ANALYSIS

Instruction Manual

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Contents

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1. Introduction

ANALYSIS is part of the Windows® ESR spectrometer software package provided to process recorded spectra. This program contains tools for rescaling, arithmetic operations, differentiation, integration, transformation, filtering and for combining spectra. The following procedures are implemented:

1. Arithmetic operations:
   - scaling factor Y[i] = A*X[i]
   - sum of spectra Y[i] = Y[i] + A*X[i + shift]
     wherein shift is a positive or negative integer in order to compensate inevitable field shifting between individual scans

2. Differentiation (first derivative)
   differential ratio (y[i+1], y[i-1])
   is calculated directly from the ordinate values of the adjacent points
   - first derivative of (Z[i]),
     wherein Z[i] denotes the interpolating polynomial of the 3rd degree over 5 data points (i-2, .., i+2)

3. Integration
   - integral of the whole spectrum $y[j] = \int_0^j y[i]di$ for j = 0,..,n-1
   - integration with offset set to zero $y[j] = \int_0^j (y[i]-b)di$ for j = 0,..,n-1

     the offset is subtracted before integration. The value of the offset is determined by FFT transforming, removing the non-periodical component of the function and FFT retransforming.

   - integration with baseline correction $y[j] = \int_0^j (y[i]-b[i])di$ for j = 0,..,n-1

     the baseline which may be tilted is subtracted before integration. The baseline is defined as a straight line through the first and last five points of the spectrum.

   - integration with polygon correction $y[j] = \int_0^j (y[i]-x[i])di$ for j = 0,..,n-1

     where a polygon curve is subtracted.
     The knots are user defined.

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4. Fourier transform
    - FFT, inverse FFT and power spectrum
    - convolution and deconvolution
    - auto and cross correlation

5. Smoothing procedures
    - moving averages of xx data points
    - 3rd degree polynomial smoothing over 5 data points
    - rectangular or Gaussian filtering
      which entails the steps of FFT transform, multiplication with the filtering function and FFT retransform of the spectrum.

      rectangular function y[x] := 1 for x = left limit .. right limit,
      y[x] := 0 for all other values of x.

      Gaussian function $y[x] := \exp(-(x/a)^2)$

      wherein $a := 2\,ñ / \pi$
      ñ denotes the filter limit set by the user (inflection point of the bell shaped curve).

      The optimal width of the filtering function can be visually defined with the help of the power spectrum of the spectrum.
    - RC low pass filtering
      simulates the traditional electronic resistor - capacity low pass filtering circuit of the old spectrometers

6. Interpolations for spectrum length adjustment

7. Special features such as reducing the length of a spectrum as indicated by the displayed window, line width and height determination and g-value calculation

ANALYSIS accepts data formats produced by the Magnettech's spectrometer control programs CU1, CU2 and DS100. Output formats are of the CU1 or CU2 type, or may be appended to existing files, so the processed spectra could be transferred directly to the presentation program MULTIPLOT in the same way as an unprocessed spectrum.

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2. System requirements

Minimum hardware requirement is an IBM compatible PC with an Intel 386DX microprocessor together with a 387 math coprocessor, or a higher type of main processor. The memory size should be at least 8 MB RAM, and a mouse should be available. The program is designed for the VGA graphic mode with 640 * 480 pixels, it also works with SuperVGA and 800 * 600 pixels if the small character size is chosen. The system software should consist of DOS 6.20 (or higher) and Windows 3.1 (or Windows for Workgroups 3.11). In the present version ANALYSIS does not work under Windows 95. Hard disk requirement is 3,5 MB free space for the program code.

