Spectroscopic Software

BRUKER

OPUS

Version 5

Reference Manual

Table of Contents

1 Starting OPUS

Before starting the OPUS installation, read the attached documentation.

To install OPUS, insert the OPUS installation CD into your CD drive. Normally, the installation starts automatically. If the Windows *Autostart* option is disabled, you have to start the installation manually by running the *Setup* program from your CD. The installation program will guide you step by step. You only need to follow the on-screen installation instructions shown in the different dialog boxes.

At the end of the installation you will be asked to restart the computer. Note that you need to restart your computer in order to complete the OPUS installation. You may also be prompted to restart your computer when you install different program components. In such a case do not restart until the OPUS setup has been completed!

When the installation has been finished, an OPUS program icon is displayed in the Windows *Start* menu. Click on this icon to start OPUS.

Figure 1: Windows start menu

The *Login dialog* box opens. Select your *User ID* from the drop-down list. OPUS provides an independent user account system which regulates the access. If you use OPUS for the first time, the *User ID* drop-down list includes two pre-defined user records *Default* and *Administrator.* Select either one of them.

Enter *OPUS* in the *Password* entry field. The password is case sensitive. Once you have assigned yourself a user record in OPUS, it is possible to determine your own *User ID* and *Password*.
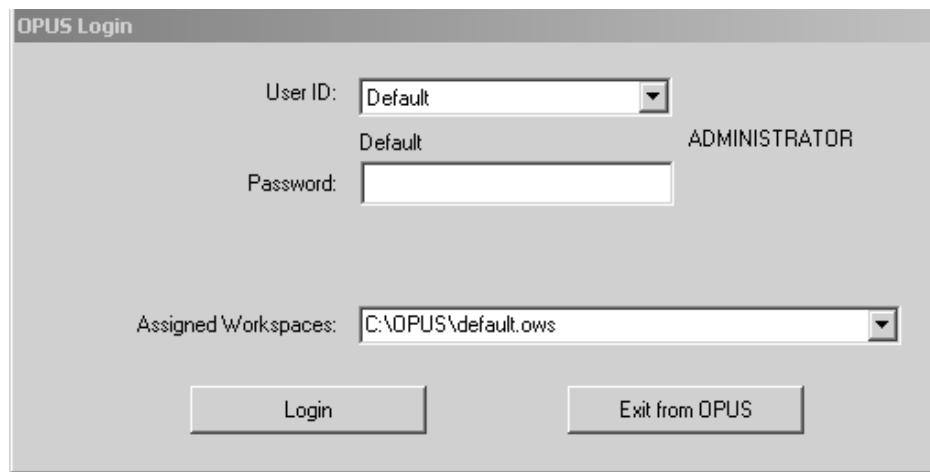
Figure 2: OPUS Login dialog

OPUS includes different accounts for operator and administrator rights. Users defined as *Operator* have limited access rights compared to users defined as *Administrator*. The rights depend on the *User ID* selected.

The *Assigned Workspaces* identify the user interface and access right. You can always select those workspaces from the drop-down list which have been defined for your *User ID*. When you use OPUS for the first time, we recommend not to change the standard *Default* workspace.

Click on the *Login* button and the *About OPUS* window opens.

It shows the serial number of your OPUS copy and the registered user name. The basic OPUS package integrates these additional licensed packages as an all-in-one application.
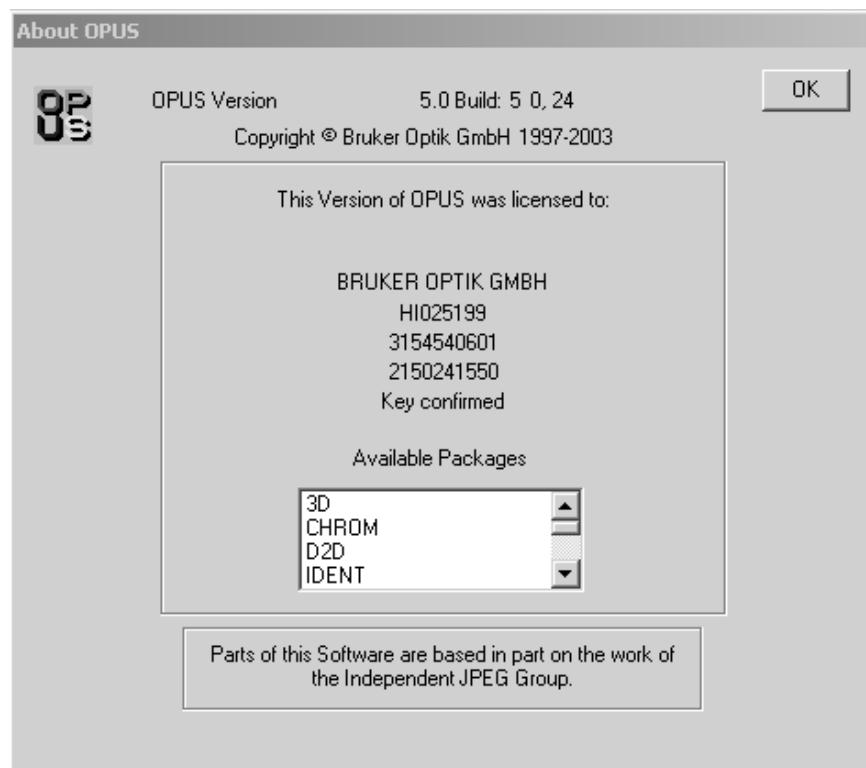
Figure 3: About OPUS dialog

Click on *OK* to open the OPUS user interface. The interface appearance depends on your screen settings and the operating system you use. Thus, the screen display of the following dialog boxes may not show exactly the screen contents displayed on your screen. BRUKER recommends a minimum graphic resolution of 800 x 600 pixel and true color.
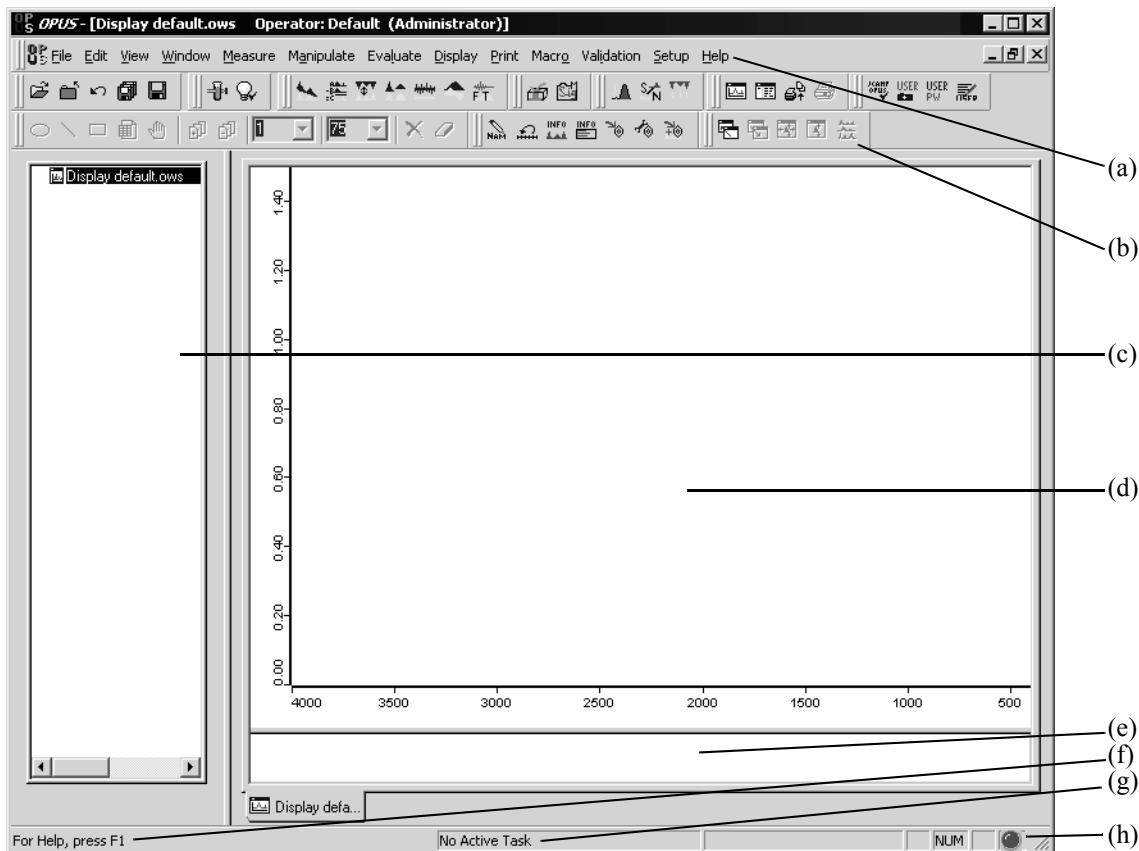
Figure 4: OPUS user interface

The OPUS user interface header shows the type and status of the operator currently logged in.

(a) The pull-down menus can be used to access all OPUS functions.

(b) The icon bars may be configured to quickly access frequently-used functions.

(c) The browser window of the OPUS file manager, similar to the Windows Explorer.

(d) The spectrum window for full views and zoom operations.

(e) The overview window always displays the full frequency range of the selected data files.

(f) A context sensitive online help.

(g) The status bar indicating background tasks.

(h) Instrument status (see section 2.9):
    Gray =   No spectrometer connected
    Green = Spectrometer connected
    Yellow = Warning
    Red   = Error

All settings (menus or icons) are individually configurable and will be reloaded when you start OPUS next time.

2 OPUS Basics

This chapter introduces the basic OPUS functions, provides general information on OPUS windows as well as on the processing of spectral data files. The remaining chapters of this manual describe in detail all OPUS functions according to their order on the different pull-down menus.

OPUS dialog boxes are similar to those of Windows. If you have already gained experience in working with Windows, it will be easy for you to use OPUS. OPUS supports drag & drop as well as shortcuts, e.g. copy (*CTRL+C*), cut (*CTRL+X*) and paste (*CTRL+V*).

To use these shortcuts, you first have to select the text or file you want to process. Drag & drop simplifies the copy and paste process, but can only be applied on files. In this case click on the files icon in the OPUS browser and press the left mouse button, while moving the file to the respective dialog box (or window). If you release the mouse button, the file will automatically be loaded into the dialog box selected.

Dialog boxes often consist of several tabs. Click on these tabs to change between them. Buttons and menu items are only active, if they are displayed in black. Grayed buttons are not available.
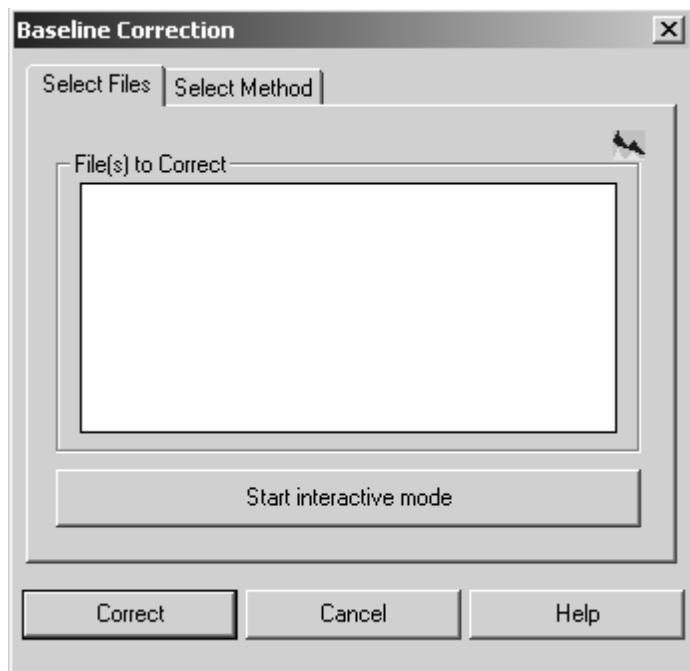
Figure 5: Example of a dialog box with two tabs

2.1   Loading and Selecting a File

Load Spectrum Dialog Box

If you load a file, either

- use the *Load File* command from the *File* menu,

- click on the [icon] icon in the tool bar or

- drag the file from the Windows Explorer into the spectrum window, OPUS browser or any OPUS dialog box.

If you select the file you want to use, the *Load Spectrum* dialog box displays the following features:
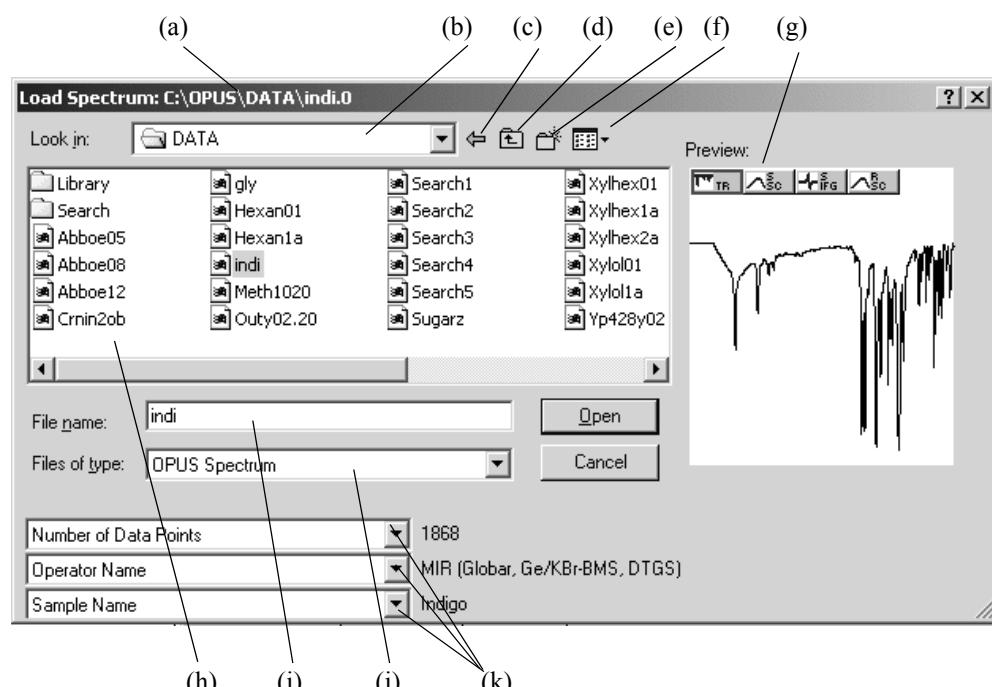
Figure 6: Load Spectrum - active preview

- a) The title bar shows the directory in which the file is stored.
- b) The drop-down list includes directory paths to search for spectra files.
- c) Using this arrow you can return to the last selection.
- d) This icon allows to return to the parent directory.
- e) Using this icon you can create a new directory.
- f) Various options to display the file list.
- g) The preview window displays a small spectrum range without indicating the axes. Data blocks are displayed on top of the preview window. They include additional information on the spectrum file.
- h) File list of the path selected.
- i) You can also manually type the name of the file you want to load into this entry field.

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j) It is also possible to load spectra of different formats, e.g. JCAMP-DX or GRAMS.SPC files. These files will automatically be converted into the OPUS file format.

k) Parameters are additional information appended to the OPUS file. Sometimes not all parameters to be selected by each drop-down list will be defined for each spectrum file. This means that some parameter fields may remain empty.

You can select several spectra in the spectra list using the *STRG* or *Shift* key while selecting the spectra. In this case the number of selected files will be shown instead of the data blocks and spectra previews. Clicking on the *Open* button will load the spectrum into OPUS and automatically close the *Load* box.

Select Files Option

You will encounter the *Select Files* option in various dialog boxes. Figure 7 shows an example of the *Select Files* tab in the *Baseline Correction* window.
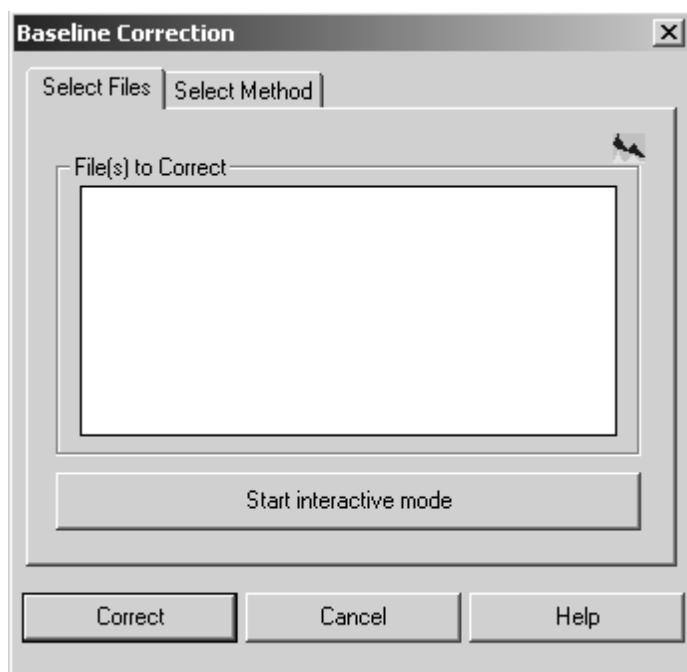
Figure 7: Example of Select Files option

Select Files tabs include *File(s) to...* fields. Spectra files to be processed have to be entered into these fields. You can use the *Drag & Drop* option to move spectra files displayed in the OPUS browser window or Windows Explorer into these selection fields. If you select spectra files **before** opening the *Select Files* tab, or if you double click on the file data block in the OPUS browser window, the spectra files will be automatically displayed in the specified entry field.

There are functions which cannot be used for all types of data. It is not possible, e.g. to apply an *AB<->TR Conversion* to an interferogram. Sometimes, the parameters of an OPUS function have to be set **prior** to loading a file, in order to be able to select the file. If selected data blocks can principally be processed by OPUS functions but the parameters do not match the data, the file name in the *File(s) to...* field will be indicated in red and a warning symbol displayed (see figure 8).

Figure 8: Convert Spectra – parameter mismatch

To remove data blocks from the *File(s) to...* field, select the data block and use the *Delete* key on your keyboard. If you press the *Shift* or *CTRL* key, you can select several files in one *File(s) to...* field.

2.2 OPUS Browser Window

The design and functionality of the OPUS browser is similar to the Windows Explorer. To enlarge the spectrum window you can reduce the OPUS browser window in size or relocate it. Left click on the upper edge of the browser window and draw it underneath the icon bar. The OPUS browser window will be displayed as drop-down list, including all the files loaded (see figure 9). To undo this view click on the upper edge of the drop-down list and move the list to the original browser window position, i.e. to the left side of the spectrum window.
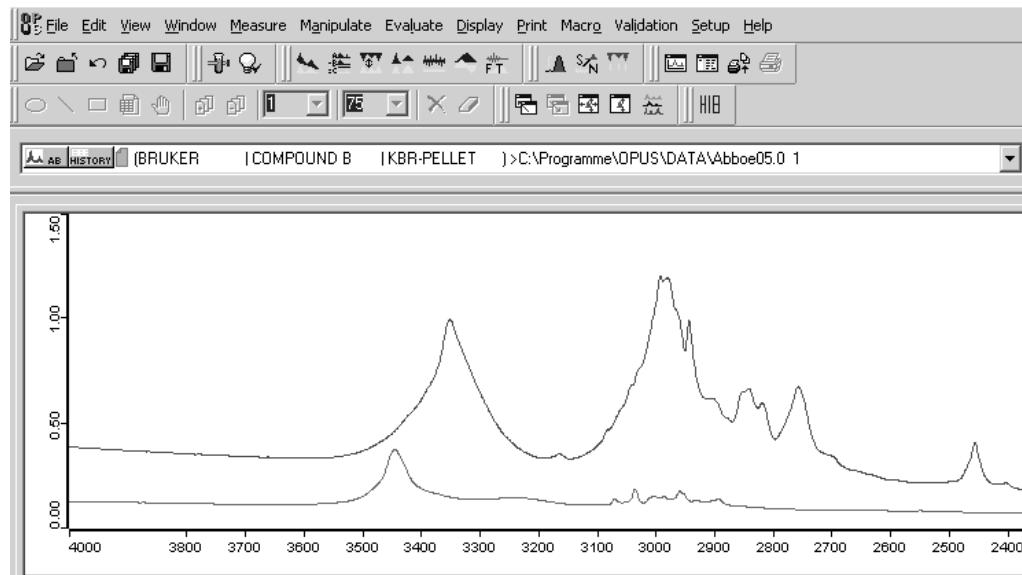
Figure 9: OPUS browser window displayed as drop-down list

When loading an OPUS file the file name, data blocks and file status information are displayed in the browser window. If you position the cursor on the file name, a small text field pops up indicating the complete data path. If you place the cursor on a data block, the text field shows the operator name, sample name and sample form.
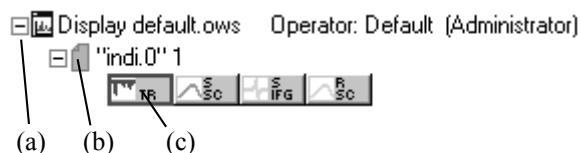
Figure 10: Browser file list

a) If you have opened several spectrum windows you can switch between them. If you click on the ⊟ sign, the file name display will be minimized.

b) The blue document symbol indicates that the file has not yet been manipulated. The number next to the file name indicates the number of copies made of the file loaded. You can load a file several times into the OPUS browser window.

c) The small icon bar underneath the file name represents data blocks which are part of the spectrum file. The data blocks displayed in figure 10 indicate a transmission spectrum, single-channel spectrum, interferogram and single-channel background spectrum. For further data blocks, see Appendix. If the data block symbols are colored, this indicates that spectra or interferograms are displayed within the spectrum window. Use the left mouse button to select one data block. If you press the *CTRL* key, you can select more than one data block. Selected data blocks are always indicated by a red frame.

The possibilities to select files are similar to those using the *Load File* option or Windows Explorer.

If you select one file using the left mouse button, press the *Shift* (⇑) key and click on a second file again. All the files between these two files will also be selected.

Additionally selected by using *STRG*
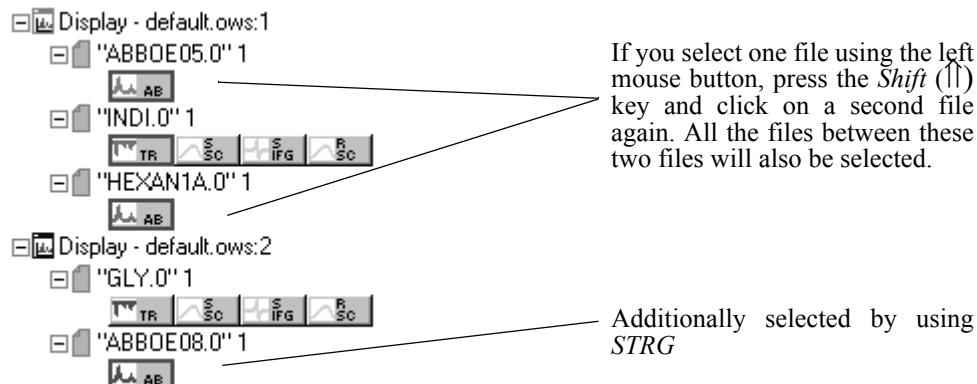
Figure 11: Select files

This kind of file selection causes the files to be automatically registered for processing functions. If you have changed or added files using a processing function, the blue document symbol will be hidden by a red one. If you have loaded the same spectrum several times, the copies will be incremented.

If you right click on a file name, a pop-up menu opens.
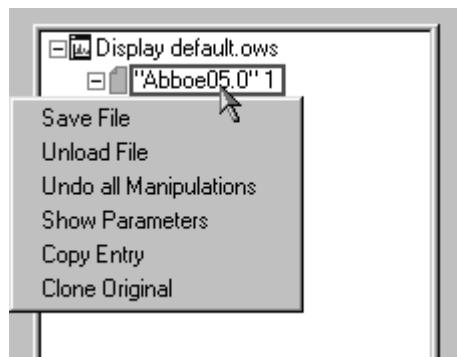
Figure 12: Pop-Up menu for file manipulation

As changes made to a file are not automatically saved in the file directory, you have to store these changes using the *Save File* option. *Unload File* means that the file is removed from the spectrum window, but is still available in the file directory. If you have modified the file using a processing function, you can *Undo all Manipulations*. The *Show Parameters* option displays all information on data acquisition which have been saved to the file. For details on parameters and information data blocks, see chapter 4.

The *Copy Entry* and *Clone Original* options are used to duplicate spectrum files. The difference between these two options is that *Copy Entry* copies a data file which has been manipulated, e.g. if a baseline correction has been performed. The *Clone Original* option copies the original spectrum file.

