



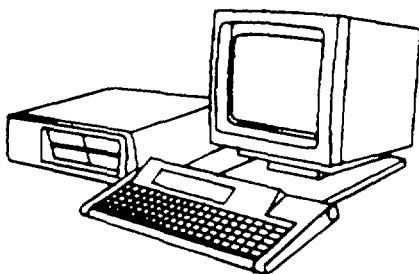
XA0102510

No.10

# **SPEDAC Pro for DOS**

## **Format Conversion of Spectral Data from Nuclear Experiments**

*User's Manual*



**32 / 37**



International Atomic Energy Agency, 1996

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# **SPEDAC Pro for DOS**

## **Format Conversion of Spectral Data from Nuclear Experiments**

### *User's Manual*

The originating Section of this publication in the IAEA was:

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FORMAT CONVERSION OF SPECTRAL DATA FROM NUCLEAR EXPERIMENTS  
USER'S MANUAL  
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## FOREWORD

During the period 1987-1996, the IAEA has been developing a software library for nuclear analysis with several software packages. The initial versions were tested in different laboratories, mainly in developing countries. On the basis of the comments and recommendations received, numerous improvements were made.

The following software packages are currently available:

- 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)
- Mössbauer spectrum analysis program (MOSA).

The complete operation manuals for all available software packages will be completed by the end of 1997.

The present publication covers the programs for transfer of spectrum from a stand-alone multichannel analyser 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 their being copied and distributed, except for commercial purposes. The source codes of all programs are available on request.

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**1****OVERVIEW**

SPEDAC Pro for DOS is a software package that allows you to convert spectral data from nuclear experiments (e.g. X ray,  $\gamma$  ray and Mössbauer spectroscopy) from one format to another. It runs on IBM compatible PCs under DOS 3.1 or higher. SPEDAC Pro has been developed under the auspices of the IAEA, Physics Section.

Spectral data acquired with multichannel analyser (MCA) cards are stored as files on disk for further processing. Every manufacturer of MCA cards uses his own format for storing the spectral data. The format used by a manufacturer often also evolves with time. On the other hand, spectrum processing software (e.g. peak fitting, nuclide identification, quantitative procedures) requires that the spectral data be in a particular format. Although some software packages can read different formats, there is generally no compatibility between the spectrum acquisition software and the spectrum evaluation software of different manufacturers.

Over the past years, the IAEA has supported the development of powerful software packages for X ray and  $\gamma$  ray spectroscopy (QXAS and GANAAS). This software uses a very flexible spectral data format known as IAEA\_SPE format (See Appendix I). The SPEDAC program uses this format as the basis for any conversion.

Tables 1 and 2 list the source and target formats that are supported by the current version. As this software package is modular in nature, other conversion modules can be added in the future without changing the basic structure of the SPEDAC software.



Although the software has been tested thoroughly, the conversion is not guaranteed to work in all cases. The various spectral data files contain, in addition to the channel content itself, additional information which cannot always be exchanged when converting from one format to another. Converting from NUCLEUS PCA to IAEA GANAAS format will produce a valid GANAAS spectral data file. Converting this file later back to NUCLEUS PCA (or another format) might result in the loss of some information, e.g. the regions of interest defined in the NUCLEUS file are lost.





If you experience any problems using SPEDAC Pro or if you have any comments, use the SOFTWARE REPLY form given in Appendix V, following the instructions given there.

**2****HISTORY**

An earlier version of SPEDAC was documented in the IAEA's publication "Computer Manual Series No. 2" in 1991. This version allowed the conversion of 8 source data formats to 10 target data formats and provided some facilities to transfer spectral data from stand-alone multichannel analyzers to PCs over serial lines.

Since then, the number of conversions between different spectral file formats has grown to such an extent that a new concept for the program was required. During a workshop in 1993, the foundations for this new concept were laid and the development started. This manual documents version 1.1 of the program called "SPEDAC Pro for DOS". SPEDAC Pro no longer deals with transfer of spectral data over serial lines, but concentrates exclusively on the conversion of spectral formats.

**3****INSTALLATION**

---

**3.1 Hardware requirements**

The software is designed to work with a minimum hardware configuration. In order to install SPEDAC PRO for DOS you need an IBM compatible PC running DOS 3.1 or higher.

The minimum configuration should contain:

- a 8086 processor
- 512 kbyte Random Access Memory
- B&W text only screen
- Hard disk with at least 1 Mbyte of free space
- a 1.2 Mbyte 5.5" floppy drive or a 1.4 Mbyte 3.25" floppy drive

With this minimum configuration, you will not be able to see the spectrum on the display; however, the spectrum conversion will proceed normally. The program supports CGA, EGA, VGA and SVGA graphics cards. It will automatically recognize this hardware and use it to display the spectrum during the conversion process.

---

**3.2 Installation procedure**

Make sure you have at least 1 Mbyte of free space on the disk to which you want to install the software.

Here, we assume you are installing the software from drive A: onto drive C:. If you are using different drives, substitute the drive letters (e.g. from A: to B:) in the commands below. The text to be entered is in bold, ↵ means that you have to press the "Enter" key.

Put the distribution diskette labeled:



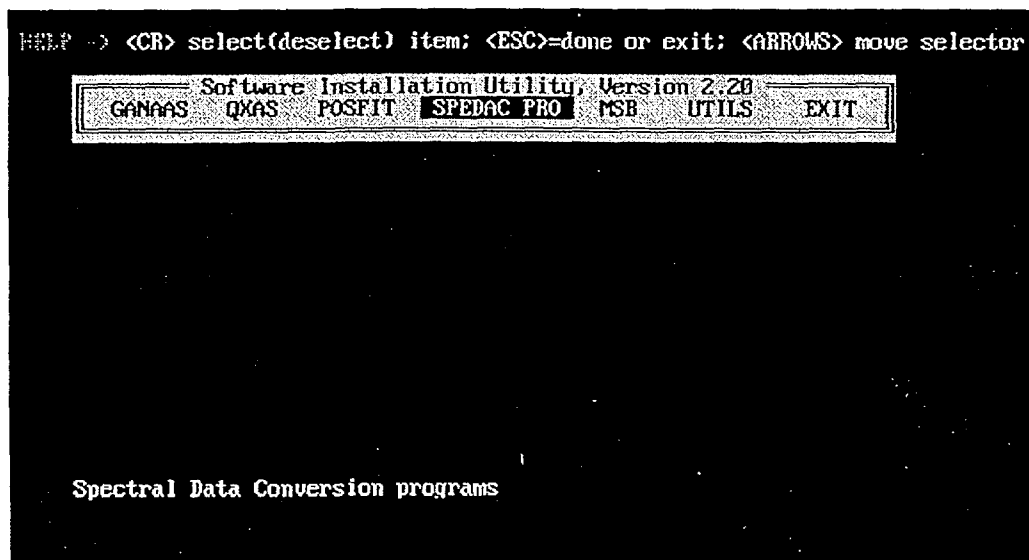
into drive A: and from the DOS prompt (C:\>) type:

```
C:\>A:↵
```

and type:

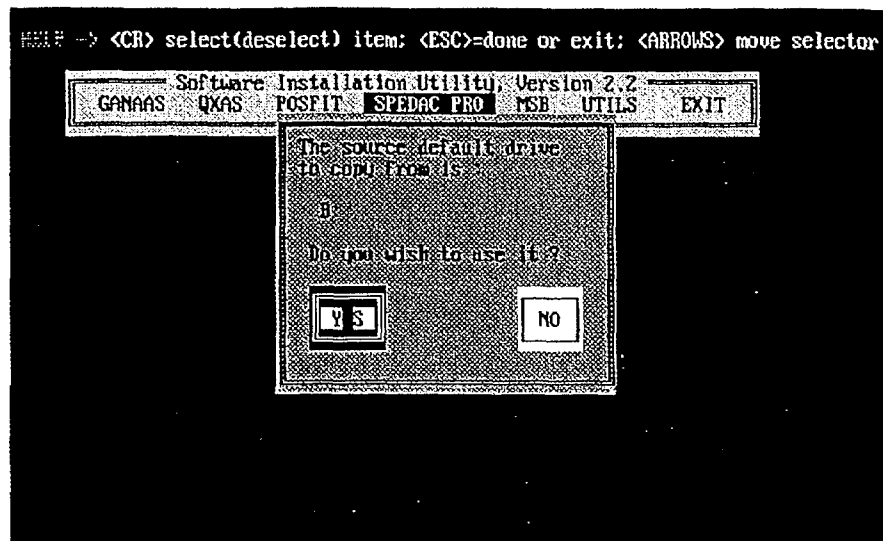
```
A:\>INSTALL.↵
```

After starting the installation program, the screen shown below will appear.

