INTERSPEC FOR WINDOWS SOFTWARE

USER'S GUIDE

INTERSPECTRUM

1 Key Features

Program

Smart data visualization
Data organised in stack and listed in the Trace Gallery
Context sensitive mouse operations
Mathematical modelling of spectra, including noise
Automatic protocols

Spectra acquisition

Selectable resolution and wavelength range
Collecting interferograms or spectra

Spectral manipulation

Calculation of transmittance, absorbance, derivative
Fourier transform zero filling
Unlimited size fast Fourier transformation
Interactive subtraction
Apodization functions
Interactive baseline correction
Smoothing filters -Savitsky-Golay, Median, Mean
Peak edit
Spectral features
Any combinations relating to the second spectra
Linear, squared or decibel Y scale
Wavenumber X scale
Peak marking
Cut and zap of the desired areas

Presentation

User compiled layout design for output graphics
JCAMP-DX, ASCII, Galactic.SPC format - export
JCAMP-DX, ASCII, Galactic.SPC format - import
600 dpi colour printing

1.1 Data visualisation

The program is designed in the same concept as Windows 95/98/XP, meaning that there are fewer controls , less windows - and greater flexibility.

For example, if you indicate a region of interest on the VDU screen using the mouse, you will see a small yellow hint indicating the possibilities within this area. The manual need only be referred to as a last resort.

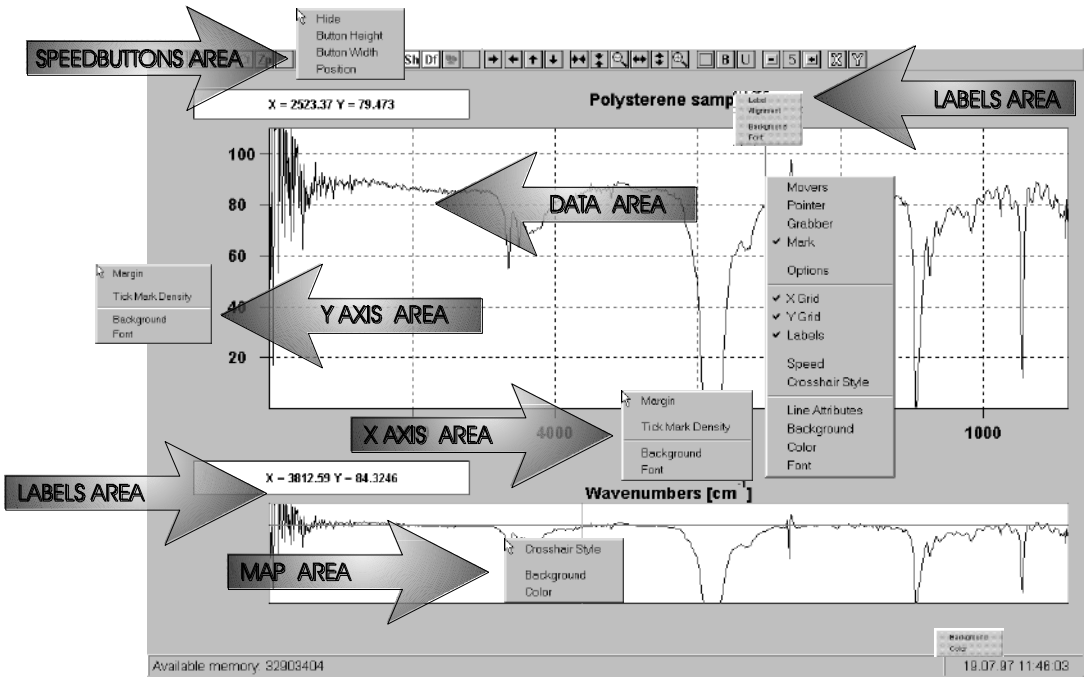


Figure 1 View screen mouse operations

All data manipulation subsystems are conceptually identical.

For example Baseline Correction selection functions are identical to Subtraction functions as displayed on the VDU screen and so minimising the number of routines that must be learned.

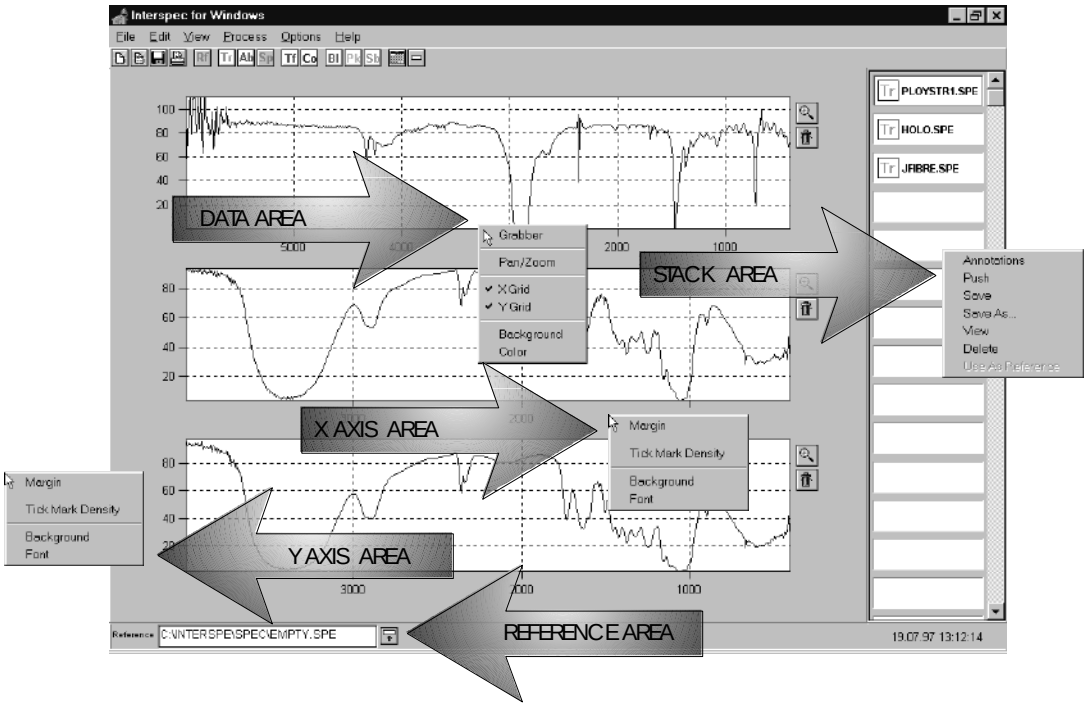


Figure 2 Main screen mouse operations

As you become familier with Interspec features you will see that compared to many other commercial software programmes, Interspec programs are very simple to use and learn. The software is also much faster than other programs and certainly more compact. We are also always working to extend the general use of our software by continuously updating features and making operations easier and faster to use.

The INTERSPEC program startup screen contains everything necessary for working with data - file operations including a special JCAMP-DX export and import feature, formatting page layouts with annotations, working with an operation journal, spectra processing, options for setting both hardware and software parameters and spectra printing. For the user's convenience we have provided icons for creating a new file, for opening, saving, printing and deleting an existing file, for determining a reference spectrum (Rf), for converting a file to transmittance (Tr), absorbance (Ab), spectrum (Sp), interferogram (In), and for such processes as Transform (Tf), Combine (Co), Baseline (Bl), Peak Edit (Pk), and Subtract Spectra (Sb). You can also select the time (date) by clicking a calendar icon, and maximise or clear the selected screen by clicking the appropriate icon between the picture and the trace gallery.

You may work in two ways . Using a traditional pull-down menu system and using speed buttons or mouse action. After each command you will see a blinking sand-glass, a magnifying glass or some other blinking icon which indicates that the system is working.

The pull-down menu commands can be activated by pressing the Alt+highlighted letter. Execution of any command can be cancelled by pressing ESC. If you want to close or delete any data set, you will always be asked for saving instructions. After making your choice in the submenu, the latter disappears. Speedbuttons are activated with a mouse click. In different context sensitive screen areas the user can find new possibilities by clicking the right hand button. The action opens the menu and you can select options as required.

The action menu is divided into five different sections:

I. Cursor Mode
- Grabber
- Crosshair
- Movers
- Mark

II. Operators
- Clear/Data
- Pan/Zoom
- Move/Resize
- Delete

III. Switches
- X Grid
- Y Grid
- X Align Data
- Y Align Data

IV. Numeric Parameters

- X Ticks
- Y Ticks
- X Margin
- Y Margin
- Speed

V. Attributes

- Background
- Color
- Font

If you move the cursor to the Move Bar and click the right mouse button, you will will be able to select changes in height (Button Height) or width (Button Width) of icons in the Move Bar. If you click Orientation, you will be offered the following choice: top, bottom, left, right, which enables one to format the screen by shifting the Toolbar and Move Bar to the top, bottom or either side of the screen, either in one or two directions , depending on the screen size - Format the screen as you wish.

If you click the upper part of the screen, you will be able to change the background colour (Background) and the line colour (Colour), choose the text font (Font) and insert the name of the spectrum (Label).

If you click the left or right border of the screen, you will be shown options for changing the background colour (Background), choosing the text font (Font) and moving or resiting the displayed image.

If you click the spectrum area, you will be able to change the background colour (Background) or the line colour (Colour), choose a text font (Font), determine the location of a chosen spectrum area within the scale division (Cross Hair), shift the spectrum in any direction (Grabber), select and zoom one part of the spectrum (Mark), mark points in the spectrum to correct the baseline (Movers), determine the crosshair as a vertical (X) or a horizontal (Y) line or a cross of two lines (X, Y) (Crosshair Style), locate labels (Labels) select the speed of move buttons within the range of 1 ... 20, depending on the capacity of your computer (Speed), shift the spectrum in any direction, enlarge or diminish it, extend or compress the spectrum either along the X or the Y axis (Pan/Zoom) and switch X and Y gridlines on and off (X Grid and Y Grid). For conventional baseline correction it is advisable to select Movers, X Grid and Y Grid.

If you click the bottom of the screen, then, in addition to the above selection you will be offered the choice of additional options- Tics Size and Tics Space enable you to format the scale of the X axis. The range of both parameters is 0 ... 1. If you choose a parameter outside of this range you will get an error message warning you that the value must be within the range of 0 ... 1.

If you click the trace gallery you can choose between Push, Save, Save As, View and Delete. Here you can move the selected spectrum to the top of the stack (Push) or perform other conventional file operations offered by Windows.

The content of selection boxes may vary with different screens but the meaning of the items within them remains the same throughout the whole program. Some screen-specific cases will be described in the corresponding chapters.

1.2 Trace Gallery

The "Interspec for Windows" software is organized in a spectral gallery format. All spectra that are measured will be piled into the spectra stack. The current spectrum is on the top of the stack. The three topmost spectra are displayed on the small displays in the main window. Each new spectrum you obtain will be piled on top and the existing stack will be shifted down. The names of the spectra in the stack are listed in the Trace Gallery. It is advisable to delete unnecessary spectra for your own convenience. You can easily recognize a modified spectrum by an asterisk in front of its name in the trace gallery. Once you have completed your work, the program will ask for your instructions, whether to save the modified spectra or not.

If you press the reference speedbutton (Rf) the current spectrum is removed from the stack and the stack is shifted up. The name of the selected reference spectrum appears in the Status Line of the screen. The reference spectrum can be returned to the Trace Gallery by clicking its name on the Status Line. It will then appear at the top, shifting other spectra down. You can also drag and drop spectra from the Trace Gallery to the display windows.

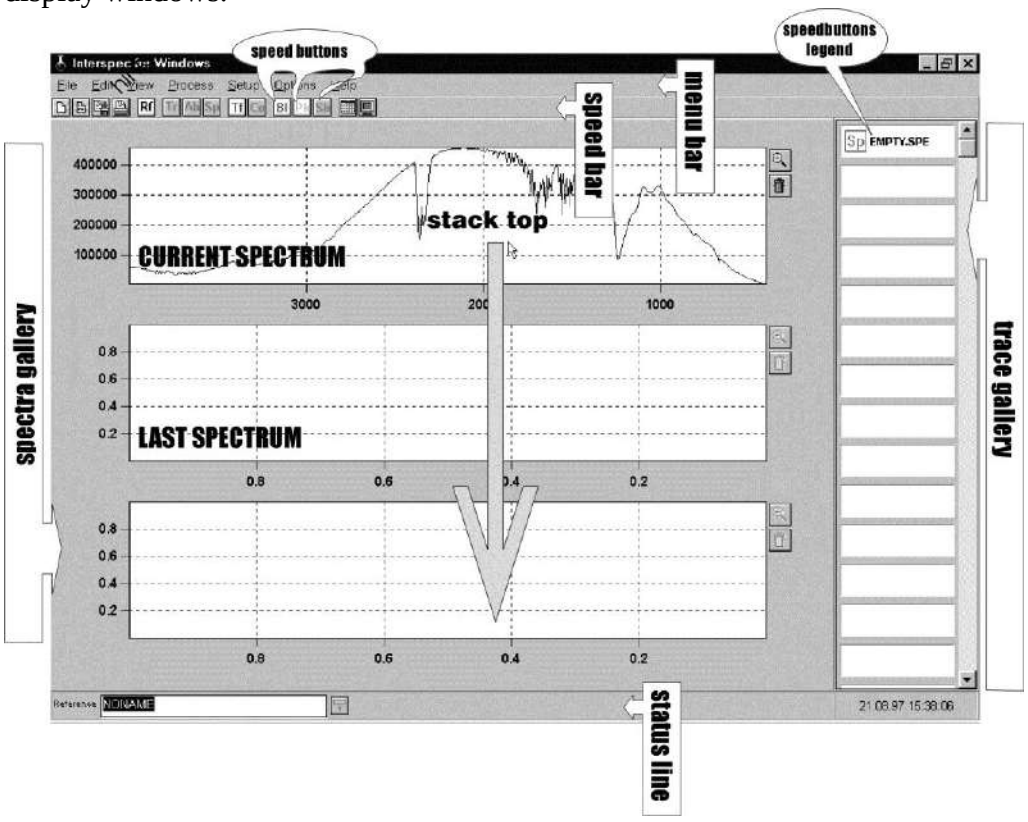


Figure 3 Interspec startup screen

If you use special editing modes such as Baseline correction or Peak Edit, then the top spectrum will be used for data input. Spectrum subtraction screen uses the two spectra from the top of the stack. The main menu is a pull-down type menu system with speedbuttons and you will see that the screen has been divided as follows:

The menu bar is displayed at all times while working with the program, except when using special spectral working modes. To open a required menu, you should press the underlined letter in the keyboard or select it by mouse. In addition you have two other possibilities to go to the next pull-down menu in the menu bar:

- Press *ESC* to close the current menu and choose a new one
- Choose a menu by arrow keys *LEFT* and *RIGHT*.

The following keys can be used for choosing the menus:

Key	**Menu Item**	**Function**
F or f	File menu	Displays the File pull-down menu (PDM)
E or e	Edit menu	Displays the Edit PDM
*V*or v	View menu	Displays the View PDM
P or p	Process menu	Displays the Process PDM
O or o	Options menu	Displays the Options PDM
H or h	Help menu	Displays the Help PDM

Each pull-down menu includes a series of commands. The command name (the highlighted letter of the keyboard) is on the left and additional information is on the right.

There are two types of commands - the first responds immediately with results displayed to the user. The others activate new submenus and ask additional information from the user. The commands are context sensitive - i.e. they are blocked with certain parameter combinations.

A choice of four possibilities are offered to the user to select a command from the opened pull-down menu by way of the keyboard

* To open the submenu use the shortcut function key (if available)
* If the submenu is opened, press the highlighted letter
* Use the arrow keys to move to the command and press ENTER.
* Move the mouse to define an area and click the mouse left button

If you wish to work with a mouse, click the menu command you require. Should you change your mind, click a part of your screen other than the displayed menu and the menu will disappear.

The working directory can be changed after the commands File/Open or File/Save (Save As). All functions relating to the data set are performed in this directory.

Example: If the working directory is C:\INTERSPE, then the FILE/OPEN command asks the user default for the file name of the spectrum, adding automatically the directory and the .SPE extension. As a result, the file with the following complete name: c:\INTERSPE\filename.SPE is opened from memory

Current Spectrum is the name of the data set last acquired, loaded or computed by the user. The current spectrum is displayed on the top display of the main window.