If you right click on a data block, the following menu pops up.
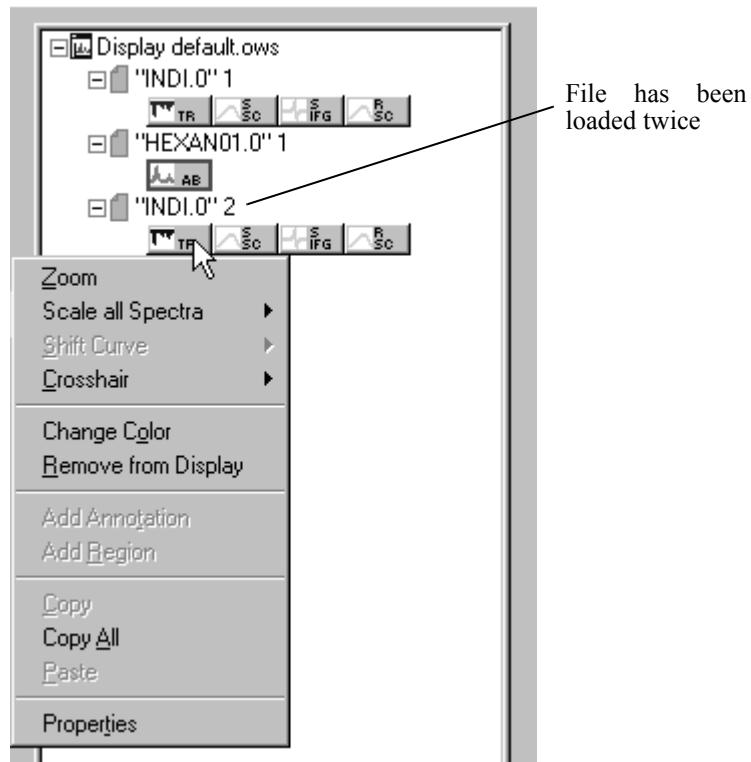
Figure 13: Pop-Up menu for spectrum manipulation

Using this menu you can change the layout of spectra within the spectrum window. Apart from changing the color you can zoom selected spectra ranges. Almost similar to this pop-up menu is the one displayed when you right click into the spectrum window. The options will be described in the next section.

2.3   Spectrum Window

The spectrum window and overview window are on the right side of the OPUS user interface. When you have loaded a file all spectra and interferograms included in this file will be displayed.

The default settings for the spectral range are from 4,000 to 400 wave numbers and from 0 to 1.5 extinction units. However, you can scale the spectrum to show the complete data range. Use the *Scale all* command in the *Display* menu or click on the [icon] icon. If a file consists of more than one data block, only the first data block is displayed in the spectrum window.

In Figure 14 the *Scale all* command has not been used. Therefore, only the overview window shows the total spectral range of data. The part shown in the spectrum window is depicted on a white background, while the remaining data range is grayed out. If you position the cursor on the gray area, the cursor will change its form from [cursor] to [cursor]. Now you can move the borders of the spectral range (white) by pressing the left mouse button.
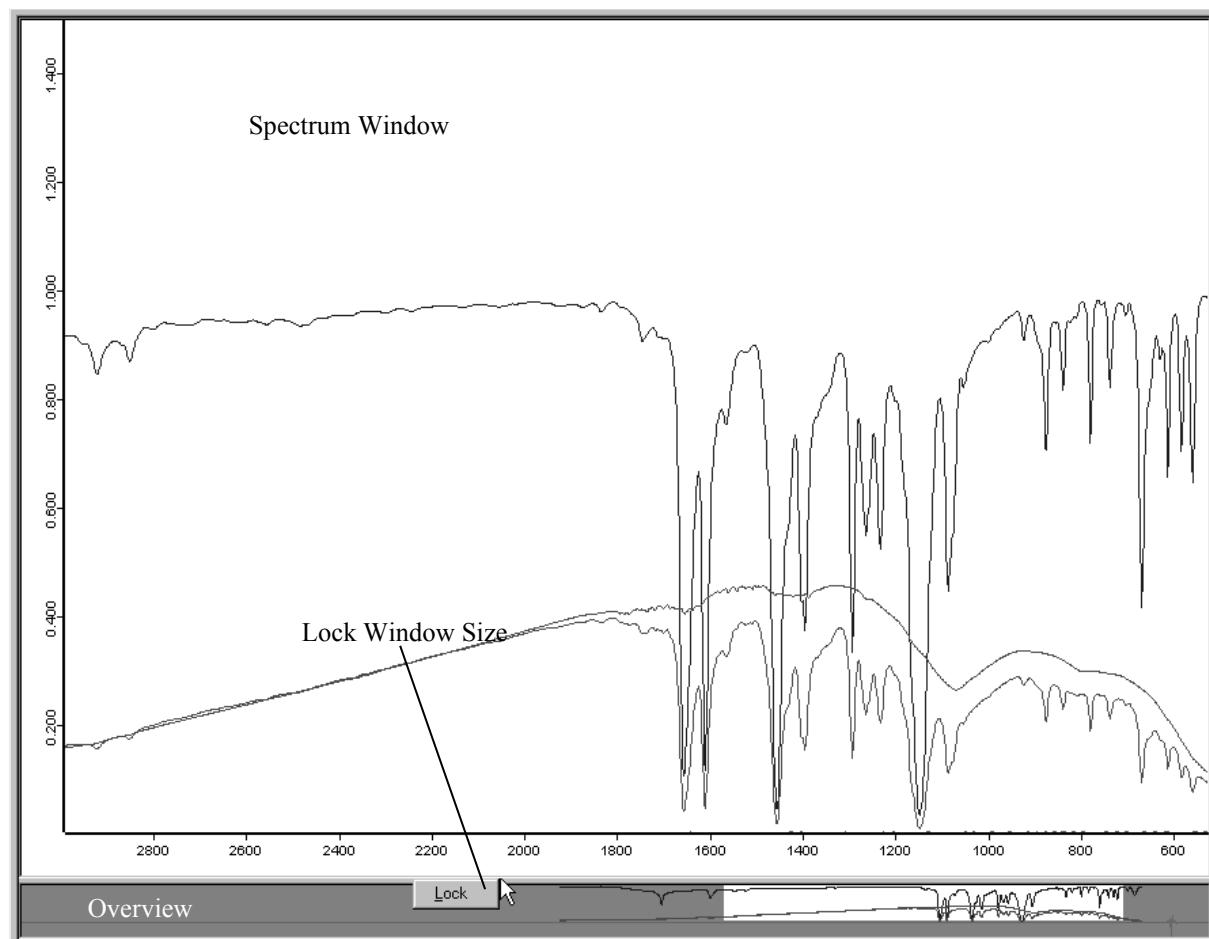
Figure 14: Spectrum and overview window showing lock button

If you position the cursor between overview and spectrum window, the cursor changes to ⬍. This allows you to re-size the windows. You can disable this function using the *Lock* button, which becomes visible if you right click on the this boundary. If the windows are looked, click again on the boundary to undo this command by selecting *Unlock*.

If you right click on a spectrum within the spectrum window, a pop-up menu will be displayed (Fig 15). This menu allows you to change the spectrum color, to zoom a specific spectral range or to shift the complete spectrum.
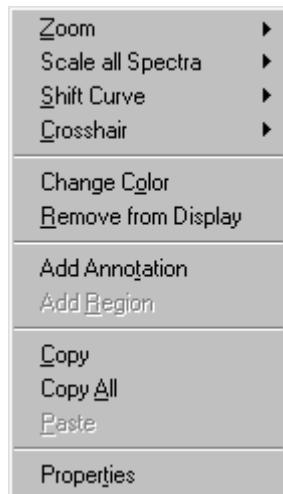
Figure 15: Pop-up menu within the spectrum window

To magnify a part of the spectrum window, select the *Zoom In* option from the pop-up menu. A crosshair is displayed in the spectrum window. Click on the left mouse button to draw a frame around the spectral range you want to magnify. If you click on the left mouse button a second time, the crosshair cursor disappears and you can reposition the frame. Now, left-click again and the spectral range selected will be resized to the spectrum window. Use the *Zoom Out* command to decrease the magnification or the *Scale all Spectra* option to go back to the original view by selecting *Show Everything (XY)* from the pop-up menu. The *Page back* option in the *Display* menu allows you to have the last 10 spectral ranges displayed again. For details on scaled spectra display, see chapter 10.

The *Shift Curve* command includes different options. You can either shift the *Whole Curve* vertically or stretch the curve to the *Top* or *Bottom* in y direction. Select the relevant option and shift the curve by clicking on the spectrum and pressing the left mouse button. If several spectra are displayed, you can shift each one of them using the *Shift Curve* option. Deactivate the *Shift* mode by right clicking. To undo these changes, select *Reset* from the *Shift Curve* option.

The *Crosshair* command also includes different options. If you select *Cursor*, a the cursor is displayed as crosshair. To follow the data points of a spectrum, use the *Follow Data* option. This option allows to display the current crosshair

position (e.g. wavelenght or absorption unit) in the upper right corner of the spectrum window. You can comfortably read out the x/y positions directly from the spectrum. If you right click, the cursor changes into its regular form.

You can change the spectrum color and remove the spectrum from the spectrum window by selecting the *Change Color* and *Remove from Display* options.

Use the *Add Annotation* command to identify peaks even more precisely. Right click on the spectrum and select *Add Annotation* from the pop-up menu. At the cursor position an arrow is inserted indicating the wave number of this data point, by default. If you position the cursor onto the arrowhead and click on the left mouse button, you can move the arrowhead.

To edit the annotation text, right click on the wave number and select *Properties* from the menu which pops up. The *Center text lines* and *With Arrows* check boxes are activated by default.

Add Region facilitates the selection of frequency ranges when using QUANT methods.

Copy and *Copy All* as well as *Paste* can be used to copy files between different spectrum windows. Special sections which have been copied can also be added to different programs.

Properties opens the *Display Settings* dialog box.

Display Settings
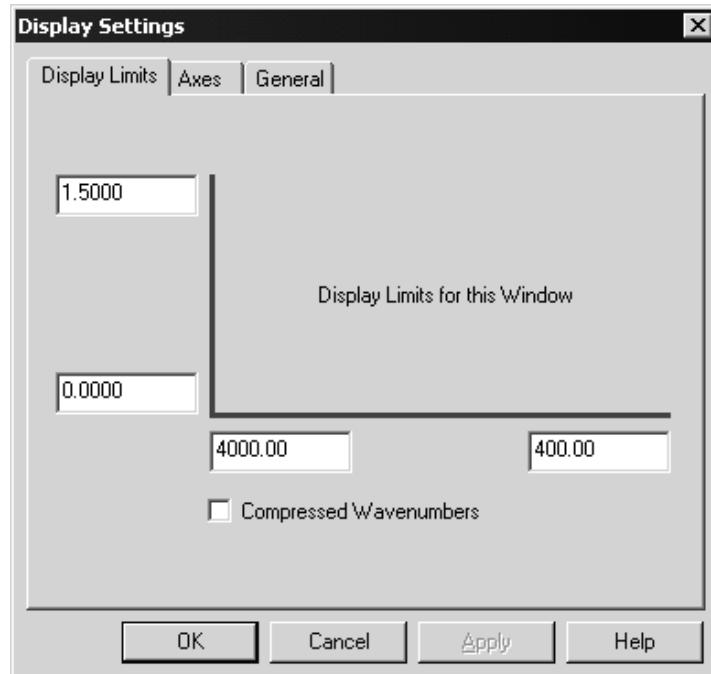
Figure 16: Display Settings – Display Limits tab

Use the *Display Limits* tab to change the size of the displayed region.
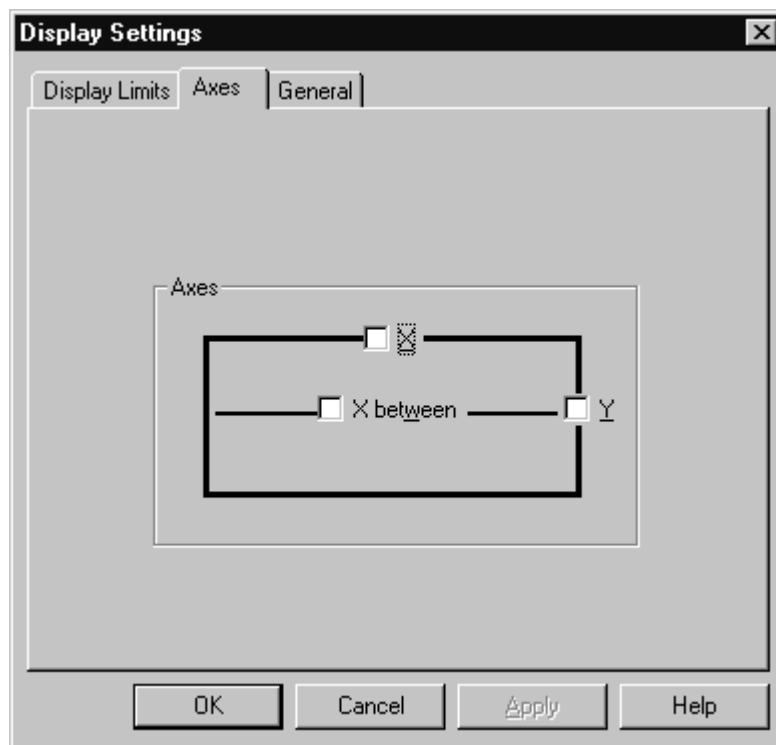
Figure 17: Display Settings – Axes tab

The *Axes* tab allows to depict each spectrum with additional axes on top and on the right side of the spectrum window. If the spectrum window includes more than one spectrum and the spectra are displayed in stacked mode, you can define separate axes for each spectrum if you select *X between*.
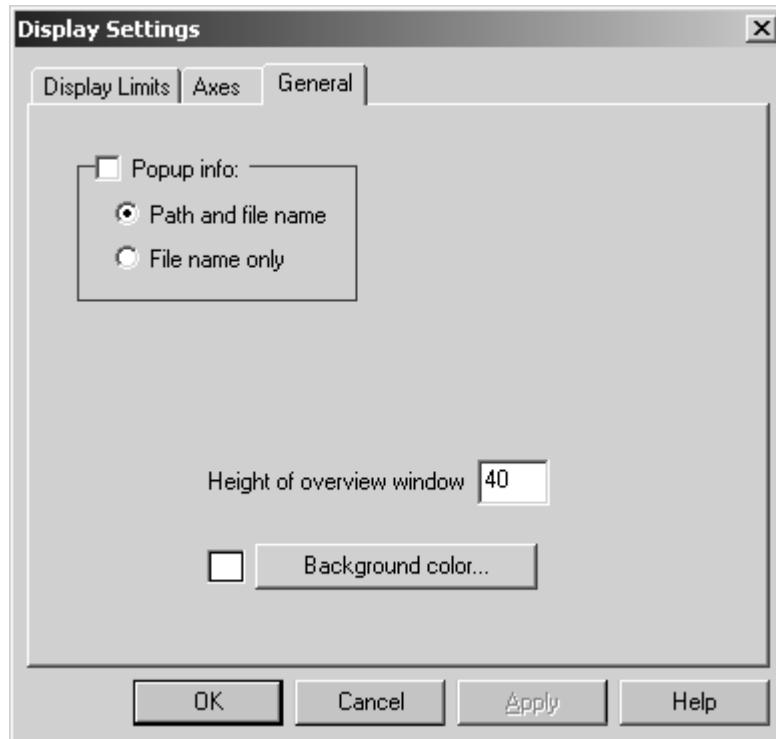
Figure 18: Display Settings – General tab

The *General* tab allows to change the background color and the default height of the overview window. If you activate the *Popup info* check box, the path and file name, or path name only, will be displayed as soon as you position the cursor on the spectrum.

You can open more than one spectrum window by selecting the *New Spectrum Window* option from the *Window* menu. You can either tile or stack windows. Tiled windows are convenient to copy data between spectrum windows. You can copy one spectrum from one window to another. Or you drag & drop the spectrum from the OPUS browser window to one specific spectrum window.

2.4   Report Window

You can use the report window to display numerical or text information, e.g. to display measurement parameters or evaluation results. This kind of information is stored in report blocks. Double click on such a report block (except for peak tables) to open a report window. A blank report window can be opened from the *Window* menu (see chapter 6.3).
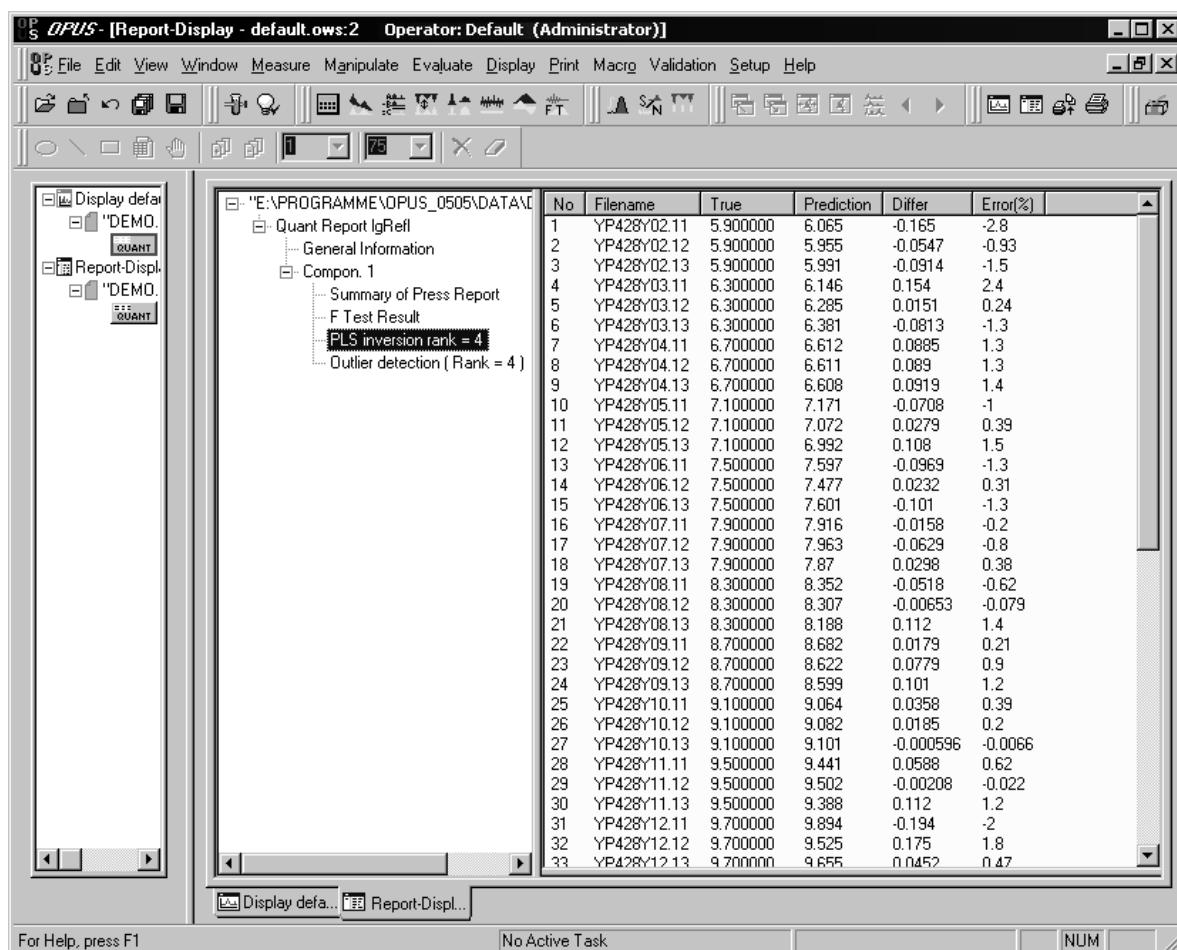
Figure 19: Report Window

The information included in the report block is displayed in form of a directory tree on the left. If you select one item in the directory tree, the specific data are displayed on the right. Click on the column title to sort the column data in ascending or descending order. For report blocks which include headers, a three-column window is opened and displays both the header and data matrix.

Right click on a report window and select *Properties* from the pop-up menu. The *View Properties* dialog box opens. You can activate the *Header preferred* check box and specify the font and font size if you click on the *Printer Font* button.
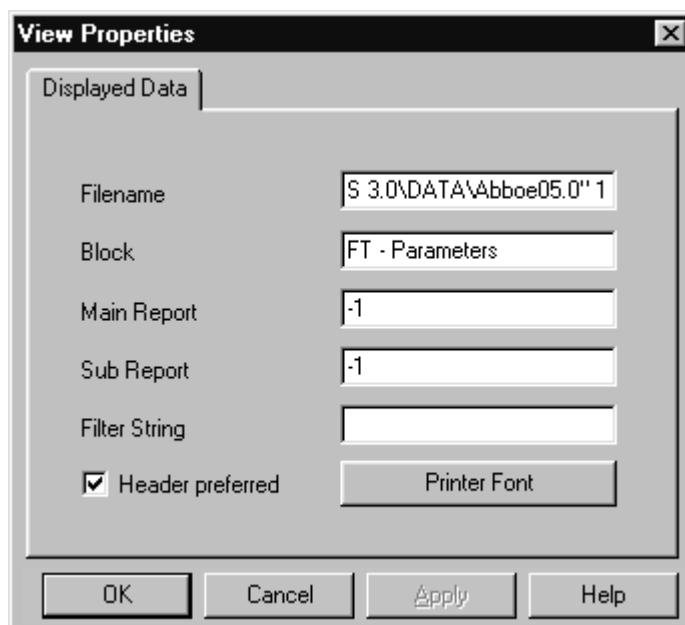
Figure 20: Report Window - View Properties

2.5   Datafile History

A special type of report window is *Datafile History*. Any manipulation made in the spectrum and even in the measurement parameters are recorded in a non-editable, non-deletable history datafile. Figure 21 shows a *Datafile History*, including several spectrum manipulations.

The first line of the *datafile history* states the operator as well as the OPUS version and the name of the spectrum. Then, all manipulations and their parameters are listed in the order of their performance.

All pieces of information are saved in a data block (HISTORY) together with the processed spectrum in one spectrum file. This ensures that all data manipulations can be reproduced, as every kind of manipulation as well as the operator name are automatically recorded.
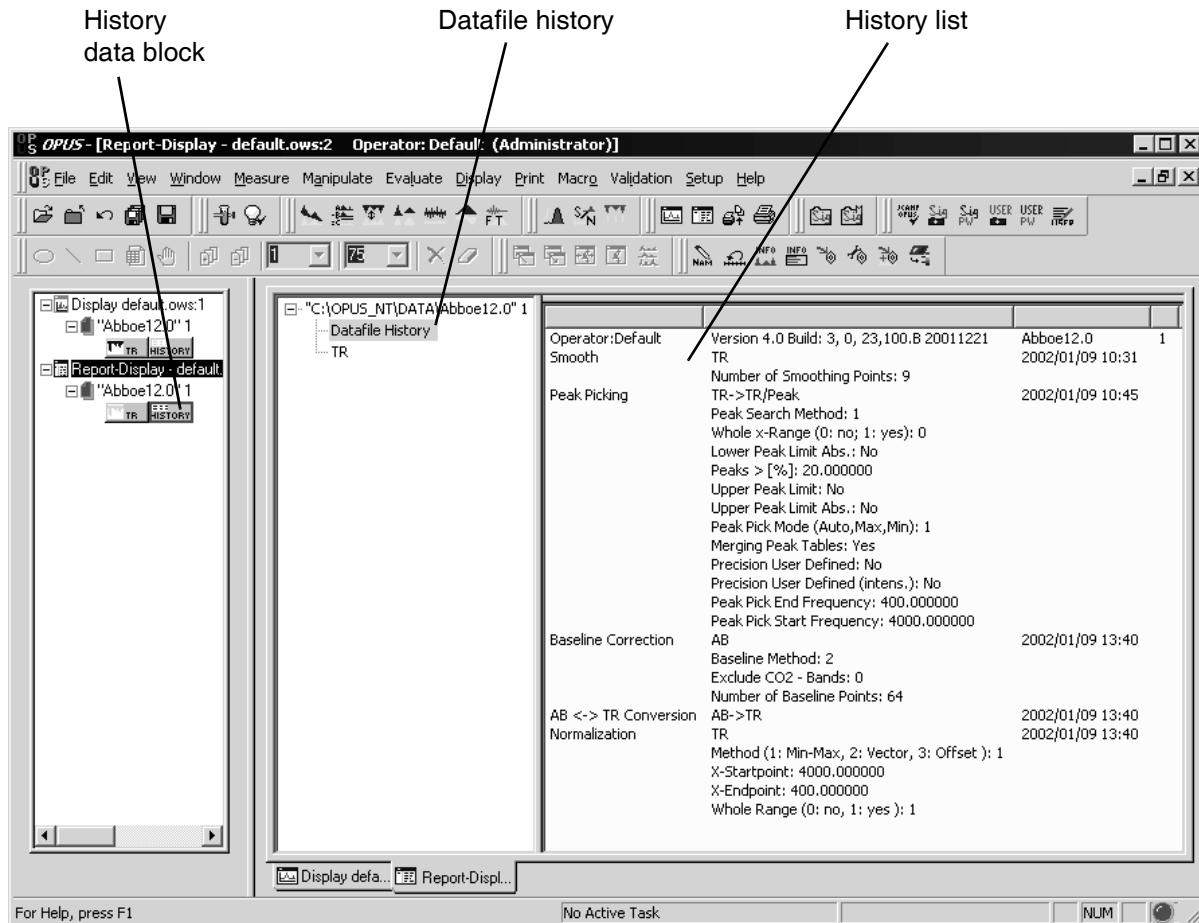
Figure 21: Report Window showing datafile history

2.6 3D Window

3D windows can be used to plot contour graphics. These windows are part of the *OPUS MAP* package and described in detail in the *OPUS MAP* manual. If you load a 3D file it will be automatically displayed in a 3D window view.