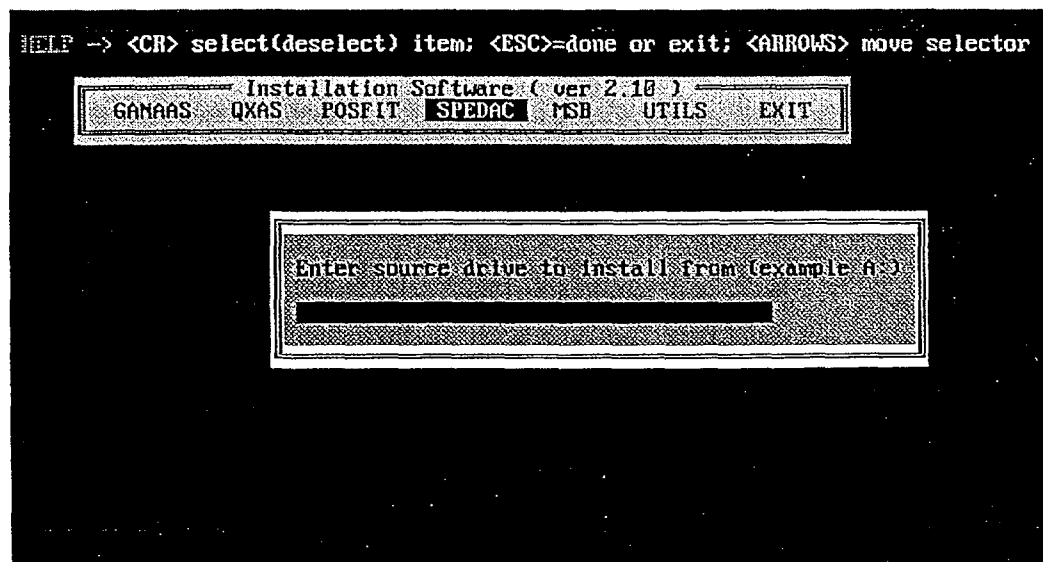


Use the left arrow <←> or right arrow <→> key to highlight SPEDAC PRO and hit the Enter key <↵>. If a mouse is installed, it can be used as the selector as well.

The next dialog selects the source drive for the installation (the drive that contains the installation floppy). By default this is the active drive.

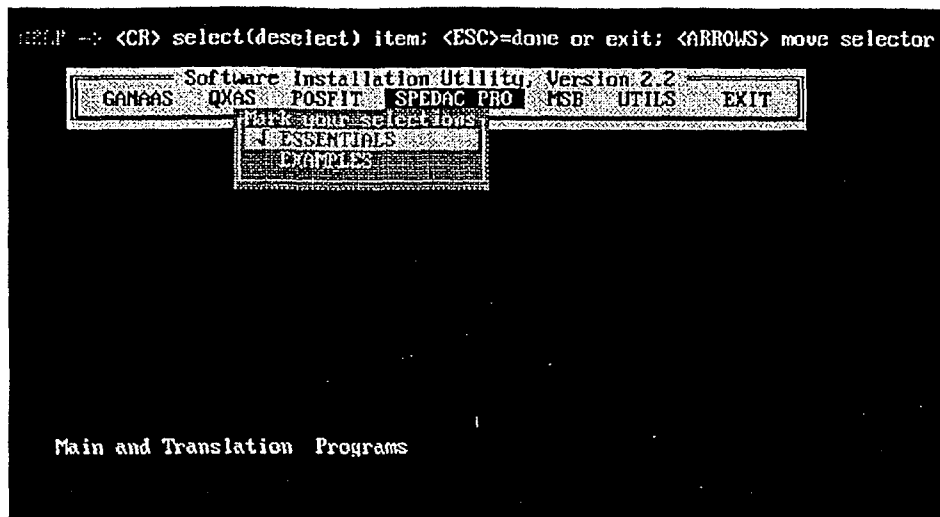


Hit the Enter key <↵> if you want to use this drive. Otherwise select NO and hit the Enter key. Fill in the drive you want to use in the dialog box as shown below.



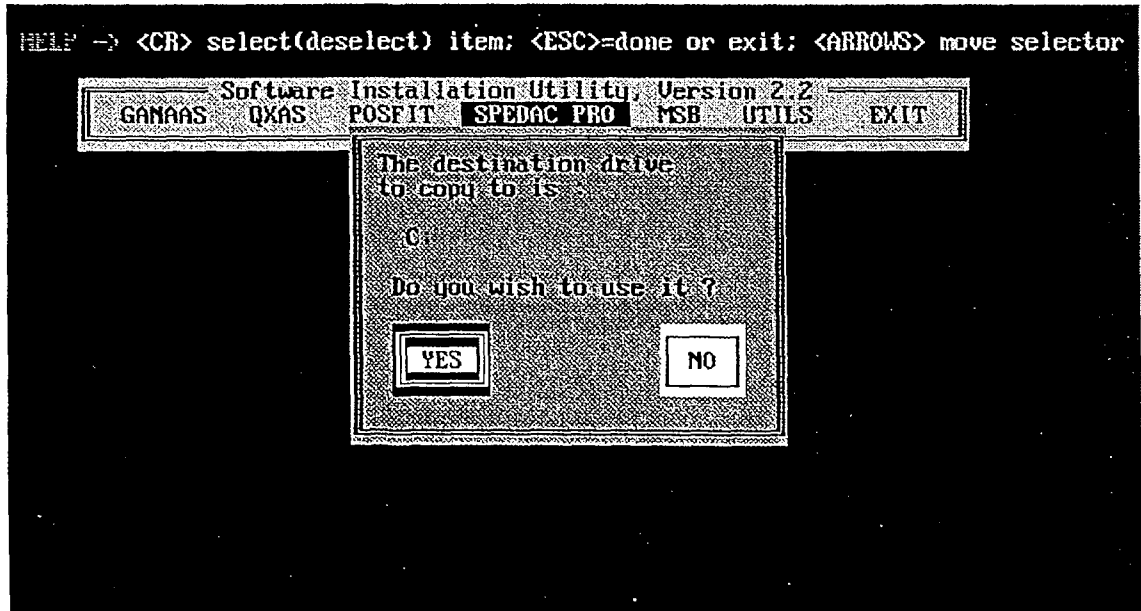
Enter a drive letter (A, B,...) followed by a colon ":". To correct typing errors, use the backspace key.

The installation procedure is common for all software packages and allows the installation of "essential" and "optional" parts of the different software packages. In the case of SPEDAC Pro, two modules are presented: ESSENTIALS and EXAMPLES. ESSENTIALS contain the main and conversion programs; EXAMPLES are spectral data files in different formats that you can use for testing. The ESSENTIALS are selected by default as shown with the check mark (✓).

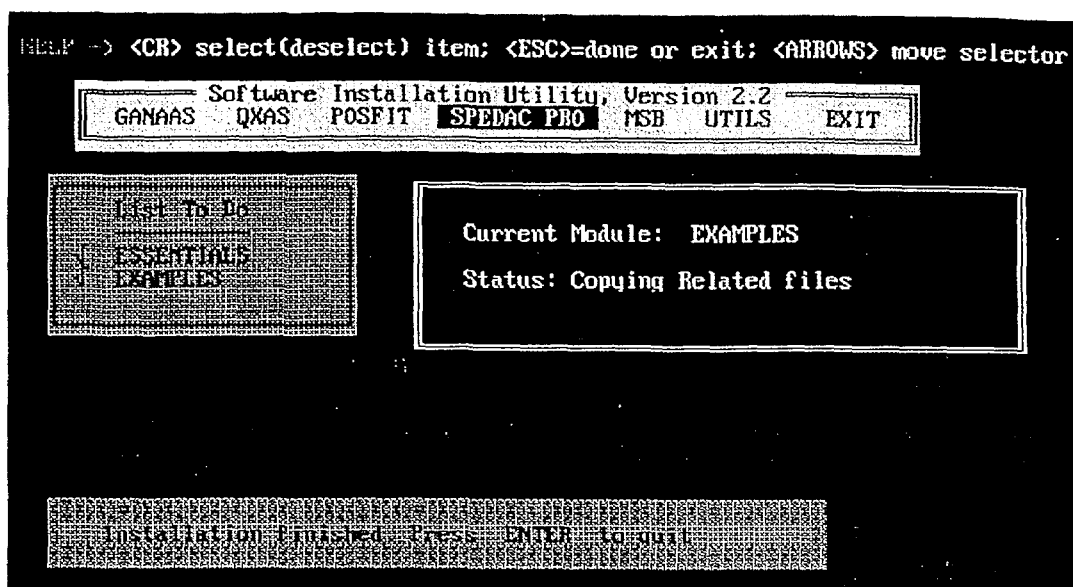


To select also the examples for installation, highlight EXAMPLES and press the Enter key. Once selections have been made, press the <Esc> key.

The next dialog box considers the destination drive for the installation (the drive on which you want to install the software). It works exactly the same as described for the source drive.



The installation program checks for the required disk space on the selected target drive. After this, the installation procedure will start, and the files related to SPEDAC Pro will be copied to the selected drive.



Hit the Enter key <J> to terminate the installation program.

The installation procedure creates a directory \P\_SPEDAC\BIN on the hard disk and puts all the files that make up the SPEDAC Pro software package in this directory. See Appendix II for a description of these files. The example spectrum files are copied to the sub-directory \P\_SPEDAC\SPECT. The files on the distribution diskette are compressed (\*.ZIP files).