3. Installation

To run ANALYSIS the program needs to be installed on the hard disk first. It comes in a compressed form on a 3.5 inch 1,44 MB floppy diskette together with the installation procedure INSTALL.BAT. As a first step you need to call this procedure with the destination drive a parameter. If „A:“ is your 3.5 inch floppy drive and „C:“ is your hard disk where you want to get your program installed, you may start as follows:

C:\>**A:**
A:\>**install C**

Then the whole program code will be written into the subdirectory „CU1“. If CU1 does not exist it will be newly created. After successful completion of the installation procedure you will find the following files in this directory:

LVDEVICE.DLL
ANALYSIS.EXE
ANALYSIS.ICO

As a next step you need to implement an icon in your Windows system. For this purpose you have to use the option „FILE/NEW“ of the Windows program manager. Just complete the appropriate program specifications (command line: C:\CU1\ANALYSIS.EXE) and do not forget to opt for the alternative symbol ANALYSIS.ICO. In any case of difficulty please refer to the Windows manual.

4. Program features

4.1 Starting the program

The most convenient start of the program is simply to double click the icon 

. Alternatively, the program may be called by the file manager or directly by the execution option of the program manager.

4.2 Closing the program

Use the pull down menu „File“, option „exit“.

4.3 Multi tasking

As with any other program running under Windows, you may temporarily leave ANALYSIS in order to switch to another task. In order to do so, you may click the „ “ symbol in the upper right corner of the window so the active window will be reduced to its corresponding icon. After completing other tasks, you may return to ANALYSIS any time by double clicking this icon.

4.4 Program details

All details of the program screen are shown in Figure 1. In principal, the display consists of the main menu bar (a), the result of the spectrum processing (b, c), a panel with the raw spectrum (i), the center field value (h), switches, buttons and displays for a grid and for cursors (d, e, f, g). The cursor and grid operating elements are only visible whenever they are active (e, g).

The bar with the pull down menus (a) contains all functions necessary to process a spectrum as shown in Table 1 ranging from file handling to all the mathematical procedures described in the introduction (see chapter 4.5.). The line below the menu bar (b) displays the actual spectrum file name and all the procedures which have been applied to this spectrum. Beyond this line the graph of the processed spectrum is shown (c), values on the abscissa represent data points, those on the ordinate digital spectrometer output. Two pairs of cursor lines, one vertical and one horizontal each, may be activated by the switch (d). All cursors may be reset to default values by pushing the adjacent „Cursor Preset“ button. They always appear together with a complete position display (e) and can be moved either directly within the graph (c) with the mouse pointer or by changing the position coordinates within the number display (e). Optionally a grid may be added to the graph by using the switch (f). Different colors may be selected for the cursors and the grid by the color buttons (g). Please remind to drag the mouse to the

color of choice after pushing the requested button with the mouse pointer. The center field value is always indicated in mT (h) and will be converted into the Landé's g-factor difference with the free unpaired electron if the microwave frequency is entered within the g-factor option of the „Special" menu. The original spectrum display (i) remains unchanged all the time.