2.7 Selecting Frequency Limits

In case of some OPUS functions you need to define frequency limits first to be able to process a data file. You have got three possibilities to select a frequency range:

• Select the frequency range interactively.
• Apply the current frequency limits of the spectrum window by clicking on the *Get Display Limits* button.
• Enter the limits manually.

If you want to interactively select the frequency range, load the spectra you want to process, select the appropriate data manipulation and click on the *Interactive* button in the *Frequency Range* tab. Figure 22 shows an example of the *Cut* manipulation.
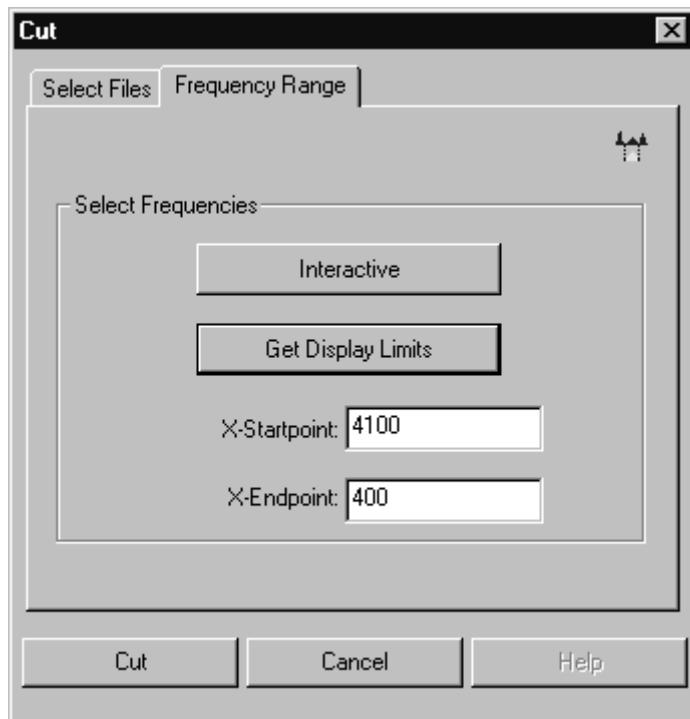
Figure 22: Frequency Range Selection

The *Select Frequency Range(s)* window opens and displays the loaded spectra. Depending on the x-startpoint and x-endpoint defined (see figure 22), the view of the *Select Frequency Range(s)* window may vary.

- If both frequency ranges are within the display limits, the area between the boundaries will be white, the background gray.
- If the frequeny range displayed completely fits the display limits, the entire range will be white.
- If the display limits are either above or below the frequency range displayed, the background will be completely gray. In this case, close the *Select Frequency Range(s)* window, define reasonable frequency ranges and start the interactive mode again.

In Figure 23 shows pre-defined display limits which do not correspond to the frequency range displayed. The frequency range between the current display limits is white.
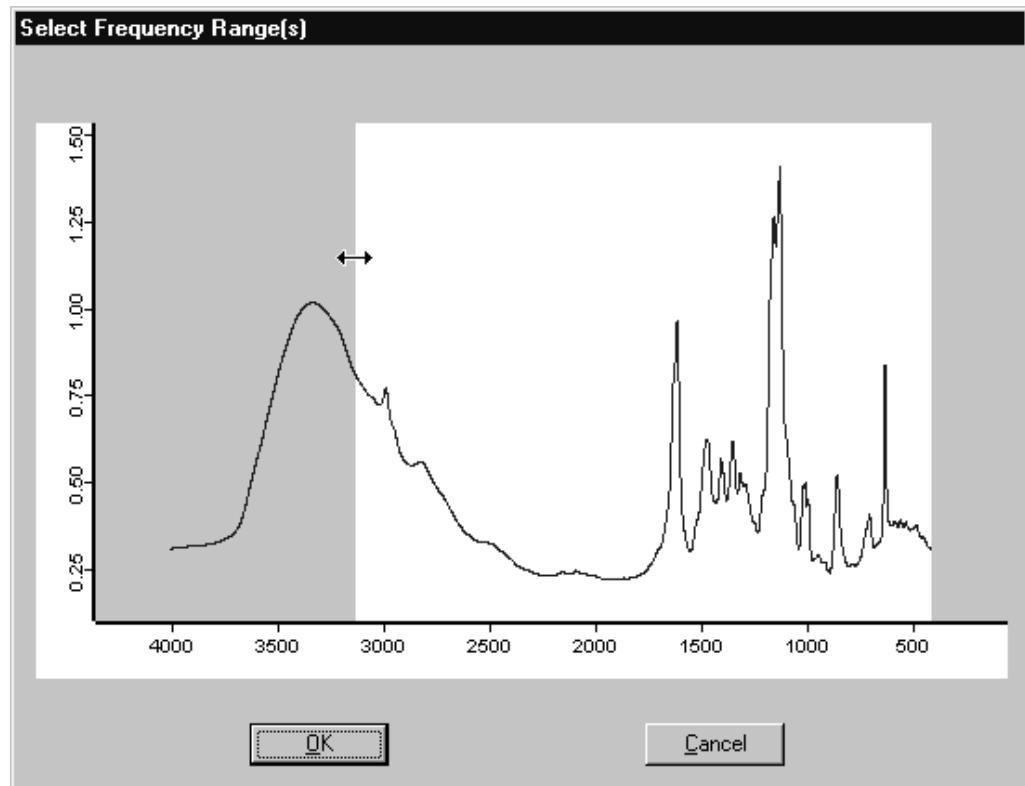
Figure 23: Select Frequency Range interactively - move frequency range

If you position the cursor on the boundary between the white and gray area, the cursor changes into a double arrow. Press the left mouse button and move the cursor to either the left or right side.

To define several frequency ranges right click on the gray area and select *Add Regions* from the pop-up menu. Within the white section the cursor changes to a cross arrow. If you press the left mouse button, you can move the entire frequency range selected.
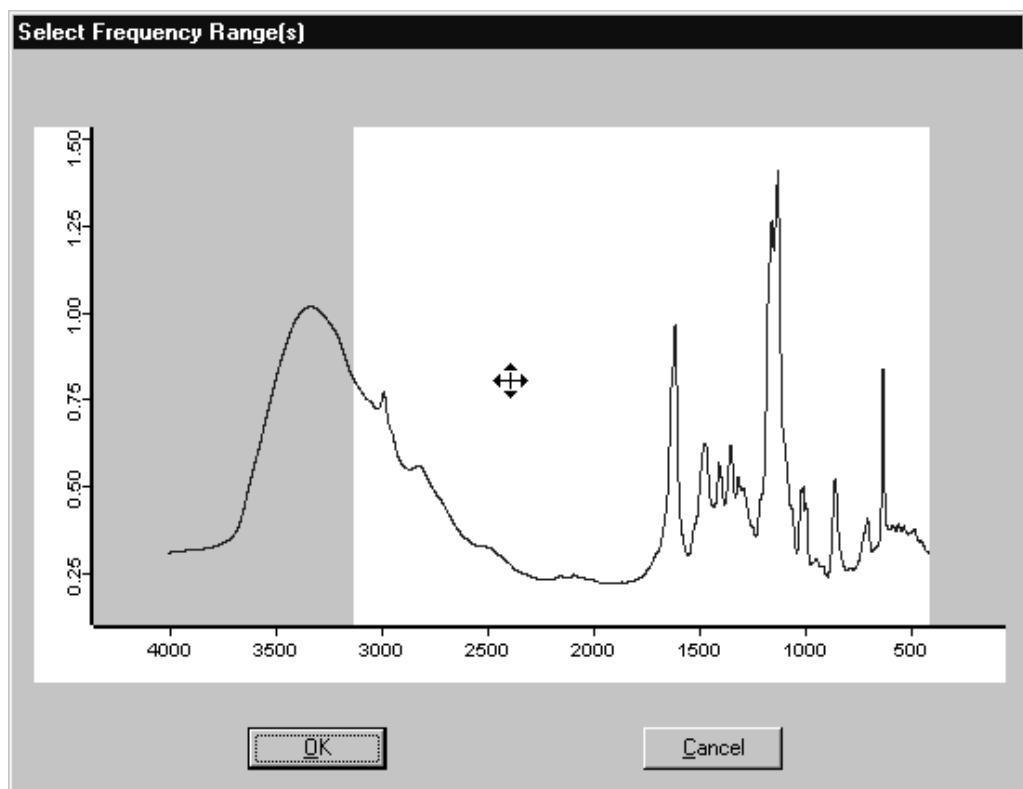
Figure 24: Select File Limits interactively – define endpoints

If you click on the *OK* button, you confirm the limits of the frequency range to be used for data processing.

2.8   Toolbars

OPUS provides toolbars which can be individually configured to quickly access frequently used functions. Next to each icon context-sensitive tooltips pop up when you position the cursor over that icon.
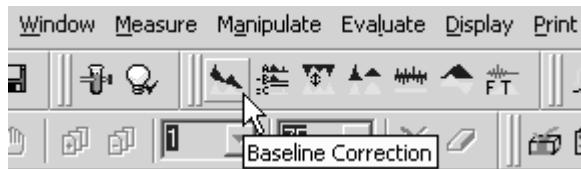
Figure 25: OPUS Toolbar showing a tooltip

A double click on the icon immediately performs the selected function. The icons are also displayed next to their respective function in the pull-down menus.

You can customize the various tool bars to best suit your personal requirements. The tool bar configurations are stored together with your workspace settings in one file which has the extension *.ows*. OPUS default settings are stored in the *DEFAULT.OWS* workspace. For details on tool bar configurations, see section 5.1 and 14.3. For a icons list, see Appendix.

2.9   Instrument Status Indicator

The instrument status is shown at the right end of the status bar (see figure 4). If no spectrometer is connected, a gray status light will be displayed. A green status light indicates that the instrument is OK and connected. When the instrument status indicator turns yellow, a warning is indicated, e.g. the instrument test has to be repeated. A red instrument status light indicates a severe error, e.g. if a spectrometer component is defective. The instrument status is also stored in a measured spectrum. If you click on the instrument status light, a *Diagnosis* dialog pops up including additional information on the status and specific help. Options for the diagnosis can be set up using the *User Settings* options in the *Setup* menu.

3 File

The *File* menu includes all features necessary for your data file management. Apart from basic commands such as loading, saving, printing and sending, the *File* menu allows to start VisualBasic scripts and external software programs.
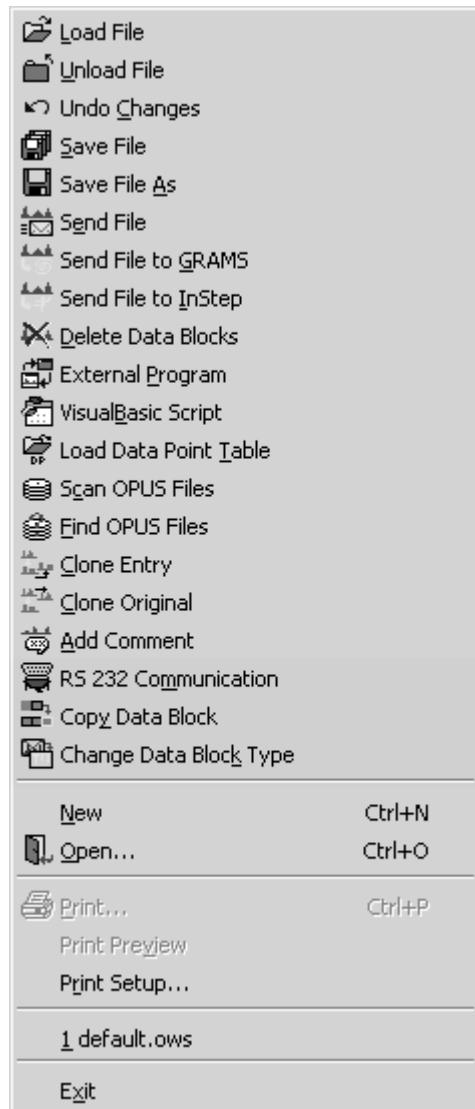
Figure 26: File Menu

3.1 Load File

The *Load File* command has already been described in section 2.1.

3.2 Unload File

The *Unload File* command removes files from the OPUS browser and spectrum window. Note that when unloading files they will not be deleted from your hard disk. Drag and drop the respective file into the *File(s) to Unload* field and click on the *Unload* button.

3.3 Undo Changes

Use this command to undo all changes made in a data file since it has been saved for the last time. The original data will be restored, but the *History* report which includes all the previous manipulations will not be reset.

3.4 Save File/Save File As

The commands *Save File* and *Save File As* provide different options to store files. Enter all files to be saved into the *File(s) to Save* entry field by drag and drop.
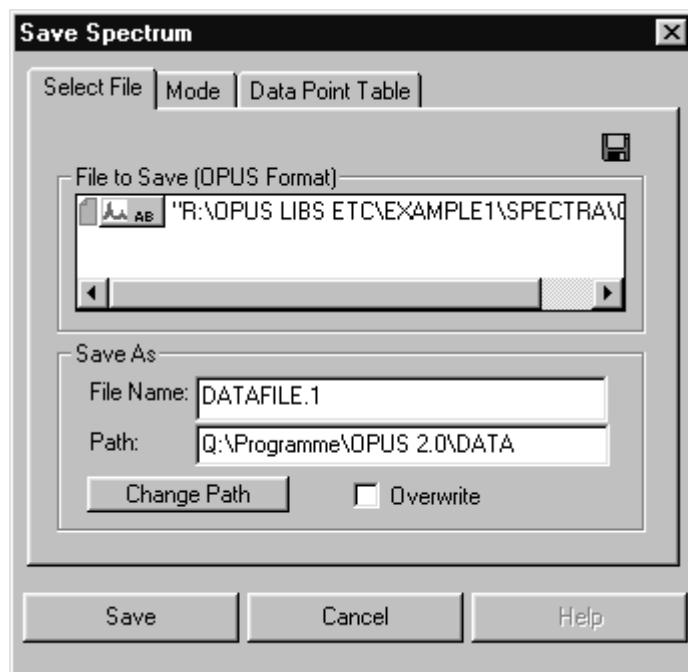
Figure 27: Save Spectrum - Select File tab

The *Select Files* tab allows you to define spectral data to be stored, and the file path. Use the *Change Path* button to browse the directory of your hard disk. If you activate the *Overwrite* check box, existing files with the same file names will be replaced by new files. This option cannot be activated when working in *GLP* mode. It is also possible to increment file names. For details, see section 14.10.

On the *Mode* tab you can set the parameters for exporting OPUS data in a file format. Apart from the OPUS and *Data Point Table* format there are also other formats available, e.g. GRAMS[1] or InStep[2]. *JCAMP.DX* as an additional ASCII format can also be used. If you activate the respective check boxes in the *Options* group field (figure 28), you can either move the original file, save all data blocks or automatically remove all copies, provided that you have checked the *OPUS Format* option box in the group field *Output*.
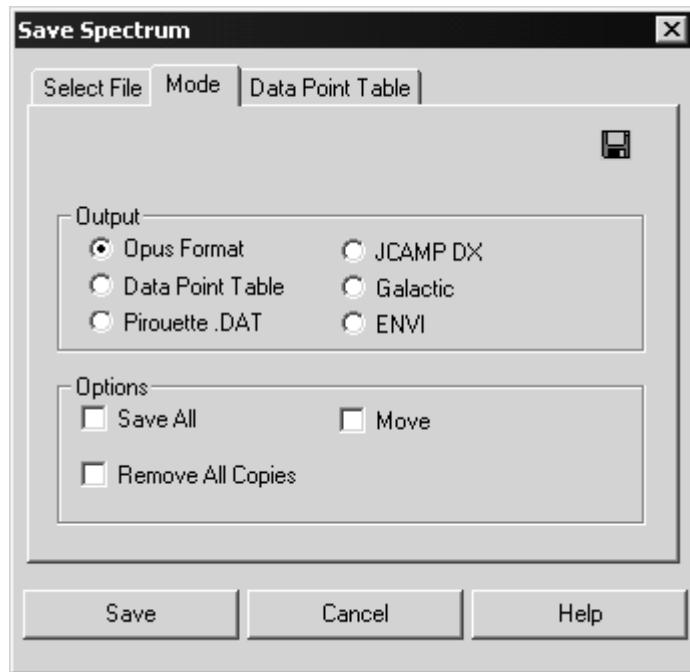
Figure 28: Save Spectrum – Mode tab

If you click on the *Data Point Table* tab, you can define the structure of the output file. Enter the number format for x and y values, the number of decimals as well as the separator format. Alternatively, you can activate the *Separator is TAB* check box, to automatically separate the columns by tabs. You can limit the output file size to 64KB by checking the *Max. 64KB* option button.

1. GRAMS is a registered trademark of Galactic Industries Corporation, 395 Main Street, Salem, NH 03079-9891.

2. InStep is a registered trademark of Infometrix Inc., 2200 Sixth Avenue, Suite 833, Seattle, WA 98121.
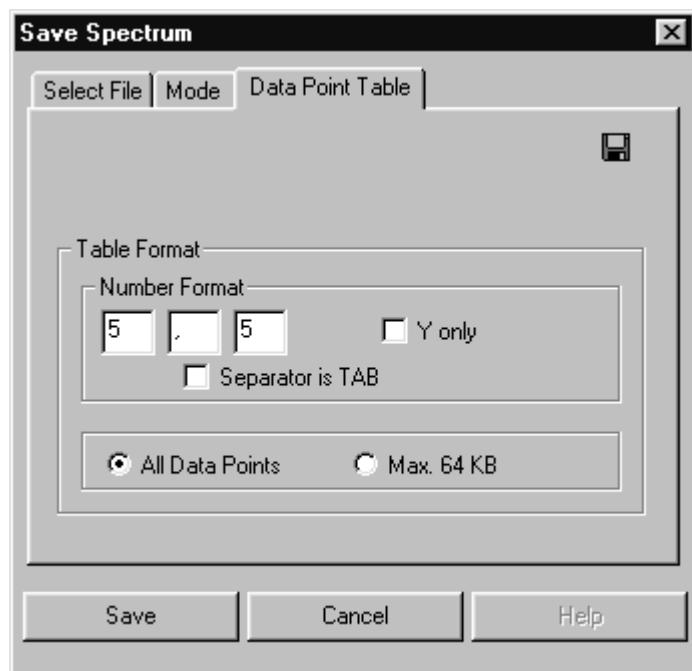
Figure 29: Save Spectrum - Data Point Table tab

3.5   Send File

You can also send OPUS files by e-mail. After loading the OPUS file into the OPUS browser window you can send the file using the *Send File* command. The respective file will be displayed in the *File(s) to Send* selection field. If not, drag and drop it from the OPUS browser window into this field.
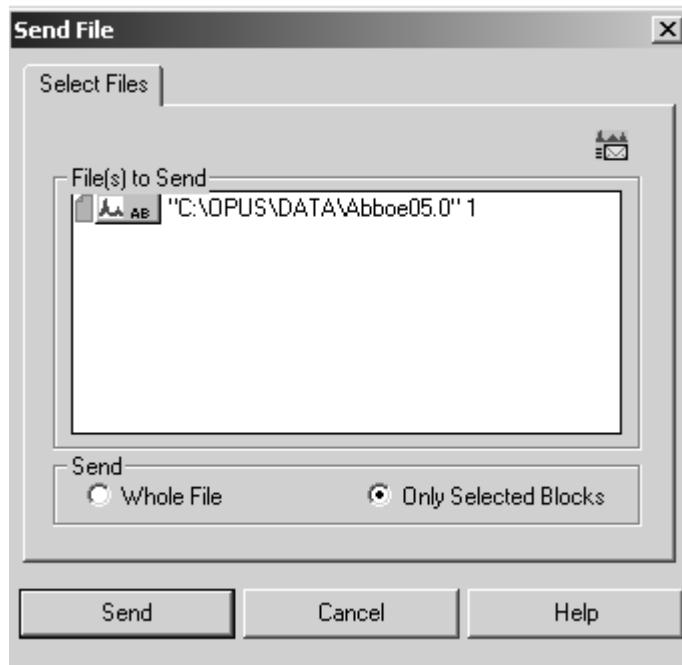
Figure 30: Send File - Select Files tab

If you check the *Whole Fil*e option, the complete file content will be sent, even if only one data block is displayed in the *File(s) to Send* selection field. Alternatively, check the *Only Selected Blocks* option button if you want to send specific data blocks only.

Clicking on the *Send* button will transfer the data to the Windows mail program. You can specify an address and write a comment. If you use the mail program for the first time, you will automatically be prompted to configure it.

The data will be attached to the letter. If the addressee uses an appropriate mail program, it is possible to drag and drop the attachment from this program directly to the OPUS spectrum window.

3.6　Send File to GRAMS

You can export a spectrum, loaded or measured by using OPUS, to GRAMS. Similar to the *Save File* command data is loaded to the *File(s) to Send* selection field and transferred to GRAMS via DDE (Dynamic Data Exchange). Make sure that the *GRAMS* program has been started on the same computer.

3.7　Send File to InStep

Analog to *Send File to GRAMS* you can also send a file to the *InStep* program.

3.8 Delete Data Blocks

An OPUS file can consist of several data blocks. Use the *Delete Data Blocks* command to delete single data blocks from an OPUS file. Peak tables, integration results and other data blocks belonging to this file will also be deleted. This does not entirely apply to GLP mode.

3.9 External Program

External programs, e.g. data evaluation programs, can be started from OPUS. For further details, refer to the OPUS *Programming* manual.

3.10 VisualBasic Scripts

VisualBasic scripts can be started from OPUS. For further details, refer to the OPUS *Programming* manual.

3.11 Load Data Point Table

The *Load Data Point Table* command enables to read in ASCII data tables. In addition to the standard load data commands, it is possible to identify the table columns, specify the data block type and limit the number of data points. Make sure that you know the type of data point table (type of spectra, configuration of x and y values). You can select the data range directly from the table by either numeric entry or interactive mode. The preview window displays the data as spectrum.

3.12 Scan OPUS Files

You can scan saved spectra selectively for character strings and text. Before you can use this search command, you have to create a database. Use the *Scan OPUS Files* command to do so.