Current Reference is the name of the reference spectrum (seen in the bottom of the screen) last specified by the user with the command USE AS REFERENCE (Rf). This is used by the program to calculate absorbance or transmittance. After entering the command Rf the current spectrum (on the top of the spectra stack) is removed from the stack and both TRANSMITTANCE (Tr) and ABSORBANCE (Ab) commands are enabled in the Speed Bar.

1.3 Context sensitive mouse operations

The menus work with both keyboard and mouse, the more often used functions have shortcut function key names.
Using the mouse you will find that it is context sensitive, i.e. you can click the mouse right button in different areas on the screen to see different context sensitive action menus. For example if you click the mouse right button on the label area you can select the command LABEL and change the label name.

A typical screen is divided as follows:

- data display
- label areas
- vertical and horizontal axis

On the data display the following tools can be applied:

- grabber - to drag data in a window
- mark - to select sub-window and display it
- zoom - "Move" toolbar appears
- crosshair - to determine the location of the chosen spectrum area in the scale division
- movers - to mark the points in the spectrum

1.4 Data input

1.4.1 Numerical Values

The numerical values in Interspec for Windows can be integers, such as

1800, -34, 600

or real values, such as

12.0, -128e-6, +22.0e+11, 0.1E-2

or perhaps shorthand

.256, 1111

Interspec for Windows software generally understands exactly what type of data is being entered. For most of the parameters being requested, the software will always indicate both upper and lower limits, but because of the somewhat complicated nature of some Interspec algorithms, it is not always possible to check all input values for consistency so care should be taken to avoid the use of absurd values.

1.4.2 Parameters

Every computation with the Interspec for Windows program depends on various parameters and options. You may, if you wish, change parameter values during the computing session (Options_Dialog). All parameter values are saved for the next session in INI File. Hovever, default values can be restored by Set Default Parameters option. You can use also standard Windows Notepad accessory to edit starting values for parameters.

1.4.3 Expressions

Expressions are entered as strings of characters with a length less than 254. All names (identifiers) must start with a letter and can contain letters, numbers and underscores. Identificators are not case sensitive.Typical identifiers

Abs f234 Cos_1

are equivalents of

```
ABS F234 COS_2
```

Expressions are made up of operators and operands. Most Interspec for Windows operators are binary, that is to say, they take two operands; the rest are unary and take only one operand. Binary operators use the usual algebraic form, for example a+b. A unary operator always precedes an operand, for example -PI.

In more complex expressions, rules of precedence clarify the order, in which operations are performed. To override precedence rules parentheses can be used.

Operands in expressions are numerical constants, names of predefined constants or variables and calls to functions.

Some examples of simple expressions

```
B-V+V

SQRT(Time)-COS(Time*Alpha)

a*b-c*d
```

Logical expressions are evaluated to 0.0 (False) or 1.0 (True):

```
a+b>4.0

min(V,1.0)=1.0

 V>2.0

V>6.1&V<6.9

Time>100.1&Weight=2
```

The rules for reading logical expressions are as follows:

If the sequence of terms are divided by the OR operators (‘|’), then the expression is true, when at least one of the terms is true.

If the sequence of terms is divided by the AND operators (‘&’), then the expression is true only when all the constituent terms are true.

If the expression contains a comparison operator which is preceded by the NOT operator, the expression is true only when the comparison gives a negative result.

Expressions inside the parentheses are evaluated first.

Table. Precedence of operators

Operators	Precedence	Categories
+, -	7	Unary operators
*. /	6	Multiplying operators
+, -	5	Adding operators
<, <=, >, =>, =, < >	4	Comparison operators
^	3	NOT operator
&	2	AND operator
|	1	OR operator

There are three basic rules of precedence:

An operand between two operators of different precedence is bound to the operator with higher precedence.

An operand between two equal operators is bound to the one on its left.

Expressions within parentheses are evaluated prior to being treated as a single operand.

Multiplying, Adding, And and Or operations with equal precedence are performed from left to right.

1.4.4 Predefined Constants and Variables

PI - always returns the 3.14....
E - always returns the 2.17....
RANDOM - returns the random value with even distribution on interval (-0.5, 0.5).
NORMAL - returns random value with normal distribution, with mean 0.0 and dispersion 1.0.

Every identificator without special meaning for Interspec for Windows is denoting current running argument for expression. For instance, when defining a new Apodization Window as

Weird=1.0-x*y

the result is equivalent to definition

Weird=1.0-x*x

or even

Weird=1.0-Sqr(x)

1.4.5 Functions

Functions with one parameter:

SQR - returns the square of the argument.
SQRT - returns the square root of the argument.
EXP - returns the exponential (e^x) of the argument.
LN - returns the natural logarithm of argument.
SIN - returns the sine of the argument.
COS - returns the cosine of the argument
ABS - returns the absolute value of the argument
FRAC - returns the fractional part of the argument.
INT - returns the integer part of the argument
POISSON - returns random step length, so that the running sum of these steps is distributed according to the Poisson law with the mean density determined by the argument.

Functions with two parameters

MAX - returns the largest of two possibilities.
MIN - returns the smallest of two possibilities.
BOX - returns the 1.0 if arg1 □ Current Argument ≤ arg2 else 0.0.
LORENTZ - position of the central part and FWHM (full width at half maximum).
GAUSS - position of the central part and FWHM (full width at half maximum).

Use of Expressions

Expressions in Interspec for Windows are used in different contexts:

when defining Model Spectra to be used in Emulation mode.

when defining Apodization Windows

when defining Transform and Combine expressions for user defined operations on spectra.

Here are some typical expressions for Model Spectra:

box(1000.0,1500.0)

0.02+box(1000.0,1010.0)

0.02+Gauss(1500.0,2000.0)-0.4*Lorentz(1800.0,200.0)

Sample of Apodization Windows:

1.0

1.0-x

cos(0.5*PI*x)

0.5+0.5*cos(PI*x)

0.543478261+0.456521739*cos(PI*x)

0.42659071+0.49656062*cos(PI*x)+0.07684867*cos(2.0*PI*x)

0.42323+0.49755*cos(PI*x)+0.07922*cos(2.0*PI*x)

1.0-sqr(x)

sin(PI*x)/((abs(PI*x))+1.0e-30)

(1-x)*cos(PI*x)+(1.0/PI)*sin(PI*x)

exp(-2.0*x)

1.0/(1.0+sqr(3.0*x))

Expressions for Transform and Combine operators tend to be very simple:

Exp(x)

-x

20.0*Ln(32000.0*x)/ln(10.0)

a+b

8.0*X+100

Syntax of Labels

Labels are used to annotate plots. In addition to ordinary text, labels may include mathematical formulas or formulas of chemical compounds. For example, if you want to add a label including the string inserted into the appropriate dialog box should be the following:

CO\-{2}

or

CO\m{2}

where both '-' and 'm' (or 'M') mean subscript.

General rules for well formed labels:

Text attributes (escapes) start with backslash ('\').

The application of attribute starts from the next symbol after attribute symbol and proceeds until the end of a label (if not interrupted by other attribute or by brackets).

The application range for an attribute can be fixed by including attributed text into brackets.

Labels with multiple of lines can be formed by concatenating separate lines with ';' symbol.

The following attributes can be used:

+ Superscript with shift of pen

- Subscript with shift of pen

p,P Superscript without shift of pen

m,M Subscript without shift of pen

i,I Italic

b,B Bold

n,N Normal

Examples

Superscript like

CO\+{2}

Subscript in Italic like

CO\-{\i{2}}

To get the result you should type the following string:

CO\p{3}\-{2}

or

CO\p{3}\m{2}

Superscript with pen shifting like

CO\-{2}\+{3} or CO\m{2}\+{3}

If you want to shift the subscript in respect to the superscript in the formula $CO^{3}{}_{2}$, type the following string:

CO\+{3}\-{2} or CO\+{3}\m{2}

Label with multiple of like lines

can be produced by entering

Purified Sample; Without Preprocessing

In the case of longer formulas with more indexes, the brackets may include several sets of brackets in them. If you use variable font styles, then, to restore normal style within the string, you should type ‘n’ before the selected parentheses.

Syntax of Macros (option)

Macro processor for Interspec for Windows is line oriented, that is every command must be fully placed on one input line in the Macro Editor Window. It is also case insensitive in general (see however DDE lines below), you can use different cases to spell command and specifier values. There can be five types of lines in macro body.

Comment

Comment lines start with “-“ symbol:

- This row is for demonstration purposes only

- Comments are used to document macros

Command

Command lines can consist from three parts: window specifier, command name and parameters. The window specifier is delimited from command name by dot as in:

View.Derivative

Command name is written as a original command from a menu, except the blanks, which must be substituted by underscores. The full set of applicable command names is described in Macro Commands. The syntax of parameters can vary from command to command, you need to check the corresponding entries in the Macro Commands section. However, for Options window the syntax is always following: after window specifier “Options” becomes the full name of one of the parameters at apropriate page of Options Window, then comes equal sign, and then parameter value:

Option.Desired_Spectrum=gauss(2000.0,200)

```
Option.Auto_Transform=False

Option.Number_Of_Scans=10

Option.Direction_Of_Scans=0
```

Here are some typical examples of command lines:

```
Save_As c:\data\spec4.spe

Engine.Scan

Pop

Option.Min_Wavelength=450.0
```

Call of other macro (option)

If on a line appears the name of the currently defined macro, it is interpretated as such, that is to say the corresponding macro is executed. The recursion depth of calls can be up to the ten levels. For instance if a macro called “Clear” has body

```
Save_As local.spe

pop
```

then if line

```
Clear
```

appears in the body of another macro, the two above lines are executed.

Call of macro in file (option)

If a line starts with “<” symbol then the rest of the line is interpreted as a filename for macro definition written into a separate file. For instance if there is a file “try.inc” in the execution directory of the Interspec for Windows then the macro line

```
<try.mac
```

will include all the lines in the "try.inc" file into current macro. It is also possible to specify the full path for macros as follows:

```
<c:\spect\macros\mac1.mac
```

The names for macro files are arbitrary, as are also their file extensions. However, it would be good practice to name them uniformly, say with extensions ".mac" or ".inc".

It is also important to note that all simple macros are saved in INI-files of Interspec for Windows. To shorten this file and to make access to it more effective, it is always reasonable to put long macro fragments into separate files and call them through "<name" construction.

Call of macro in DDE server (option)

Every line which starts with a symbol ">" is not interpreted by Interspec software, but is sent to the DDE Server.

Inserts in macro parameters (option)

Every macro parameter (that is text that follows a macro name) can contain inserts. Inserts are constructs which are reformatted or filtered before an actual macro command is executed. Inserts are written between two "%" symbols. For instance:

```
option.%Enter Number of Scans:Int,1,1,100%

write Name of Sample = %Enter Sample Name:NoName%

write Current Apodization Window  = %Apodization_Window%
```

First line activates Input Dialog where the user can enter the number of scans to be performed. The second line writes into Journal sample name from dialog. The "NoName" is default for sample name. Third line outputs to journal current expression for the Apodization Window.
The following formats of inserts are recognized by Interspec for Windows :

- Name of the variable (%Number_Of_Scans%, %Min_Wavelength% etc.)
- Inserts which activate Input Dialog must contain ":" symbol.

The inserts which activate an Input Dialog must the follow general pattern:

```
%Dialog Caption : Parameter Type, Parameter Default, Parameter Minimum, Parameter Maximum%
```

where Parameter Type can be “String”, “Integer” or “Float” (case is not important). There are many shorthands available to this general pattern.

- The “String”, “Integer” and “Float” can be shortened to “S”,”I” and “F” or “s”, “I” and “f”.

%Enter Minimum Wavenumber:Float,400.0,100.0,1000.0%

%Enter Minimum Wavenumber:F,400.0,100.0,1000.0%

For “String” type inserts, Parameter Minimum and Parameter Maximum are not needed, if Parameter Type is not given then it is assumed to be “String” and the characters after “:” symbol are considered to be default value. If there is nothing after “:” symbol the empty string is considered as default.

%Sample Name:String,NoName%

%Sample Name:S,NoName%

%Sample Name:NoName%

%Sample Name:%

If Parameter Default, Parameter Minimum or Parameter Maximum is absent, then zero or empty value is assumed.

%Number of Scans:Integer,1,1,100%

%Number of Scans:I,1,1,100%

%Number of Scans:I,1% **Default is 1, Min and Max are not specified.**

%Number of Scans:I% **Default will be zero (dangerous here!)**

1.4.6 Mathematical modelling of desired spectra (emulation)

INTERSPEC programs contain a unique feature for modelling the spectra allowing the user to work with computed data using software routines only. You may also check your results with the help of mathematical methods. For example, if you require a Gaussian spectrum, simply set the check button Emulation in the

Spectrometer Operations dialog, specify Gaussian expression in the Options/Emulation section. Then run "Virtual Spectrometer" with the command Start. The result is a perfect Gaussian spectrum. If you want to see the interferogram of this Gaussian spectrum, remove the Auto Transform check button in the Options/Scan section before starting the scan.

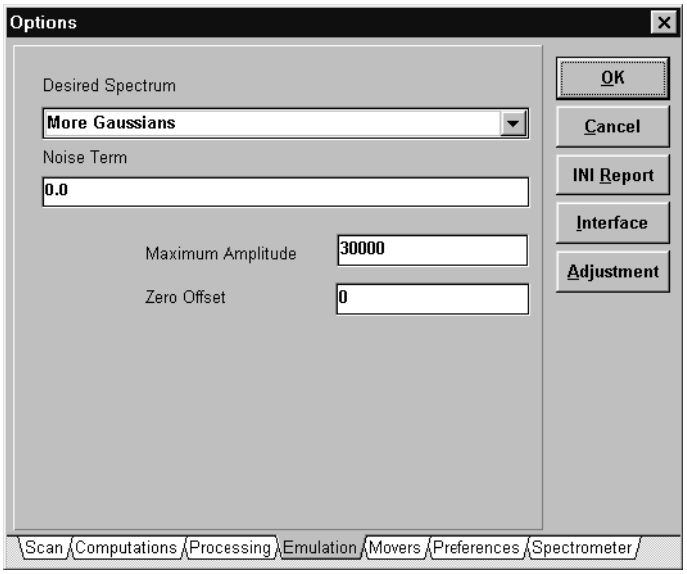


Figure 4 Emulation page in Options menu

With this feature it is very simple to teach other users the value or use of simulated data. You can specify expressions to generate spectra. You may, if you wish, add noise to this spectrum and specify the amplitude of the interferogram or perhaps define the ZPD stability.

In the Options dialog there is a special section to set modelling parameters. Simply run Options and select the Emulation page from the notebook.

1.5 Automatic journal

All actions in INTERSPEC are written into the Journal. To track work done so far you can use the View/Journal command.

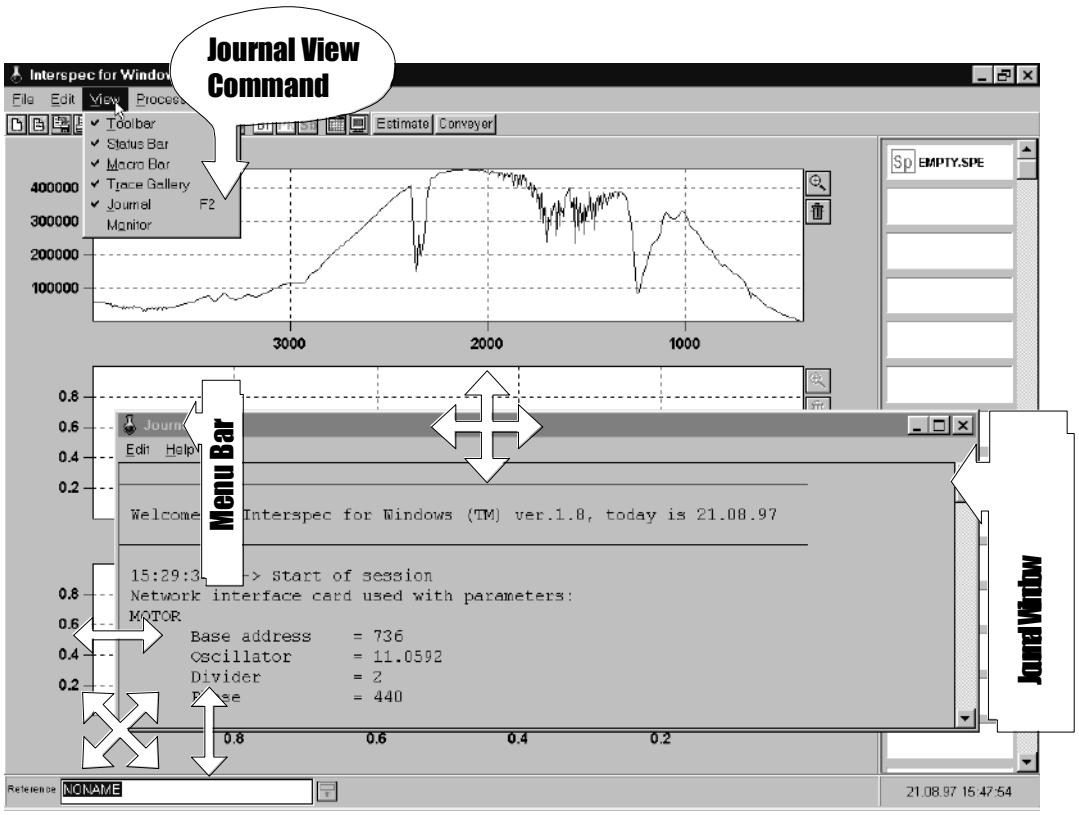


Figure 5 Intespec journal viewer - editor

The maximum size of the Journal is not limited. Journal is not a permanent file and is removed from memory after the session has ended.