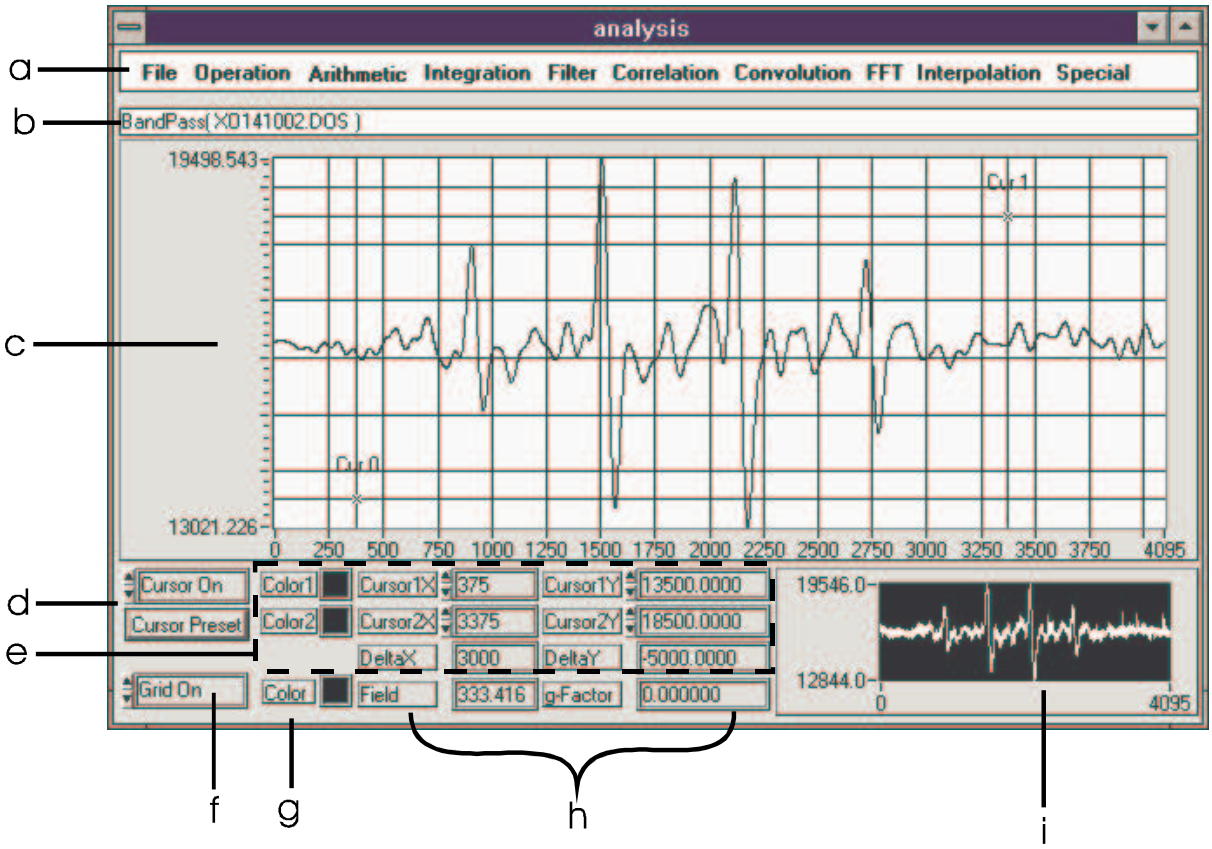

Figure 1: Main screen

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4.5 The menu bar

In difference to the majority of Windows programs the menu works in a dragging mode, i.e., you have to keep the left mouse button pushed while selecting. You have to drag the mouse pointer to the desired option. Releasing the mouse button will select the chosen item and start the selected routine. All program functions are summarized in Table 1.

Table 1: menu bar

menu item	option		function
File	new		selects a spectrum file
	reload		reloads selected spectrum file
	save		saves processed spectrum
	print		prints processed spectrum
	parameter		shows spectrum parameters
	exit		quits this program
Operation	xy-scale		changes axis scaling on the display
	zoom in	1	displays only the frame formed by the cursors
	zoom out		reverses zooming in
Arithmetic	summation	2	addition of another spectrum
	difference	2	subtracts a spectrum
	scaling		multiplies spectrum with a constant factor
Integration	DERIVATIVE 1		differential ratio
	DERIVATIVE 2		forming derivative from interpolating polynomial
	Y=INT(Y)		direct integration
	Y=INT(Y-ZERO)		integration after subtracting zero line
	Y=INT(Y-BASE)		integration after subtracting base line
	Y=INT(Y-POLY)	3	integration after subtracting base polygon line
Filter	moving average		shapes a spectrum with averaged data points
	polynomial filter		fits 5 data points to a 3rd degree polynomial
	window	3	smoothes a spectrum by user defined filtering
	RC Low Pass	3	applies a time constant to smooth the spectrum
Correlation	auto correlation		product of the complex conjugate (same or other spectrum)
	cross correlation	2	in the transformed domain
Convolution	convolution	2	product in the transformed domain (Faltung)
	deconvolution	2	division in the transformed domain (cave!)
FFT	FFT		executes the fast Fourier transform (FFT)
	inverse FFT		executes the inverse FFT
	power spectrum		shows the squared FFT (power spectrum)
Interpolation	.. to next BAS 2		inserts as much interpolated data points as necessary
	.. up to 512		to reach a length of the next power of 2
	.. up to 1024		or to the specified number.
	.. up to 2048		
	.. up to 4096		
Special	window	1	cuts spectrum length to distance between cursors
	line width		determines height and width of the largest peak
	g-factor		converts center field value and MW frequency into g-value
		1	requires active cursor
		2	operates with a further spectrum file
		3	switches to another screen

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The mathematical details of the functions are listed in the introduction (chapter 1). Please remind that any fast Fourier transform requires a set of data points exactly in the length of a power of 2. Any zero padding (a common technique) may result in distortions whenever the offset of the spectrum is different from zero.