The option UTILS on the main menu of the installation program contains a standard ASCII editor. You might use this editor to change any variable (e.g. PATH variable) or parameter in your "autoexec.bat" or "config.sys" files. For the editor's commands, use on-line help by typing **ALT-H** combination keys while you are editing a file.

**4****STARTING SPEDAC  
Pro**

---

**4.1 Quick start**

You can start SPEDAC Pro immediately after installation. Make sure that the current directory is set to \P\_SPEDAC\BIN. You can do this by typing the following DOS command (Change Directory):

```
C:\>CD \P_SPEDAC\BIN.␣
```

Next you enter the name of the program to start it:

```
C:\>P_SPEDAC\BIN>P_SPEDAC.␣
```

Another way to start the program while you are in a different directory is to enter the full path name of the program, e.g.:

```
C:\MYDIR>\P_SPEDAC\BIN\P_SPEDAC.␣
```

---

**4.2 Setting the path**

It is most efficient to include the directory \P\_SPEDAC\BIN in the DOS PATH. To see the current path setting, type the following DOS command:

```
C:\>PATH.␣
```

The path will be displayed on the screen, e.g.

```
C:\>PATH=C:\;C:\DOS;C:\MYPROG
```

To include the directory of SPEDAC in the path, enter the path that was displayed on your screen and add ";C:\P\_SPEDAC\BIN", e.g.

```
C:\>PATH=C:\;C:\DOS;C:\MYPROG;C:\P_SPEDAC\BIN.␣
```



This change of the path will however only remain effective until you switch off your computer (or until you change the path again).

To set the path permanently, change the path as explained above in the AUTOEXEC.BAT file using a text editor (e.g. EDIT of MS DOS).

---

### 4.3 Disk space requirements while running

Make sure that during the execution of the program there is always at least 500 Kbyte of free disk space. SPEDAC uses disk space to store temporary files and also needs disk space to save the converted spectral data.

---

### 4.4 Memory requirements while running

To run the program, you need about 300 Kbytes of free RAM (Random Access Memory; see your DOS Manual). The amount depends on the conversion module that is loaded and the spectrum size. If not enough memory is available you will receive an error message of the type:

"Cannot start <program name>"

where <program name> is the name of any of the conversion programs. Check how much DOS memory (RAM) is available using the DOS program MEM (DOS version 5.0 or higher). If less than 300 Kbytes is available, try to free memory by unloading memory resident programs or by moving parts of DOS to high memory area (UMB, see your DOS Manual).

## 5

## USING SPEDAC Pro

In this section the use of the program is explained. We first give an overview of the program flow. Next, each step is discussed in detail.

---

### 5.1 Program flow

The program converts spectral data from a source format to a target format. The functioning of SPEDAC Pro is shown in Fig. 1. The following logical sequences are executed:

1. Select format of spectrum to be converted from (source).
2. Select format of spectrum to convert to (target).
3. Select directory and filenames of all source spectra.
4. Select directory for target spectra.  
For each selected source file:
  - 4.1. Read the spectrum in the source format.
  - 4.2. Display the spectrum (for visual inspection).
  - 4.3. Save the spectrum in the target format.
5. Stop

---

### 5.2 Detailed discussion of each step

After starting the program (by typing P\_SPEDAC at the DOS command prompt, as explained in Section 4), a full screen will be displayed.

```

===== INFO - SPEDAC PRO Version 1.01 - DEC 1993 =====
SOURCE format: 1

Select format of spectrum to be converted from (source):
1. APTEC
2. APTEC Version 4.5
3. ASCII
4. ASCII (with 1000 points)
5. ASCII (with 10000 points)
6. ASCII (with 100000 points)
7. ASCII (with 1000000 points)
8. ASCII (with 10000000 points)
9. ASCII (with 100000000 points)
10. ASCII (with 1000000000 points)
11. ASCII (with 10000000000 points)
12. ASCII (with 100000000000 points)
13. ASCII (with 1000000000000 points)
14. ASCII (with 10000000000000 points)
15. ASCII (with 100000000000000 points)
16. ASCII (with 1000000000000000 points)
17. ASCII (with 10000000000000000 points)
18. ASCII (with 100000000000000000 points)
19. ASCII (with 1000000000000000000 points)
20. ASCII (with 10000000000000000000 points)
21. ASCII (with 100000000000000000000 points)
22. ASCII (with 1000000000000000000000 points)
23. ASCII (with 10000000000000000000000 points)
24. ASCII (with 100000000000000000000000 points)
25. ASCII (with 1000000000000000000000000 points)
26. ASCII (with 10000000000000000000000000 points)
27. ASCII (with 100000000000000000000000000 points)
28. ASCII (with 1000000000000000000000000000 points)
29. ASCII (with 10000000000000000000000000000 points)
30. ASCII (with 100000000000000000000000000000 points)
31. ASCII (with 1000000000000000000000000000000 points)
32. ASCII (with 10000000000000000000000000000000 points)
33. ASCII (with 100000000000000000000000000000000 points)
34. ASCII (with 1000000000000000000000000000000000 points)
35. ASCII (with 10000000000000000000000000000000000 points)
36. ASCII (with 100000000000000000000000000000000000 points)
37. ASCII (with 1000000000000000000000000000000000000 points)
38. ASCII (with 10000000000000000000000000000000000000 points)
39. ASCII (with 100000000000000000000000000000000000000 points)
40. ASCII (with 1000000000000000000000000000000000000000 points)
41. ASCII (with 10000000000000000000000000000000000000000 points)
42. ASCII (with 100000000000000000000000000000000000000000 points)
43. ASCII (with 1000000000000000000000000000000000000000000 points)
44. ASCII (with 10000000000000000000000000000000000000000000 points)
45. ASCII (with 100000000000000000000000000000000000000000000 points)
46. ASCII (with 1000000000000000000000000000000000000000000000 points)
47. ASCII (with 10000000000000000000000000000000000000000000000 points)
48. ASCII (with 100000000000000000000000000000000000000000000000 points)
49. ASCII (with 1000000000000000000000000000000000000000000000000 points)
50. ASCII (with 10000000000000000000000000000000000000000000000000 points)
51. ASCII (with 100000000000000000000000000000000000000000000000000 points)
52. ASCII (with 1000000000000000000000000000000000000000000000000000 points)
53. ASCII (with 10000000000000000000000000000000000000000000000000000 points)
54. ASCII (with 100000000000000000000000000000000000000000000000000000 points)
55. ASCII (with 1000000000000000000000000000000000000000000000000000000 points)
56. ASCII (with 10000000000000000000000000000000000000000000000000000000 points)
57. ASCII (with 100000000000000000000000000000000000000000000000000000000 points)
58. ASCII (with 1000000000000000000000000000000000000000000000000000000000 points)
59. ASCII (with 10000000000000000000000000000000000000000000000000000000000 points)
60. ASCII (with 100000000000000000000000000000000000000000000000000000000000 points)
61. ASCII (with 1000000000000000000000000000000000000000000000000000000000000 points)
62. ASCII (with 10000000000000000000000000000000000000000000000000000000000000 points)
63. ASCII (with 100000000000000000000000000000000000000000000000000000000000000 points)
64. ASCII (with 1000000000000000000000000000000000000000000000000000000000000000 points)
65. ASCII (with 10000000000000000000000000000000000000000000000000000000000000000 points)
66. ASCII (with 100000000000000000000000000000000000000000000000000000000000000000 points)
67. ASCII (with 1000000000000000000000000000000000000000000000000000000000000000000 points)
68. ASCII (with 10000000000000000000000000000000000000000000000000000000000000000000 points)
69. ASCII (with 100000000000000000000000000000000000000000000000000000000000000000000 points)
70. ASCII (with 1000000000000000000000000000000000000000000000000000000000000000000000 points)
71. ASCII (with 10000000000000000000000000000000000000000000000000000000000000000000000 points)
72. ASCII (with 100000000000000000000000000000000000000000000000000000000000000000000000 points)
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74. ASCII (with 10000000000000000000000000000000000000000000000000000000000000000000000000 points)
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77. ASCII (with 10000000000000000000000000000000000000000000000000000000000000000000000000000 points)
78. ASCII (with 100000000000000000000000000000000000000000000000000000000000000000000000000000 points)
79. ASCII (with 1000000000000000000000000000000000000000000000000000000000000000000000000000000 points)
80. ASCII (with 10000000000000000000000000000000000000000000000000000000000000000000000000000000 points)
81. ASCII (with 100000000000000000000000000000000000000000000000000000000000000000000000000000000 points)
82. ASCII (with 1000000000000000000000000000000000000000000000000000000000000000000000000000000000 points)
83. ASCII (with 10000000000000000000000000000000000000000000000000000000000000000000000000000000000 points)
84. ASCII (with 100000000000000000000000000000000000000000000000000000000000000000000000000000000000 points)
85. ASCII (with 1000000000000000000000000000000000000000000000000000000000000000000000000000000000000 points)
86. ASCII (with 10000000000000000000000000000000000000000000000000000000000000000000000000000000000000 points)
87. ASCII (with 100000000000000000000000000000000000000000000000000000000000000000000000000000000000000 points)
88. ASCII (with 1000000000000000000000000000000000000000000000000000000000000000000000000000000000000000 points)
89. ASCII (with 10000000000000000000000000000000000000000000000000000000000000000000000000000000000000000 points)
90. ASCII (with 100000000000000000000000000000000000000000000000000000000000000000000000000000000000000000 points)
91. ASCII (with 1000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000 points)
92. ASCII (with 10000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000 points)
93. ASCII (with 100000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000 points)
94. ASCII (with 1000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000 points)
95. ASCII (with 10000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000 points)
96. ASCII (with 100000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000 points)
97. ASCII (with 1000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000 points)
98. ASCII (with 10000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000 points)
99. ASCII (with 100000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000 points)
100. ASCII (with 1000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000 points)

Current dir: C:\
Using table: C:\SPEDAC\BIN\SPEDAC.TAB