Before closing the INTERSPEC program you will notice that the dialog box will ask if you wish to "Save your results or not". To save your results, you must enter the correct file name and click OK.

You will also be asked for the "Append" checkbox in the dialog screen. If you check this, all of the data in the listing will then be added to the end of the file with the name that has just been entered. If such a file is absent, then it can be created. The default name for output is INTERSPE.REP.

The journal viewer is a very simple text editor like for example MS Windows Notepad. All actions that can be made in the Notepad, can also be made in the Journal.

As you will see, the names of the keys relate to moving the screen relative to the data, not the data relative to the screen. This is quite traditional for text editors and other similar programs. The Journal width is 80 columns. Data is normally not shifted to the extreme left because, as a rule, the most important numbers are always displayed on the left side of the row.

Marking is very simply made by following the standard Windows procedure. Move the Cursor to the beginning of the segment and then, keeping your finger on the left

mouse button, slide across the text to the end of the selected segment. The whole segment changes its color from gray to blue and you can distinguish it visually.

After marking, the Output Listing contains the lines of two colours: normal and selected. When you now press the F2 Print key the lines with selected color will not only be output to the file but will also be deleted from memory. When you press the Delete key, the selected lines only will be deleted.

1.5.1 Output Listing in Online Mode

You can resize the window and move it to the desired place on the screen.

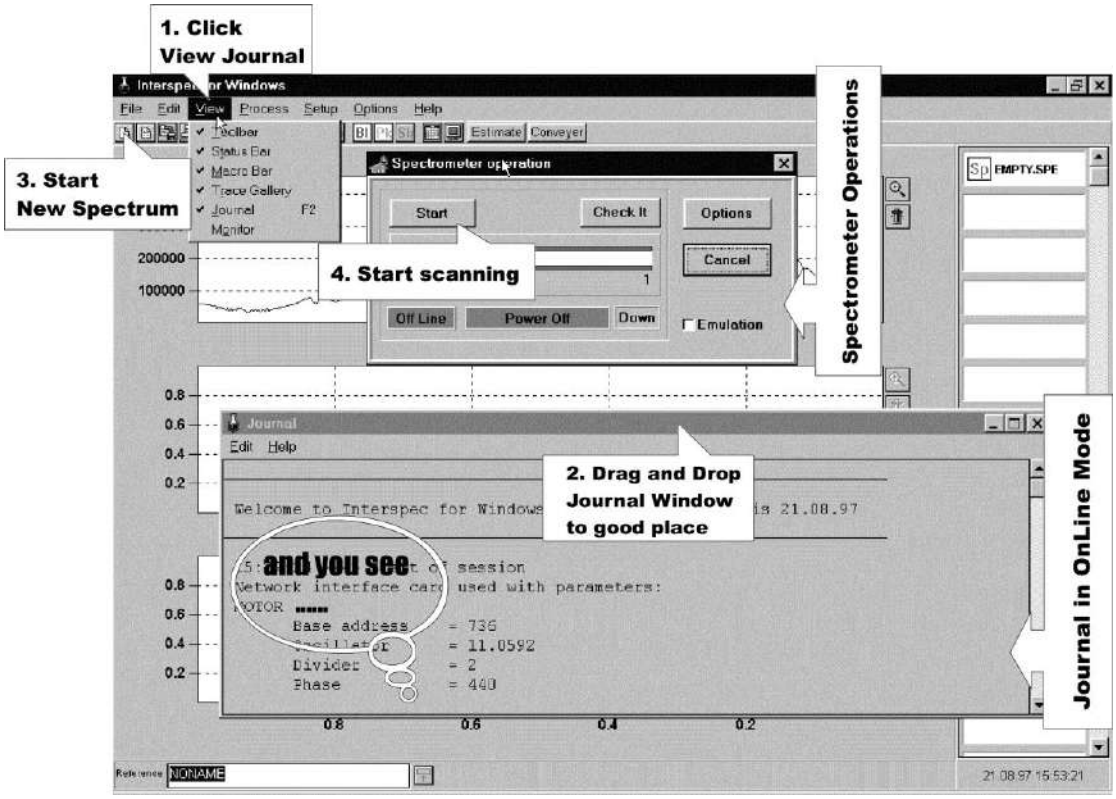


Figure 6 Setting journal to online mode

Some algorithms (like the "New" command in the INTERSPEC software) work iteratively and it is useful to scan computed results in time with actual calculations. This is because if the INTERSPEC program does not close the Output Window in time for some calculations to be completed, then you may follow computations visually.

The second method is defining automatic parameters in the Options /Preferences page.

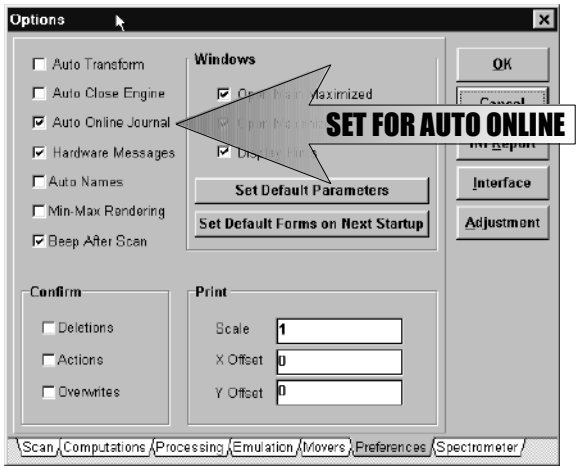


Figure 7 Checkbutton for setting journal to automatic online mode

2 Quick Guide

How to obtain a simple polystyrene or similar spectrum.

2.1 STEP 0. Start

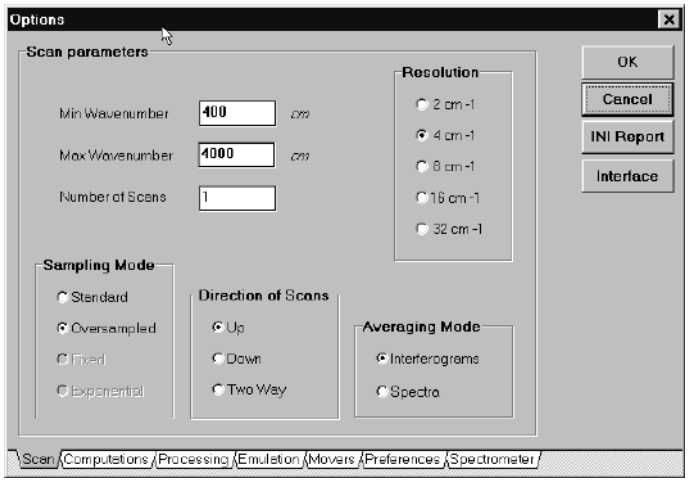
Turn on your spectrometer.

2.2 STEP 1. Testing the spectrometer

Command (File)/New/Check It For testing spectrometer.
If you wish to see more detail then open before Browser (Options/Preferences/Auto Online Journal)
If you are not able to observe this information you will not be able to obtain a spectrum and you should use the Trouble shooting procedure.

2.3 STEP 2. Checking parameters.

Run INTERSPEC for Windows. Check the Scan Page in Options dialog. The parameters must be seen to be correct. The following setting will normally give acceptable results with 1 scan and 4 cm-1 resolution in the UP or Down direction.
Example parameters: **New/Spectrometer Operation page** - Emulation-off. **Options/Scan page** - Min. Wavenumber-400; Max. Wavenumber-7000; Number of Scans-1; Resolution-4; Sampling Mode-Oversampled; Direction of Scan-Up.
Options/Computations page - Zero Filling-2; Apodization-on; Window-cos4.



.

Figure 8 Scan page in Options menu

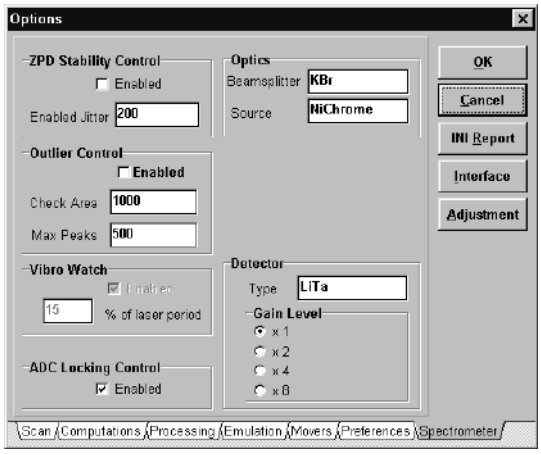


Figure 9 Spectrometer page in Options menu

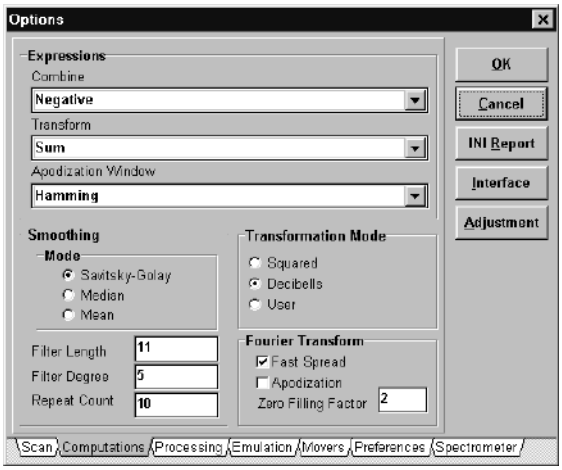


Figure 10 Computations page in Options menu

All other parameters are unimportant at this stage.

2.4 STEP 3. Taking a reference spectrum

Close the cover with an empty sample chamber. You will now be able to obtain a reference spectrum.

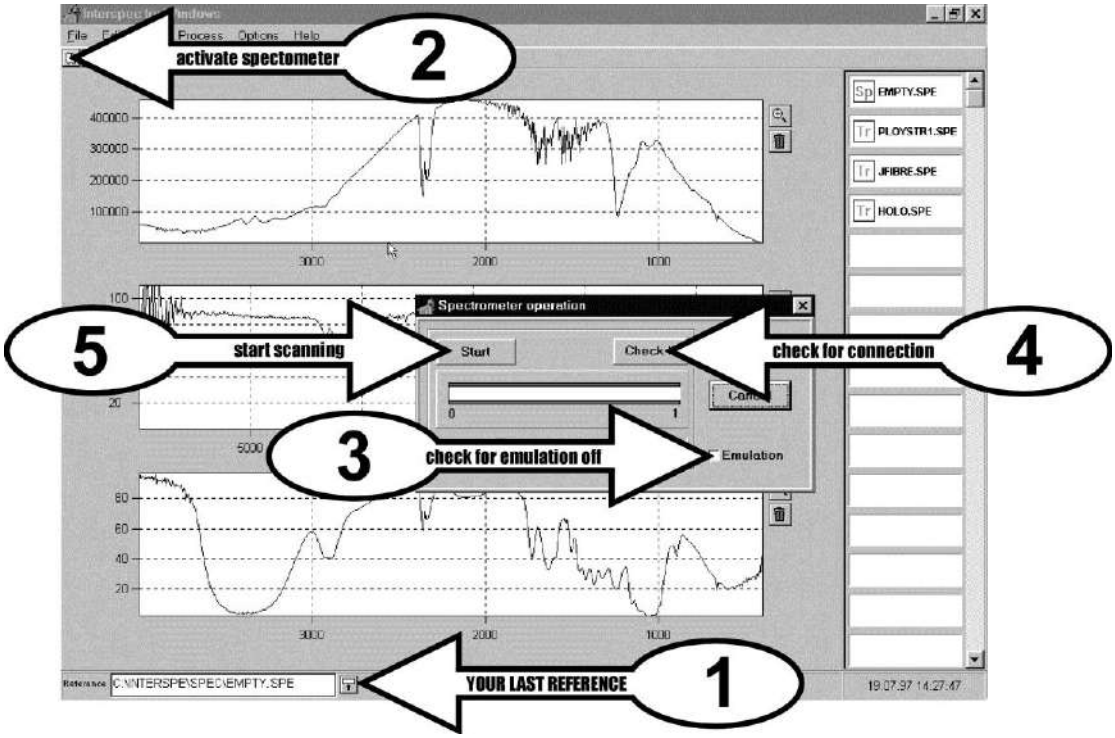


Figure 11 Start scanning procedure example

Click New/Start and you will see the spectrometer status "Wait for scan 1" - this is a normal operation. The progress bar indicates how many scans have been performed. After 1 scan you will see a new spectrum on the top of the stack. This is an empty sample chamber spectrum.
You will need to define this spectrum as a reference. Press Use As Reference (Rf) speedbutton. The spectrum will be hidden from the stack. You may now obtain the spectrum of interest - Polystyrene in the present case.

2.5 STEP 4. Making a polystyrene spectrum

Insert the polystyrene test sample into the sample holder. Close the covers. Then try to make STEP 3 once more. After the end of the scanning period you will see the scanned polystyrene spectrum on top of the stack. Press the Convert To Transmittance (Tr) speedbutton. On the top of the stack is now displayed the transmittance spectrum of polystyrene. Examine wavenumber values of polystyrene spectrum at 2849.5, 1601.2 and 1028.3 cm^{-1}. Check the wavelength setting of reference laser if polystyrene spectrum is not in a good match (+/- 1 cm^{-1}) with these values.

2.6 STEP 5. Saving the result

If you do not wish to use Windows in this way, then we would suggest that you look at the previous File Operations section of the Data Manipulation paragraph.

The default spectrum to be saved is the current spectrum at the top of the stack. Enter the command File/Save or use the speedbutton Save. You will see the Windows standard file operations dialog box. Select the folder you want to store your spectrum in, enter the name of the spectrum (up to 256 in Windows 95). Then press OK button. Your spectrum is now stored on hard disk for future use.
The same operation can be made using the mouse right button and clicking the appropriate window in the trace gallery. Now enter the command Save and follow the above mentioned instruction.

2.7 STEP 6. Printing

Print options, including scaling, orientation and plot colours can be set in the File/Print Setup or Options/Preferences/Windows. In the same page you can click and mark the following options:

*Open Main Max - when you start the program, the main screen will be opened to its maximum size

*Open Maximized - all screens will be opened in their maximum size

*Display Hints - a small yellow box with the name of the icon or short cut key in it will be displayed when pointed at by the mouse.

If unmarked, the screens will be opened in their minimized version and the hints will not be displayed.

The program uses the Windows default printer and settings for this printer. You can change these settings with the command File/Print Setup. If you use the speedbutton for printing, the screen is printed without a preview, if you want to see the preview, then enter the File/Print Preview command.

The program prints on a one to one basis of the image you see in the working area of the screen. Before printing it is recommended to add labels, select fonts and tick the size of your choice in File/Page Layout. If you have a color or a good laser printer you can change colors as you wish, including line, foreground and background colors. Simply click your mouse right button in the desired area and make your choice.

2.8 STEP 7. Exit from the program

Select the command File/Exit or simply click "x" in the upper right part of the screen. The program will ask if “You want to save your results”. This means that the program will try to save both the Journal and all files in the spectra stack. If you want to save the Journal, enter the filename for the output listing text file and click the OK button. Then the program will ask first for the modified spectra marked with an asterisk and then for the unnamed spectra on the stack - starting with the topmost spectra. You can if you wish, cancel this facility in Options/Preferences.