Select the drive on which the spectrum files are saved. Generally, you should select all drives which contain spectrum files. Click on the *Scan Files* button to start creating the database. Depending on the number of spectrum files being stored, the scanning can take a while. During scanning, the status bar indicates this background task by *Scan OPUS Files*.
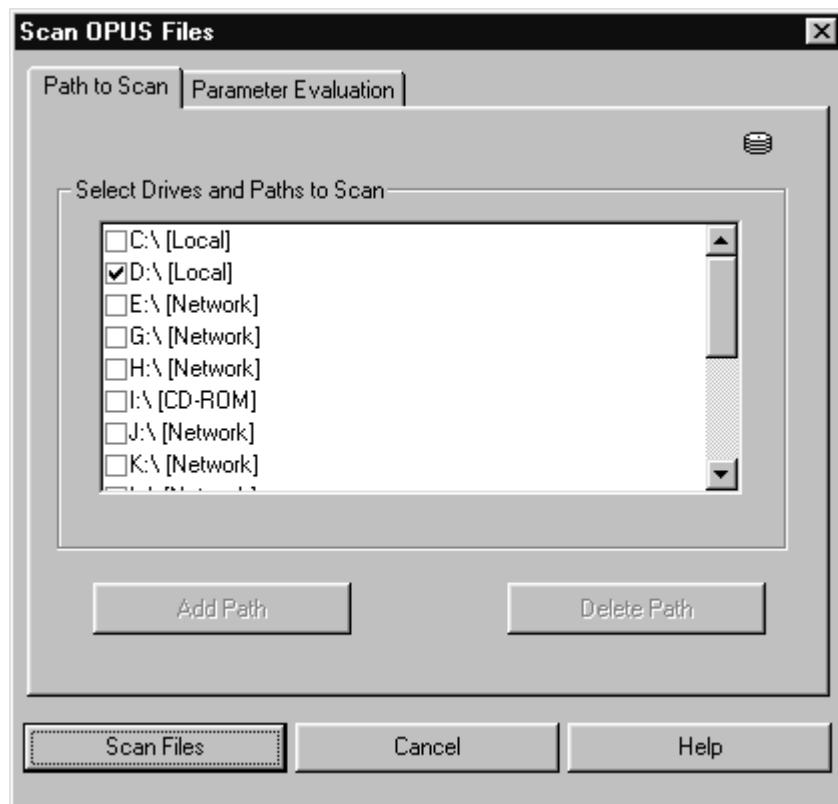
Figure 31: Scan OPUS Files – Path to Scan tab

If you click on the *Parameter Evaluation* tab you can limit the information stored in the database by selecting the parameters you want to add or remove. The smaller the number of parameters, the smaller the database.
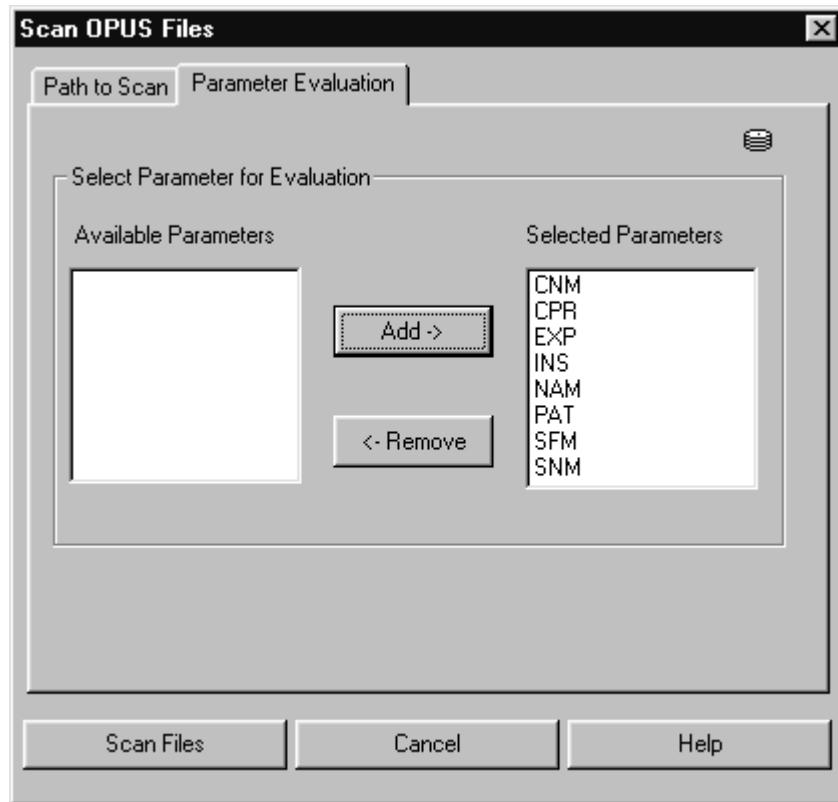
Figure 32: Scan OPUS Files – Parameter Evaluation tab

3.13   Find OPUS Files

All spectrum files found are displayed in the *Select File(s) to load* selection box. If you point the cursor on a spectrum, the selected parameters and information from the info block are listed in the field on the right. Select a file from the selection box and load it into the spectrum window by clicking on the *Load Selected Files Load* button. If you have selected too many files, you will be informed that the list has been shortened.

As soon as a database has been generated you can search for file names, text strings in files or file parameters. In case you added spectra to your hard drive after the database has already been generated, it is recommended to update the database. Click on the *Update Database now* button prior to a search run. Date and time of the last update is displayed to the left of this button.

Enter the string to be searched for in the *Find Text in Files* line. You can specify whether to find *exact wording* only, *any word*, or *all words* you have entered. You can even further narrow down the search by activating the *Find in Period* check box. Specify the date and select between *after*, *before* or *between* this date to narrow down your search. Start the query by clicking on the *Update Database now* button.
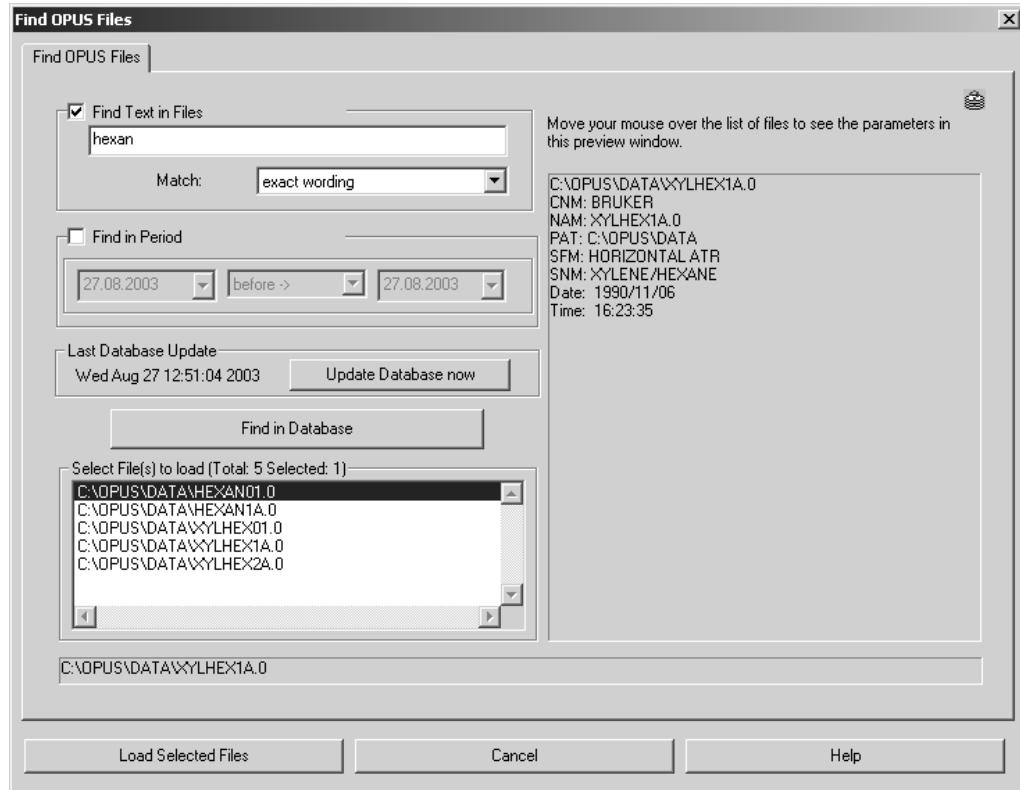
Figure 33: Scan OPUS Files tab

3.14   Clone Entry and Clone Original

Clone Entry and *Clone Original* are used to duplicate spectrum files. Use *Clone Entry* to make a copy of a data file that has been manipulated (e.g. by baseline correction). If you use the *Clone Original* command, you create a copy of the original data file (manipulations made will not be stored). In either case drag & drop the respective data file to the *File(s) to Clone* selection field. Click on the *Clone* button.
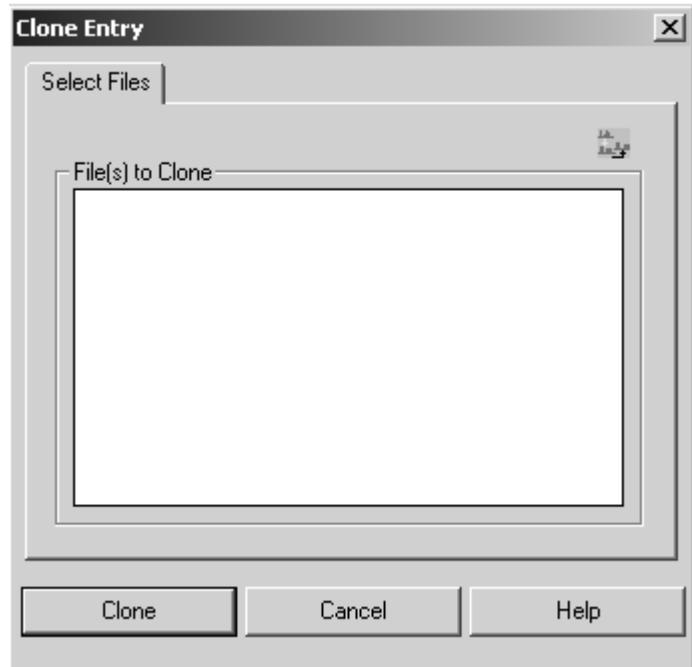
Figure 34: Clone Entry - Select Files tab

3.15   Add Comment

If you want to add a comment to a spectrum, click on the *Add Comment* command. Select the file(s) and drag and drop the file(s) into the selection field File(s) to Comment. Then, enter the comment into the *Comment Text* entry field. The comment will be displayed in the *Report Display* under *Datafile History*.
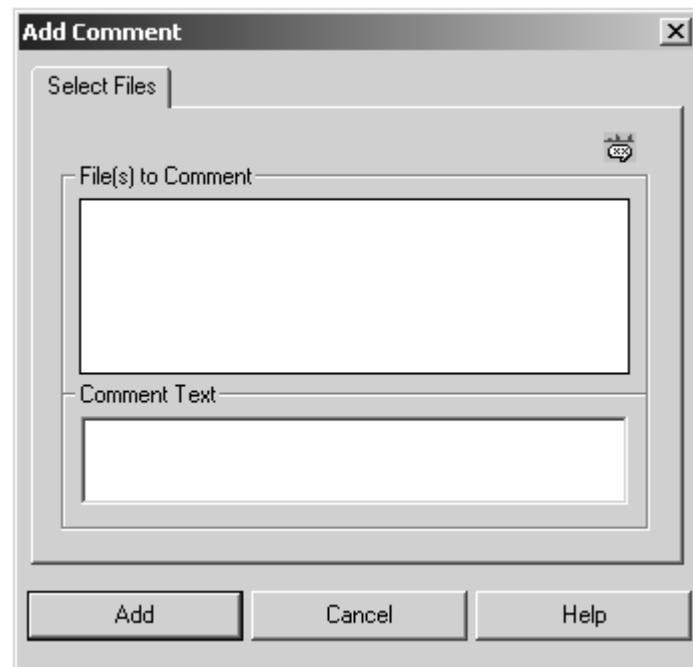
Figure 35: Add Comment - Select Files tab

3.16   RS 232 Communication

RS 232 Communication is a command which allows to communicate with external devices using the serial port(s) of your PC (COM 1, COM 2, etc.).

In general, it is recommended not to use this command interactively, but in combination with a macro or VB-Script. The interactive mode can be used to test the communication.

3.16.1   RS 232 Write/Read

If you start the command interactively, the following dialog window will be displayed:
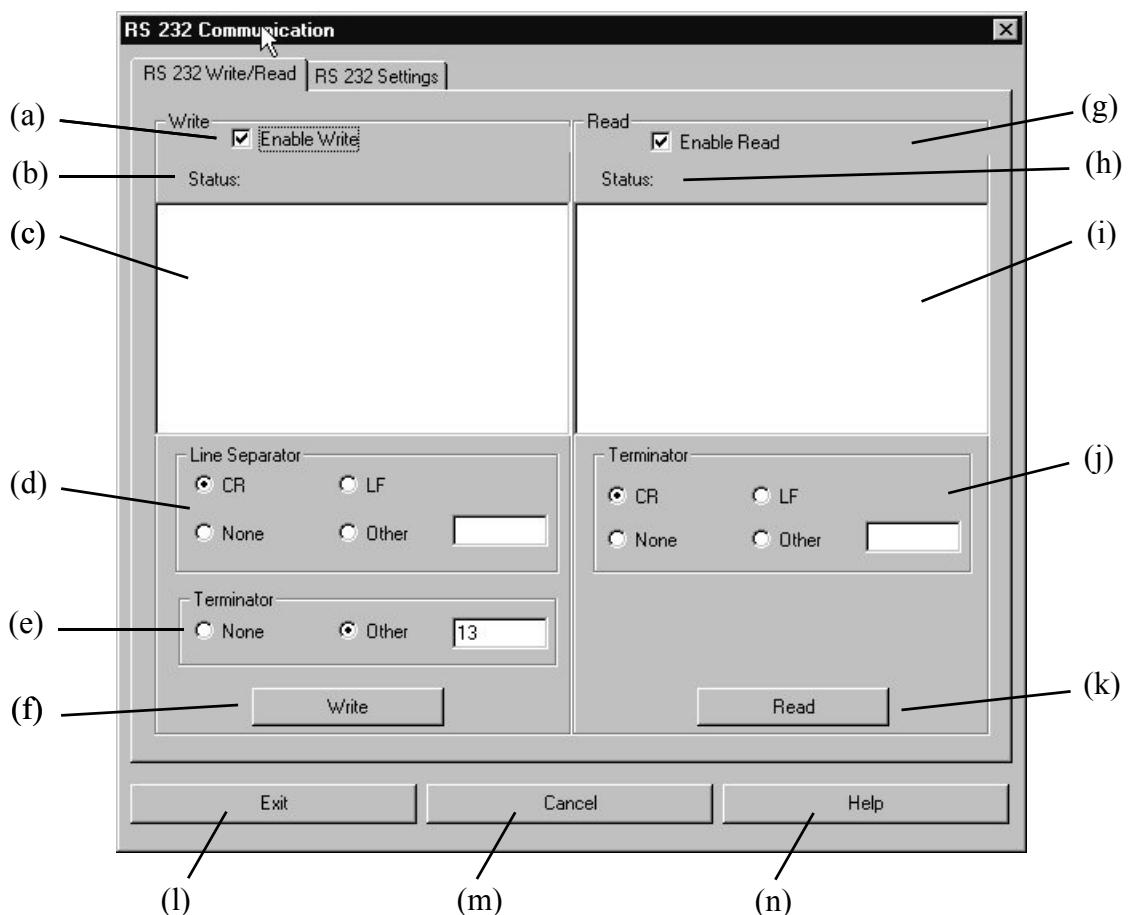
Figure 36: RS 232 Communication - RS 232 Write/Read tab

(a) This check box enables or disables the *Write* command.

(b) Indicates the status of the *Write* command (e.g. Writing..., Time-out etc.)

(c) Enter the text line(s) which are to be written to the external device. If you enter more than one line, each line will be optionally terminated by the specified end-of-line character. If you want to send single special characters to RS 232, which cannot be used as strings as they are reserved for special purposes e.g. ' (single quote),{} (braces) etc., enter **@(#)** followed by the three digit ASCII code of this special character.

Example: **ABC@(#)039DEF** will be sent as **ABC'DEF**

(d) The *Line Separator* options are used to specify the *Line Separator* for the *Write* command. Whenever the specified line separator is detected the lines will be separated accordingly. Carriage Return (*CR*) and Line Feed (*LF*) are already pre-defined. If you need a different kind of line separator, check the *Other* option button and enter the ASCII code of the desired line separator into the entry field next to the option button. If no line separator is to be used, check the *None* option button.

(e) You can specify a *Terminator* to be sent after the last character has been entered. Either select *None,* if no character should be sent, or *Other*. In the latter case you have to enter the ASCII code of the terminator into the entry field next to the option.

(f) If you click on the *Write* button, the text entered in (c) will be sent to the RS 232 interface.

(g) This check box enables or disables the *Read* command.

(h) The status of the *Read* command is indicated here (e.g. Reading..., Time-out etc.)

(i) The answer sent by the external device is displayed in this entry field

(j) These options are used to specify the *Terminator* for the *Read* command. Whenever this terminator is detected the *Read* command will stop. Carriage Return (*CR*) and Line Feed (*LF*) are already pre-defined. If you need a different kind of terminator, check the *Other* option button and enter the ASCII code of the desired terminator into the entry field next to the option button. If you check the *None* option button, the *Read* command waits for answers until the *time-out* has been reached.

(k) If you click on the *Read* button you activate the read command only.

(l) Exits the *RS 232 Communication* command and stores the current settings. No write or read activity is started.

(m) Exits the *RS 232 Communication* command without saving the current settings.

(n) Shows the online help.

3.16.2   RS 232 Settings

The *RS 232 Settings* tab allows to set the different options for the serial interface:
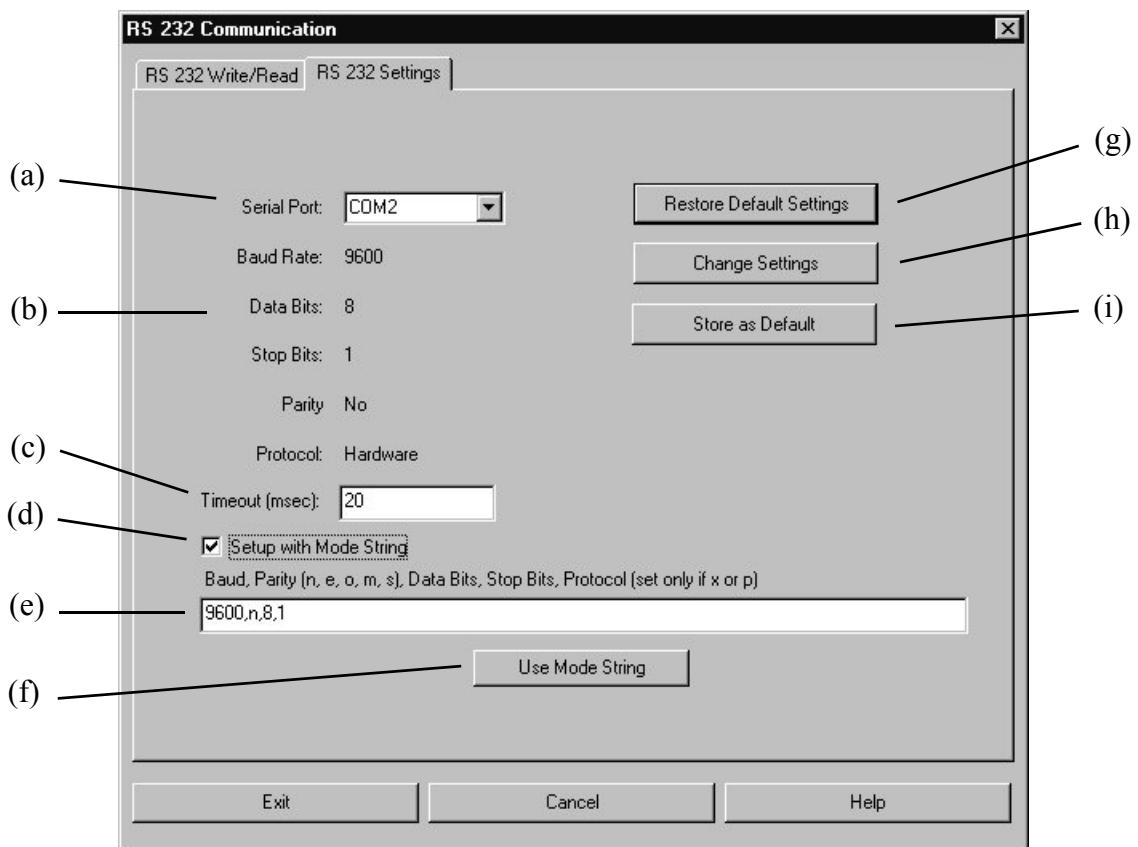
Figure 37: RS 232 Communication - RS 232 Settings tab

   (a) The drop-down list includes all serial interfaces currently available. If a serial interface is not available (e.g. if the mouse is connected to COM 1) this interface will not be included in the drop-down list.

   (b) The current interface settings are displayed.

   (c) Enter an appropriate time-out value in milliseconds.

   (d) If you activate this check box, the interface will be configured with a *Mode* string. For details on the *Mode* command, refer to the operating system manual. If the check box is deactivated, (e) and (f) will be disabled.

   (e) Enter the mode string to be used for configuration (without specifying the serial port) into this entry field.

   (f) If you click on this button, the current settings according to the mode string. The settings will be shown in (b).

   (g) The *Restore Default Settings* button reads the current settings which have been specified in the operating system as default.

   (h) The *Change Settings* button activates the setup dialog of the operating system. See section 3.16.3.

   (i) The *Store as Default* button overwrites the operating system settings by using the current settings.

3.16.3   COM1 Properties

The *COM1 Properties* dialog will be displayed if you click on the *Change Settings* button (see section 3.16.2):
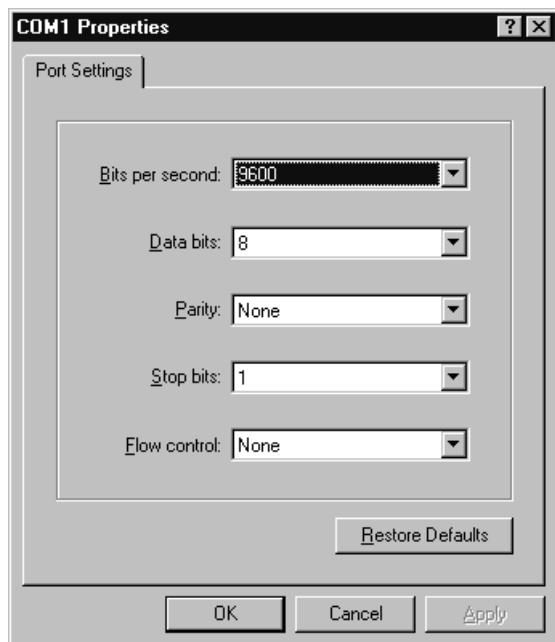
Figure 38: RS 232 Communication - Port Settings tab

Use this dialog to specify the following communication parameters:

- Bits per second
- Data bits
- Parity
- Stop bits
- Flow control

The same dialog opens if you set up the parameters of the serial interface by using the *System Settings* command of the operating system.

3.17   Copy Data Block

Single data blocks can be copied from one OPUS file to another. This, however, is only possible when using definite block types, e.g. INFO.
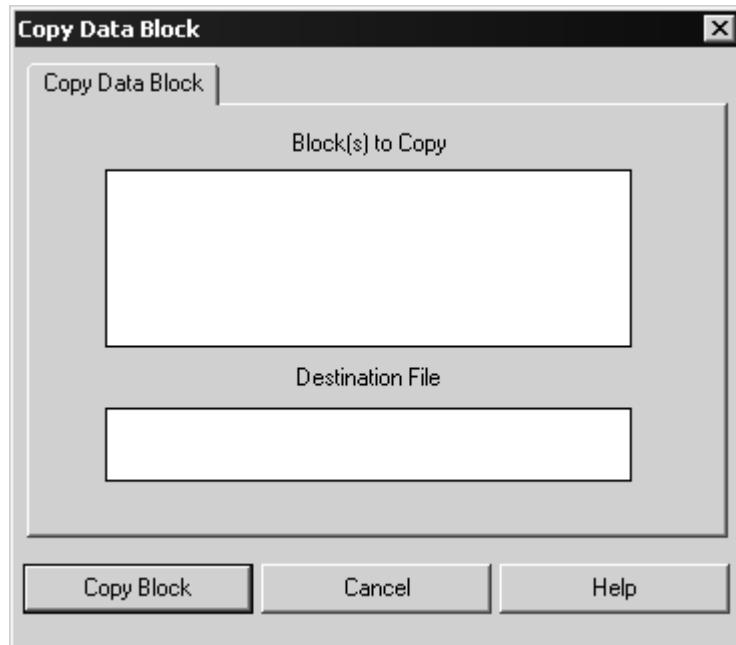
Figure 39: Copy Data Block

Data blocks to be copied are entered into the *Block(s) to Copy* selection field, e.g. by drag & drop from the OPUS browser window. Specify where to copy the data blocks in the *Destination File* field.

3.18   Change Data Block Type

Changing the data block type is not required very often. Macros, however, may need a definite data block type. If you select the *Change Data Block Type* command, the data block type will only be renamed. The data, however, will not be changed.