```

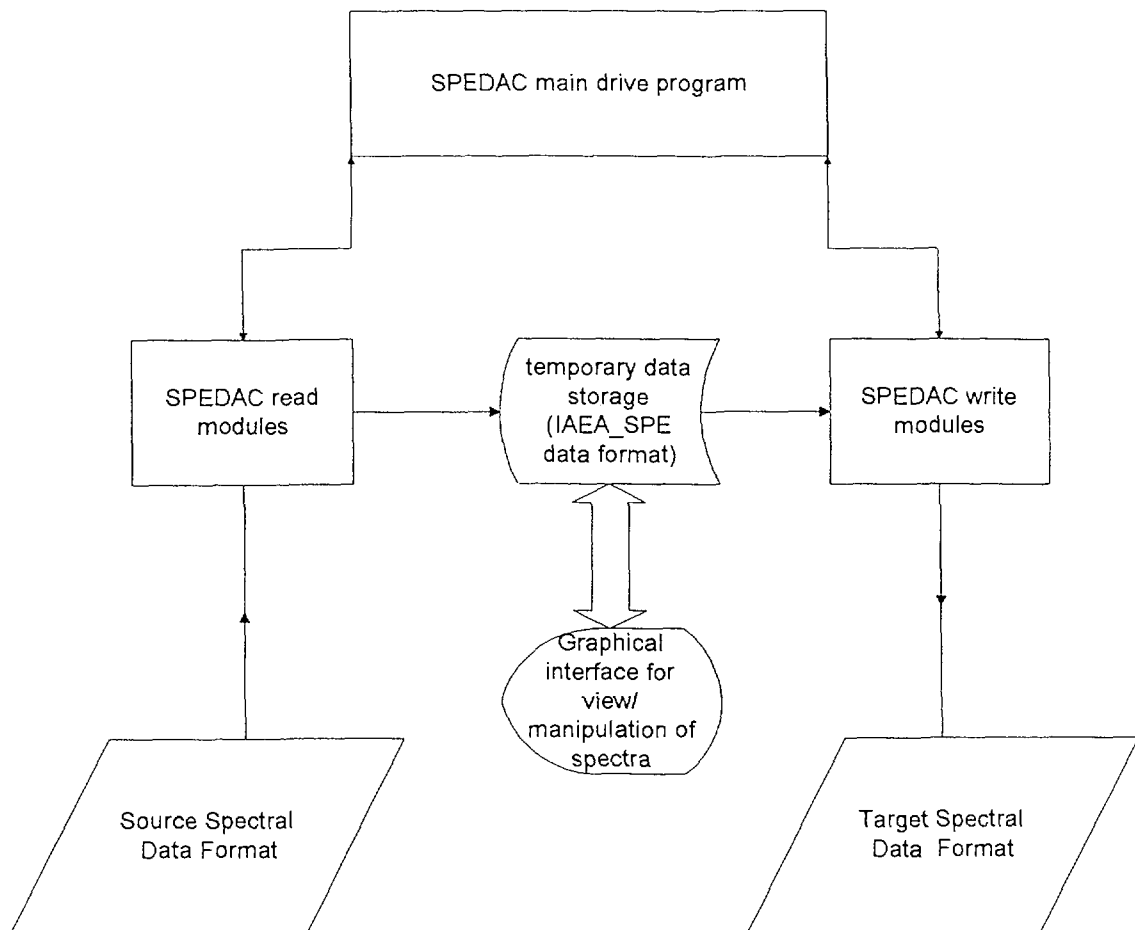


FIG. 1: Spedac Pro Operational Flowchart.

The first line contains the program identification, version number and production date:

```
== IAEA - SPEDAC PRO Version 1.01 - Dec 1993 ==
```

Below the scroll box (bottom of the screen) two lines are visible. The first indicates the current directory, e.g.

```
Current dir: C:\
```

This is the directory that was current when you started the program. The second line indicates which table SPEDAC is using for the conversions (see later). This should normally read:

```
Using table: C:\P_SPEDAC\BIN\SPEDAC.TAB
```

The scroll box itself, labeled "Select format of source data" contains all the possible sources you can select to convert from, in alphabetic order. Use the up arrow <↑> or down arrow <↓> to highlight the desired source, e.g. "APTEC Version 4.3". Once the right choice is made, press the Enter key <J>. (If you press the <Esc> key, no selection is made and the program terminates). The selected source format is indicated below the line SOURCE.

A scroll box to select the target of your conversion is displayed. The label of this scroll box is "Select format of target data". In the same way as for the source, highlight the desired target format and press <J>. (If you press <Esc> the program will terminate.) As an example, we will select "IAEA Ganaas" as the target format, as shown on the next screen picture.

```

== IAEA - SPEDAC PRO Version 1.01 - DEC 1993 ==
SOURCE format:                                TARGET format:
APTEC Version 4.3
Select format of source data:                 Select format of target data:
APTEC                                         APTEC
APTEC Version 4.3                             APTEC Version 4.3
ASCII                                         ASCII
CANBERRA S100 PCA Card                       CANBERRA Cebas-C
IAEA GANAAS                                  CANBERRA Spectra-RT
IAEA Spain                                   CANBERRA MicroSAMCO
IAEA OXAS                                     CANBERRA Gamma-RT
NUCECARE DRUM Record                         IAEA Ganaas
NUCLEONIS PCA                                 IAEA Spain
ORTEC PC4                                     IAEA Oxas
Current dir: C:\
Using table: C:\P_SPEDAC\BIN\SPEDAC.TAB
Prompt: Move  Ctrl= Select  Alt= InSelect  Esc= Done

```

The bottom line of the screen (in reverse colors) always indicates what you can do at a certain moment while input is active.

The program now allows you to select one or more (up to 10) source files. It displays a frame labeled "Select SOURCE files".

```

== IAEA - SPEDAC PRO Version 1.01 - DEC 1993 ==
SOURCE format:          TARGET format:
APTEC Version 4.3      IAEA Ganaas

Select SOURCE files
C:\WINDOWS\APTEC
  MCARDV
  QCY48.S0
  QCY48CAL.S0
  QCY48G.S0
  QCY48L.S0
  QCY48M.S0
  QCY48R.S0
  QCY48S0

Current dir: C:\
Using table: C:\NP_SPEDAC\BIN\SPEDAC.TAB
[REVERSE]

```

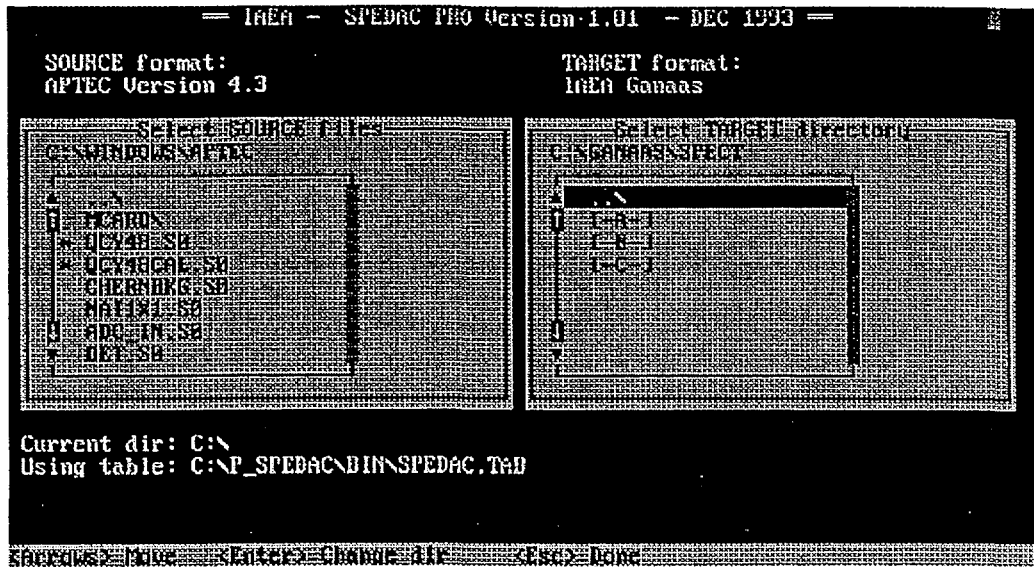
In the frame, you see the current directory for selecting spectrum files. In this example C:\WINDOWS\APTEC is displayed because this is the default directory where the APTEC Version 4.3 spectrum files (\*.S0) are located.