3 Functionality

3.1 Spectrometer Operations

This section includes a description of the commands necessary for operating the spectrometer. For this you can activate the Spectrometer Operation dialog box with the possibility of direct access to parameter options.

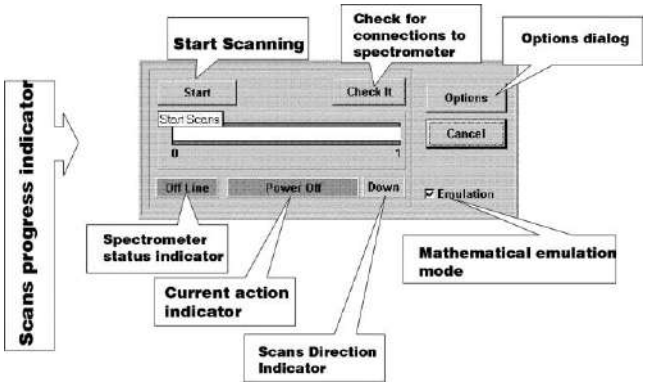


Figure 12 Spectrometer operations menu window

You can activate the spectrometer operations to all screen modes and editors. For this there is a command called NEW. Asking for a new spectrum will open the Spectrometer Operations dialog box.
The Options settings are described in the section 5.2 for "Obtaining a spectrum".
"CHECK IT" is the parameter used to start the spectrometer test procedures. First the interface cable reliability is tested and then the data transfer quality. The last is a test to ensure that the interrupts have been installed correctly. If these test results are correct then the spectrometer status indicator light is seen to be green "On Line", if something is incorrect, the indicator will show red "Off Line". The current action indicator displays the current state of the spectrometer.

"START" starts the collection of data sets. Preconditions for starting are:

- The spectrometer is switched on (Emulation=off) or the spectrum modelling system is turned on (Emulation = on)
- All Options parameters relate to your requirements

Execution of the Scan command can differ depending on the state of the checkbox EMULATION.

During a Scan, data from the spectrometer is carefully controlled by the INTERSPEC system including the ZPD of the interferogram and system stability . The stability of the spectrometer PLS™ motor is also controlled and any imperfect data is rejected.

All control system levels can be changed or switched out as required (Options dialog Spectrometer page).

Emulation ≡OFF is the main mode of the program. Entering the command START will initialize the spectrometer and will always result in a spectrum. Now you have to wait for the spectra to be measured as defined by your selected number of scans. Further activity will be seen on the screen unless you wish to see the interferogram. Should this be required the user can clear the checkbox in the Options/Preferences/Auto Transform. By entering this mode you will be able to see the last collected interferogram. You can convert this manually to a spectrum with the command SPECTRUM (Sp) in the Speed Bar.

Emulation ≡ON - here the mathematical modelling of spectra is defined. The spectrometer itself is not addressed at all. The acquired spectrum is determined by your choice of Options dialog Emulation section parameters and the user defined expression of Model Spectrum. In this mode the START command works, the only difference being that data comes from the defined spectrum generator instead of the spectrometer.

3.2 Obtaining a spectrum

3.2.1 Parameters

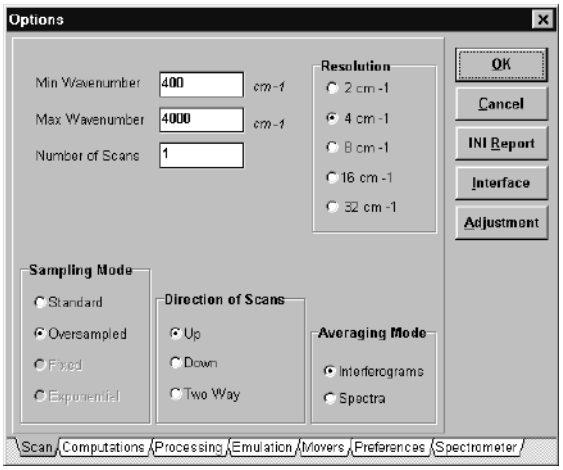


Figure 13 Scan page in Options dialog

Resolution is the smallest frequency or wavelength separation by which two distinct spectral lines of equal intensity can be distinguished. The resolution offered allows a selection between 2, 4, 8, 16, 32 cm-1 in the INTERSPEC IR spectrometer and between 8, 16, 32 cm-1 in the INTERSPEC NIR spectrometer.

Max. Wavenumber enables one to select the desired max. wavenumber within $0 < x < 16.000$ (for IR = 8000)

Min. Wavenumber enables to select the desired min. wavenumber within $0 < x < 16.000$ (for IR = 350)

Number of Scans gives the number of measurements $1 < x < 5000$ (optimal 4-10) averaged by the spectrometer.

Direction of Scans. Scanning of an interferogram is performed in both scan directions from -x to x (up) (x - the farthest point from ZPD) and from x to -x (down). The interferograms are therefore accumulated in both directions relative to ZPD. In practice this produces slight phase anomalies which the system must take into account when calculating spectral features. As the spectral features can be optimized, the user has the opportunity to choose the shape of the interferogram. As the Fourier transform is calculated for a double-sided interferogram, errors may only arise with the summation of interferograms taken from different directions and to correct for these possible errors, the interferograms are stored in different accumulators. The user now has the unique possibility to measure interferograms either in one direction (up or down) or in two directions (up and down).

Averaging Mode. This selects the object of summation of measured data or results and can be either to sum a number of interferograms or to sum a number of already transformed spectra. It should be noted that an improved signal-to-noise ratio is achieved with summation of interferograms, when the SNR is about $\sqrt{2}$ times better than the Nyquist level. Interferogram averaging is the usual mode, spectrum averaging is recommended only when the spectrum consists of narrow spectral lines or features. The interferogram of such a spectrum may theoretically have no recognizable maximum energy limit for the summation algorithm (it may resemble a sine for example). In this case the summation of spectra will exclude incorrect summation.

The signal-to-noise ratio of an interferogram acquired by signal averaging improves proportionally by the square root of the number of scans, if all other parameters are constant.

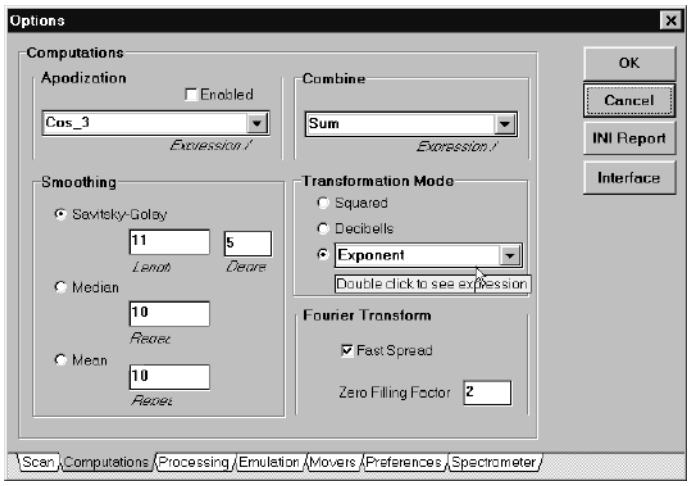


Figure 14 Computations page in Options menu

3.2.2 Annotations

The INTERSPEC software offers a very wide selection of JCAMP standard annotations, such as Afactor, Alias, Aunits, Beilstein Lawson No, Blocks, BP, Cas Name, Cas Register No, Class, Concentrations, Cross Reference, Data Processing, Data Type, Date, Deltar, Deltax, Density, End, Firsta, Firstr, First x, First Y, Spectrometeral Parameters, JCAMP-DX, Lastr, Lastx, Maxa, Maxx, Maxy, Miny, Molform, MP, MW, Names, Npoints, Origin, Owner, PathLength, Peak Assignments, Peak Table, Pressure, Radata, Refractive Index, Resolution, Rfactor, Runits, Sample-Description, Sampling Procedure, Source Reference, Spectrometer / Data System, State, Temperature, Time, Title, Wiswesser, X Factor, XLabel, XUnits, XYData, XYPoints, YFactor, YLabel, YUnits.

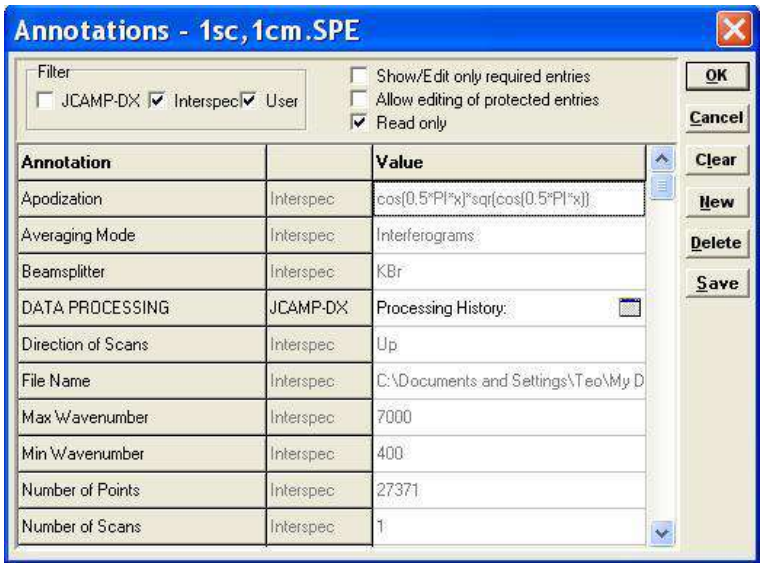


Figure 15 System page in Annotations menu

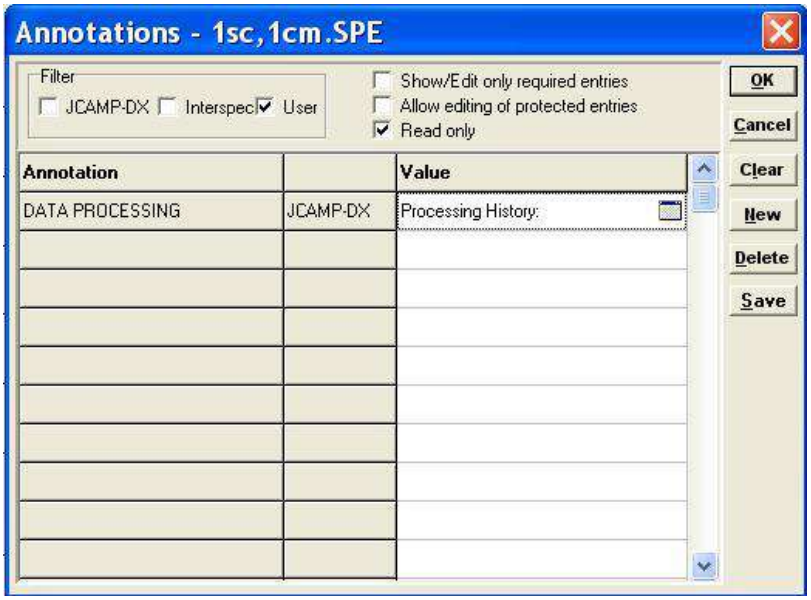


Figure 16 User page in Annotations menu

You will find Annotations dialog by clicking mouse right button in the chosen spectrum box within the spectra stack. You may choose between three annotation screens - System, User and Filter. System screen shows the content of the last saved file. User screen gives only user determined parameters. If you click the selected line, you will be able to insert information. TAB key enables you to move from one column to another, arrow keys enable you to move up and down, and to the left or to the right. If you click Move, you will be able to import the user inserted parameters from the View screen to the Edit screen. The Filter screen shows a table with four columns:

- Annotations
- Type
- Plot
- JCAMP

The annotations column includes a list of annotations; Type column distinguishes three different types of parameters - User (user defined parameters), System (parameters, calculated by the INTERSPEC software) and Constant (parameters, either defined by the program or taken from the .INI file); Plot column allows to mark parameters to be plotted out; JCAMP shows the parameters to be saved in JCAMP files.

Filter screen gives you a possibility to choose what annotations to use in connection with your spectrum. Click the button Filter and you have three options: standard annotations, Interspec defined annotations or user defined annotations. You may choose one, two or all of them. OK button closes the filter window and you see these annotations you just chosen. "v" marks the annotation in the Plot column you wish to plot out with your spectrum in File / Page Layout Annotaion box. "v" marks in the JCAMP column the annotations which will be connected to your spectrum in JCAMP file format for data export.

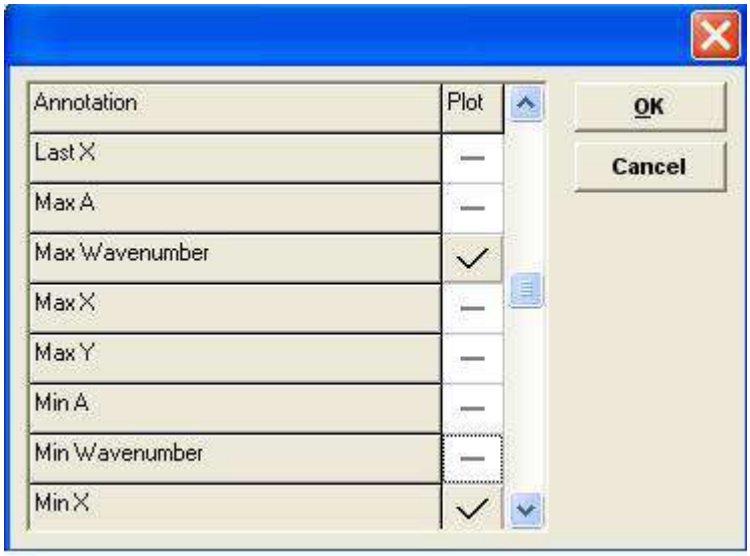


Figure 17 Filters page in Annotations menu

The parameters in the annotations table are marked in two different ways: "□" marks the parameters selected by the user to be calculated and saved, "-" marks the parameters which the user has decided to leave out. To move the Filter screen you can use either arrow keys or the mouse.

Edit Annotations is a three page dialog which allows one to inspect and edit annotations and select subsets of annotations for printing and including into the files to be exported.
The System Page allows to inspect annotations which are generated by Interspec for Windows and to use the Scroll Bar to navigate among the entries.
The User Page allows one to enter and edit annotations which must be set by user. Use Scroll Bar to navigate among the entries. Click on the entry to be inspected or edited. Click on the edit field in the bottom of the page to enter or edit current values.
The Filter Page displays a full set (determined by general filter setting) of annotations. Use Scroll Bar to navigate among the entries. Click on the entries in Plot or JCAMP column to change terms of annotation. The entries in Filter Page can be in four states:

Excluded by System
Excluded by User
Included by System
Included by User

You can change the term Excluded by User to Included by User and *vice versa*. You can not change terms set by the system. There is a column of buttons in the Edit Annotations Dialog. They function as follows:
OK. - Press this button to leave dialog so that the current value in edit field is accepted.
Canc. - Press this button to leave dialog so that the current value in edit field is rejected.
Clear. - By pressing this button you can clear all entries in the User Page or set all Plot and JCAMP column entries to an excluded state.

Add. - This button opens the Input Dialog and you can enter the name for a new user defined annotation. After that the entered name is included into the permanent list and you can work with it as with every other annotation. The names for all annotations are saved in .INI files, and correspondingly, you can also edit them there.
Save. - Save buttons save the current state of user annotations as a pattern. When annotations are generated for a spectra, they will be included automatically. You may wish to save in this way annotations about your general experiment setup, laboratory, etc. in this way.
Filter. - This button opens the Annotations Filter Dialog from which you can select subsets of annotations to be displayed in dialog. The annotations by themselves are not influenced by this choice. The sole purpose of this filtering is to make browsing among annotations more convenient.
Spread. - If you press this button when User Page is open the current annotation an its value is spread to all data sets in the Data Stack. It allows the user to define and fix certain annotation values.
This dialog allows you to select one annotation from the current set of annotations. If you click on the entry already included an annotation will not be selected. (In the context of page the layout design this means that the current label will display an arbitray label and not mirror an annotation).
The full set of annotations is divided into three groups: Standard, Interspec and User. You can include or exclude any of them from displaying in the Annotations Editor. The annotations themselves are not affected by this choice. This option allows one to work with smaller subsets of annotations in the editor.