Drag & drop data blocks to be changed into the *Block(s) to Change* selection field. Select the desired block type from the *Choose Block Type* drop-down list. It may be possible that not all data block types are included in the list.
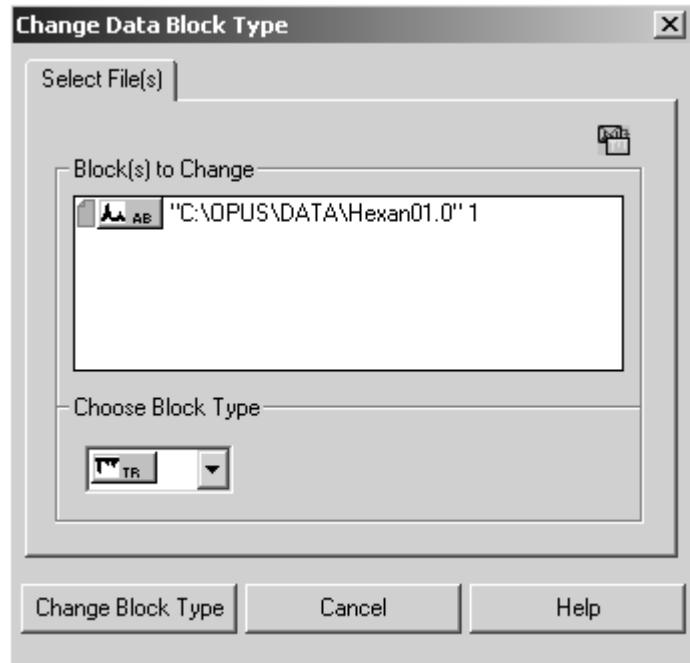
Figure 40: Change Data Block Type

3.19 New/Open

If you select the *New* command, a dialog opens which includes the *OPUS*, *PLE* or *VBScript* options. *OPUS* generates a new OPUS workspace (see sections 14.10 and 14.11), *PLE* a blank template for the Plot Layout Editor (see chapter 11.5), and *VBScript* a blank VisualBasic script form. For details on how to write VB Scripts, refer to the OPUS *Programming* manual.

Use the *Open* command to open available OPUS workspaces.

3.20 Print

You can print any report on your default printer using the *Print* command. The report data are either printed on the printer or into another file.

3.21 Print Preview

This command is only available if a report window is displayed. You can print a preview of a print-out by using the *Print Preview* command.

3.22   Print Setup

The default printing dialog can be used to define printer settings. You can define the paper size and print-out format. These settings will be standard for future OPUS print-outs. As the dialog box appearance depends on the printer selected, it is not shown in this section.

3.23   Exit

If you select the *Exit* command, the OPUS program will close.

4 Edit

The *Edit* menu includes features for information input, options to edit structures as well as the standard Windows commands such as *Copy* and *Paste*.
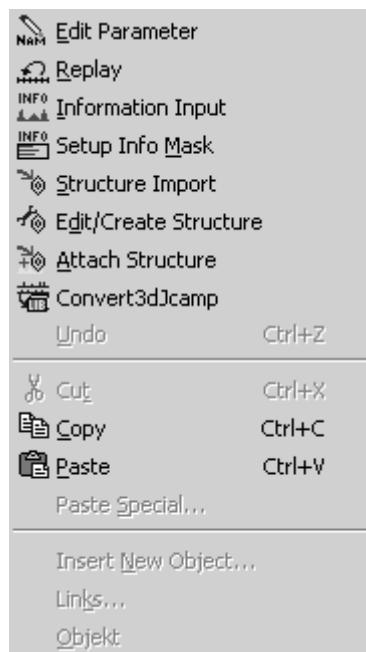
Figure 41: Edit Menu

4.1 Edit Parameter

Use the *Edit Parameter* command to edit the most important sample parameters, e.g. sample name, sample form, operator name and sample number. First, load the spectrum the parameters of which you want to edit into the OPUS browser window. Select the *Edit Parameter* command. The following dialog box opens:

Figure 42: Edit Parameter – Enter Parameter tab

Now, change the parameters accordingly. Note that you will not be able to change these parameters if working in GLP mode.

On the *Axes Labels* tab you can set the axes labels and a scaling factor for the axes. These settings are used when the spectra are printed out. The scaling factors will only be considered in case of 3D spectra.
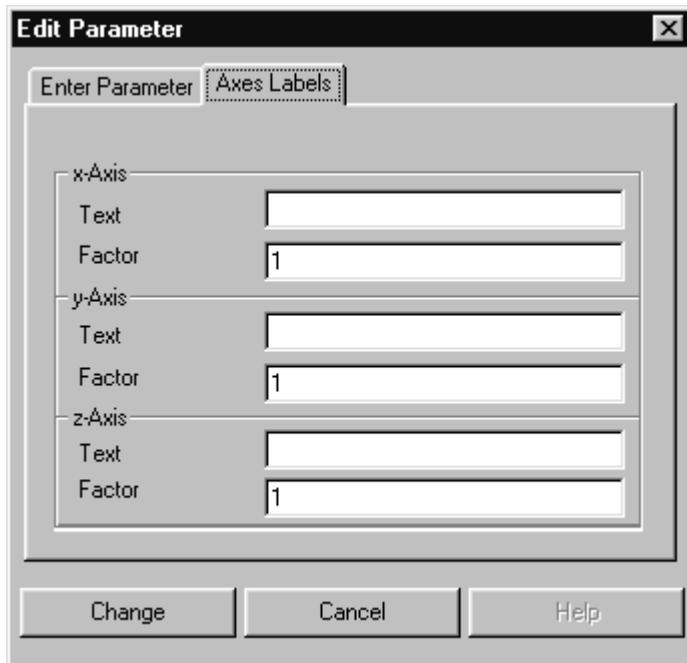
Figure 43: Edit Parameter – Axes Labels tab

4.2 Replay

When working in GLP mode a copy of the original spectrum is saved together with the corresponding data. On the basis ofthis original spectrum, you can repeat some of the manipulations performed.

Drag and drop the spectrum from the OPUS browser window to the *File for Replay* entry field to repete some manipulations.
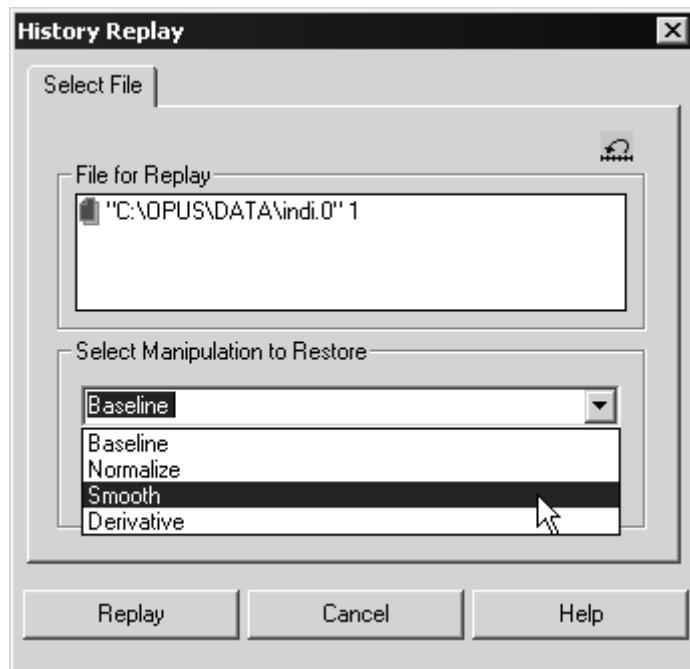
Figure 44: History Replay - Select File tab

Select the manipulation command up to which you want to restore the file. If you select *Smooth,* as exemplified in figure 44, *Baseline*, *Normalize* and *Smooth* manipulation command will be performed on the original spectrum, except the *Derivative* command.

4.3 Information Input

Apart from OPUS parameters you can also save additional information, using the *Information Input* command. This kind of information will be saved in a separate *INFO* (information) data block ⊞INFO , and can be integrated both into a report window and in a plot. If you want to save spectra in your own search libraries, information input is mandatory.

The so-called *Info Mask* (see section 4.4) includes the descriptions of up to 99 lines which can be saved in one *INFO* data block. You can define this *Info Mask* according to your individual needs.

4.3.1   First-Time Information Input

Load a spectrum into the OPUS browser window and select the *Information Input* command. The following dialog opens:
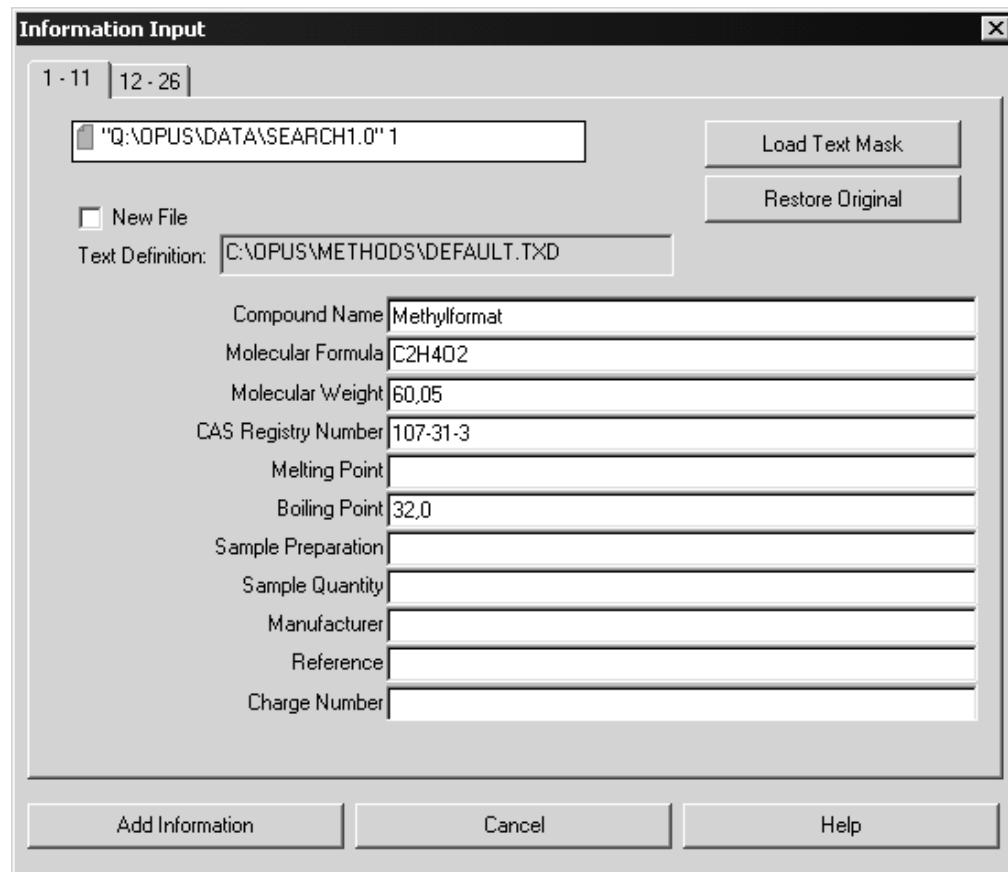
Figure 45: Information Input

You can only select one spectrum file at a time to enter additional information. The name of the information mask, a file with the extension *TXD* is displayed in the *Text Definition* field. To use a different information mask, click on the *Load Text Mask* button. The *Load Info Text Mask* dialog pops up which you can select a different information mask from.

Depending on the number of lines defined for the *Info Mask* selected, the *Information Input* dialog (see figure 45) can include up to 7 pages. Enter the requested information. You do not need to fill in all the fields.

Clicking on the *Add Information* button will create or modify the *INFO* data block for the file selected. This new data block will be attached to your spectrum file and displayed in the OPUS browser window. Right click on this data block and select *Show Report* from the pop-up window. The report window only includes data which have been filled into the lines of the *Information Input* dialog (see figure 45).
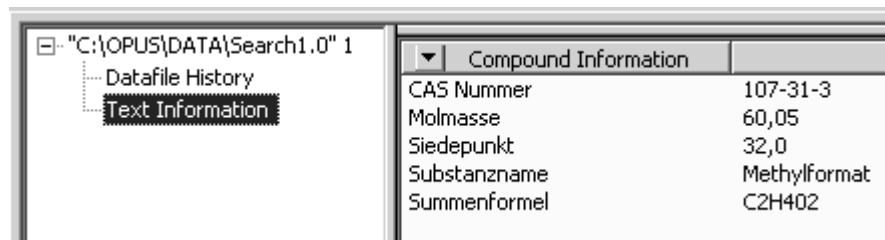
Figure 46: Report window with text information

4.3.2   Editing Existing INFO Blocks

If you load a spectrum file which already includes an *INFO* data block, the information added to this data block will be displayed in the *Information Input* dialog (figure 45) together with the appropriate information mask.

However, it may occur that the appropriate information mask cannot be found on your data structure. Maybe the mask is based on a different data structure or you have copied the information mask into a different directory, or even deleted it. In this case the information mask reference will be highlighted in red in the *Text Definition* field (figure 45).

Now, you can edit existing data or add new data. Alternatively, you can select a different kind of information mask. In this case all inputs made so far will be deleted in the dialog. If you have deleted or overwritten entry fields by accident, click on the *Restore Original* button to read the original data again.

4.3.3   Creating a New File

Instead of attaching an *INFO* data block to an existing OPUS file you can also create a new file, which only consists of an *INFO* data block. In this case activate the *New File* check box (see figure 45). A new file, *INFOx.0,* will be created, with *x* being either a single or multi-digit number.

4.3.4   Displaying and Printing INFO Data Blocks

As already mentioned the *INFO* data block can be displayed in a report window. To print the *INFO* data block each data line of the block can be addressed as OPUS parameter, using the parameter name I*nn* with *nn* being the line number (e.g. I01 = first line, I12 = twelfth line). Similarly, you can also include information mask texts into the plot, using T*nn* as parameter name (e.g. T01 = text in first line, T12 = text in twelfth line).

4.4 Setup Info Mask

When creating an information mask you define the kind of information available for information input. Depending on the field of application you can create different kinds of information masks. The contents and file name of the information mask will be saved during information input. This enables all data to be displayed on data systems which do not contain the appropriate *Info Mask*.

If you select the *Setup Info Mask* command, the corresponding dialog will be displayed (figure 47), and the last-accessed *Info Mask* is automatically loaded. The file name and path of the *Info Mask* is displayed in the *Current Info Mask* line.
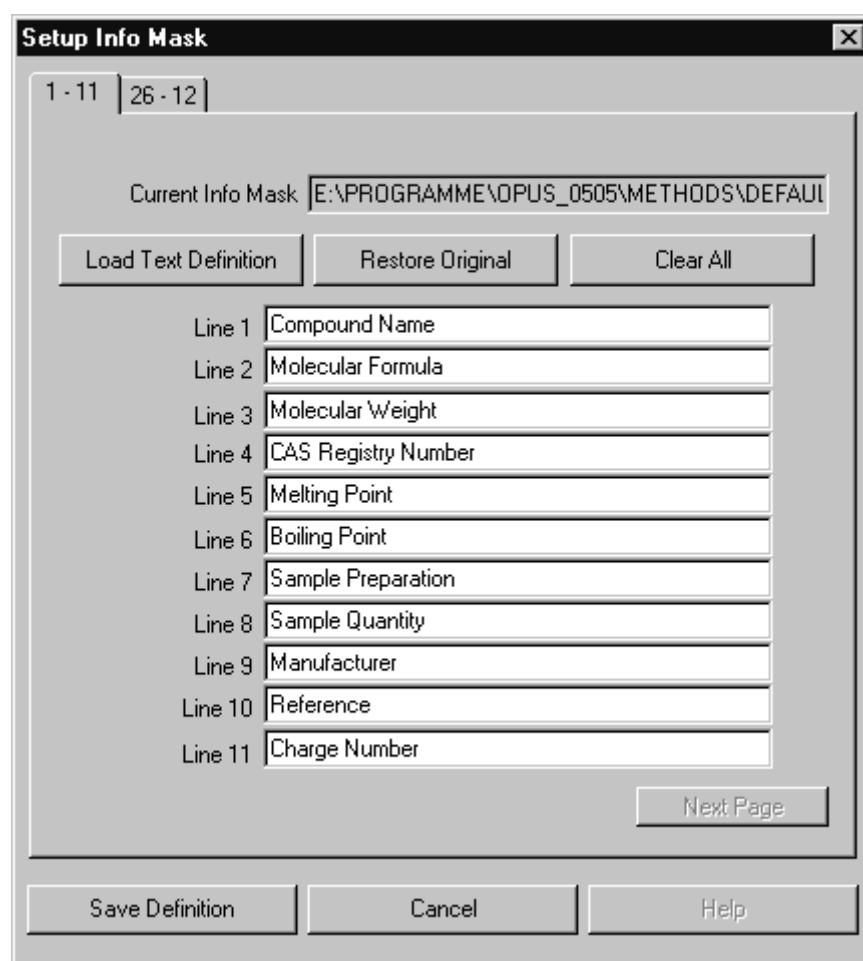
Figure 47: Setup Info Mask

Depending on the number of lines up to 7 pages can be displayed, similar to the *Information Input* dialog. To create a new information mask click on the *Clear All* button. All entries will be deleted and only the first page is available. All entry fields will all be highlighted in red (see figure 48).
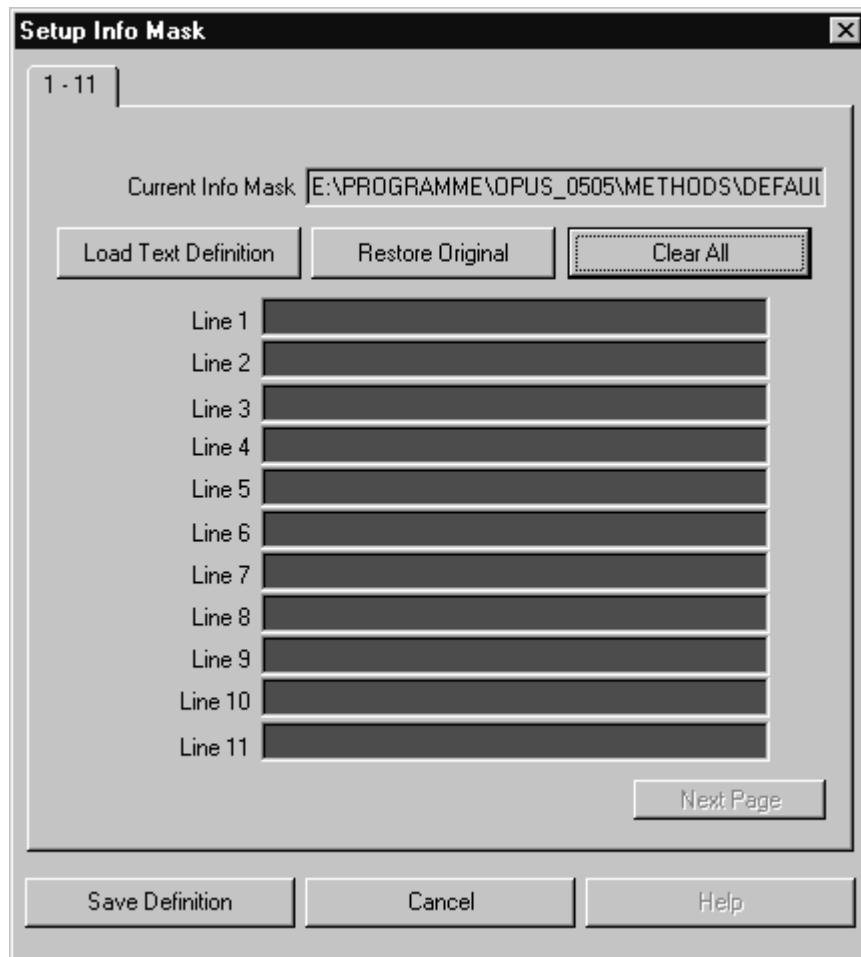
Figure 48: Setup Info Mask - defining entry fields

As soon as you have started to enter data, the entry field color will change to white. When entering data, make sure that the entry fields are filled in one after the other. Be careful not to skip a line.
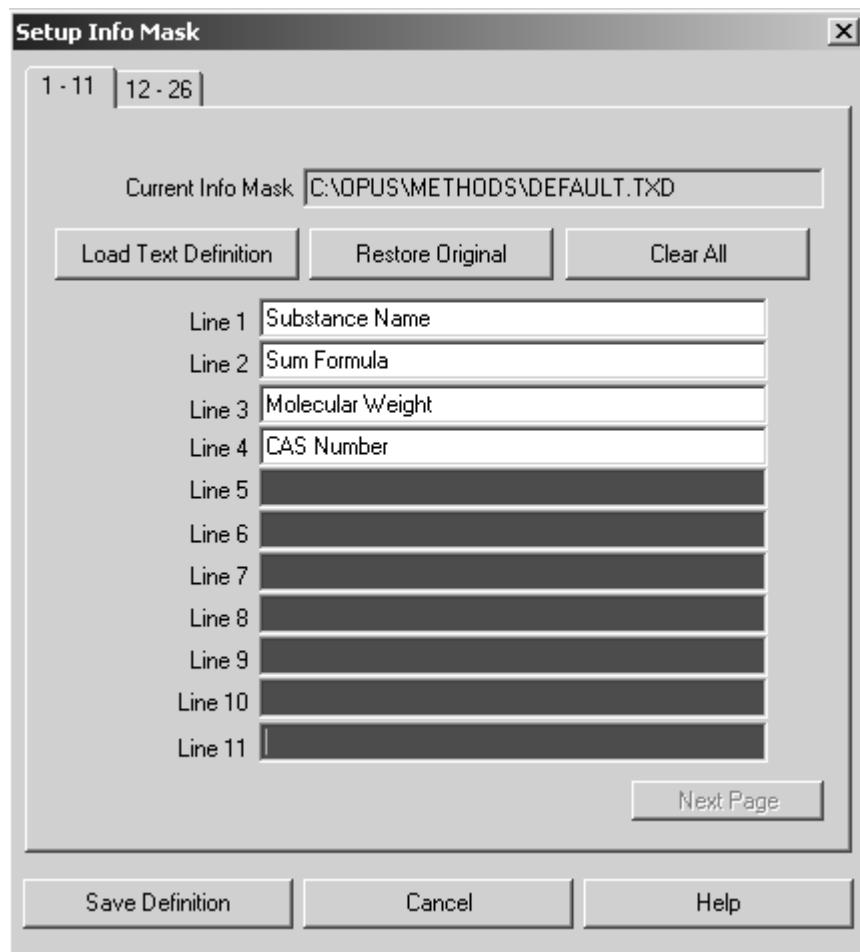
Figure 49: Setup Info Mask - defining entry fields

You have to define all entry fields on the first page before being able to open a new page by the *Next Page* button. Save the information mask by clicking on the *Save Definition* button. If an information mask with the same name already exists, you will be asked whether you wish to overwrite the existing mask.

To load and edit an existing mask click on the *Load Text Definition* button. Changes can easily be undone by clicking on the *Restore Original* button.

4.5   Structure Import

The *Stucture Import* command can be used for chemical structural formulae created in Molfile format. These formulae can be imported to OPUS. If you select the *Structure Import* command, the *Structure Import* dialog opens. Load the corresponding files.

Files in Molfile format have the extension **.MOL*. An OPUS file is created for each structural file, using the same file name and a consecutively numbered extension (starting with 0). This OPUS file is automatically loaded into the

OPUS browser window. Double click on the *Structure* data block to have the structural formula displayed within the *Structure* window type registered in OPUS. For details on how to attach a structural formula to an OPUS file, see section 4.7.

4.6   Edit/Create Structure

The *Edit/Create Structure* command provides a general interface to any software that supports the Molfile format. You can use an editor of your own choice. Bruker provides an editor suited for this interface.