The scroll box lets you change to other directories as well as selecting the spectrum files in a directory. If you highlight the entry "MCARDV" and press the Enter key, you will move to that directory. If you highlight the entry "..\", you move to the parent directory of the current directory (one up in the hierarchy). If you move the highlighted bar of the scroll box all the way down you will see entries for other drives like [-A-]. If you highlight this entry and press the Enter key, this drive will be activated. Only the files with the correct extension, in this case \*.S0, will be displayed as you move through the directories.

Once the correct directory has been found, you can start selecting the files you want to convert. Highlight the file name and press the Enter key. This will select the file, and an "\*" is put in front of the name. Pressing the Enter key while a selected file is highlighted will un-select this file. After selecting one or more files, press the <Esc> key. In the example, we have selected "QCY48.S0" and "QCY48CAL.S0".

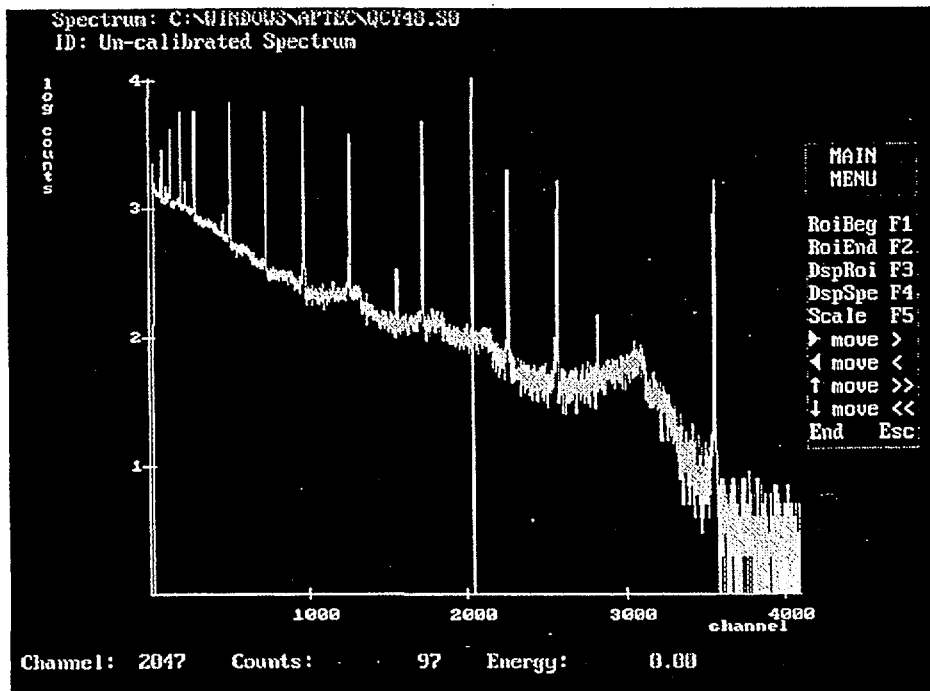
You can only select files in one directory. If you press the <Esc> key without selecting any files, the program will terminate.

The next form allows you to set the target directory.



This is the directory on which all converted spectra will be stored. The directory displayed is the default directory. For IAEA Ganaas spectra this is C:\GANAAS\SPECT. You can select another directory or drive by moving the highlight bar and pressing the Enter key.

Now, for a short time the message "Reading Source..." and "Displaying Spectrum..." will appear after which the source spectrum is displayed on the screen.



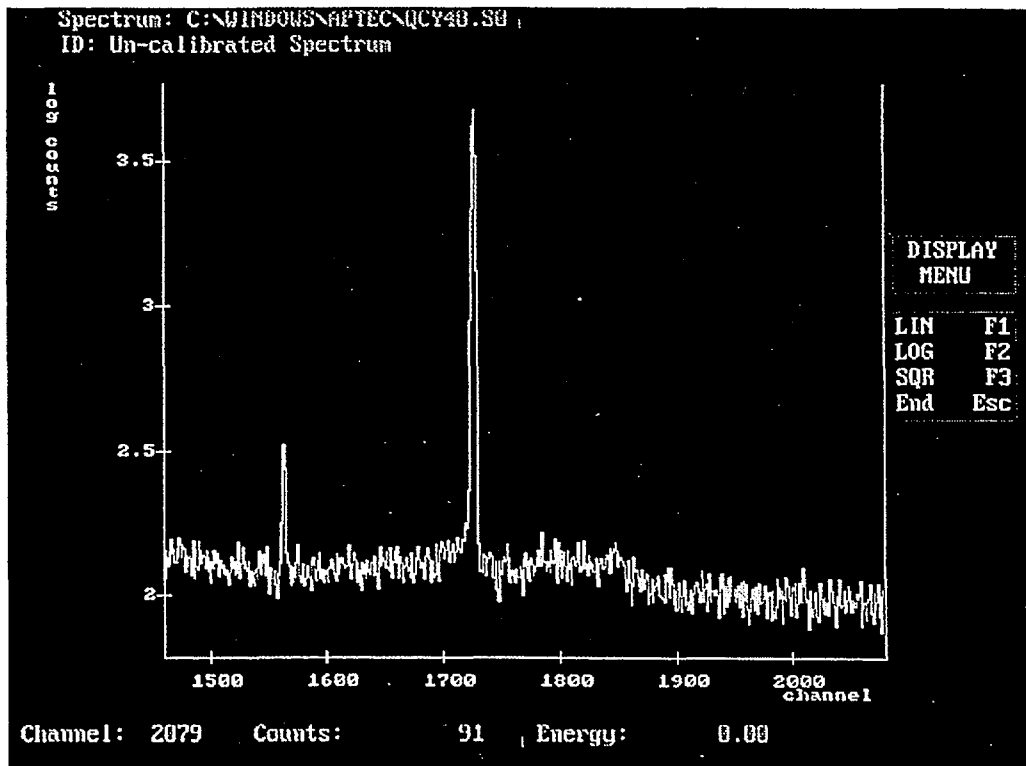
The top line shows the spectrum file name, the next line the spectrum identification (ID) if any, e.g.

Spectrum: C:\WINDOWS\APTEC\QCY48.S0

ID: Un-calibrated Spectrum

The main menu on the left tells you what you can do. <Esc> terminates the display of the spectrum and SPEDAC continues as explained below. With the left and right arrow keys <←>, <→> you move the spectrum cursor one channel; the channel, its content and its energy are displayed on the bottom line. The energy is only correct if the spectral data contains energy calibration parameters. With the up arrow and down arrow keys <↑>, <↓> the cursor moves in larger steps (10 channels). You can also use the mouse to move the cursor and to point to the menu, providing the mouse driver is installed.

Pressing <F1> (RoiBeg) marks the current cursor position as the beginning of the region of interest (ROI). Pressing <F2> (RoiEnd) sets the end of the region of interest to the current cursor position. If a region of interest has been defined in this way, pressing the <F3> key will display the region of interest. With <F4> the entire spectrum is displayed. Finally using <F5> (Scale) you can change the vertical scale mode. A sub-menu appears.



F1 sets the vertical scale to linear; F2, to logarithmic; and F3, to square root.

Very often you will not need to use these options; the spectrum is displayed to let you verify if indeed the right spectrum was selected for conversion and to indicate that the spectrum was read correctly. When you press the <Esc> key from the main menu, the display function terminates.

Now a form is displayed as shown below

```

= IAEA - SPEDAC PRO Version 1.01 - DEC 1993 =
SOURCE format:          TARGET format:
APTEC Version 4.3      IAEA Ganaas

Processing file 2
SOURCE: C:\WINDOWS\APTEC\QCY48.S0
First channel: 0      Last channel: 1023
ID: Uncalibrated Spectro
TARGET dir: C:\GANAAS\SPECT
TARGET Name: QCY48.SPE

Copying from channel 0      to 1023      Squeezing factor 1
Cont. in batch mode: OFF
Graphics displayed: ON
Overwrite protection: OFF

Current dir: C:\
Using table: C:\P_SPEDAC\BIN\SPEDAC.TAB

Options: move <Enter> Save Channel <Esc> Done <Enter> on <Ins>

```

The label of the form shows the number of the spectrum you are currently processing out of the list of selected files. The first 3 lines in the form identify the source spectrum by its full file name, the first and last channel number, and the (optional) ID. The line below this identifies the target directory you have chosen.

There are a number of fields you can alter on this form. The first one is the name of the target spectrum to be saved:

**TARGET Name:**

The program gives by default the same name as the source and changes the extension according to the selected target format, e.g. if the source spectrum is the APTEC spectrum QCY48.S0 and the target is an IAEA Ganaas spectrum, then the file name will be QCY48.SPE, since .SPE is the default file name extension for this file format. You can alter the name and extension as you wish. If a file with the same name and extension already exists on the target directory, a warning will be given when you try to save the spectrum. At that moment you have the option to not write the spectrum to the disk.