3.2.3 Sampling modes

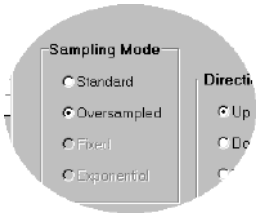


Figure 18 Sampling mode parameters

The INTERSPEC spectrometer offers you several other features for measuring sampling parameters allowing complete optimisation of data acquisition.

They include:

Standard
Oversampled

Standard

In the standard (classical) sampling mode the interferogram is sampled at equal intervals of optical retardation. The sampling interval is based on the laser zero crossing points and is determined by one half of the shortest wavelength of any spectral feature in the spectrum. In the infrared region (4000 - 400 cm-1) the sampling interval is ~ 1,2 microns, in the near infrared region (15 800 - 3000 cm-1) the interval is 0,3 microns.

Oversampled

This is similar to the standard sampling mode with the exception that the sampling interval is shorter than in the standard sampling mode. Here it is possible to obtain better measured results if there is minimum noise outside the short wavelength region to be measured.

3.2.4 Collecting Interferograms

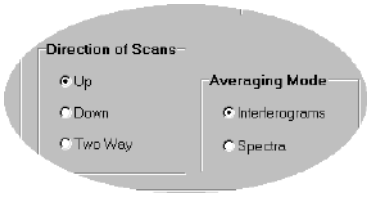


Figure 19 Averaging mode and Scan Direction parameters

Direction of Scans

Scanning of an interferogram is performed in both scan directions from -x to x (up) (x - the farthest point from ZPD) and from x to -x (down). The interferograms are therefore accumulated in both directions relative to ZPD. In practice this produces slight phase anomalies which the system must take into account when calculating spectral features. As the spectral features can be optimized, the user has the opportunity to choose the shape of the interferogram. As the Fourier transform is calculated for a double-sided interferogram, errors may only arise with the summation of interferograms taken from different directions and to correct for these possible errors, the interferograms are stored in different accumulators. The user now has the unique possibility to measure interferograms either in one direction (up or down) or in two directions (up and down).

Averaging Mode

This selects the object of summation of measured data or results and can be either to sum a number of interferograms or to sum a number of already transformed spectra. It should be noted that an improved signal-to-noise ratio is achieved with summation of interferograms, when the S: N ratio is about 2 times better than the Nyquist value. Interferogram averaging is the usual mode, spectrum averaging is recommended only when the spectrum consists of narrow spectral lines or features. The interferogram of such a spectrum may theoretically have no recognizable maximum energy limit for the summation algorithm (it may resemble a sine for example). In this case the summation of spectra will exclude incorrect summation.

3.2.5 Apodization functions

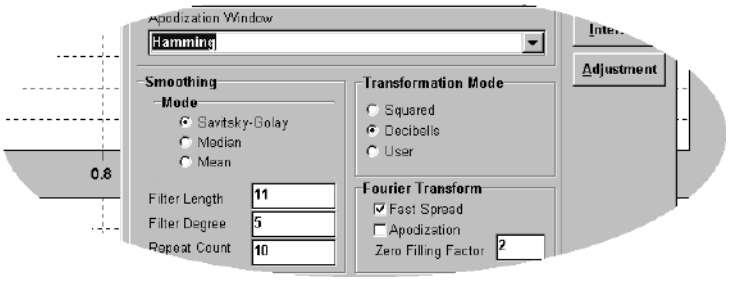


Figure 20 Apodizations expression input line

The user can specify his or her own apodization function or select them from the list provided Apodization Window Box. Apodizations can be enabled or disabled by using the Apodization option. All settings can be changed in the Options dialog Computations page.

Apodization is a mathematical process used to remove side lobes (or feet, hence the name). This will of course slightly reduce the actual resolution. A number of apodization functions are available and the two types commonly employed are:

Triangular or Fejer: This gives slightly lower resolution with no negative side-lobes and somewhat lower noise. It is used for liquid or solid phase samples. The bandwidth is increased by a factor of 1.47.

Boxcar or Dirichlet or no apodization: This allows best resolution with some negative side-lobes and slightly higher noise. It is used in those instances when higher resolution is required (for example, gas phase samples). When data is collected, the interferogram is sampled over a finite distance and effectively truncated to zero at the end of the data file and all information that would be present at longer distances (or

greater optical retardation) relative to ZPD is lost. This causes some distortion in the shape of narrow lines because the information for these lines was truncated at the limit of resolution. The data collected over a finite distance includes in its essence the boxcar function.

When comparing or ratioing spectra the same apodization must be used.

You can choose the following apodization functions:

Dirichlet or Boxcar or no apodization
1.0
Fejer or Triangular
1.0-x
Cos_1
cos(0.5*PI*x)
Cos_2
sqr(cos(0.5*PI*x))
Cos_3
cos(0.5*PI*x)*sqr(cos(0.5*PI*x))
Cos_4
sqr(sqr(cos(0.5*PI*x)))
Hann
0.5+0.5*cos(PI*x)
Hamming
0.543478261+0.456521739*cos(PI*x)
Blackman
0.42659071+0.49656062*cos(PI*x)+0.07684867*cos(2.0*PI*x)
Harris_1
0.42323+0.49755*cos(PI*x)+0.07922*cos(2.0*PI*x)
Harris_2
0.44959+0.49364*cos(PI*x)+0.05677*cos(2.0*PI*x)
Harris_3
0.35875+0.48829*cos(PI*x)+0.14128*cos(2.0*PI*x)+0.01168*cos(3.0*PI*x)
Harris_4
0.40217+0.49703*cos(PI*x)+0.09392*cos(2.0*PI*x)+0.00183*cos(3.0*PI*x)
Riss
1.0-sqr(x)
Rieman
sin(PI*x)/(PI*x+1.0e-30)
Boman
(1-x)*cos(PI*x)+(1.0/PI)*sin(PI*x)
Poisson_2
exp(-2.0*x)
Poisson_3
exp(-3.0*x)
Poisson_4
exp(-3.0*x)
Cauchy_3
1.0/(1.0+sqr(3.0*x))
Cauchy_4

1.0/(1.0+sqr(4.0*x))
Cauchy_5
1.0/(1.0+sqr(5.0*x))
Gauss
exp(-5*x*x)

Whenever you choose a specific apodization function in the Apodization window of the Computation page in the Options dialog, you will see the name of the selected function in that window. When you next come to use the Interspec software, you will not see the usual name, but instead the apodization window will show the formula of the last selected apodization function.

3.2.6 Zero filling

Zero - Filling Factor

When a complex Fourier transform of n interferogram points is obtained, the real output (spectrum) array contains n/2 points and the imaginary array also contains n/2 points. If n zeros are added to the input array, then the real and imaginary output arrays each contain n points, n/2 of which are linearly independent and the rest represent sinc x interpolation between these points. This zero filling smoothes data by calculating more spectral points.

Figure 21 Zero filling input line

For example, if (m-1)n zeros are added to an n point interferogram, the real array in the spectrum contains n/2 points, which are linearly independent and the rest are interpolated. This procedure is known as zero-filling and results in a smoother spectrum. Actual resolution is not improved.

The minimum number of m is 1 and this means that in a normal Fourier transform no zeros are added. The maximum number is 16 and that means that 15n zeros are added to the end of the interferogram. Zero-filling obviously increases the computation time, so there is a trade-off between the computation time and a smoother spectrum.

3.2.7 Spectrometer control

Figure 22 Gain control and optics dialog

The Option dialog for the Spectrometer provides information about the status of the spectrometer and the possibility to change parameters. You can see what type of beamsplitter and radiation source are present in the spectrometer.
Detector type determines what type of detector is used in the spectrometer: LiTa, DTGS, MCT etc.
Gain Level provides an opportunity to raise the output signal level of the detector and is useful for low transmitting samples. Normally gain 1 is used.

3.2.8 Interferogram monitor

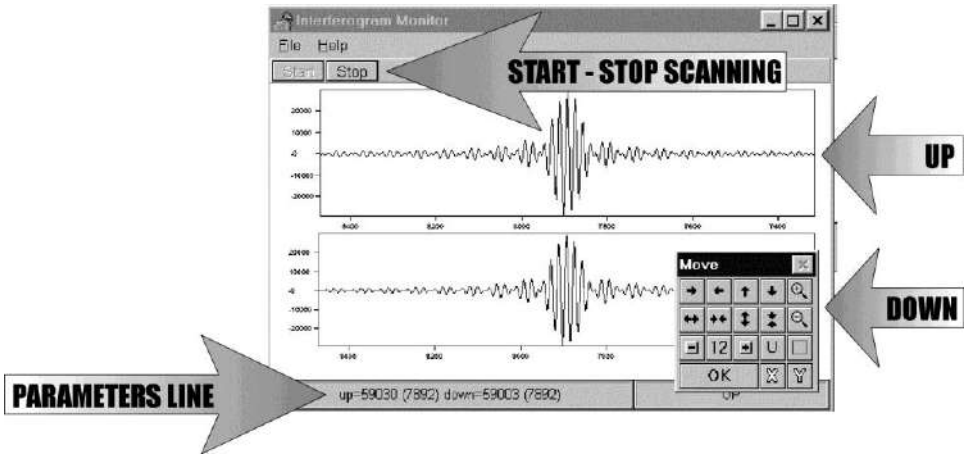


Figure 23 Interferogram monitor screen

There is an icon "Interferogram monitor" in the speed bar of the main screen and this provides an opportunity to look at the interferograms. If you use low resolution scan parameters (Option/Scan/Resolution) for example 16 or 32 cm-1 with a two-way scanning mode, you can obtain a quick display of interferograms. This is especially useful as an aid for accessory alignment.

3.2.9 Tools

There are four types of tools in the Interspec for Windows software:
Movers are small colored rectangles on the Data Display which allow one to edit or label different graphical elements connected to the data or data models.

- **Switch on or off** Movers Tool using Movers Item in Popup Menu.
- **Add** movers by clicking on Data Display.
- **Remove** mover by pressing Alt key and clicking with mouse on the mover.
- **Move** mover by Mouse Dragging.
- **Click** mover with Right Mouse Button to open local Shortcut Menu.
- **Change color** of movers by setting Colors property on Movers Page in Options Dialog.

Movers for feature labels

Depending on the state of the Movers Style option there are one or two movers per feature label on the Data Display. You can drag the movers, but their actual movement depends on the value of the Movers Force Mode option.

Movers for baseline editing

In Baseline Window, movers are use as pivot points to define the model curve for a baseline. Depending on the Interpolation Mode they indicate either the endpoints of local interpolating cubic curves (spline interpolation) or they are corner points for multiline interpolation.

Movers for peak editing

Typically there are three movers for every defined spectral line. The middle mover marks center and amplitude of the corresponding line. The right mover determines the Gaussian component of the composite line profile (Voigt profile) and left mover determines the Lorentzian component. When peak is marked the Lorentzian component is set to zero.

- **Change position and amplitude** of the peak by dragging central mover.
- **Change Gaussian width** component by dragging right mover.
- **Change Lorentzian width** component by dragging left mover.
- **Add** movers by clicking on Data Display
- **Remove** peak by pressing Alt key and clicking with mouse on any of the movers connected to the peak.
- **Click** mover with the Right Mouse Button to open Local Shortcut Menues.
- **Change color** of movers by setting Colors on the Movers Page in the Options Dialog.

Movers for subtracting spectra

Movers in the Subtract Spectra window are used to mark selected points in a spectra to be subtracted.

Grabber allows one to adjust the position of data within Data Window. You can switch Grabber on and off by clicking the Right Mouse button to open the Shortcut menu, and then selecting Grabber. To move data simply drag Grabber along the screen.

Pointer is a tool which allows one to add Movers on the screen. If the Mouse Cursor is used as a Pointer you can click with the left Mouse button to add new movers (Peaks, Feature Labels, subtraction markers etc.).

Mark tool allows one to remove rectangular subsections in the Data Window. Press the mouse left button on the upper left corner of the displayed rectangle and drag the display using mouse to the bottom right corner. After releasing the button the rectangular region will fill the Data Display. You can switch Mark tool on and off by using the Shortcut menu item Mark.

3.3 Spectra manipulating

3.3.1 Calculating Transmittance, Absorbance, Derivatives

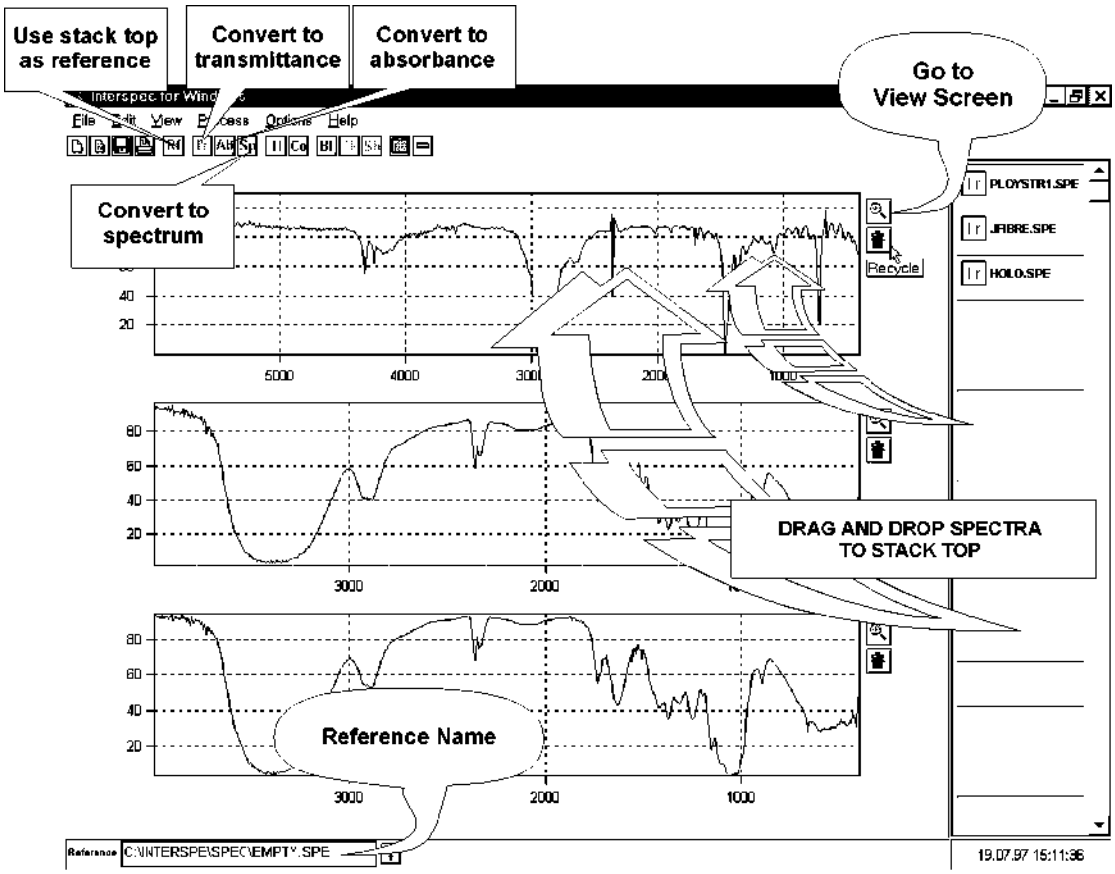


Figure 24 Manipulating with data sets

Spectrum (Sp)

The Spectrum command is carried out automatically when you switch on the Automatic Transform mode in the Options/Preferences section. When the Automatic Transform is switched off you will obtain after a scan, an interferogram. Using the spectrum (Sp) icon you can transform the interferogram into its spectrum.

Absorbance (Ab)

For this calculation you must determine the reference spectrum with the command Set Reference (Rf) on the speed bar. For better results it is advisable to use the same measurement parameters as the current ones.

The absorbance (A) for a sample is the logarithm of the intensities of the incident light (Io) and the transmitted light (I). It is a dimensionless quantity the value of which can be calculated according to the equation:

$$A = \log_{10} \frac{I_o}{I} = \varepsilon cl = \log_{10} \frac{1}{T}$$

where (is molar absorption coefficient, c is molar concentration and l is path length through the sample.

Transmittance (Tr)

The procedure is similar to calculating Absorbance. Determine the reference spectrum by clicking "Rf" icon on the speed bar. If you now click "Tr" icon the uppermost spectrum will be converted into the transmittance spectrum. Transmittance is the ratio of the radiant energy transmitted by a sample to the radiant energy incident upon that sample

$$T = \frac{I}{I_0}.$$

The values obtained for transmittance are given as percentages.