OPUS files with structural formulae are automatically converted into Molfile format and stored in the *Search* sub-directory, using the *BIRSY.MOL* file name. The file name, including the path, is transferred to the editor using the command line. If your editor supports command line parameters, the structural formula will automatically be displayed. You can edit the structural formula and store it in Molfile format. The file edited in Molfile format will automatically be converted into the OPUS format.
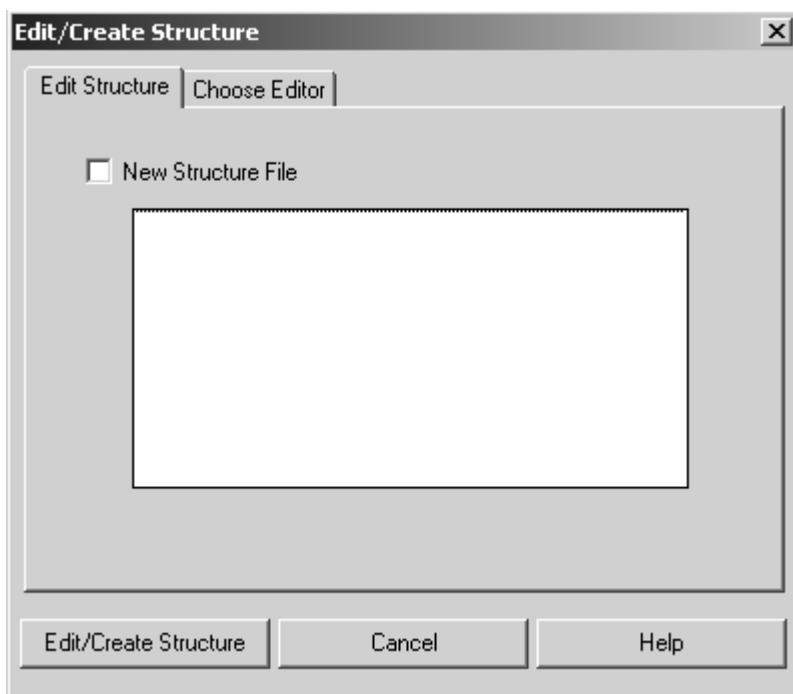
Figure 50: Edit/Create Structure – Edit Structure tab

On the *Edit Structure* tab you can create a new structural formula, or edit an existing one. In the first case, activate the *New Structure File* check box. An empty file will be created and transferred to the structure editor. Define the file name, including the path. To edit an existing structural formula drag and drop the file into the entry field displayed (see figure 50), and click on the *Edit/Create Structure* button.
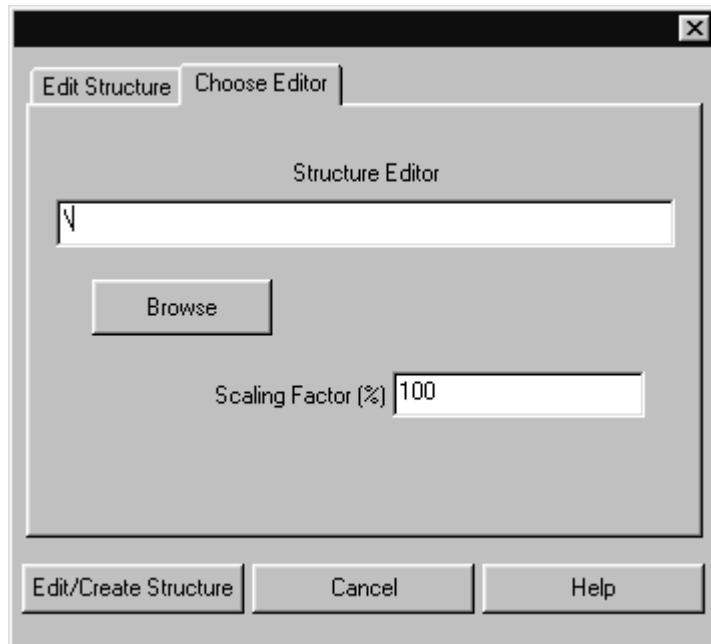
Figure 51: Edit/Create Structure – Choose Editor tab

Click on the *Choose Editor* tab to specify which structure editor you want to use in combination with the *Edit/Create Structure* interface. Enter the program name, including the path, into the *Structure Editor* entry field or use the *Browse* button to search the directories for the editor program. The *Scaling Factor* determines the size of an imported structural formula.

4.7 Attach Structure

Having imported a structural formula you can assign this formula to an OPUS spectrum file. The structural formula will automatically be converted into the OPUS format.
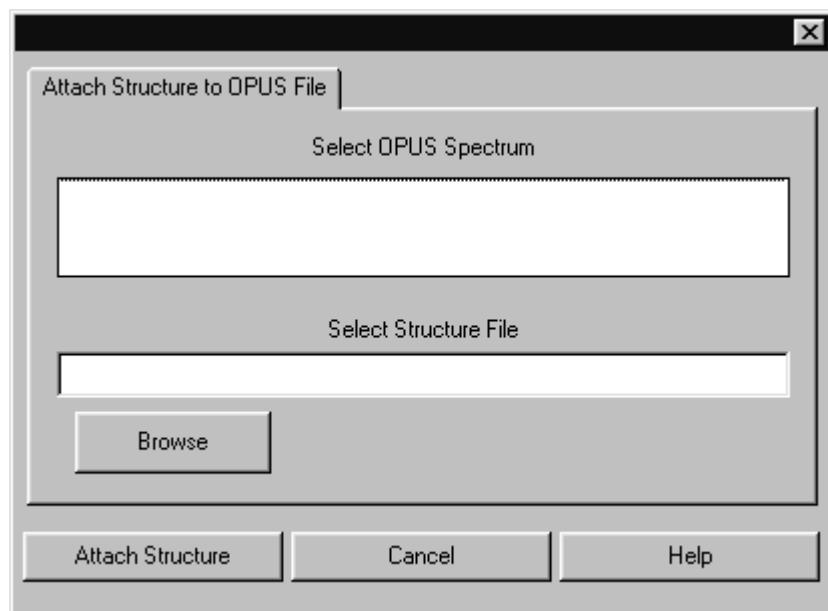
Figure 52: Attach Structure

Load the spectrum into the OPUS browser window and drag and drop it into the *Select OPUS Spectrum* entry field. Specify the name of the structural formula file. You can also use the *Browse* button to locate the file. Click on the *Attach Structure* button to include the structural formula into the OPUS file.

4.8   Convert 3dJcamp

The *Convert 3dJcamp* command allows to convert JCAMP spectra files into the OPUS format. A JCAMP file can consist of several spectra. Each spectrum of a JCAMP file has to have a specific format. The following file extract exemplifies such a format:

```
##TITLE=Butanoic acid
...
...
##CAS REGISTRY NO=107-92-6
...
450.0 637 638 621 624 638 665 702 723 741 798
490.0 839 862 888 935 928 967 1021 1000 996 1098
530.0 1133 1222 1328 1382 1488 1531 1571 1558 1559 1570
570.0 1572 1637 1678 1756 1802 1942 1924 1905 1927 1920
...
```

The "..."characters represent additional information lines, all starting with "##" (exceptions see below), or additional lines of data points.

For further details on how to convert information lines into OPUS parameters, refer to chapter 14.2.

The CAS REGISTRY NO information line is obligatory if a structure formula JCAMP file also exists. For the reason that the spectrum is assigned to the molecular structure according to the CAS number. The structure of this spectrum is available in OPUS in the form of the *STR* (structure) data block (![STR icon]).

If you click on the *Convert3dJcamp* command, the following dialog opens:
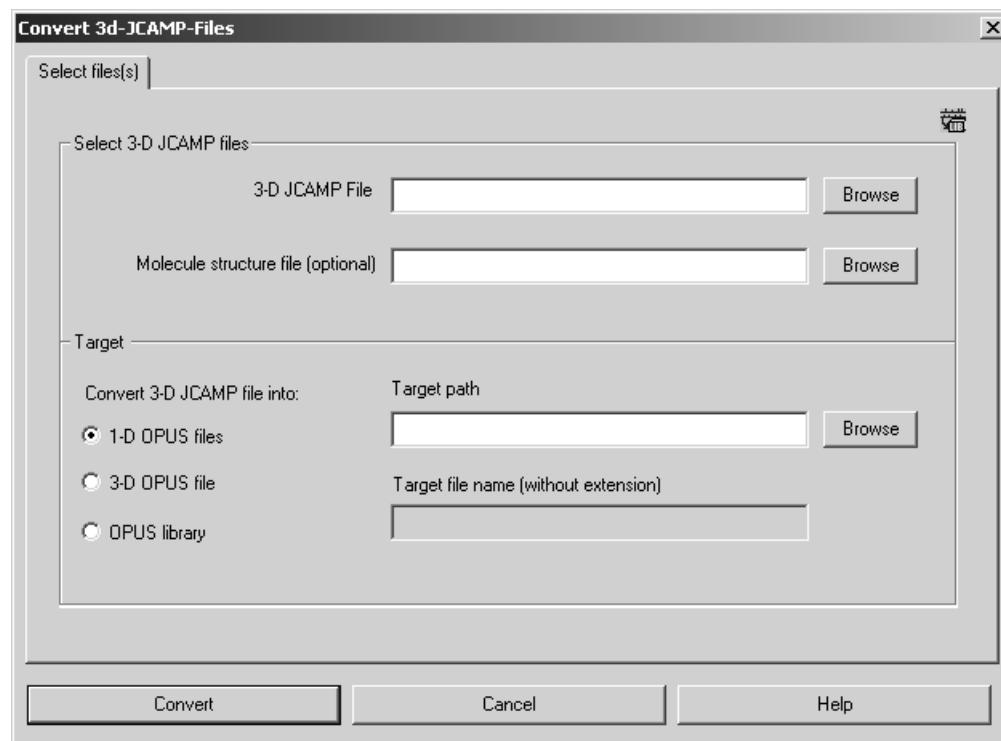
Figure 53: Convert 3d-JCAMP-Files - Select File(s) tab

In the *Select 3-D JCAMP files* group field you define the file name of the 3-D JCAMP file which includes the spectra information. You either type in the file name manually with the complete path or click on the *Browse* button to select the file in the directory structure.

Optionally, you can enter the file name of the molecule structure file. If you skip the *Molecule structure file* entry line, the OPUS spectra created will not include a *STR* data block.

Format of JCAMP structure formulae

The format of a molecular structure may be as follows:

```
c:75014
C2H3Cl
2:(303,155,320,165;2)(337,156,320,165;1)
1:(3,Cl)
0:
```

The first line includes the CAS number followed by the sum formula, bonding data and the names of foreign atoms.

You can also add the melting and boiling points of the different substances to the OPUS file *INFO* data block. Make sure that you add the data at the end of the JCAMP structure file, line by line as follows:

```
,CAS_NO,MELTINGPOINT,BOILINGPOINT,
```

Example:

```
,1571864,75.0,263.0,
```

Always write a comma at the beginning and at the end of the lines.

In the *Target* group field (figure 53) you specify the OPUS format which the JCAMP spectra have to be converted to. You can select between three option buttons:

- **1-D OPUS files:**

  Each JCAMP spectrum is stored separately as OPUS spectrum. The file name is a combination of the *TITLE* and *CAS REGISTRY NO* information lines used in the JCAMP file. If you check the *1-D OPUS files* option button, you also have to specify the target path. Either type in the target path name manually or click on the *Browse* button to select the path from the directory structure.

- **3-D OPUS files:**

  The 3-D-JCAMP file is converted into a 3-D-OPUS file. This is useful if the spectra have been acquired by chromatography, or if all spectra are a compound of always the same substance which comes in different concentrations. You can also define this substance concentration in the information line for each spectrum. The format in the JCAMP file must be as follows:

  ```
  ##CONCENTRATIONS= (NCU)
  (<Glucose>,    2.100, %)
  (<Lnvisco104>,    1.131, %)
  ```

  In this case the substance name, quantity and quantity unit will be included in a text file (in table format) which will be created apart from the OPUS file and with the same file name. This is helpful if the data are used to perform a QUANT analysis. In this case the

concentration data can be used from the text file by means of the clipboard.

Either type in the target path name manually or click on the *Browse* button to select the path from the directory structure. You also have to specify the OPUS target file name without extension. If the 3-D OPUS file already exists, it will not be overwritten, but the name incremented.

- **OPUS library**

   All spectra are stored in an OPUS library, including spectra information and possible structure data blocks. Either type in the target path name manually or click on the *Browse* button to select the path from the directory structure. You also have to specify the OPUS target file name without extension. If the OPUS library already exists, it will be overwritten.

Click on the *Convert* button to start the conversion. The conversion progress will be indicated by the status bar on the bottom right. If one of the information lines includes the sum formula, the molecular mass will be calculated from this formula, indicated in atomic units and entered in the *INFO* data block of the respective spectrum.

To undo the settings click on the *Cancel* button and the dialog will be closed.

5 View

The *View* menu allows to configure the OPUS user interface. You can define the toolbars, hide or unhide the status bar or the browser window.
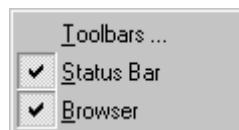
Figure 54: View Menu

5.1 Toolbars

Use the *Toolbars* option from the *View* menu or right click onto the OPUS toolbar to open the *Toolbars* dialog box. This dialog box allows to configure single icons or even complete toolbars.
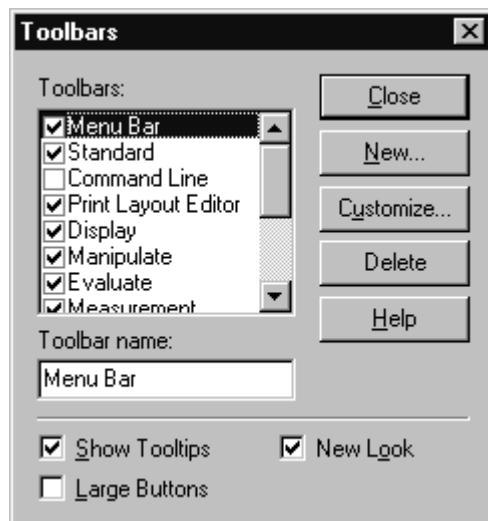
Figure 55: Toolbars Configuration

If you check the different boxes, you activate or deactivate the different toolbars on the user interface. Click on the *New* button to create a new toolbar. *Customize* allows you to adjust the toolbar according to your individual preferences. A second dialog box will open, see figure 56.
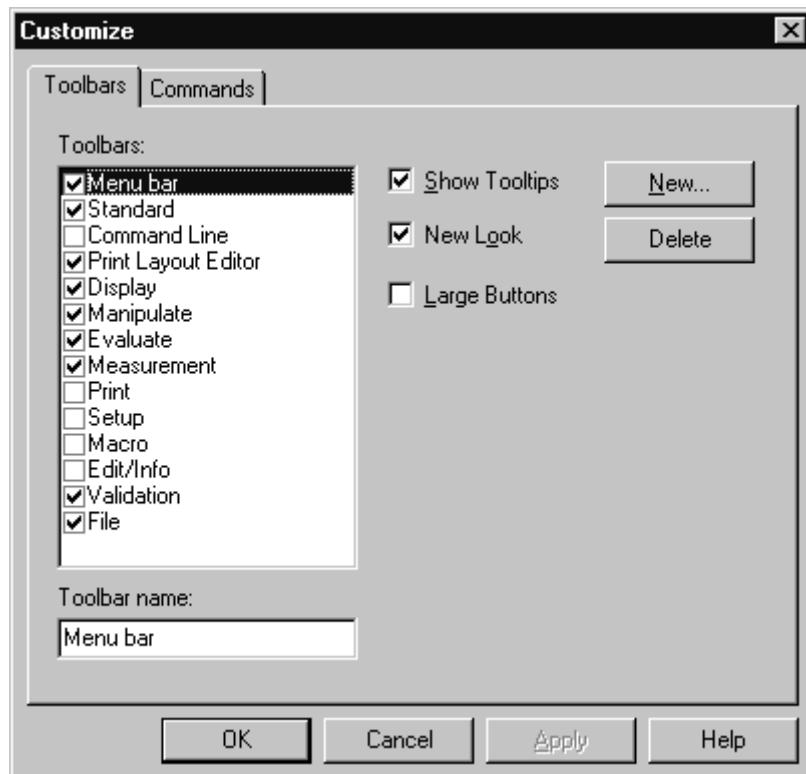
Figure 56: Customize Dialog

Click on the *Toolbars* tab and select the toolbar you want to customize. If you activate the *Show Tooltips* check box, additional info text pops up which describes the function of a specific icon when you position the cursor on it. *New Look* means that the line between the icons on the toolbar will not be displayed. This is set by default. To enlarge the icons displayed, activate the *Large Buttons* check box.

Click on the *Commands* tab and select the categories you want to customize. Each category selected is exactly described on the lower part of the dialog box, see figure 57. You can drag the icons directly into the toolbar. If you want to remove an icon from the toolbar, simply drag the specific icon from the toolbar and drop it outside the bar.
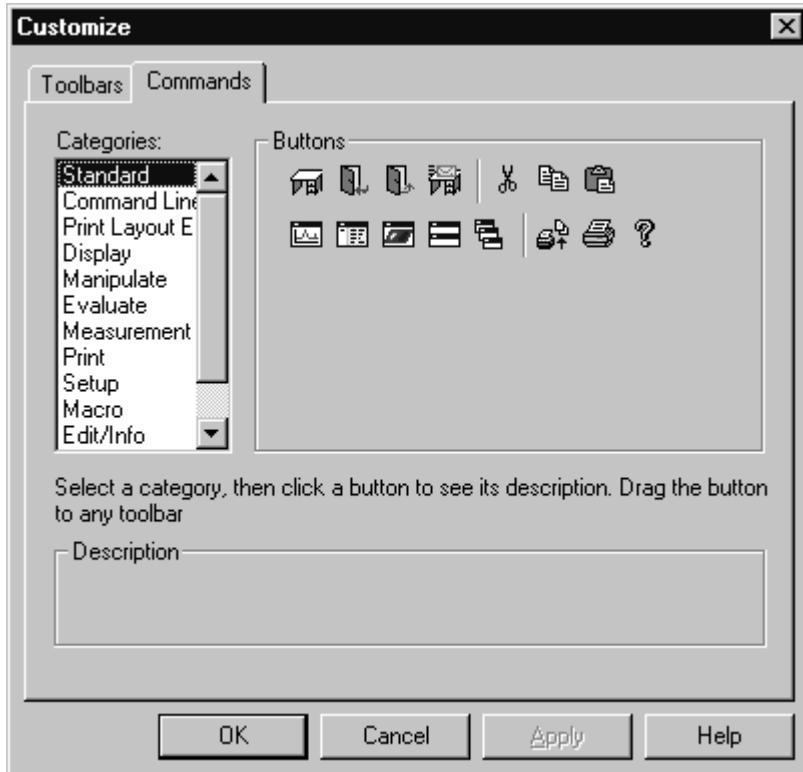
Figure 57: Customize – Commands

5.2 Status Bar

The status bar informs you about the background tasks of programs running in the OPUS, and displays their current status. To activate or deactivate the status bar, check or uncheck the *Status Bar* option.

5.3 Browser

By default, the OPUS user interface always displays the browser window on the left side. If you deactivate the *Browser* option, only the spectrum and overview window will be displayed on the screen. Apart from this option you can also reposition the OPUS browser window (see section 6.4).

6 Window

The *Window* menu allows you to open new windows and to customize their position and appearance. If you load a file, OPUS automatically opens the appropriate window to this file. For example, if you open a 3D file, OPUS directly opens a 3D window and displays the spectrum accordingly.
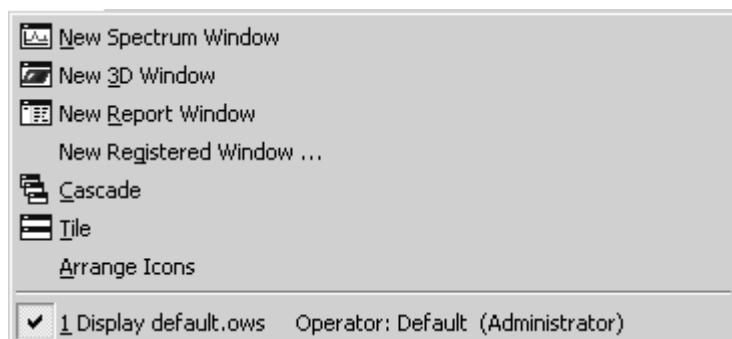
Figure 58: Window Menu

6.1 New Spectrum Window

OPUS allows to display several spectra in one spectrum window, and to display spectra in different windows. If you select the *New Spectrum Window* option, a new spectrum window opens, indicated by the [Display defa...] tab at the bottom of the spectrum window. Click on the respective tab to switch between the windows.

6.2 New Report Window

Apart from spectra and interferograms OPUS files store different data as well. For example, the results of a peak picking evaluation and its parameters used can be listed numerically. The data are displayed by dragging the *PEAKS* (peak pick) data block [PEAKS] into the report window.

6.3 New Registered Window

If you click on the *New Registered Window* option, a drop-down list opens which includes all possible types of OPUS windows. The number of windows may vary, according to the additional software packages installed. Therefore, the list in this manual may not exactly reflect the list contents displayed on your

screen. You can open any type of blank window by selecting the window from this list.

Window Name	Type
3d, 3d+	To display three-dimensional plots.
Cluster Analysis	To display a dendrogram or histogram (part of OPUS IDENT).
Display	To display spectra.
Library	To display libraries and their detailed information.
OldReport	Shows report in the OPUS/OS2 format.
Process Control	To display a standard trend chart (part of OPUS PROCESS).
Report	To display report blocks.
SearchResults	To display the result of a search performed using Spectrum Search and other Search functions.
SingleReport	To display a report without the tree structure.
Structure	To display molecular structures, generated with a structure editor (part of OPUS SEARCH).
Text View	To enter text. See section 6.3.1.

6.3.1   Text View

Select *Text View* from the drop-down list. The *Text View* window is indicated by the ⬚ Text View de... tab. There are three possibilities to enter text into the OPUS *Text View* window:

1) **Keyboard**

    Place the cursor into the window and enter text using your keyboard.

2) **Copy and Paste**

    It is possible to copy and paste text in the *Text View* using the shortcuts *Ctrl+C* and *Ctrl+V*.

3) **Drag and Drop a text file**

    Drag and drop a text file into the *Text View* window.

    You can only drag one file into the *Text View* window. If there has already been a text file in the *Text View* window, this file will be replaced and the text is overwritten unless you press the *CTRL* key during the *Drag and Drop* operation. In this case the text of the dragged file is appended to the content of the file which has already been open.

To select a text passage within the *Text View* window, move the cursor to the relevant text passage and press the left mouse button. You can also use the *Shift* and one arrow key to mark a text passage. If you want to delete a text passage, you can either use the *Backspace* (←) or *Delete* key, or you select the text and use the *CTRL+X* shortcut. It is also possible to use the *Cut* command from the *Edit* menu.

To save a text file, right click on the *Text View* window and select the *Save* option from the pop-up menu.

6.4 Cascade and Tile Windows

You can either cascade or tile the different windows, see Figure 59 and 60.
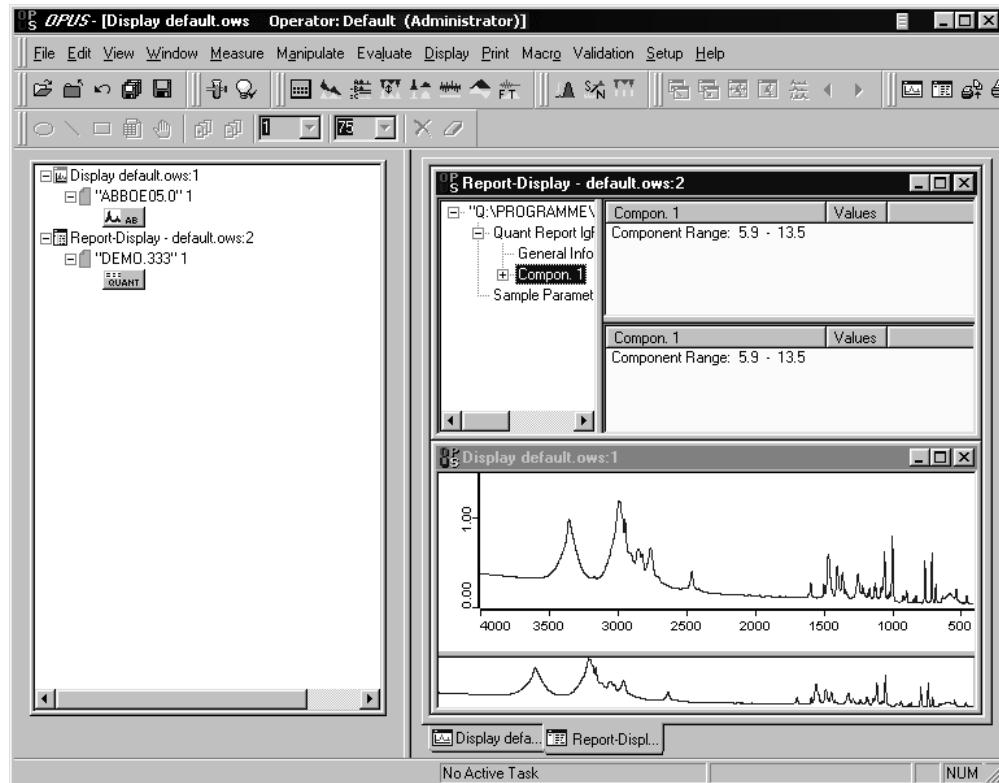
Figure 59: OPUS User Interface – Tiled Windows
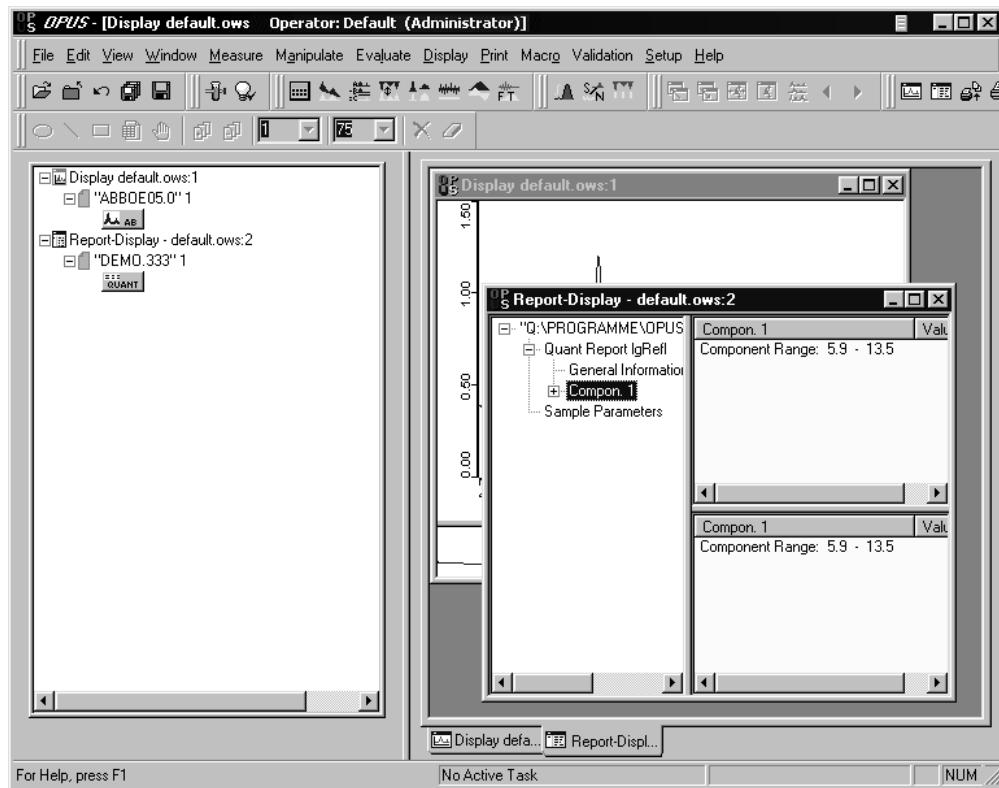
Figure 60: OPUS User Interface – Cascaded Windows

In connection with the OPUS browser pop-up menu you can further configure the appearance of your OPUS interface. Right click on the browser window. The following menu pops up:

Figure 61: Browser Pop-Up Menu

If you select *Allow Docking*, the windows (browser, spectrum and overview window) are displayed next to each other within the OPUS interface. If you deactivate this option, you can remove the browser window from the OPUS interface and position it somewhere else on the Windows desktop.