The next line of the form holds three fields:

Copying from channel 0 to 1023 Squeezing factor 1



Changing these values allow you to save only part of the source spectrum in the target file, by altering the beginning channel (default 0) and/or the ending channel (the default is the last channel in the source spectrum). The squeeze factor can be used to reduce the number of channels in the spectrum. With a squeeze factor of 1 (the default) each channel in the source corresponds to one channel in the target. If the squeeze factor is two, the sum of two channels in the source spectrum will be stored into one channel of the target spectrum, and so on. This option might be interesting, as some software products are not able to work on very large spectra. An 8K spectrum can then be stored as a 4K spectrum.

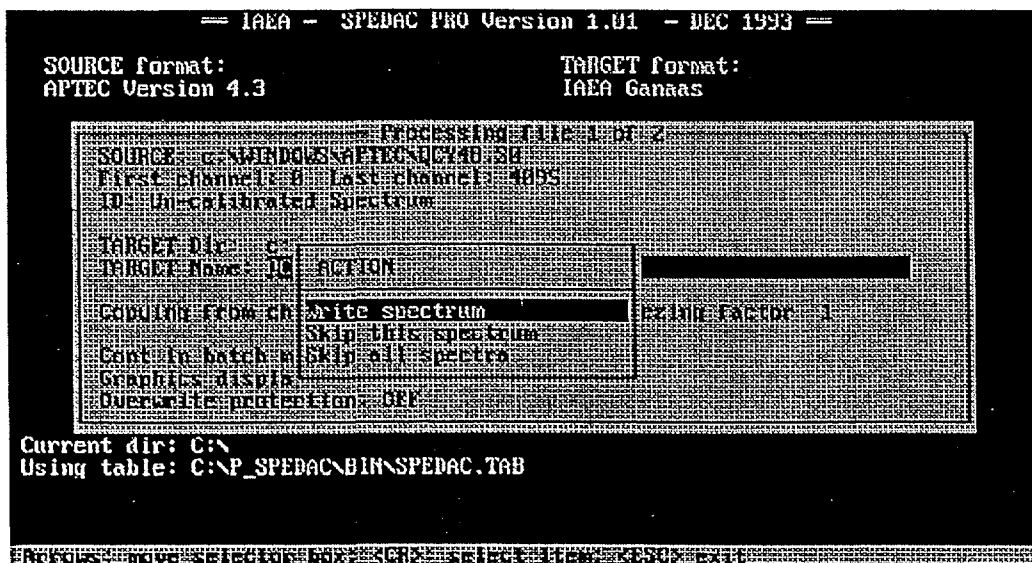
If more than one spectrum has been selected for conversion, three more fields appear in this form:

```
Cont in batch mode  OFF
Graphics display:   ON
Overwrite protection: OFF
```

You can move to these fields using the up and down arrow keys, pressing the Enter key or pointing with the mouse. Since these are toggle fields, you can switch between ON and OFF by pressing the + or - keys or the Space bar.

If "*Continue in batch mode*" is ON, the current and the remaining selected files will be converted without further intervention of the user. If "*Graphics display*" is OFF, the remaining spectra will not be shown on the screen during conversion in batch mode. And finally, if "*Overwrite protection*" is ON, any file with the same name will not be overwritten during batch mode operation.

The final dialog determines the action to be taken.



Use the arrow keys to highlight one of the three options and press <Enter>. "Write spectrum" writes the spectrum in the selected format. "Skip this spectrum" will not write the current spectrum to disk. "Skip all spectra" will skip the current and all other selected spectra, and the program will terminate. In both other cases, the program will continue to process the next spectrum of the list you have selected, if any.

---

### 5.3 Advanced options

SPEDAC Pro uses intermediate files during the conversion process. By default, these temporary files are written in the program startup directory \P\_SPEDAC\BIN. However, if the environment variable TMP (or TEMP) is assigned to a drive, it will write the temporary files there. The execution of the conversion will speed up considerably if you assign to TMP or TEMP a RAM disk. To create a RAM disk see your DOS manual. To see the environment variables, type the DOS command SET:

```
C:\>SET
```

The following will typically be displayed on the screen after this command:

```
COMSPEC=C:\DOS\COMMAND.COM
PATH=C:\;C:\DOS;C:\MYPROG;C:\P_SPEDAC
...
```

To set the environment variables TMP to a RAM disk D: use the DOS command SET in the following way:

```
C:\>SET TMP=D:\
```

SPEDAC will look first for the environment variable TMP; if this is not assigned to a drive, it will look for the environment variable TEMP

SPEDAC uses a file containing information on the various conversion modules. For each source and each target, it contains the identification, the file extension, the default directory and the name of the conversion program. The contents of this file are listed in Appendix III. The installation program has copied this file, called SPEDAC.TAB to the directory \P\_SPEDAC\BIN.

When the program is started as described above, it will, by default, use this table (\P\_SPEDAC\BIN\SPEDAC.TAB). When you change the directory of the source spectra or target spectra during the execution of the program (see chapter 5) the table will be updated with these changes, so that the directories

last used will become the default when you run the program again. In some cases it might be interesting to have your own table; e.g. if you are working with different people on the same computer and you want to avoid interferences from other users. Make a copy of the original table, e.g. :

```
C:>COPY \P_SPEDAC\BIN\SPEDAC.TAB \MYDIR\MYTABLE.TAB
```

If you now start SPEDAC Pro with the full path name of the table as argument, e.g.,

```
C:>P_SPEDAC \MYDIR\MYTABLE.TAB
```

the program will use and update this table.

The program uses the following logic in relation to locating the table:

1. If there is a command line argument that does not start with a minus sign (these are switches, see further), use this command line argument as the full file name of the table.
2. Otherwise, use the table located in the same directory where the program itself is (\P\_SPEDAC\BIN).
3. If the table file as defined in 1 or 2 cannot be opened, look for any occurrence of the file SPEDAC.TAB in the directories specified in the path.
4. If all fails, the program terminates with the error message

"File SPEDAC.TAB not found, Re-install program"

Re-installation of the program will put the original table SPEDAC.TAB back into the directory \P\_SPEDAC\BIN. You can also copy a saved version of this table to this directory.

SPEDAC Pro recognizes the type of display adapter you have on your computer. In some cases, it might be useful to overwrite this default. You can specify two (mutually exclusive) switches on the command line. "-b" (or "-B") will insure that the program operates in B&W mode even if you have a color display. The switch "-c" (or "-C") forces the use of colors. An example of the use of these switches on the command line, in combination with your own table, is:

```
C:\>P_SPEDAC -B \MYDIR\MYTABLE.TAB
```

---

## 5.4 Using individual modules

The program P\_SPEDAC that you start is a control program that calls other programs to do the actual conversion. You can use the individual conversion program as any other DOS program if you wish.

The general name for the programs that convert between a specific format and the IAEA\_SPE format is "XXX\_SPE.EXE" where "XXX" identifies the source; e.g. the program ASC\_SPE converts from ASCII to IAEA\_SPE format. See table 1 for all possible conversion programs from a specific format to IAEA\_SPE format. The programs are located in the directory \P\_SPEDAC\BIN. All these programs accept two arguments on the command line, the first one is the source file name; the second one, the name of the converted spectrum. e.g. to convert a Canberra S100 spectrum "CANTEST1.MCA" to a spectrum in IAEA\_SPE format, saving it with the name "TEST.SPE" in the directory "MYDIR", you can use the following command:

```
C:\>\P_SPEDAC\BIN\S100_SPE WINDOWS\S100\CANTES1.MCA MYDIR\TEST.SPE
```

You can convert a large number of spectra using a DOS command line similar to the one shown here:

```
C:\WINDOWS\S100>FOR %A in (*.MCA) DO \P_SPEDAC\BIN\S100_SPE %A.MCA %A.SPE
```

The programs that convert from IAEA\_SPE format to any specific format have names such as "SPE\_XXX.EXE". They are also located in the directory \P\_SPEDAC\BIN and are used in the same way; e.g. the command:

```
C:\>\P_SPEDAC\BIN\SPE_S100 TEST.SPE TEST.MCA
```

will read the spectrum file "TEST.SPE" in IAEA\_SPE format in the current directory and produce a spectrum file "TEST.MCA" in Canberra S100 format in the same directory. See table 2 for a list of all conversion programs that convert from the IAEA\_SPE format to any specific format.

Note that there are no default directories and file extensions when you use the conversion programs in this way. The defaults are handled by the main program P\_SPEDAC.