*If you want to find out the positions of the absorption bands in your transmittance spectrum go to the View screen by clicking the magnifier icon in the right upper part of the spectrum screen. Click mouse right button and choose "Movers". Select Options on the Movers page. By clicking the mouse left button near absorption bands of interest both wavenumber and absorption values will be displayed.

*If you click Find Peaks icon Fp, the program will indicate absorption bands and their value. The result depends on values you select for three parameters - threshold global, threshold local and noise. You will find them in the Option menu Processing page. Threshold global determines the value of the transmittance band and may be between 1 and 0. For example, value 0 corresponds to 100% and value 1 to 0%. If select a threshold (glb) value 0.2 absorption bands deeper than 20% will be labeled. Threshold local determines the distance from the absorption minima to a straight line connecting two neighbouring absorption minima. Noise values may be up to 10% and determine the absorption minima where other absorption bands are seen as noise and are ignored

View Window

The view or main screen or window is the most suitable place for manipulating a spectrum. You can move from the main screen or window to the view screen by clicking the icon "View" on the right side of a spectrum. In the View Screen you can manipulate one or more spectra using speed bar icons or the right mouse button menu and dragging spectra from the trace gallery into the view screen. You can erase spectra brought into the view screen starting from the last spectrum using icon "Erase Last Spectrum". Use movers under the right mouse button to mark the spectral features in the view screen. To delete all movers click the icon "Clear Movers". When

you have separated or enlarged a part of your spectrum you may use the icon "Backup Window" for memorising this area of interest. This icon also gives you the possibility to memorise up to five different spectra or parts of a spectrum. You can see them using the icon "Undo Window". When you wish to return to initial spectrum use the icon "Show All".

Derivative (Df)

In "View" window this calculates the derivative of the data set. This function is used to enhance fine structures within a spectrum. If you click once on the "Df" icon you will get the first derivative of the spectrum. Clicking for the second time you get the second derivative. In this way you are able to calculate up to the sixth derivative.
In spectroscopy the technique is used to magnify fine spectral features. It involves calculating the first, the second and higher order derivatives and plotting them in addition to or instead of the normal spectrum. The main advantage of the derivative approach lies in the enhanced spectral features that are obtained, and as the order of the derivative increases, this advantage grows, although the signal-to-noise ratio will decrease.

3.3.2 Baseline correction

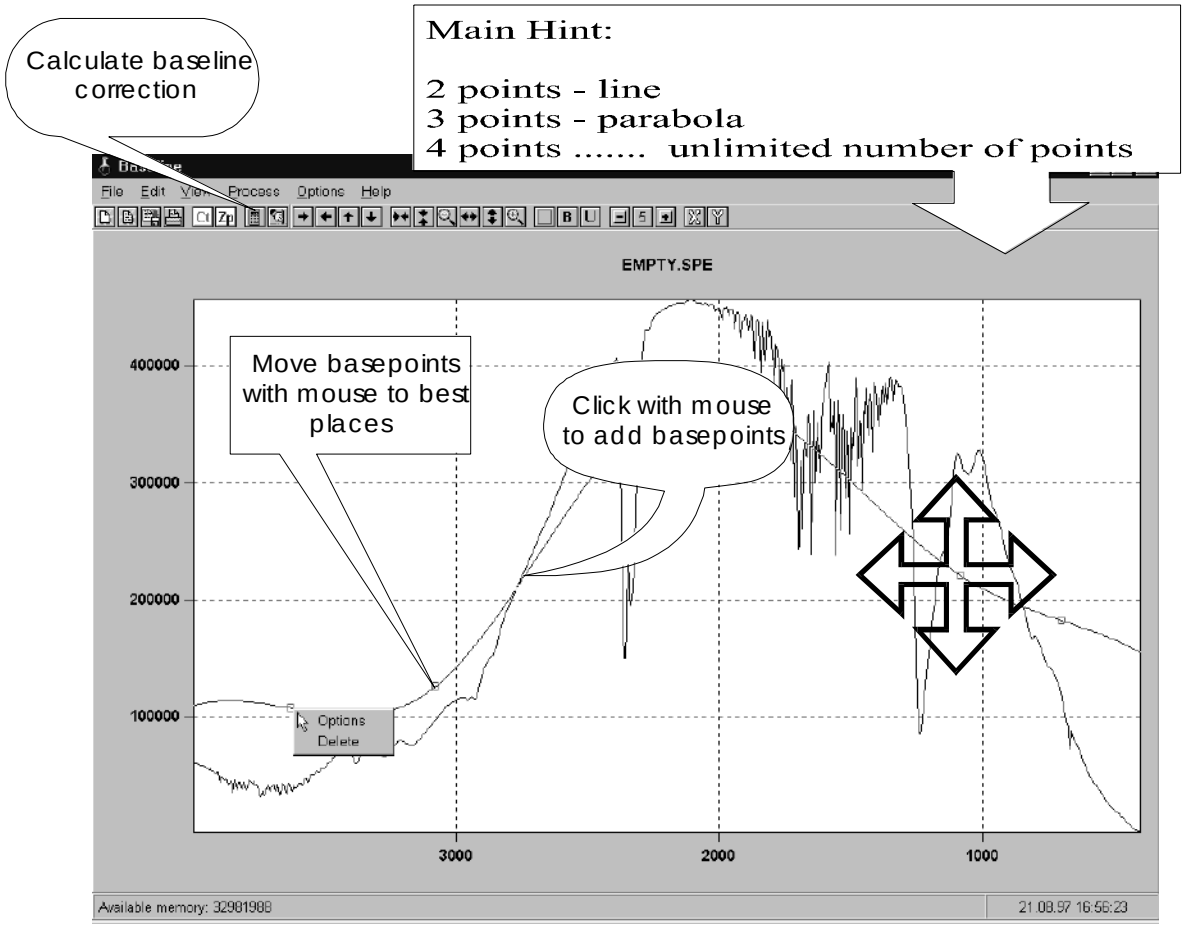


Figure 25 Baseline editor screen

Baseline ("Bl" icon in the menu bar) is an unique INTERSPEC software function, which allows a baseline to be interactively generated from a set of line segments. You can then subtract this new baseline from the displayed spectrum and display both the initial and the resulting spectra. This function can be useful to correct irregular baselines of spectra.

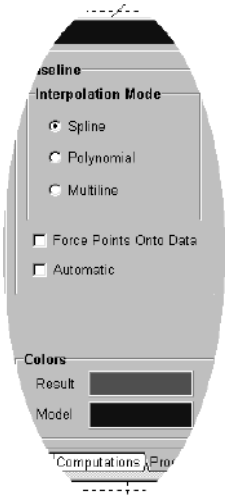


Figure 26 Baseline parameters

To edit the baseline

1. You must have one spectrum on the top of the spectra stack.

2. Click the Bl icon in the main screen. As the system works in a multiple spectra mode, it will use the current spectrum for baseline correction, and temporarily hide other spectra.

3. Besides the Menu Bar and the Speed Bar (see Smart Data Visualization) the opened screen shows the Move Bar, which includes icons with arrows for moving the displayed spectrum in any desired direction. In addition there are icons such as: Back Up (B) - for saving selected screens (maximum memory - 5 screens); Undo (U) - for undoing either the last or one of the previously saved 5 screens (a step-by-step circular action) and Full Screen ( ) - for restoring the initial screen.

4. The baseline screen with the selected spectrum is context sensitive, which means that if you click the right mouse button on any part of the screen you will see different options displayed.

5. Click Options/Processing and choose the baseline interpolation mode - either Spline, Polynomial or Multiline. Spline will give you a smoother line. Multiline will connect the selected points with a straight line. You can select one of the two other options - Force points onto data (forces the selected points onto the spectral line independent of how far above the line they have actually been marked) or Automatic.

Automatic performs the baseline correction without any user interaction, making it the easiest method to use. It automatically fits the best straight baseline to the "non-peak" areas of the data. **It should be noted however, that the automatic method is optimized for use with absorbance data.** The algorithm used here is the following: A least squares line is made to fit through all the points in the spectrum. The number of points above and below the line are counted. If there are less points above the line than below, they are considered peaks and discarded. The process is then repeated until the number of points above the line is less than or equal to those below the line. The calculated line is then used as the baseline and on command, it is subtracted from the spectrum.

6. Mark as many points on the spectrum baseline as may be required. You will see small red boxes (movers) connected with a blue line (the user can make his own choice of colors). If you want to delete one or several points, move the cursor onto the selected point, hold Alt and click the mouse left button. If you want to delete all movers, click the Clear Movers icon in the toolbar and then click Y (yes) or N (no) to confirm or cancel the command in the Confirm Window. The baseline is automatically updated when points are added or deleted. To change endpoints, click near the end of the baseline and drag up or down. X movement is not allowed for endpoints and will be ignored if attempted. Having obtained a new line click the Calculate icon in the menu bar for the calculation of baseline correction.

7. Wait for a few seconds for the baseline corrected spectrum.

8. Leave the baseline screen by File/Exit to return to the main screen. You will now see displayed two spectra - the original and immediately above it the baseline corrected spectrum. The name of the baseline corrected spectrum will appear in the Trace Gallery marked with an asterisk to distinguish the modified spectrum.

9. If you want to make other changes to the output result, follow the above baseline correction procedure. For a more detailed inspection go to the view mode by clicking the view icon on the right of the upper spectrum. You will have displayed two views - the lower one shows the complete spectrum and the upper one shows the enlarged section marked in the complete view. The icons in the menu bar offer you the following possibilities:

Smooth (Sh)
Transform (Tr)
Derivative (Df)
Cut (Ct)
Zap (Zp)

Smooth treats the spectrum with the filter selected in the (Smoothing/Filter Type) section of the Computations parameters in the Options menu. Transform, treats the spectrum with the transform selected from the Transform Expression section of the Computations parameters in the Options menu. Derivative is a mathematical function showing the places, where the function changes. The quicker the changes the bigger the value of the derivative. Here only the marked section of the spectrum is being observed. You can mark a section either in the upper window or in the lower window.

Cut enlarges the selected part of the spectrum to the upper screen for further treatment. Zap enables one to mark and delete a selected section of the spectrum.

10. Having obtained the desired visual result, return to the main screen by File/Exit.

If you save the Baseline screen before calculating the baseline correction, the main screen will display the initial spectral line without the edited line, but if you open the baseline screen again, you will see both the original and the edited lines.

3.3.3 Smoothing

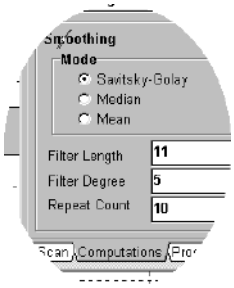


Figure 27 Smoothing parameters

In "View" window you can use three smoothing functions clicking the icon "Sh". The smoothing icon activates the user defined filter in Option/Computation page - Savitsky-Golay, median or mean type filter.

Savitsky-Golay smoothing is based on the method described by Savitsky-Golay (Savitsky and Golay, Analytical Chemistry, vol. 36, p. 1627, 1964.). This method uses a convolution approach which performs a least squares fit to a specified "window" of data points. Smoothing is controlled by the degree of "polynomial" and the length of smoothing segment. The degree of "polynomial" specifies the order of the polynomial to fit over the specified length of smoothing points. Thus, the larger the length of points specified and the lower the order of the polynomial, the heavier the smoothing. The length and number of smoothing points must be one more than the "degree of polynomial". The value of the "length" can range from 2 to 100 and that of the "degree" may range from1 to 99.

Median smoothing activates the "window" consisting of three points and determining the "median" value of these three points. Suppose for example you have the following sequence - 2, 7, 5, 11, 15, 3. Four median values are - 5, 5, 11, 11. "Repeat" parameter determines how many times such a filter makes to the smoothing operation over the data set. "Repeat" parameter can range from 1 to 500.

Mean smoothing activates the "window" consisting of three points and determining the mean value of these three points. It will let you have the above mentioned data sequence - 2, 7, 5, 11, 15, 3. Four mean values are - 4.66; 7.66; 10.33; 9.66. "Repeat" parameter can range from 1 to 500.

3.3.4 Peak edit

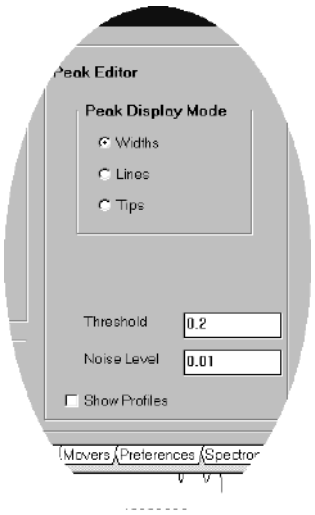


Figure 28 Peak editor parameters

Peak editing also known as Curve fitting or Deconvolution, allows overlapping bands to be analysed and modeled as the sum of fully-resolved ideal peak functions. Peaks can be modeled as Gaussian, Lorentzian or Voigt curves. Peak Edit allows you to point on the screen with a mouse to approximate the peak locations while showing the residual curve. You can see displayed the original (black line) and the fitted profile curve (a green line connecting small red squares - peak points) and also the calculated summary curve (blue line) as the application operates. If the profile curve and the calculated curve coincide, the result is a red line. (The given default colours can be changed by the user.) This process is very fast. The maximum number of peaks is limited only by the available memory.

The conventional peak editing procedure is as follows:

* Select a saved spectrum with File/Open or take a new spectrum with File/New. The spectrum will appear in the topmost view box.

* Click the Pk (Peak Edit) icon in the main screen. If you have more than one spectrum displayed in the main screen, the topmost will be chosen and displayed in the peak editing screen for peak editing and the multiple spectra mode will temporarily hide the other spectra.

* The peak editing screen is context sensitive offering selection boxes. (For more information see Smart Data Visualization). Click the mouse right button in the

central part of the screen to get the selection box and click Movers before you start to mark the selected peaks. If you click options / Processing / Peak Editor you will be offered the following choice of Peak Display Mode for the convenience of the user: Width, Lines and Tip.

* Now click the approximate peaks which will be displayed as red squares connected by a green line. To delete a selected peak press Alt and click the red square or click the right mouse button on the peak and select Delete. If you want to delete all marked peaks, click the Clear Movers icon in the toolbar. You will also see a blue line above the spectrum showing the summary of the user selected peaks (the user can make his own choice of colours). If you click the right mouse button on a peak box, the selection box will show the choice of Info/Delete. Delete clears the selected peak, Info saves such data in the journal as position, height, Lorentz FWHM and Gauss FWHM. To see this information open Peak Edit/View/Journal. You can also choose either continuous tracking (the numerical value of each mouse movement can be followed in the Crosshair Display) or Profile.

- If you click the Peak Edit icon Fp (find peaks), the program will perform the peak finding operation itself. The result depends on the values you give to three parameters - threshold global, threshold local and noise. You will find them in Option menu Processing page. Threshold global determines the overall level under which the transmittance or absorbance peaks are situated and may be between 1 and 0. For example, value 0 corresponds to 100% and value 1 to 0%. If you give to threshold (glb) a value 0.2 it means that absorption bands deeper than 20% will be labeled. Threshold local determines the distance from the absorption minima to a straight line connecting two neighbouring absorption minima. Noise values may be up to 10% and determine the point where other absorption bands are taken as noise and are neglected.

*For the best results you should first try to resolve the bands. To start with, you should determine the section you want to "clean". Mark 3 to 5 points and try to achieve manually the best possible result by moving the peaks so that the blue line coincides with the initial spectrum as much as possible. To do so click and hold (drag) the selected red square and shift it in the desired direction. In the beginning you see two little red boxes and one cross in the centre of the user inserted peak. The inserted peak has a Voigt type spectral curve consisting of Lorentzian and Gaussian components. In the initial stage the Lorentzian curve is zero and the inserted peak is a pure Gaussian type spectral peak. If you drag the centre cross to the left you get Voigt type curvature. In this case you have three red boxes. The left one determines the Lorentzian component of the spectral peak, the right box determines Gaussian components of the curvature and the topmost box determines the height of the peak. For fitting the peak you can drag all three boxes to reach the best coincidence. When your peak has a red box on the left and a cross in the centre of the peak you have a pure Lorentzian type curvature. If you now click the curve fit icon Cf, the program will try to model the best combination and fit the new line into the original one.