The *Hide* option makes the browser window invisible. To undo this setting, activate *Browser* in the *View* menu.

Float In Main Window opens the browser and spectrum window in equal size on the OPUS user interface. You can switch between these two windows by clicking on the corresponding tabs at the bottom.

6.5   Arrange Icons

If you have minimized several spectrum or report windows, you can have their icons arranged according to the Windows settings. By default, the icons are arranged at the bottom of the OPUS user interface.

7 Measure

OPUS supports the configuration and adjustment of spectrometers. You can immediately start measurements as well as define, save and reload measurement experiments. Additionally, you can use OPUS to control external spectroscopic devices, and you can have your data acquisition triggered by external signals. If an Ethernet interface is used to communicate with the spectrometer, you have to install the Microsoft Internet Explorer 5.0 or higher.
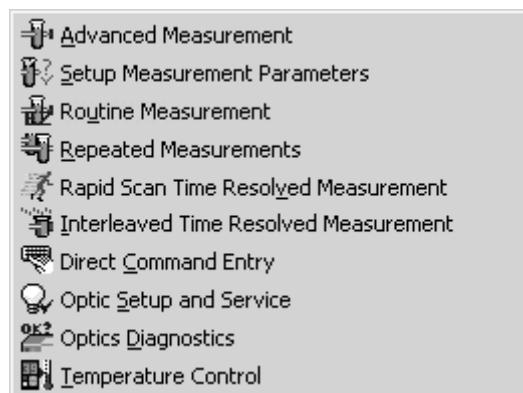
Figure 62: Measure Menu

When installing the optics a Bruker service engineer has already saved the optics configuration in OPUS. If you change or modify the spectrometer, you have to adjust these settings accordingly.

7.1 Configuring the Optics

To define the type of your spectrometer use the *Configuration* selection box on the *Optical Bench* tab of the *Optic Setup and Service* command. Figure 63 shows *Vector 22* as configuration. If a spectrometer is connected to the PC, it signalizes the firmware version (i.e. software inside the spectrometer) to OPUS. Additionally, the acquisition processor (AQP) type, AQP software version number and AQP memory size are displayed (see figure 63), provided no Ethernet connection has been used.

7.1.1 Optical Bench
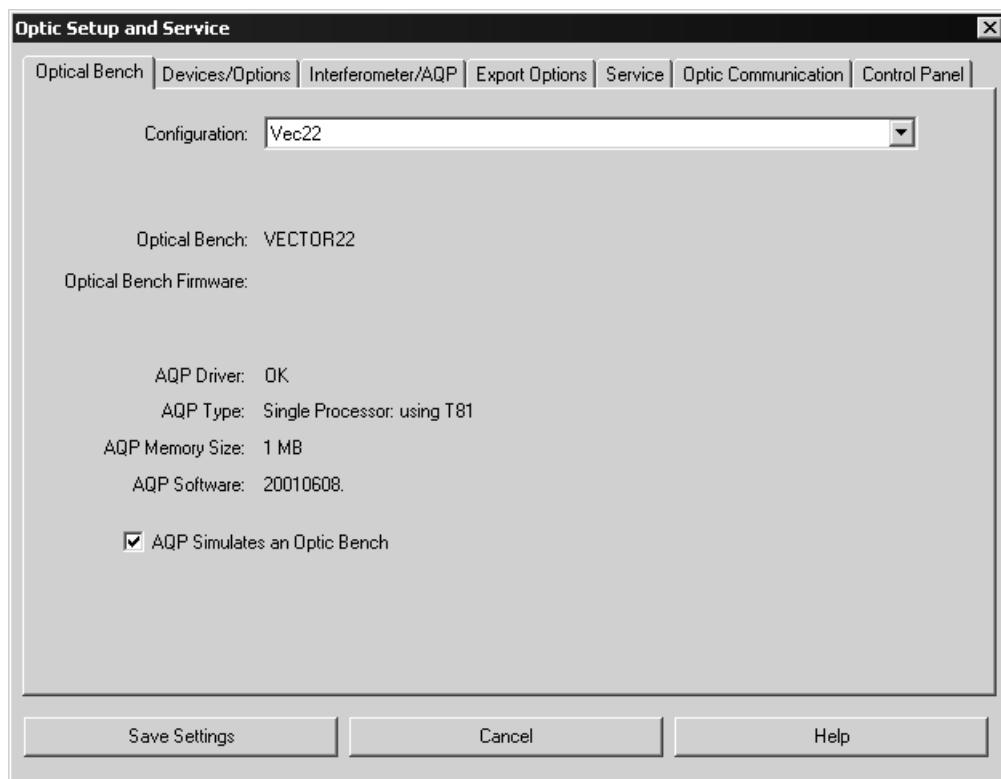
Figure 63: Optic Setup and Service – Optical Bench tab with VECTOR configuration

If the *AQP simulates an Optic Bench* check box is activated, the communication between OPUS and your spectrometer will be disabled. This check box is used for test purposes only, as all measurement commands are performed in simulation mode and not on the optics bench. The AQP generates interferograms which include a simulated noise signal.

Spectrometers with Ethernet connection, e.g. MATRIX or TENSOR series have no AQP installed. These instruments are connected via a network and use a URL (Uniform Resource Locator) that needs to be defined during the setup. The *Optical Bench* tab looks slightly different in case of these spectrometers (see figure 64).
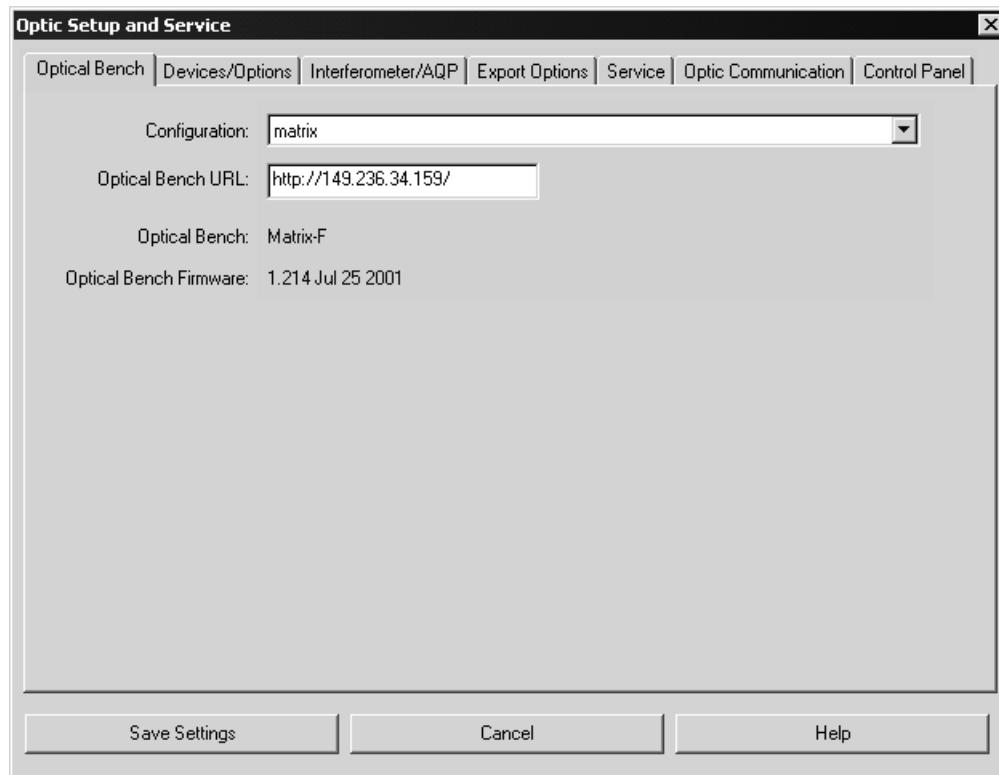
Figure 64: Optic Setup and Service – Optical Bench tab with MATRIX configuration

7.1.2 Devices/Options

On the *Devices/Options* tab you specify the components installed in your spectrometer. Make sure that the settings correspond to the spectrometer configuration. To activate a component, select the respective check box (see figure 65).
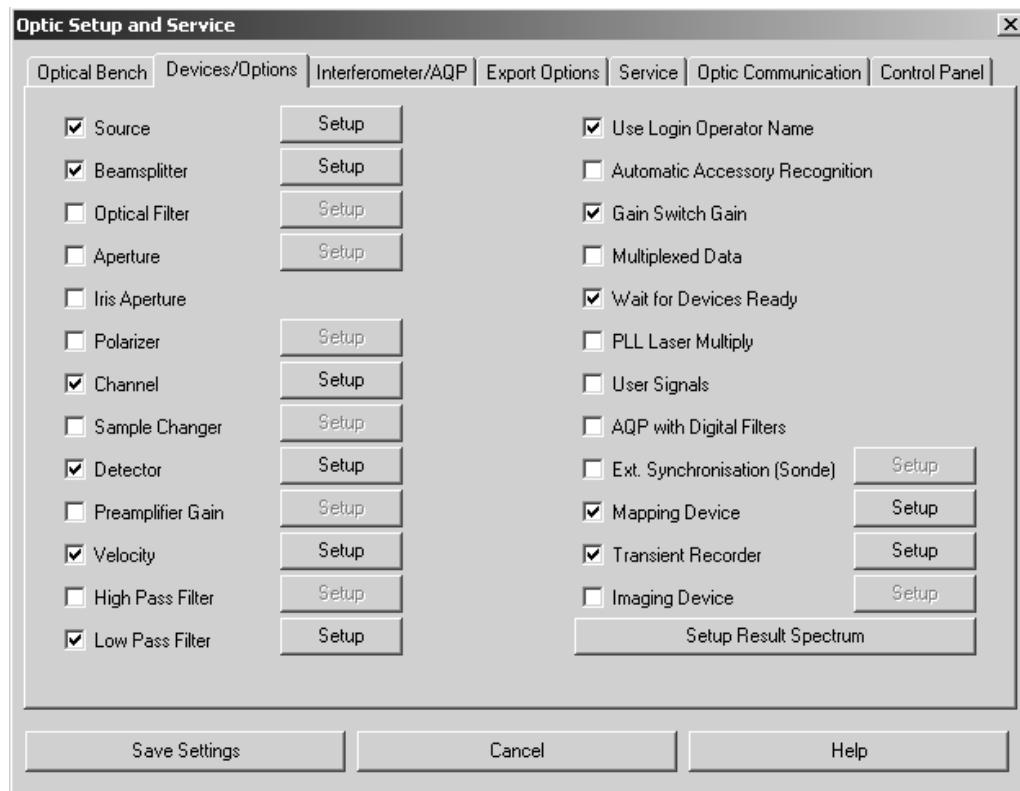
Figure 65: Optic Setup and Service – Devices/Options tab

All available options can be configured using the *Setup* button. Figure 66 exemplifies a detector configuration.
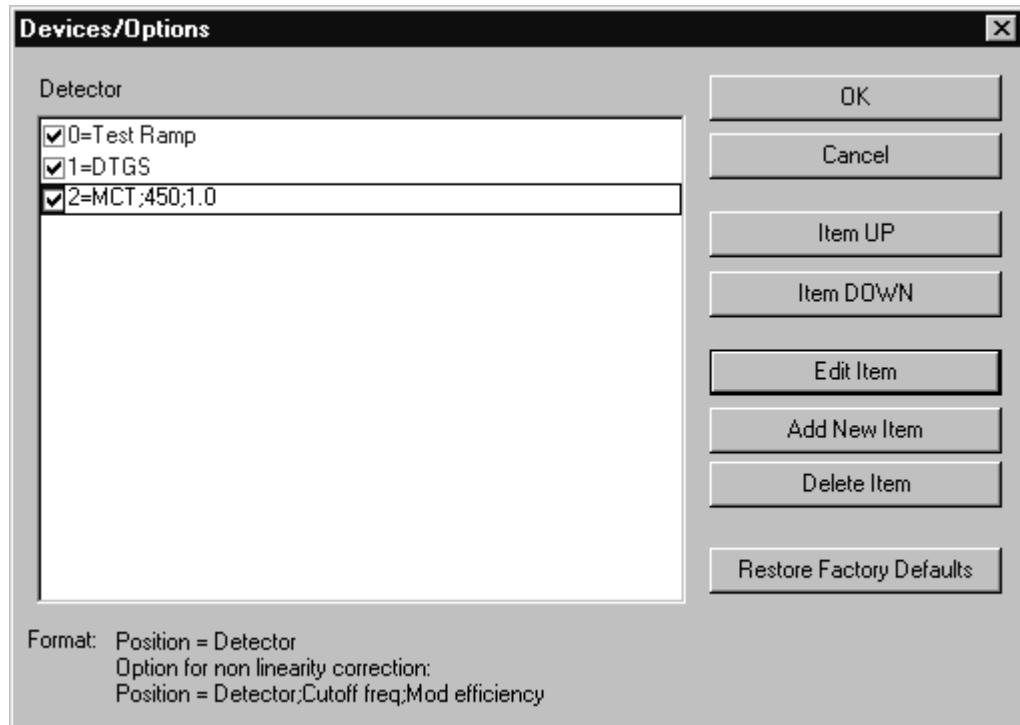
Figure 66: Detector Configuration

Figure 66 shows as common configuration a *Test Ramp* for test purposes, and a DTGS detector for measurements. These options are displayed in blue. As special feature the spectrometer defined has been equipped with an MCT detector.

Click on the *Add New Item* button and enter the *2=MCT* definition into the respective line. This entry is now displayed in black. Entries displayed in black can always be edited and deleted. If an option has not yet been available (or should not to be used at the moment), deactivate the respective check box.

Some detectors, e.g. MCT detectors, show non-linearity between sample concentration and peak intensity. If these detectors are used to perform a quantitative analysis, it is necessary to know this non-linearity to be able to correct it.

If you edit a line, it will be displayed inversely (e.g. white on black). A line selected can be vertically moved by clicking on the *Item UP* and *Item DOWN* buttons. Confirm your changes by clicking on the *OK* button, or discard them by clicking on the *Cancel* button.

The direct result of a data acquisition is always an interferogram. This interferogram can be transformed into spectra of various types, e.g. absorbance, transmittance or reflectance spectra. A result spectrum type will only be available if you activate the respective result type check box in the *Setup Result Spectrum* list (figure 67).
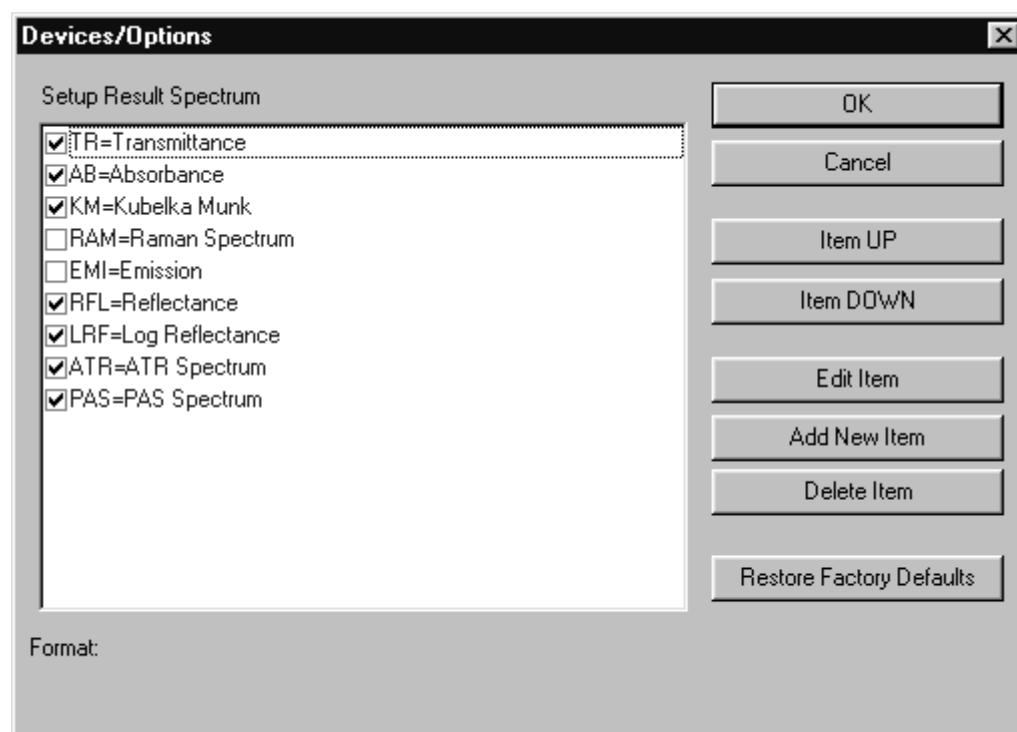
Figure 67: Setup Result Spectrum

If a result spectrum type is not available in the list or deactivated, it cannot be requested in the method.

> **Note:** If you have created a measurement method and subsequently edited the optics configuration, this may cause the method to be incompatible to the optics settings. A red error symbol on the different *Measurement* dialog tabs indicates this kind of problem.

Special features in case of Raman experiments

If you use a laser as light source, you have to define its wavelength and maximum power output. A special format is required for this kind of entries. Click on the *Devices/Options* tab of the *Optic Setup and Service* dialog. Activate the *Source* check box and click on the *Setup* button. The special format will be displayed on the bottom of the dialog box (see figure 68).
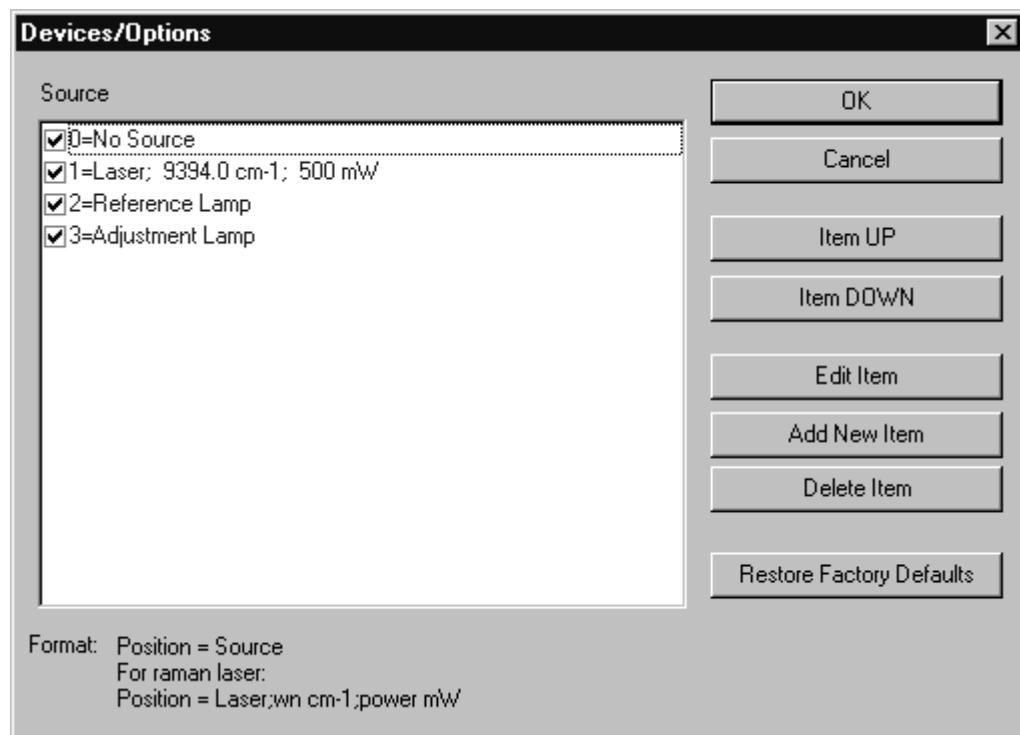
Figure 68: Source settings in case of Raman instruments

7.1.3   Interferometer/AQP

On the *Interferometer/AQP* tab of the *Optic Setup and Service* dialog (see figure 69) you can set the values for the absolute peak position, laser wave number, resolution, data rate and the maximum FT size.
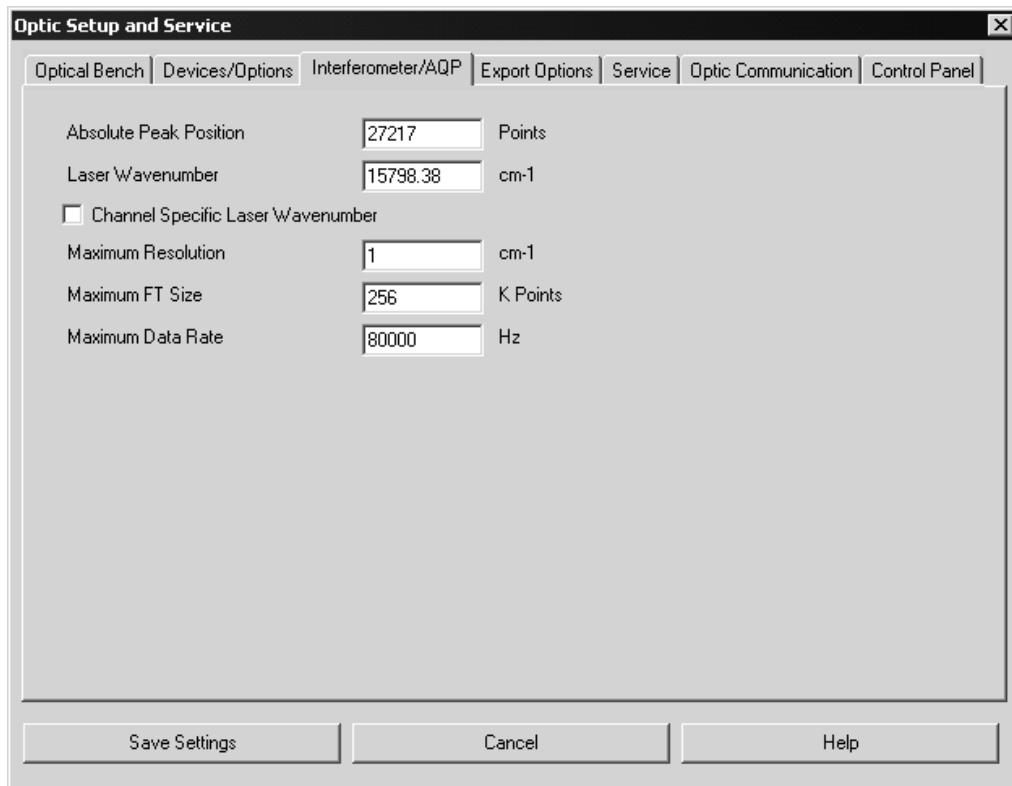
Figure 69: Optic Setup and Service - Interferometer/AQP tab

You have to experimentally evaluate the *Absolute Peak Position* of your system by using the *Check Signal* tab of the *Measurement* dialog. This value has to be re-adjusted if the detector or laser have been replaced, or if the optics has been completely re-adjusted. In case of multi-channel measurement, the laser wave number can be specified individually for each channel if a channel-specific IT-Test is possible.