In the case of deconvolution (cave!) it is in the responsibility to avoid division by zero. In such circumstances spectral information may have been lost in a previous convolution so there is no mathematical way to regain the original data.

5. Functions in detail

5.1 File

5.1.1 new

This is the first menu option to be used in the program, it opens the file dialogue (see below 5.12). After completing the file dialogue the file name of the spectrum appears in the line below the menu bar (Fig. 1: b). The default colour for drawing the spectrum line is black.

5.1.2 reload

If the processing of a spectrum has not lead to the expected result this option gives the user the opportunity to return to the original unprocessed spectrum. The identification line (Fig. 1: b) shows only the file name without any addition as a result of this procedure.

5.1.3 save

The processed spectrum may be stored as a file on disk with this procedure opening the file dialogue (see below 5.12).

5.1.4 print

The spectrum display (Fig. 1: c) will be printed as shown on the screen.

5.1.5 parameter

A window will be opened which shows the instrument parameters of the actual spectrum, i.e. the B0-field, field sweep, sweep time, number of samples, modulation amplitude, gain and time constant.

5.1.6 exit

Quits program execution.

5.2 Operation

5.2.1 xy-scale

This option opens a window to define ranges and tick distances of both axis's. Auto scaling can be switched on and off by clicking the appropriate boxes with the mouse pointer. Minimum, maximum and precision (tick distances) can be entered with the numeric boxes in this window. „OK" will accept the values entered whereas „Cancel" will return to the previous ones.

5.2.2 zoom in

This blows up the area surrounded by the pointers to the full size of the diagram (Fig 1: c).

5.2.3 zoom out

The zoom in function is canceled and the whole spectrum will return onto the display.

5.3 Arithmetic

5.3.1 summation

Another spectrum will be added to the actual one. The file dialogue window (see 5.1.1) will be opened in order to select the spectrum to be added.

5.3.2 difference

Another spectrum will be subtracted from the actual one. The file dialogue window (see 5.1.1) will be opened in order to select the spectrum to be subtracted.

5.3.3 scaling factor

Within the representation of the spectrum the gain factor is multiplied with the scaling factor in order to spread or shrink the amplitude. The value of this factor will be entered into a numerical box within a separate window which appears on the screen. It also shows the spectrum and the axis's together with the actual tick labels.

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5.4 Integration

5.4.1 Derivative method 1

The first derivative will be calculated directly by differential ratios of the adjacent data points (see Introduction, item No. 2). The resulting graph will appear auto scaled on the screen.

5.4.2 Derivative method 2

The first derivative will be calculated from an interpolating third order polynomial through five data points, i.e. the actual point and the two adjacent once to the left and to the right (see Introduction). The resulting graph will appear auto scaled on the screen.

5.4.3 direct integration

An integral curve will appear on screen directly after selecting this menu item.

5.4.4 integration after subtracting zero line

The spectrum will be integrated after subtracting the offset which represents the non-periodic component of the spectral curve (see Introduction, item No. 3).

5.4.5 integration after subtracting base line

The spectrum will be integrated after subtracting the base line which is defined by a straight line through the first and last five points of the spectrum.

5.4.6 integration after subtracting base polygon line

A submenu window will appear to allow defining the base line as a polynomial spline curve. The knots of the spline will be set within the upper panel of this window using the mouse pointer, the degree of polynomials can be entered into the provided numerical box. „OK“ will continue integration whereas „Cancel“ leaves the displayed spectrum unaltered.