TABLE 1: SOURCE FORMATS

| Name                    | File<br>Extension | Default<br>Directory | Conversion<br>Program |
|-------------------------|-------------------|----------------------|-----------------------|
| APTEC                   | *.S0              | \APTEC               | APT1_SPE.EXE          |
| APTEC Version 4.3       | *.S0              | \WINDOWS\APTEC       | APT_SPE.EXE           |
| ASCII                   | *.*               | \DATA                | ASC_SPE.SPE           |
| CANBERRA S100 MCA Card  | *.MCA             | \WINDOWS\S100        | S100_SPE.EXE          |
| IAEA GANAAS             | *.SPE             | \GANAAS\SPECT        | SPE_SPE               |
| IAEA QXAS               | *.SPE             | \AXIL\SPECT          | SPE_SPE               |
| NUCLEAR DATA AccuSpec   | *.DAT             | \ND                  | ACS_SPE.EXE           |
| NUCLEUS PCA             | *.SPM             | \NUCLEUS             | PCA_SPE.EXE           |
| ORTEC ACE               | *.CHN             | \ORTEC               | ACE_SPE.EXE           |
| SILENA EMCplus          | *.DAT             | \SILGAMMA            | SIL_SPE.EXE           |
| SILENA                  | *.DAT             | \SILGAMMA            | SIL1_SPE.EXE          |
| TRACOR (Spectrace 5000) | SPECTRUM.*        | \EDXRF               | TR5_SPE.EXE           |

TABLE 2: TARGET FORMATS

| Name                      | File<br>Extension | Default<br>Directory | Conversion<br>Program |
|---------------------------|-------------------|----------------------|-----------------------|
| APTEC                     | *.S0              | \APTEC               | SPE_APT1.EXE          |
| APTEC Version 4.3         | *.S0              | \WINDOWS\APTEC       | SPE_APT.EXE           |
| ASCII                     | *.ASC             | \DATA                | SPE_ASC.EXE           |
| CANBERRA Cebas-G          | *.SPC             | \CEBASG              | SPE_CEB.EXE           |
| CANBERRA Spectran-AT      | *.MCA             | \WINDOWS\S100        | SPE_S100.EXE          |
| CANBERRA MicroSAMPO       | *.MCA             | \SAMPO               | SPE_S100.EXE          |
| CANBERRA Gamma-AT         | *.SCA             | WINDOWS\S100         | SPE_S100.EXE          |
| IAEA GANAAS               | *.SPE             | \GANAAS\SPECT        | SPE_SPE               |
| IAEA QXAS                 | *.SPE             | \AXIL\SPECT          | SPE_SPE               |
| INTERTECHNIQUE InterGamma | *.SPE             | \GAMMA.SPE           | SPE_IGAM.EXE          |
| NUCLEAR DATA Asap         | *.DAT             | \ASAP                | SPE_ACS.EXE           |
| ORTEC MiniGam II          | *.CHN             | \USER                | SPE_ACE.EXE           |
| QUANTUM TECHNOLOGY GDR    | *.SPM             | \GDR                 | SPE_GDR.EXE           |
| SILENA SilGamma           | *.DAT             | \SILGAMMA            | SPE_SIL1EXE           |
| SILENA EMCplus            | *.DAT             | \SILGAMMA            | SPE_SIL.EXE           |

# APPENDIX I

## IAEA\_SPE (GANAAS, QXAS) SPECTRAL DATA FORMAT

In the IAEA\_SPE format, spectral data is stored in so-called BLOCK STRUCTURED ASCII files (BSA-file). A BSA-file is an ASCII file, so its content can be viewed with any text editor and can be printed, as well.

A BSA-file is divided into blocks. Each block is identified by a string that starts with a dollar sign (\$) and ends with a colon (:), thus, \$BLOCK\_NAME:. The total length of the block identifier, inclusive the \$ and : should not exceed 64 characters. The block name is case sensitive, upper case letters are recommended. The structure of the data in each block is uniquely defined; the order in which blocks appear in the file is, however, not defined. Programs can add or modify blocks by copying all other blocks and then append the new or modified block. The advantage of this is that the programs which operate on BSA-files need not have knowledge about all the blocks. Moreover, the file can contain much more information than relevant for a particular program.

The IAEA\_SPE spectral data files are block structured ASCII files that contain at least one block "\$DATA:". This block contains the channel content of the spectrum. An overview of all defined blocks and their structure is given below.

### NECESSARY BLOCK

```
$DATA:                (spectral data)
first_chan last_chan
chan_cont[first_chan] ...
...chan_cont[last_chan]
```

### OPTIONAL BLOCKS

```
$SPEC_ID:            (spectrum identification, max. 64 char)
spectrum_id
```

```
$MEAS_TIM:          (spectrum measurement time in seconds)
lifetime truetime
```

```
$DATE_MEA:          (start date of measurement)
month day year hour min sec
```

\$DATE\_END\_MEA (end date of measurement)  
month day year hour min sec

\$COOLING\_TIME: (spectrum cooling time)  
days hours min sec

\$DATE\_IRRAD: (date of irradiation, NAA)  
month day year hour min sec  
\$TUBE\_CURRENT: (X-ray tube current in mA)  
current

\$SHAPE\_CAL: (peak shape calibration parameters)  
num\_param (number of peak shape parameters)  
shap\_par[0] ... shap\_par[num\_param-1]

\$MCA\_CAL: (energy calibration data)  
num\_param (number of parameters)  
cal\_par[0] ... cal\_par[num\_param-1]

\$FWHM\_CAL: (FWHM calibration data)  
num\_param (number of parameters)  
fwhm\_cal[0] ... fwhm\_cal[num\_param-1]

Additional blocks can be added, provided they comply with the above criteria.

**APPENDIX II****SPEDAC Pro FILES**

The following files will be in the directory \P\_SPEDAC\BIN after successful installation on the SPEDAC Pro software:

|              |  |
|--------------|--|
| SPEDAC.TAB   | SPEDAC table file, see also appendix III   |
| P_SPEDAC.EXE | SPEDAC Pro main program                    |
| APT1_SPE.EXE | Converts from APTEC format                 |
| APT_SPE.EXE  | Converts from APTEC Version 4.3 format     |
| ASC_SPE.EXE  | Converts from ASCII (text) format          |
| S100_SPE.EXE | Converts from Canberra S100 format         |
| ACS_SPE.EXE  | Converts from Nuclear Data AccuSpec format |
| PCA_SPE.EXE  | Converts from Nucleus PCA format           |
| ACE_SPE.EXE  | Converts from Ortec ACE format             |
| SEL_SPE.EXE  | Converts from Silena EMCAplus format       |
| SEL1_SPE.EXE | Converts from Silena format                |
| TR5_SPE.EXE  | Converts from Tracor Spectrace 5000 format |
| SPE_SPE.BAT  | Copies IAEA_SPE files                      |
| SPE_APT1.EXE | Converts to APTEC format                   |
| SPE_APT.EXE  | Converts to APTEC Version 4.3 format       |
| SPE_ASC.EXE  | Converts to ASCII (text) format            |
| SPE_S100.EXE | Converts to Canberra S100 format           |
| SPE_ACS.EXE  | Converts to Nuclear Data ASAP format       |
| SPE_ACE.EXE  | Converts to Ortec ACE format               |
| SPE_SIL1.EXE | Converts to Silena format                  |
| SPE_SIL.EXE  | Converts to Silena EMCAplus format         |



**APPENDIX III**

**LISTING OF FILE "SPEDAC.TAB"**

\$SPEDAC\_SOURCES:

APTEC  
 \*.S0  
 \APTEC  
 APT\_SPE.EXE  
 APTEC Version 4.3  
 \*.S0  
 \WINDOWS\APTEC  
 APT4\_SPE.EXE  
 ASCII  
 \*\*  
 \DATA  
 ASC\_SPE.EXE  
 CANBERRA S100 MCA Card  
 \*.MCA  
 \WINDOWS\S100  
 S100\_SPE.EXE  
 IAEA Ganaas  
 \*.SPE  
 \GANAAS\SPECT  
 SPE\_SPE  
 IAEA Span  
 \*.SPN  
 \SPAN\DATA  
 SPAN\_SPE.EXE  
 IAEA Qxas  
 \*.SPE  
 \AXIL\SPECT  
 SPE\_SPE  
 NUCLEAR DATA AccuSpec  
 \*.DAT  
 \ND  
 ACS\_SPE.EXE  
 NUCLEUS PCA  
 \*.SPM  
 \NUCLEUS  
 PCA\_SPE.EXE  
 ORTEC ACE  
 \*.CHN  
 \ORTEC  
 ACE\_SPE.EXE  
 SILENA  
 \*.DAT  
 \SILGAMMA  
 SIL\_SPE.EXE  
 TRACOR (Spectrace 5000)  
 SPECTRUM.\*  
 \EDXRF  
 TR5\_SPE.EXE

\$SPEDAC\_TARGETS:

APTEC  
 \*.S0  
 \APTEC  
 SPE\_APT.EXE  
 APTEC Version 4.3

**Information on SOURCES**

Label  
 File Extension  
 Default Directory  
 Conversion Program  
 ...