* Click the Calculate icon for the resultant spectrum which is the original spectrum minus peak summary.

* Leave the Peak Editing screen with File/Exit and return to the main screen. The edited spectrum will be displayed in the topmost viewbox and its name will appear in the Trace Gallery marked with an asterisk.

* For further treatment go to the view screen by clicking the upper icon on the right of the view box. Follow the procedure as presented in Baseline Correction.

* In Peak Edit screen near the bottom you have an option F or O. F means focus and when F is displayed you can use the keyboard to move the cursor emulating mouse movements. O means otherwise and in this case you can use for cursor movements only by the mouse. To shift focus use the Tab Tab key as in a Windows environment.

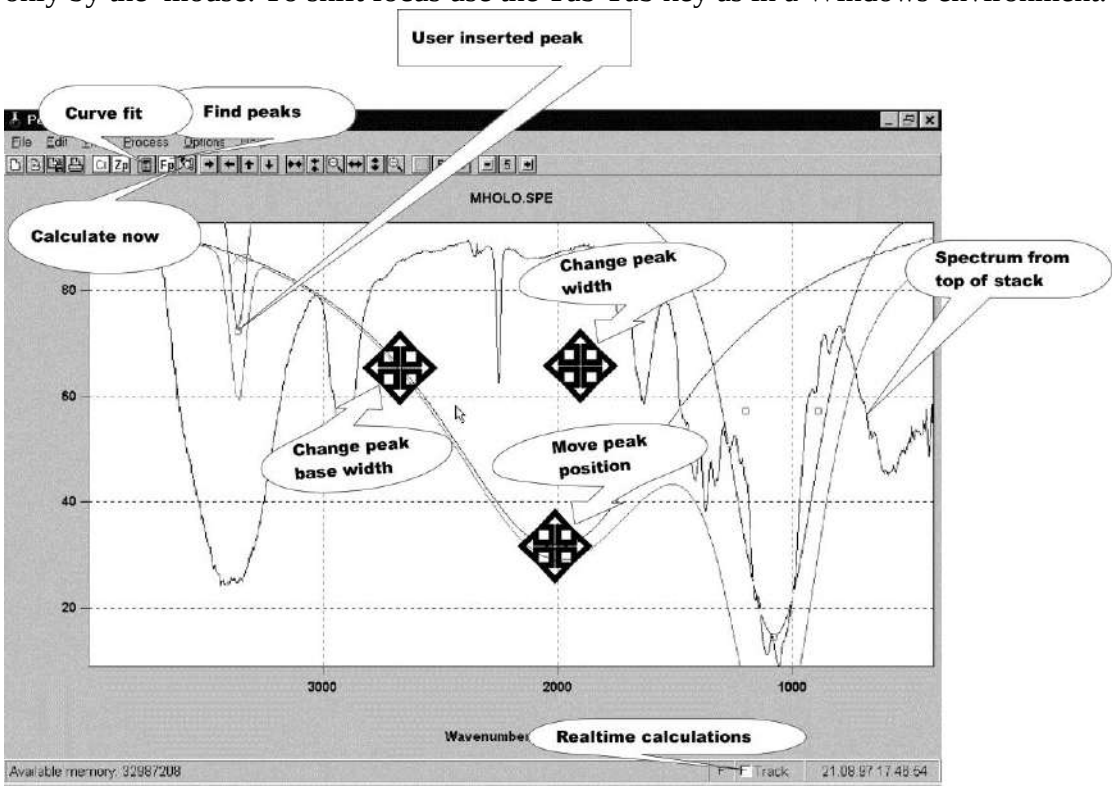


Figure 29 Peak editor screen

3.3.5 Subtraction

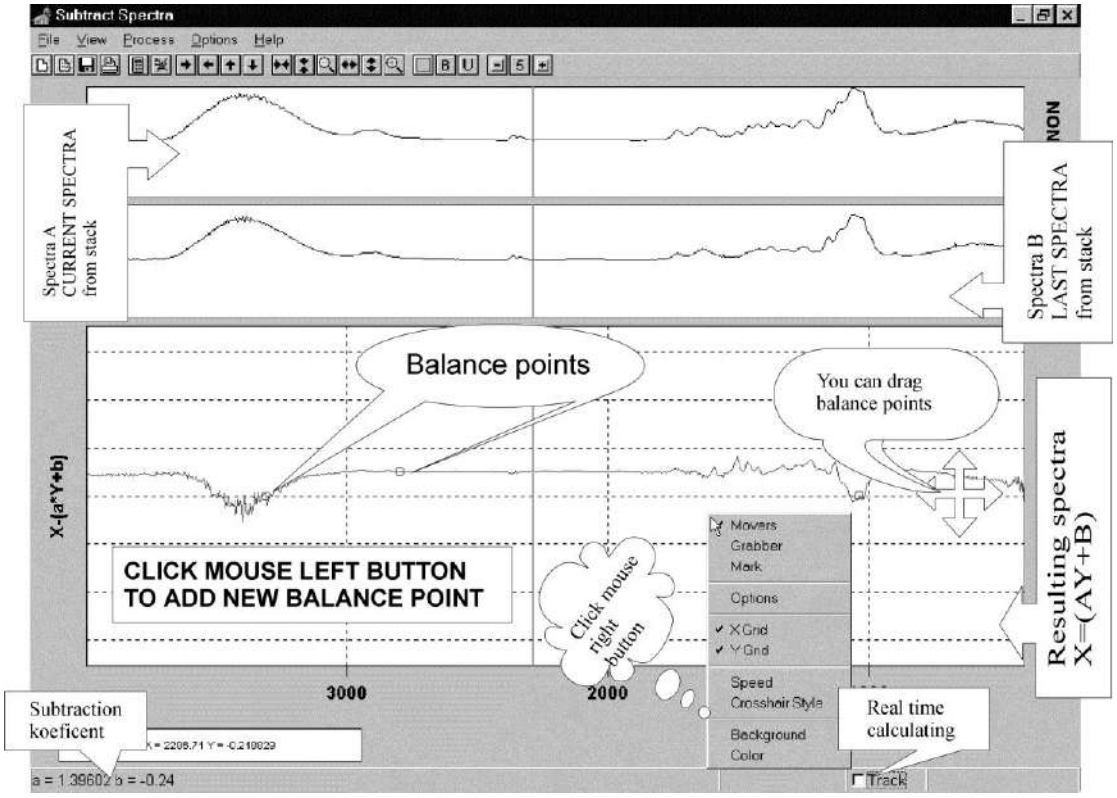


Figure 30 Subtraction screen

Spectral subtraction, also known as solvent subtraction or spectral stripping, enables the user to subtract spectra from one another, especially the spectra of pure components from those of mixtures to derive the underlying peaks for unseparated substances. Interspec software allows quick adjustment for differences in sample concentration and thickness by modifying the scaling factor.

This is useful, for example, for the removal of absorption bands caused by solvents.

The conventional procedure for spectral subtraction is as follows:

Select two spectra either from the top of the trace gallery of the main screen or with File/Open from among the stored spectra;

Click the Sb icon in the menu bar of the main screen which will take you to the context sensitive subtract screen. You will now see three viewboxes. The uppermost will show the user a specified input spectrum labeled X, the middle viewbox will show the spectrum to be subtracted from the upper spectrum - labeled Y, the third and the lowest viewbox will show the resultant spectrum subtracted according to the

formula X-(aY+b). The numerical values of a and b are given in the bottom left hand corner. In the beginning a=1 and b=0. You can change these values marking the resultant spectrum as follows.

Mark and click at least two points in the third spectrum. The marked points will fall onto the spectral curve
Make your choice in the selection box. Having marked the selected points you will be able to drag one of the points, say (xk,yk) to achieve the minimum difference between two curves that are interesting to you. The exact values of a and b parameters can be observed at the bottom of the screen. The difference between the X and Y curve is minimized according to the formula

$$\min_{a,b} \sum_{i=1}^{N} [x_i - (ay_i + b)]^2$$

where constraint for the selected point (xk,yk) holds

$$[x_k - (ay_k + b)]^2 = 0$$

3.3.6 Evaluation of expressions with spectra

Transform Command (Tf) - allows you to apply more complex mathematical expressions to displayed data. The result of the command will depends on the value of the Transform Expression selection in the Options/ Computations. The current data is transformed as follows:

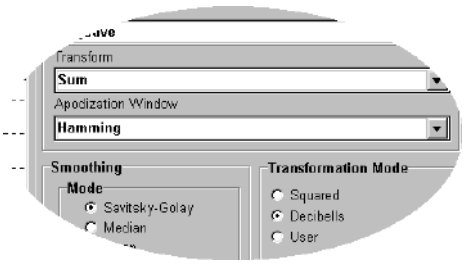


Figure 31 Transform parameters

Amplitude : Y=Abs(Y)
Squared : Y:=Y*Y
Decibells : Y=10.0*log(Y)
Expression : Y=F(Y)

Where F(Y) is the expression entered into the Transform Expression entry box in the Options/Computations page. You can insert your own formula into the transform expression entry box simply printing a new formula into this box. For example x-20, x+0.5, x*1.5, x/3, etc. where x is the spectrum to be transformed.

3.3.7 Combination with a second spectra

Figure 32 Combination expression input line

Combine Command (Co) - enables one to combine two topmost spectra as displayed in the trace gallery. It is very much recommended that you do not forget, which data set you have used for combining, otherwise you might get incorrect results. Combining expressions can be found in the Options / Computations page. Combined expression syntax is described in the 2.4 Data Input paragraph. You can insert your own formula simply printing into the expression entry box a new formula.
For example x/y, x*1.5/y, (x-20)/(y+3), x*3-y, etc.

3.3.8 Cut and zap the desired areas

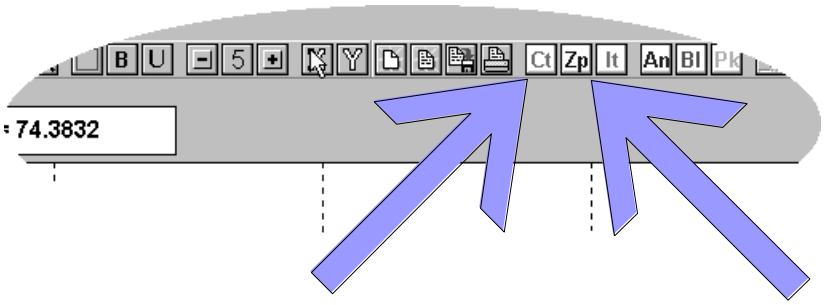


Figure 33 Cut and Zap buttons

The "View" window is the most convenient place for treating a spectrum i.e. to select the required part of a spectrum to be enlarged, reduced, shifted, smoothed etc. When the treatment is finished and you wish to save the result you must use the "Ct" icon.

Cut ("Ct") icon activates the process of cutting the treated spectral region from the whole spectrum and deleting parts of a spectrum. Now you can make smoothing on

this part of spectrum and insert it back to the previous spectrum using icon "It". After cutting you may save the new processed spectral data set.

Zap ("Zp") allows you (contrary to "cut" function) to "blank out" the spectral region you have chosen from the whole spectrum. In this case the selected spectral region is going to be deleated and the remaining part of the spectral data, can be saved.

3.4 Data manipulation

3.4.1 File Operations

File menu includes all activities related to MS Windows file system - creating a new file, opening, saving and printing an existing and current data set. The file menu also includes a special ASCII import/export feature and the JCAMP-DX format import/export and also Galactic.SPC format feature to link the INTERSPEC spectra files with other software or libraries.

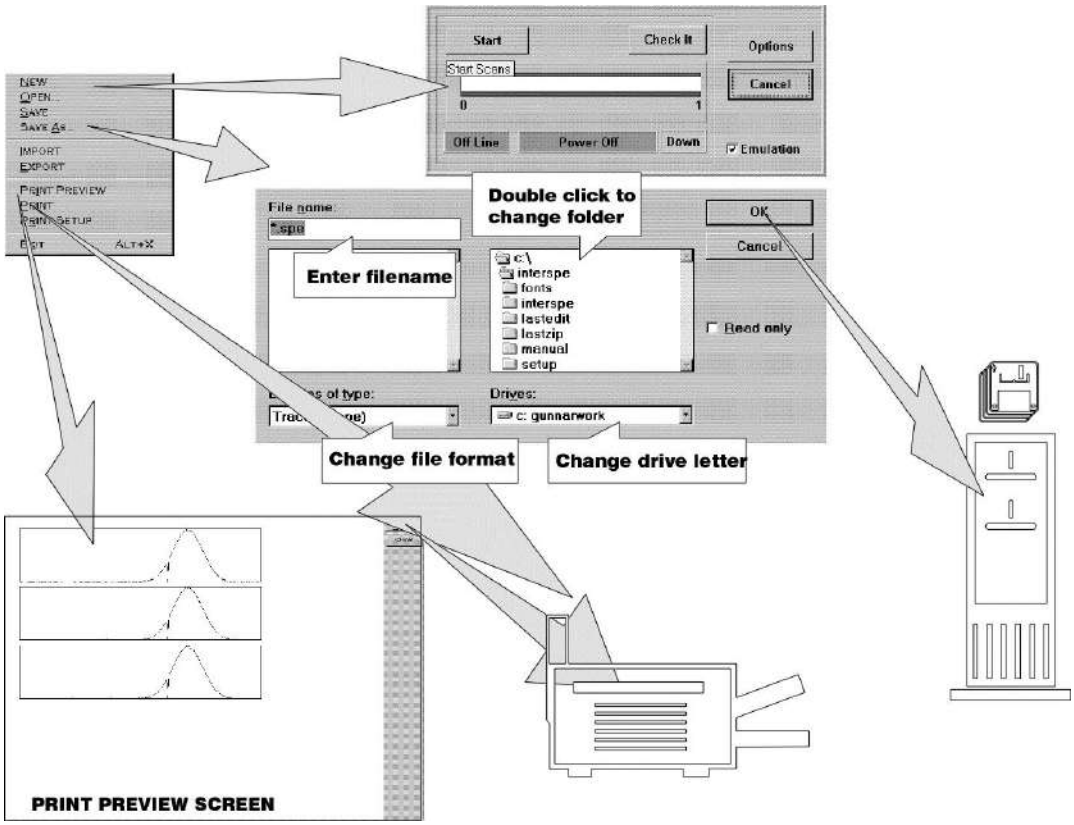


Figure 34 Basic file operations

Open

opens the user specified spectral data with the extension .SPE (INTERSPEC spectra format described on the distribution diskette in file\format\format.txt) using the Windows standard FILE/OPEN menu box. The file is opened from the working directory last defined by the user. After the program startup the default directory is the program working directory. The current directory can be seen on the top of the directory box.

Example: If you wish to save a data set INTERF from directory C:\INTERSPE\SPEC.

be sure that Dir: C:\INTERSPE\SPEC is on the top of the directory box. If not, use the Up and Down arrows to select the right directory.

Now select or type the file name - INTERF. Extension .SPE will be added automatically. Click OK..

There is a list of the most recently used files in the bottom of the File menu. The maximum number of recenly used files is 15. Default number is 4. You can change this in the Option menu Preferences page typing the required number into the MRU box.
You can also open a set of files in the following way. Resize the Interspec software so that you can open Windows Explorer. Activate the required set of files in Windows Explorer and drag it into the trace gallery of the Interspec software.

Save

Saves the current data set in the top of the stack using the Windows standard FILE / SAVE AS dialog box. The same directory rules should be observed as with the OPEN command.

As default, the program inserts the data set name last used. If you do not want to overwrite the previous data set, use a new name (the rules are the same as with the Windows files). Extension .SPE will be added automatically. If a filename has not changed, an overwriting warning will be displayed. If you want to overwrite, press Y, if not, then any other key.

You can change the folder by following the standard Windows procedure in FILE/OPEN or FILE/SAVE AS menu box.

Import

There are 5 types of text formats:

FORMAT	DATA SEQUENCE	VALUES	Extension
format I	Mode	0 – spectrum 1 – transmittance 2 – absorbance 3 – interferogram	.ASP
	Number of points Xmin Xmax y data		
format II	x y pairs		.TXT
format III	x,y pairs		.CSV (comma separated value)
format IV	JCAMP-DX		.DX
format V	Galactic.SPC files		.SPC

File/Import takes you to the File/Open menu box, where you can select a saved JCAMP-DX, ASCII (*.ASP,*.PRN,*.CSV), Galactic.SPC or All (*.*) file and import it to the topmost view box of the main screen. The file with an unspecified extension in the table is treated as a format II file.