5.5 Filtering

5.5.1 moving averages

The spectrum will be smoothed by replacing each data point by the average of ... points of the original curve.

5.5.2 polynomial filtering

The spectrum is replaced by a series of interpolating polynomials.

5.5.3 window smoothing

A submenu window will be opened to define the kind and size of filtering function (see application example below). Both, a rectangular and a Gaussian function are provided as filters (see Introduction, No. 5). In case of the Gaussian function the full bell shape or the positive half of the function can be used for filtering. The kind of filter can be selected from a list which appears in a pull down menu. The dialogue window entails two graphs, the power spectrum of the ESR spectral curve in the upper panel and the original spectrum in the lower one. The smoothed spectrum will appear on top of the original in red. The size of the filtering function is defined by setting the pointers in the power spectrum within the upper panel, or the limits may be entered via the numerical boxes. Since the smoothed spectral curve is instantaneously adapted to the limits set in this dialogue optimal filtering can be achieved easily by moving the pointers within the power spectrum accordingly.

Practical hint: The power spectrum should clearly show distinct intensities within the signal area well above the noise level. The upper limit of the filtering function should be selected ad the borderline between signal and noise frequencies.

5.5.4 RC low pass filtering

This option mimicks the electronic resistor - capacity circuit for low pass filtering.

5.6 Correlation

5.6.1 auto correlation

An auto correlation of the spectrum will be calculated directly without any transform. As a consequence the result comes with twice the number of original data points.

5.6.2 cross correlation

The correlation between the present spectrum and a further one will be calculated. The file dialogue will be opened to choose the second spectrum. Like the auto correlation function the cross correlation is calculated directly without any transform so the total length of the spectrum will be extended by the length of the second one.

5.7 Convolution

5.7.1 convolution

The spectrum will be convolved directly with a function which must be available as another spectrum file („Faltung“). The file dialogue allows to select the function file.

5.7.2 deconvolution

This is the reverse function of the convolution and needs also a second operand in form of a spectrum data file which will be identified within the file dialogue window.

5.8 Fourier transform

5.8.1 FFT

The spectrum on display is Fourier transformed and the real part of it appears on screen. Since a fast Fourier algorithm is used the length of the spectrum must be a power of 2 (e.g. 1024, 2048 or 4096 data points).

5.8.2 inverse FFT

The fast Fourier transform will be reversed with this function. The untransformed spectrum will return onto the screen.

5.8.3 power spectrum

This makes the power spectrum of the displayed ESR spectral curve.

5.9 Interpolation

It may be necessary to extend the total length of a spectrum e.g. for a FFT or to compare spectra recorded with different sampling rates. The interpolation function serves to fill the spectrum to the requested size.

5.10 Special

5.10.1 Resizing spectrum to actual window size

A subarea of the displayed spectrum may be of particular interest so an enlarged presentation is desired. The area of interest can be surrounded with the cursors and blown up to the full size of the display with this function.

5.10.2 line width

Since in quantitative spectroscopy line height and width are key parameters for interpretation of a spectral measurement this function provides a convenient tool for reading these values. The cursors have to be switched on first. Then they only need to be set near to the area to be interpreted. Pressing the line witdth function of this menu will automatically set the pointers to the maximum and minimum of the part of the spectral curve wich is included between the actual x-axis cursors. The values of the peak to peak distances are shown in a separate window.

5.10.3 g factor

If the exact frequency of the microwave is known, i.e. separately measured, then the corresponding g-value difference can be calculated with this function. A separate window is opened to enter the microwave frequency and to show the result of the calculation. The magnetic field value is taken from the present cursor settings but may be altered within the numerical box of this menu if desired.

Alternatively, the g -factor can be determined in reference to a standard with a known g-value. For this purpose the switch „field frequency“ has to be toggeld to „reference sample“. Then the g - value and the magnetic field of the line position of the reference needs to be entered into the appropriate boxes.

5.11 file dialogue

The windows of the file dialogue are shown in Fig. 2 in sequence of their appearance. First the file type has to be selected from the three available formats CU1, CU2 and MS100. The choice is completed by ticking the appropriate box with the mouse pointer.

