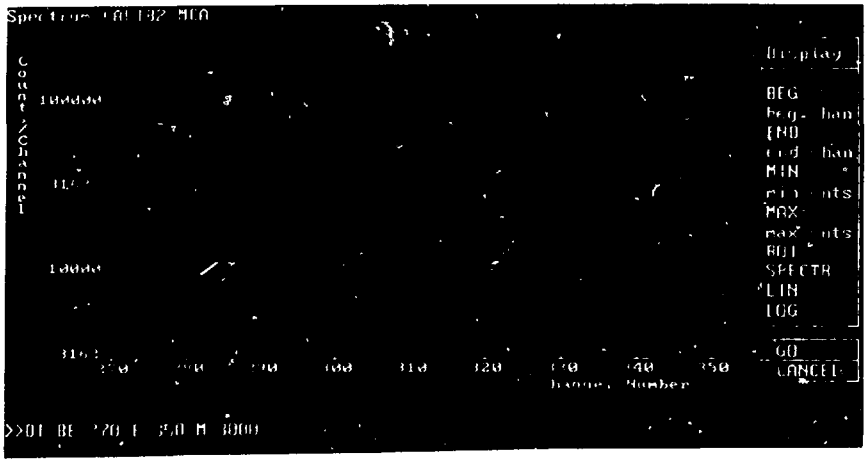
Selecting this instruction will display a new command box, as shown on the left. Here, you have the opportunity to set a region of interest in three different ways:

- Typing **BEG=** and **END=** instructions to the bottom line.
- Moving the vertical cursor line with the arrow keys. A particularly useful function is performed with the up and down arrow keys. Pressing the up arrow key will instruct the cursor to jump to the next peak at a higher energy. With the down arrow, it will jump to the next lower energy peak. Once in the desired position, the beginning and the end of the ROI can be set with the **F1** and **F2** keys.
- Using the mouse. Place the mouse cursor to the channel which will define the beginning of ROI. Press left button. Select **F1**, either by pressing the corresponing key, or by clicking this function in the command box. The same with the **F2** for the end of ROI. Clicking on GO will implement your selection.

The spectrum display with ROI indicated (white vertical lines), and with cursor line (black) is shown on the previous page.

The results of the **ROI** setting procedure can be seen if you implement the ROI command in the **DISPLAY** box.

As an example, a spectrum is shownabove: the **ROI** has been set to include one peak only, and the **MIN** and **MAX** were selected to include only the informative part of the spectrum.



PLOT. This command is used to plot the spectrum with a printer. In the present version, only matrix printers are supported.

EXIT returns to the previous menu of SPEDAC.

Notes:

Annex 1

DEFAULT DIRECTORIES AND FILE EXTENSIONS

Multichannel analyzer	Default directory	File extension
Canberra stand alone analyzers	any	*.MCA
Innovator add-on card	\INNOVAT	*.ASC
Canberra/Nuclear Data stand alone MCA	\ND66	*.DAT
Canberra\Nuclear Data add-on cards	\ND	*.DAT
NUCLEUS add-on cards	\NUCLEUS	*.SPM
ORTEC, all MCA and cards	\ORTEC	*.CHN
SILENA, all MCA and card	\SILGAMMA	*.DAT
APTEC add-on cards	\APTEC	*.S0
TRACOR add-on card	\TRACOR	SPECTRUM.*

Spectrum analysis programmes	Default directory	File extension
Canberra :CEBASG	\CEBASG	*.SPC
Canberra: SPECTRAN	\SPECTRAN	*.MCA
Canberra: SAMPO	\SAMPO	*.MAC
Canberra: GAMMA-AT	\GAMMA-AT	*.SCA
Canberra/Nuclear Data: ASAP	\ASAP	*.DAT
Nucleus: GDR	\GRD	*.SPM
ORTEC: MINIGAM	\USER	*.CHN
INTERTECHNIQUE	\GAMMA.SPE	*.SPE
SILENA: SILGAMMA	\SILGAMMA	*.DAT
IAEA: SPAN	\SPAN\DATA	*.SPN
IAEA: QXAS	\AXIL\SPECT	*.SPE
IAEA: GANAAS	GANAAS\SPECT	*.SPE

Notes:

INTERNATIONAL
ATOMIC ENERGY AGENCY
VIENNA, 1991