Export

FILE/EXPORT takes you to the File/Save As menu box, where you can save the topmost spectrum of the main screen as a JCAMP-DX, ASCII (*.ASP,*.PRN,*.CSV) or Galactic.SPC file format. If you specify other extensions, then format II will be assumed.

Clipboard

You can take your text, data and spectra into the other Windows program using the Cut or Copy command. Using the Main Screen click Setup menu Server page default

Extensions .WMF or .EMF. Now copy your main screen, view screen or page layout screen. After opening a new Windows program for example Windows Word you can insert into this program using the Copy command your selected screen from Interspec software.

Page Layout

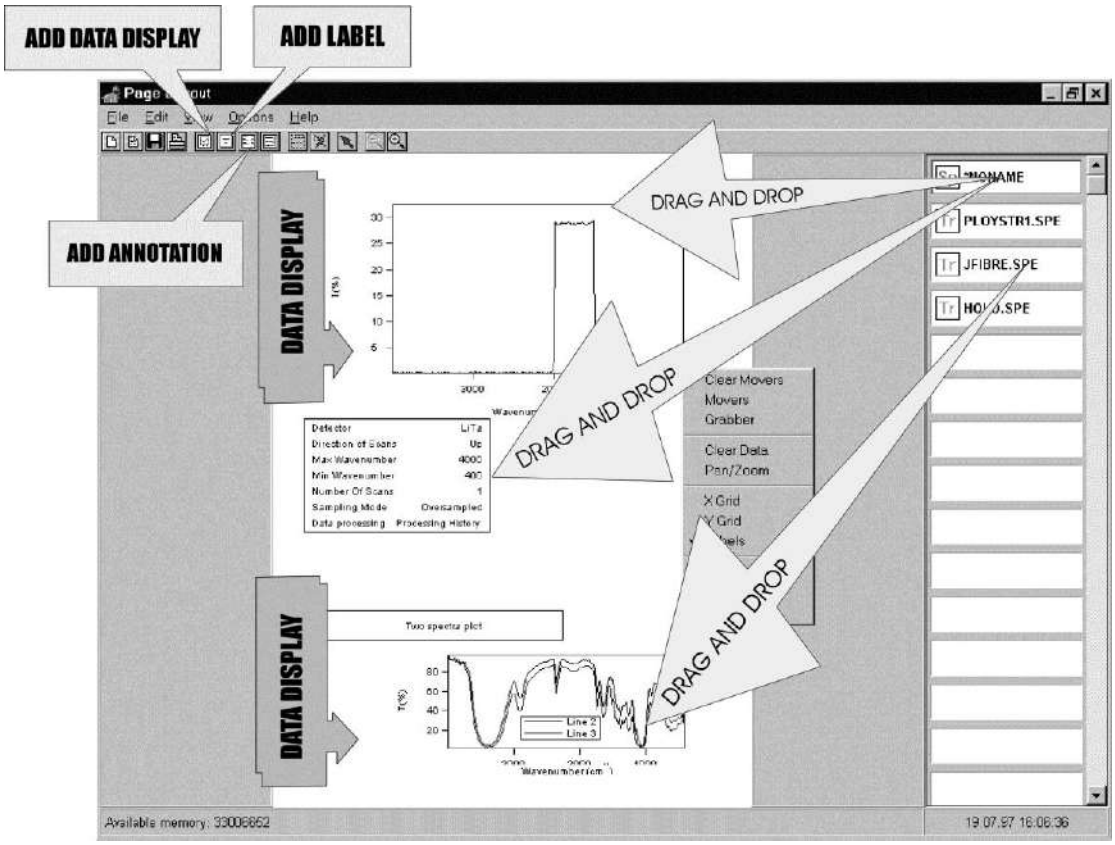


Figure 35 Page layout features

FILE/PAGE LAYOUT enables the user to format the page layout. You are offered such options as: Add Data Display, Add Label, Add Annotations, Add Line Attributes, Object Borders, Select Object, Zoom Out, Zoom In. After clicking the icon (Add Data Display) you have to format one or more data display boxes to the desired size and location. The available spectra are listed in the trace gallery, from where you can bring them into the formatted data display box simply by dragging the spectrum. You can drag into the one data display box up to six spectra. If you click the Object Borders icon you will see different areas around the data display box. It is possible to enter into a dialog with each area surrounded by a dotted line box separately by clicking the right mouse button in a chosen area and then, in addition to the previously mentioned possibilities, you will also find the possibility to edit of the text inside these areas. There is also an opportunity to choose different scales (linear, logarithmic, inverse) concerning X and Y axis. There is also a possibility to change the scaling factor of X (wavenumber) axis. If you choose Map Mode/User Data you

will have the possibility to define the place to break the X axis (Map Break) as well as how many times these two axis differ in scale from each other (Map Slope).
In the same way as making a data display box you also have to format additional boxes for Labels and Annotation. It is recommended to format these boxes after the data display box. You can format these boxes both inside or outside of the data display box. If you format them inside the data display box the additional boxes will move along with the data display box.
To print a new label text click mouse right button inside this label box and chose the Label. If you wish to form more than one line from your text inside the label box you can use ";" to separate the printed text. In addition to ordinary text, labels may include mathematical formula of chemical compounds. For example, if you want to add a label including the formula for carbon dioxide you will need to print into the label box the following CO\-{2} or CO\m{2}. General rules for well formed label printing are found in this manual, in the chapter Syntax of Labels. In case you need to write a special label formula for use within this formula or within brackets click the option "Raw".
You can use the label box also as an annotation box only for one annotation. Click right mouse button in the label box field and choose annotation. Now you have the possibility to select one annotation which will be displayed in this label box when you drag information from trace gallery into the label box. If you choose "Auto Load" the annotation will be displayed in the label box automatically after dragging the spectrum from trace gallery to the Data Display. You can make several label boxes and all of them may be filled with selected annotations.
Annotation box is filled with data either simply dragging it from the trace gallery or by "Auto Load".
Line Attributes Box is recommended to be formatted inside the Data Display Box. If you have more than one spectrum in the data display box (six is maximum) you will see as many numbered lines inside the Line Attribute Box as you have dragged spectra. To give these lines different colours, styles and names click the right mouse button in the area of the data display box and chose Line Attributes. Now you can make decisions about the line style, colour and name. Simply print a new name of the line into the Caption window.
In Page Layout screen near the bottom you have an option F or O. F means focus and when F is displayed you can use the keyboard to move the cursor emulating mouse movement. O means otherwise and in this case you can only use the mouse for cursor movement. To shift focus use Tab key as in a Windows environment.

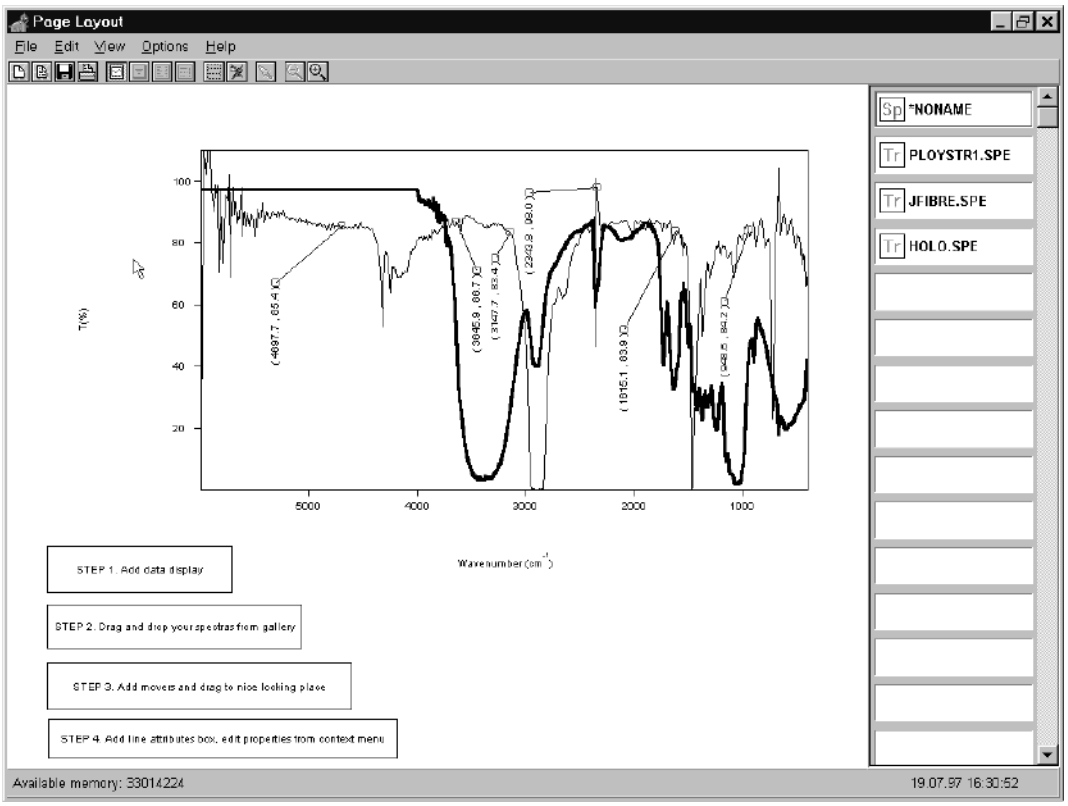


Figure 36 Multiple spectra plot preparing

The formatted screen can be saved only as a layout (FILE/SAVE LAYOUT AS). Later it can be opened as a saved layout (FILE/OPEN LAYOUT). If you click Clear, the program will ask you for the confirmation of the action selected. For the convenience of comparison you may drag two or more spectra one upon another into the same data display box, providing they have the same scale. If you select File/Print Setup you can choose the displayed screen corresponding to an A4 format sheet in portrait or landscape

3.4.2 Printing

In the Interspec software, printing is a standard Windows printing procedure. It has been made very easy for the user. It is possible to print the new or saved spectra at any stage of your work or in any displayed screen.

The three printing possibilities are as follows:

1) Click the PRINT icon in the menu bar, or
2) Select the PRINT command from the FILE menu, or
3) Select PRINT PREVIEW from the FILE menu and then click PRINT in the top right hand corner.

For higher print quality open PRINT SETUP from the FILE menu and specify the parameters of your printer, the orientation (portrait or landscape) the paper size and source (Tractor, Manual Feed, Sheet Feeder - Bin 1 or Sheet Feeder - Bin 2).

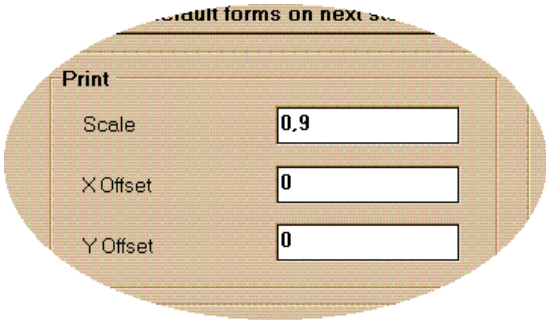


Figure 37 Print setup parameters

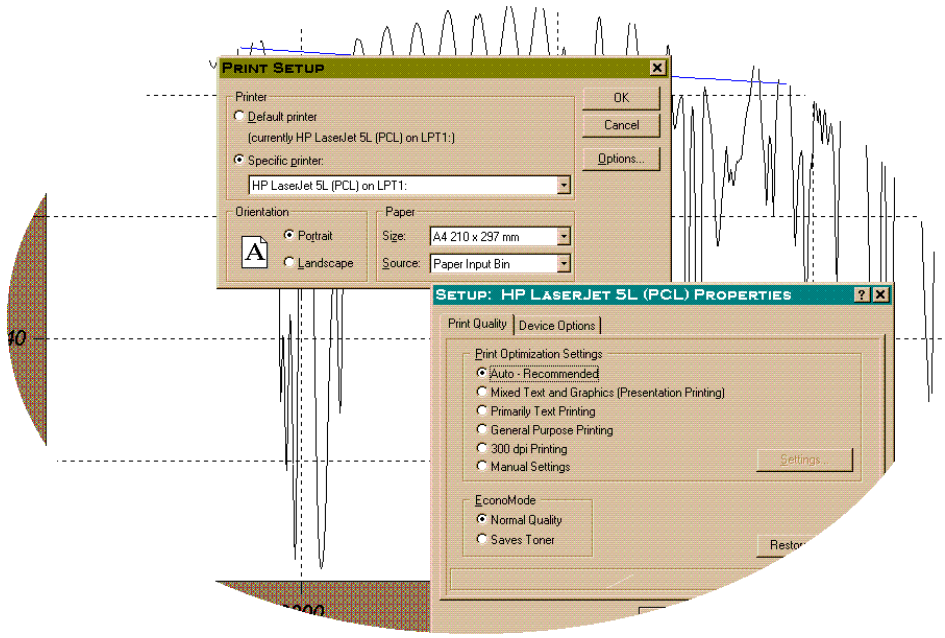


Figure 38 Printer Setup Options (HP5 L Printer Properties)

Labels can be added and fonts selected while editing the displayed screen. Just click the right mouse button either in the upper part of the screen (for labels and fonts) or in any other part (for fonts) and make your choice from the menu.

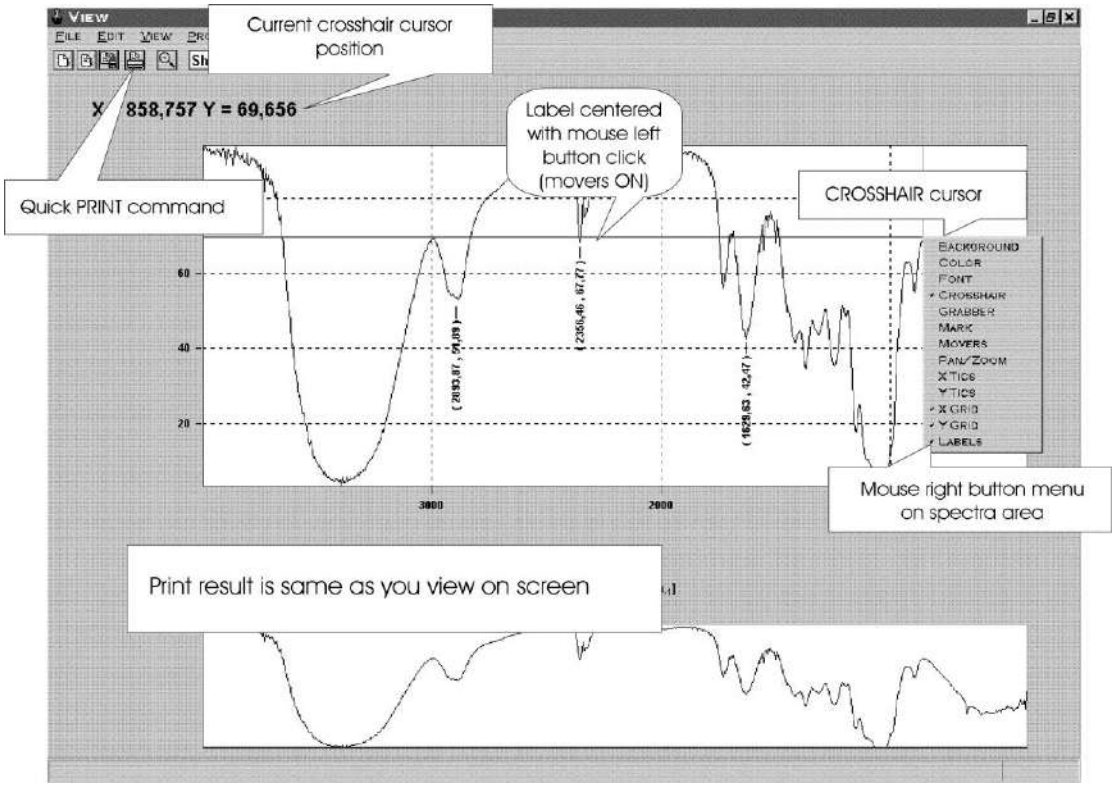


Figure 39 Preparing View screen for printing

You can make changes to any screen except PRINT PREVIEW. If you are not satisfied with the displayed picture in the PRINT PREVIEW screen, click CANCEL, make the required changes, return to PRINT PREVIEW and if the results meet your expectations, click PRINT.