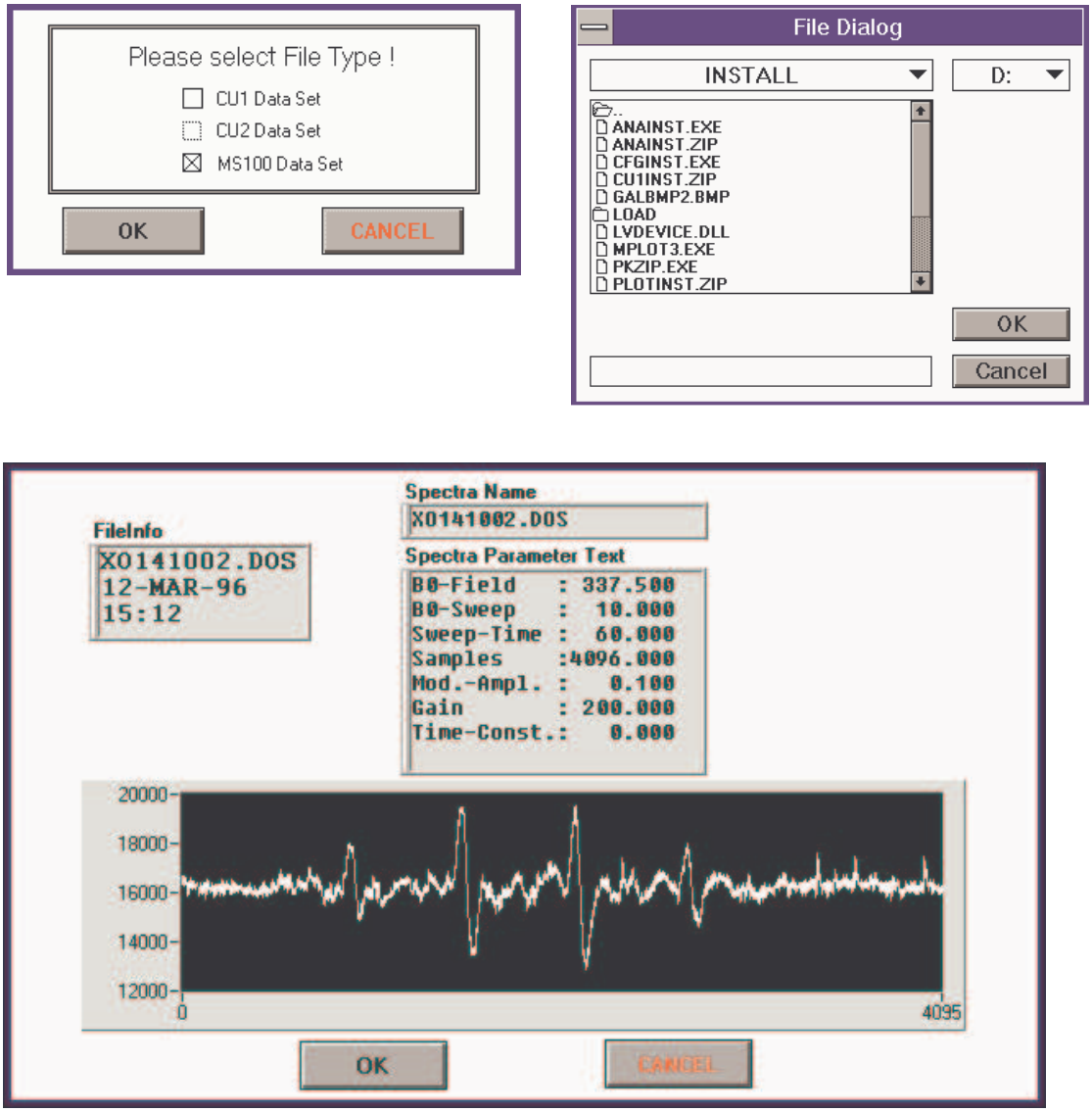

Figure 2: File dialogue (MS100 file type)

Caution: The appropriate file type must be selected correctly since not any format can be automatically checked.