**Information on TARGETS**

Identification  
 File Extension  
 Default Directory  
 Conversion Program  
 ...

```

*.SO
\WINDOWS\APTEC
SPE_APT4.EXE
ASCII
*.ASC
\DATA
SPE_ASC.EXE
CANBERRA Cebas-G
*.SPC
\CEBASG
SPE_CEB.EXE
CANBERRA Spectran-AT
*.MCA
\WINDOWS\S100
SPE_SAT.EXE
CANBERRA MicroSAMPO
*.MCA
\SAMPO
SPE_SAM.EXE
CANBERRA Gamma-AT
*.SCA
WINDOWS\S100
SPE_GAT.EXE
IAEA Ganaas
*.SPE
\GANAAS\SPECT
SPE_SPE
IAEA Span
*.SPN
\SPAN
SPE_SPAN.EXE
IAEA Qxas
*.SPE
\AXIL\SPECT
SPE_SPE
INTERTECHNIQUE InterGamma
*.SPE
\GAMMA.SPE
SPE_IGAM.EXE
NUCLEAR DATA Asap
*.DAT
\ASAP
SPE_ASAP.EXE
ORTEC MiniGam II
*.CHN
\USER
SPE_MGAM.EXE
QUANTUM TECHNOLOGY GDR
*.SPM
\GDR
SPE_GDR.EXE
SILENA SilGamma
*.DAT
\SILGAMMA
SPE_SGAM.EXE
$SPEDAC_SHOSPE:
SHOSPE.EXE
$SPEDAC_CUTSPE:
CUTSPE.EXE
$SPEDAC_SQUSPE:
SQUSPE.EXE

```

**Name of spectrum display program**

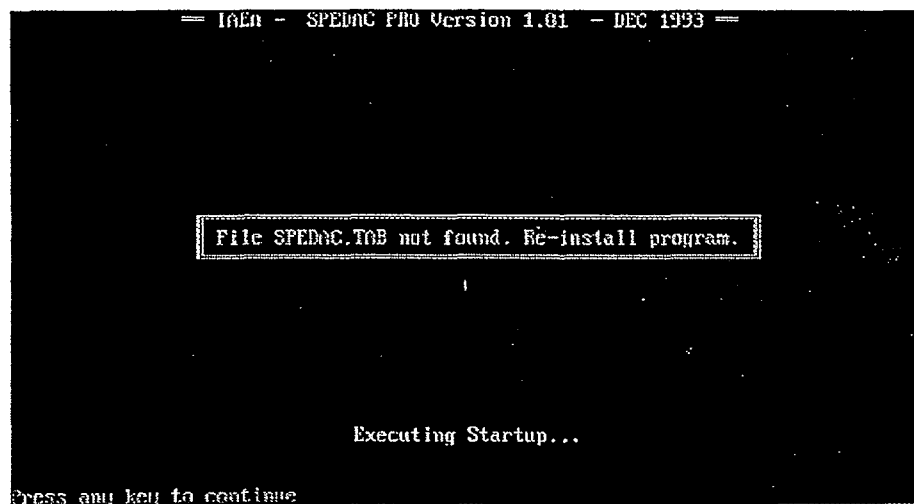
**Name of spectrum cut utility program**

**Name of spectrum squeeze utility program**

## APPENDIX IV

### ERROR MESSAGES

While running SPEDAC Pro, error messages can appear in a box:



Below is a list of all the error messages and their most likely cause.

#### Error messages related to starting and running SPEDAC Pro

These are error messages issued by the SPEDAC Pro main program P\_SPEDAC.EXE.

##### "File SPEDAC.TAB not found. Re-install program"

The program could not find the SPEDAC table. This could be either the file name specified on the command line when you started SPEDAC Pro or the file SPEDAC.TAB in the directory \P\_SPEDAC\BIN or in any directory in the path. Make sure that the file SPEDAC.TAB is in the directory \P\_SPEDAC\BIN (or in another directory in the current path) or that the file name specified as argument is correct.

**"File <filename> is corrupt. Re-install program"**

SPEDAC could locate the table file but while processing (reading and interpreting) this file an error was found. This might indicate that this file, which is a BLOCK STRUCTURED ASCII file, has been altered in an inappropriate way, e.g. by editing the file with a text processor or other text editor. The best thing to do is to re-install the program. This will put the original file SPEDAC.TAB in directory \P\_SPEDAC\BIN.

---

**Error messages related to starting the conversion and spectrum display modules.**

For the conversion and the display of spectral data, SPEDAC Pro starts other programs. This process is known as spawning. The following error messages relate to this process. Instead of <programe> the actual name of the spawned process is given.

**"SPAWN: Not enough memory to run <programe>"**

There is not enough free DOS memory (RAM) available to load the program. Increase DOS memory by removing memory resident programs, or moving parts of DOS to high memory (see DOS manual). This error might also occur if you try to run SPEDAC Pro from within another DOS shell (PCTOOLS, XTREE....).

**"SPAWN: <programe> not found"**

The program that needs to be loaded is not in the same directory where the main program P\_SPEDAC.EXE is located and the program is also not found in any other directory in the current path. Normally all executable files of SPEDAC Pro must be in the directory \P\_SPEDAC\BIN. Move the program in this directory or re-install SPEDAC Pro. This could also happen if the SPEDAC table SPEDAC.TAB is corrupted. The program name will then be different from those listed in Appendix II. Re-install SPEDAC in this case.

**"SPAWN: <programe> has wrong format"**

Although a program with the correct name was found, this program could not be started because it is not a DOS executable file. It could be a Windows program with the same name.

**"SPAWN: Argument list too long"**

This error occurs when the argument list exceeds 256 bytes, when DOS runs out of environment space (by default 256 bytes).

Make sure that your path names are not too long:

```
C:\MYDIR\MYSPECT\MYEXAM\TODAY\MORNING\GOOD
```

or use the DOS SUBST function to reduce the path length (See DOS manual). Remove unnecessary variables from the environment (See DOS command SET) or increase the environment space (to 512 bytes or more) with a line in CONFIG.SYS similar to the one below:

```
SHELL=C:\DOS\COMMAND.COM C:\DOS\ /E=512 /P
```

**"SPAWN: Invalid argument"**

This error is very unlikely; if it occurs, re-install SPEDAC Pro. If the error persists, use the reply form in Appendix V.

**"SPAWN: Error number = <number>"**

This error is very unlikely; if it occurs, re-install SPEDAC Pro. If the error persists, use the reply form in Appendix V. Indicate the number of the error on the form.

---

**Error messages related to conversion and spectrum display modules.**

These error messages are produced by the conversion and display modules while running. The error terminates the module and the message is displayed by the main program.

**"FORMAT\_NOT\_CORRECT"**

The conversion program was given the task to convert a spectral data file; however, the conversion program cannot read the format of the spectral data. This might happen because you have selected the conversion of APTEC files and then selected a file that was not in the APTEC format, although the file extension was correct. Also the spectral data file might be corrupted.

**"INVALID\_CHANNEL\_RANGE"**

The conversion program failed to find a reasonable value for the first and last channel number in the spectrum; e.g. the channel number is negative, or the first channel is bigger than the last channel. The spectral data file is corrupted or has the wrong format.

**"CANNOT\_ALLOC\_MEM"**

Although the conversion program could be started, while running it could not allocate enough memory (heap) to operate properly. The programs allocate memory e.g. to read the spectral data. See "SPAWN: Not enough memory to run" to cure this problem.

**"CANNOT\_ALLOC\_HMEM"**

Same as above (but this program needed huge memory, >64 KByte).

**"NO\_GRAPHICS\_MODE"**

The spectrum display program found that your computer has no graphics card to display the spectrum. The rest of the programs will however, continue to work correctly.

The remaining error messages are very unlikely. If they occur, re-install SPEDAC Pro. If they persist, use the Reply Form in Appendix V.

**"CANNOT\_OPEN\_FILE\_FOR\_WRITE"**

The program failed to open a file for writing, the file name is probably illegal.

**"CANNOT\_OPEN\_FILE\_FOR\_READ"**

The program failed to open a file for reading; the file does not exist.

**"MISSING\_CMD\_LINE\_ARG"**

The conversion module expected a number of command line arguments; because of a failure in the spawning process they were, however, not present.

**"INVALID\_CMD\_LINE\_ARG"**

The command line argument given to the conversion program cannot be interpreted.

**"FAIL\_OPEN\_READ"**

The module failed to open a file for reading.

**"INTERNAL\_ERROR"**

Any other error.

**APPENDIX V****SOFTWARE REPLY FORM**

SPEDAC Pro Version 1.1 JAN 1995

If you experience any problems using this software or have any suggestions for improvement, make a copy of the form, fill it in as completely and as accurately as possible and send it to the address listed below.

-----&

RETURN ADDRESS :

Physics Section, IAEA  
P.O. BOX 100  
A-1400 VIENNA  
AUSTRIA

USER IDENTIFICATION:

Name:  
Institute:  
Address:

Phone:  
Fax:

**PROBLEM EXPERIENCED:**

Describe in as much detail as possible the problem you experienced while using SPEDAC Pro. If relevant, include a floppy with the spectral data file with which you experienced problems.

Note: You could also send your comments/problems through e-mail to:  
FAZINIC@RIPO1.IAEA.OR.AT on *INTERNET*.