The file name can be picked from a listing of a selected directory like in any common Windows program. The spectrum and its characteristics appear in a third window once a file is selected. At this point the choice can be either confirmed with „OK“ or rejected with „Cancel“. The program control will return to the main menu.

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6. A practical example: smoothing a spectrum.

The use of ANALYSIS will be demonstrated step by step starting with a spectrum file from one of Magnettech's spectrometers. This file is supposed to be present either on a floppy disk or in one of the directories of the hard disk. Having started ANALYSIS with a mouse double click only the File menu is active within the menu bar on top of the program screen. You may switch on or off the cursors or the grid any time during the program run whenever the main screen is shown (Figure 1).

Step 1: Reading the experimental spectral data

The File menu option „new" initializes loading a new spectrum. A window to select the file type will pop up first, the appropriate data set format has to be chosen. Next a file dialog window allows you to select the desired spectrum file from the disk or diskette. The content of the picked file is shown on screen in separate panels for file information, name of the spectrum, experimental parameters and for a graph of the spectrum (Figure 2). In case of CU1 or CU2 types of spectra additional panels will appear displaying spectra number, index, recording date and time and free text originally supplied from the experimental run.

At this point you may either accept the spectrum for loading or cancel this procedure. In the latter case you have to repeat the selection procedure. The successfully loaded spectrum is now displayed in both graph panels of the screen (Figure 1), its name occurs in line (b).

Step 2: Selecting the filtering procedure

The „window" option of the Filter menu opens a separate Filter Window with two graph panels, cursor position displays and a roll up menu for selecting a filter type (Figure 3). In the lower panel two curves are shown simultaneously, the original raw spectrum (green color) and the result of the smoothing procedure (red color). The graph in the upper panel represents the power spectrum of the original data together with two movable cursors marking the edges of the filter window. The Pulse type of filter cuts abruptly at the limits set by cursor positions whereas the bell shaped Gauss filter gradually suppresses information towards the limits outside the band pass window. The Half Gauss filter cuts abruptly only on the left side of the window.

Having selected the appropriate type of filter the band pass window has to be defined by setting the cursors which mark the limits in the upper graph panel. The cursor can be set either by dragging with the mouse directly in the upper graph or by changing the numbers in the corresponding display. The result of the limit definition is immediately shown in the lower panel as a red curve on top of the original data drawn as a green line. As soon as the filter settings reach a satisfactory result the smoothed curve can be saved by pressing „OK" or rejected by hitting „cancel". This action will bring you back to the main screen where the smoothed curve is displayed in the big center panel and the small graph down right on the screen still shows the original raw spectrum for comparison. The spectrum

name in the line between menu bar and graph panel is set into brackets and preceded by „BandPass“ in order to indicate the completed procedure.

Figure 3: Filter Window for smoothing

Step 3: reconsidering the smoothing procedure

If doubts are rising that the result may be really satisfactory the whole procedure may be repeated after reloading the original spectrum. For this purpose the „reload“ option is available in the File menu.

Step 4: saving the result

The „save“ option of the File menu provides a way to store the processed spectrum either in the CU1 or in the CU2 data set format. Alternatively it may be appended to an existing file. A pop up window leaves you to select the desired format. When storing as a single file a comment can be added to the data as free text. You may leave the program by selecting the „exit“ option within the File menu.

7. Concise guide for immediate use

- Start program by double clicking the ANALYSIS icon,
- Load your file with „File/new“,
  - Select data set format,
  - Pick data file,
  - Verify choice of data,
- Switch on and reset the cursors if desired, you may pick different colors for each pair,
  - move the cursor by dragging with the mouse or entering numerically the positions,
- Switch on the grid and choose a color for it, if desired,
- Select an option from the pull down menu bar,
  - enter prompts as appropriate, some applications open a separate window,
- Restart processing with „File/reload“,
- Repeat selecting any program function,
- Save your result with „File/save“,
- Print your result with „File/print“,
- Quit the program with „File/exit“.

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