7.1.4   Export Options

You define the file format of an OPUS data file on the *Export Options* tab (see figure 70). The *OPUS* option box is checked by default. Optionally, you can also export the data to GRAMS format. Make sure that the GRAMS software runs on the main memory of your computer, together with OPUS, while exporting data.
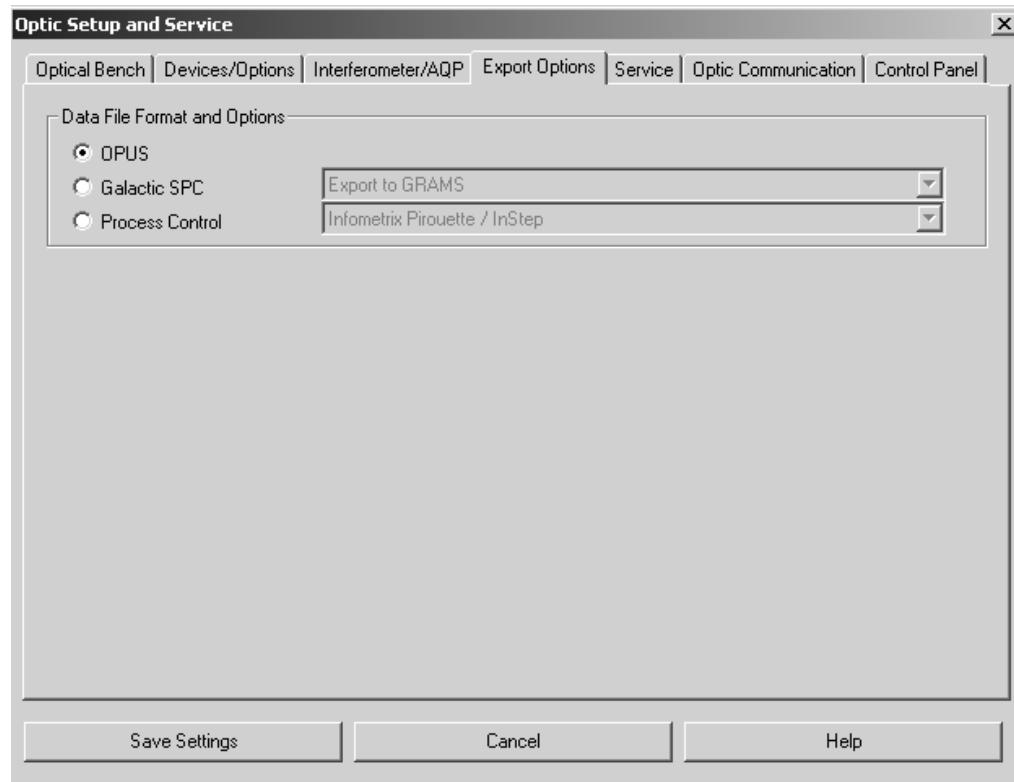
Figure 70: Optic Setup and Service - Export Options tab

7.1.5   Service

The *Service* tab (see figure 71) includes the OPUS diagnostic functions, i.e. diagnostic results and statistics of the spectrometer. Clicking on the buttons on the right side resets the parameters displayed. Note that the diagnostics test must have been performed at least once after the installation of OPUS, otherwise no test results will be available. You can repeat the diagnostics test by clicking on the *Repeat Diagnostics Test* button.
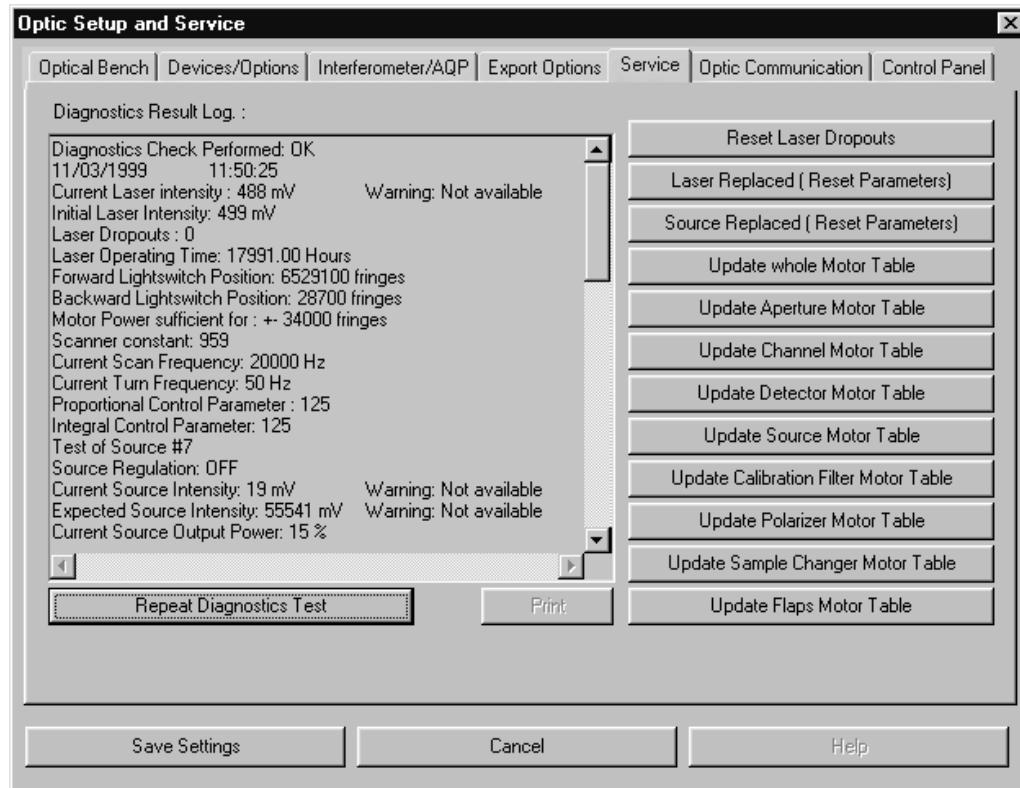
Figure 71: Optic Setup and Service - Service tab

The upper two buttons refer to the HeNe laser parameters. Some lasers show sporadic power fluctuations during operation, which influence the interferometer control. These fluctuations are automatically recorded by an internal counter. The fluctuation value should always be 0, other values would indicate an error. If the fluctuations increase, you have to replace the laser. Use the *Reset Laser Dropouts* button to reset this counter to 0.

If you have replaced the laser, you can set the laser operating time meter to 0 by using the *Laser Replaced (Reset Parameters)* button. At the same time, the value of the laser start intensity is read again.

The *Source Replaced (Reset Parameters)* button resets both the counter of the total source operating time and the counter of the on/off source cycles if you have replaced the source.

The remaining buttons determine the control parameters of the spectrometer stepper motors. The number and position of stepper motors depend on the spectrometer type. To read the parameters of all motors click on the *Update whole Motor Table* button. The other buttons read the status of specific motors:

- *Update Aperture Motor Table* – motor to control the aperture
- *Update Channel Motor Table* – motor to switch beam ports
- *Update Detector Motor Table* – motor to switch detectors
- *Update Source Motor Table* – motor to switch sources
- *Update Calibration Filter Motor Table* – motor to control the calibration filter
- *Update Polarizer Motor Table* – motor to control the polarizer
- *Update Sample Changer Motor Table* – motor to move the sample wheel
- *Update Flaps Motor Table* – motor to control the flaps

7.1.6   Optic Communication

To monitor the AQP communication click on the *Optic Communication* tab (figure 72). Check the *Auto Scroll* box if you want the list to automatically scroll.
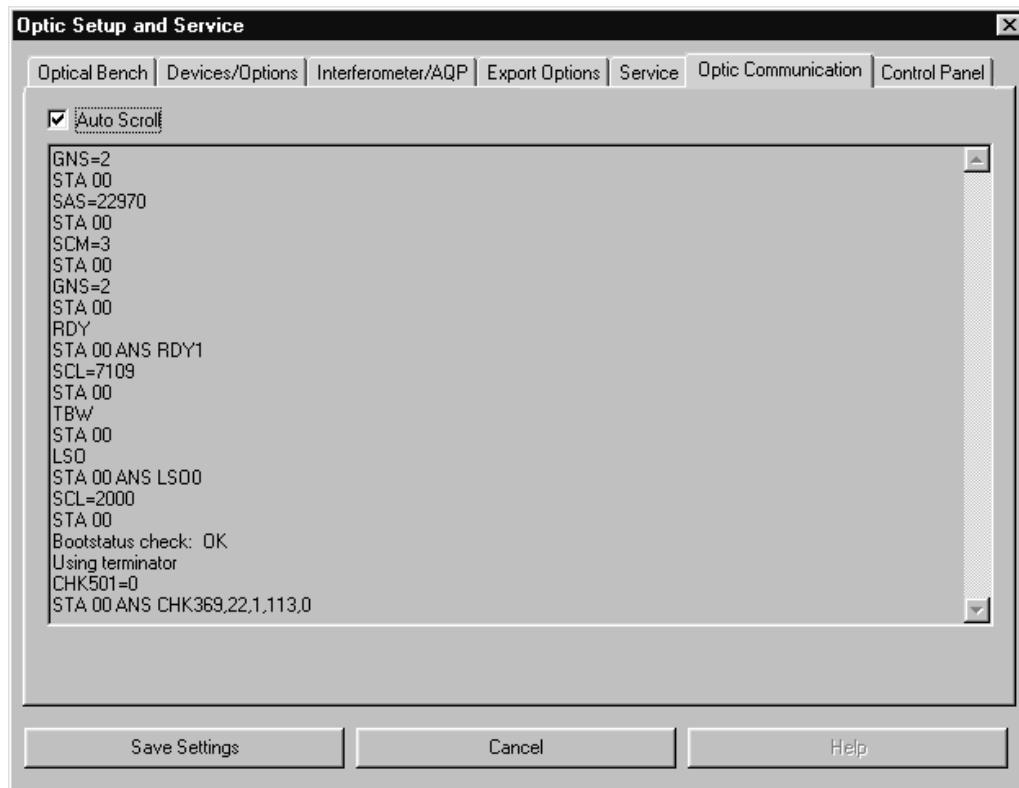
Figure 72: Optic Setup and Service - Optic Communication tab

In case of spectrometers connected by a network the *Optic Communication* tab includes the appropriate URLs.
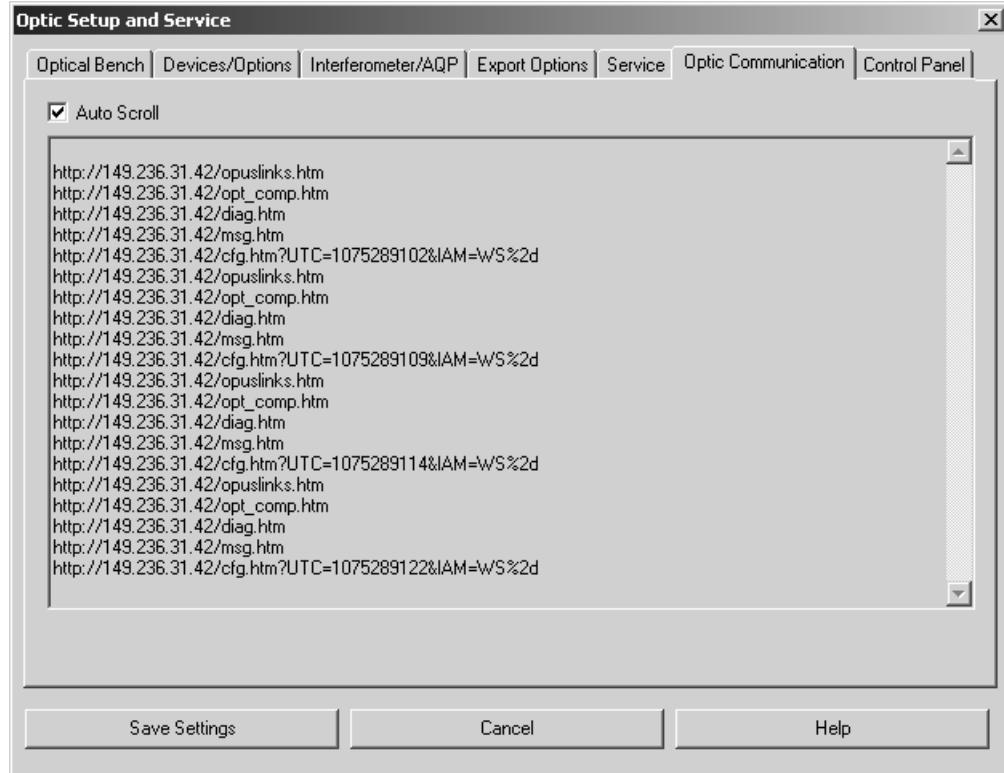
Figure 73: Optic Setup and Service - Optic Communication With URLs

7.1.7   Control Panel

This option applies to the IFS 125HR spectrometer only and is described in the IFS 125HR user manual.

7.2   Measurement

After you have configured your spectrometer you can start to set up an experiment. Basically, two types of measurement modes are possible: *Advanced Measurement* and *Routine Measurement*. The difference between these two modes is the number of parameters to be set up. The *Advanced Measurement* mode provides access to all parameters, and the *Routine Measurement* mode provides only a pre-selection of parameters most reasonable for the spectrometer. In this case you only have to select very few parameters to perform a measurement. Note that the *Routine Measurement* mode is not available for all instruments.

When working in a validated environment (see chapter 14.10), the *Setup Measurement Parameters* command allows to load and edit a measurement without actually performing this measurement.

Special considerations and conditions in case of Raman measurements will be explained in section 7.2.11.

If you start OPUS, the parameters used for the last OPUS experiment will be loaded by default. If this is exactly the experiment you want to use, just continue, otherwise you will have to load a new experiment.

By clicking on the *Exit* button you save all parameter settings made in the *Measurement* dialog box, except the interferogram peak position. The peak position has to be saved separately by clicking on the *Save Peak Position* button on the *Check Signal* tab (see figure 88). If you click on the *Cancel* button, you exit the dialog box without saving the changes made. You can use the *Cancel* command as an *Undo* command for all changes made, except for peak positions saved.

7.2.1   Error and Warning Symbols

Configuration errors are indicated by colored entry fields, and warning symbols on the corresponding tab. Errors during measurement may be caused by:

a) The method loaded is not compatible with the spectrometer configuration.
b) A parameter value is beyond the allowed limit.

Example 1:
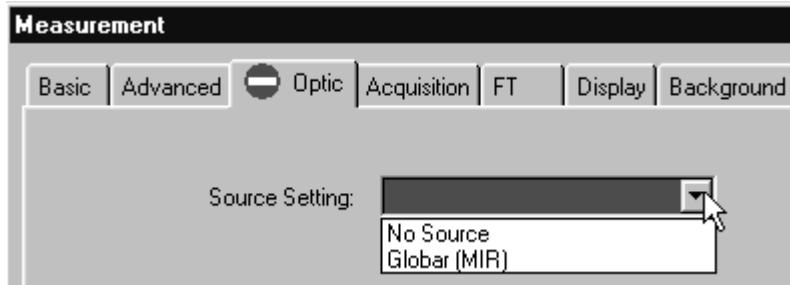
Figure 74: Error caused by wrong selection

The red ⊖ symbol on the *Optic* tab indicates a parameter mismatch with the existing hardware. The *Source Setting* entry field is marked in red. If you place the cursor on the drop-down list, a help text pops up indicating *Globar (MIR)*. This means, that *Globar (MIR)* has been entered as source in the method, but the spectrometer is not equipped with a globar. Open the *Source Setting* drop-down list to see the sources available. After correcting the entry, the warning symbol will disappear.
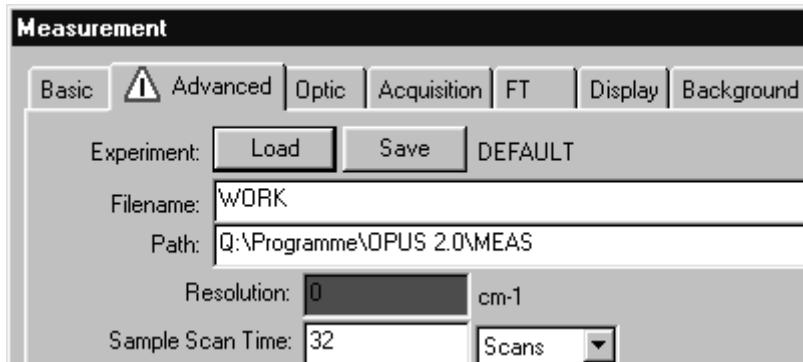
Example 2:

Figure 75: Error caused by wrong parameter

If the value of a parameter is beyond the allowed limits, the ⚠ symbol will be displayed. If you place the cursor on the respective entry field, a help text pops up indicating the cause of error. In the example shown in figure 75 the resolution of $0cm^{-1}$ is too small as the resolution has been set to $0.25cm^{-1}$ in the optics configuration for the spectrometer.

Example 3:

A warning symbol will not necessarily be displayed on the tab on which the last change has been made. In the following example the *Wanted High Frequency Limit* on the *Acquisition* tab has been changed from

to

Consequently, the ⚠ symbol will be displayed on the *Advanced* tab. Place the cursor on the respective entry field, to have the help text displayed.
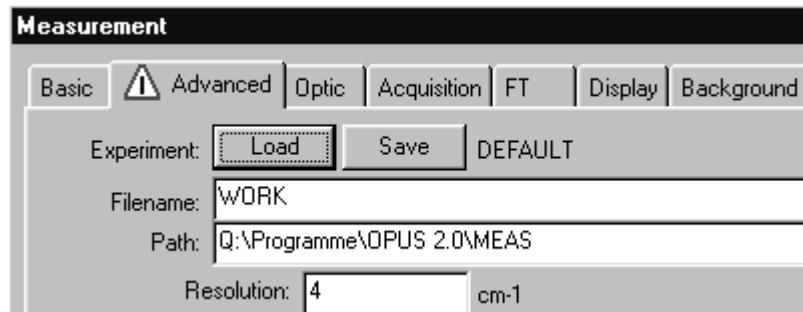
Figure 76: Error caused by wrong frequency limit

Example 4:

In this example the resolution has been set to 1cm^{-1} on the *Advanced* tab, and the frequency range has been set from 4000cm^{-1} to 400cm^{-1}. In the *Aperture Setting* drop-down list an aperture size of 10mm has been selected.
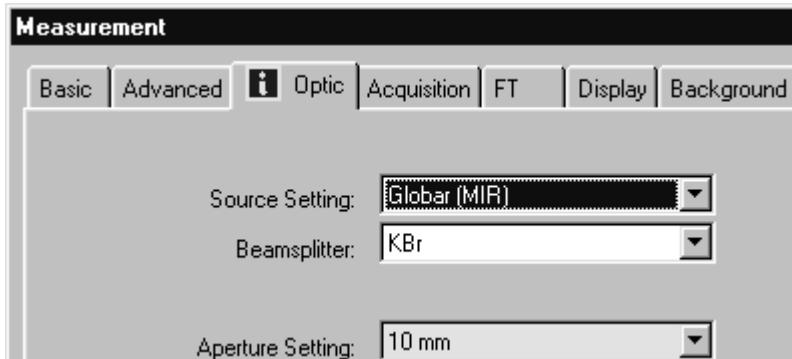
Figure 77: Information about restrictions on measurement

The measurement can be performed, but the resolution desired cannot be achieved above a wave number of more than 1300. This will be indicated by the symbol on the *Optic* tab, and a yellow entry field.

Example 5:

If you select *User settings* from the *Setup* menu, you can disable the parameter change function. Deactivate the *Change Parameters* check box on the *Rights* tab.

This may cause that a wrong parameter cannot be corrected. In this case the error will be indicated by the symbol.
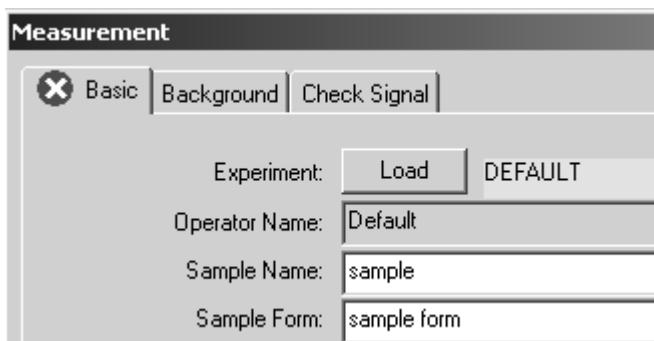
Figure 78: Error caused by limited user rights

Use a different measurement experiment.

7.2.2 Basic

The basic parameters for data acquisition can be found on the *Basic* tab of the *Measurement* dialog box.
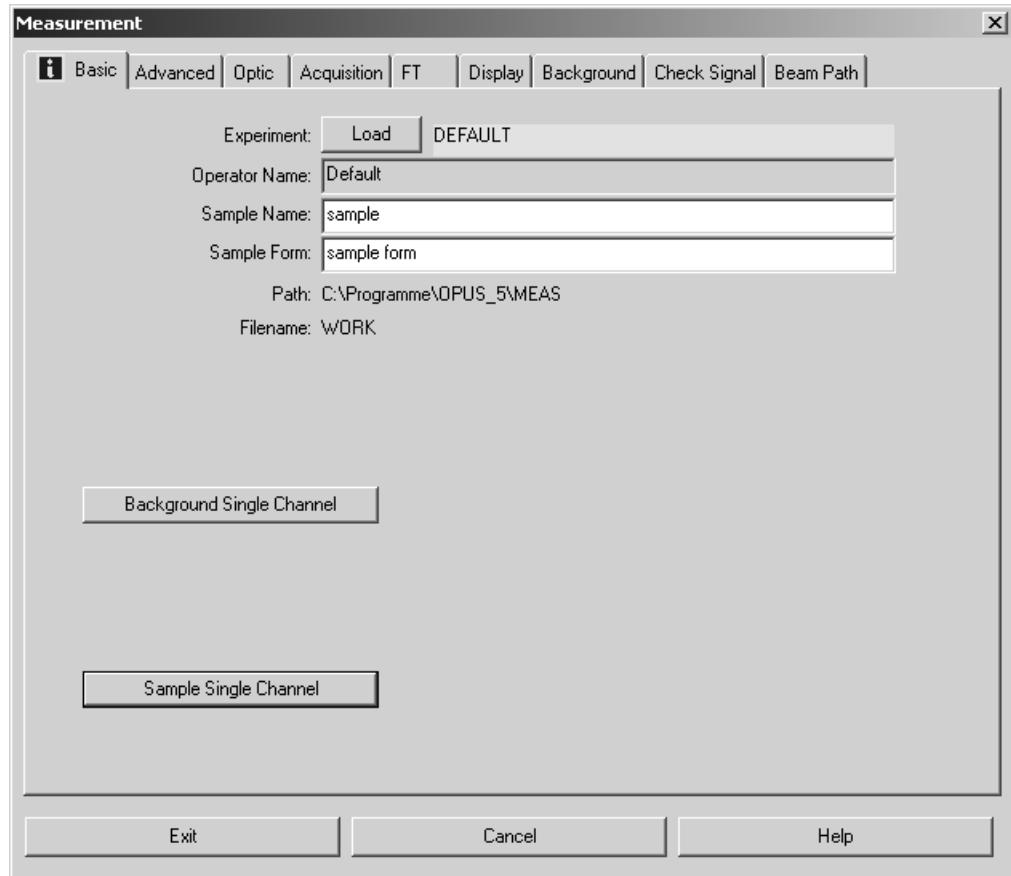
Figure 79: Measurement – Basic tab

On the *Basic* tab you specify:

- Experiment
- Operator name
- Sample name (e.g. identification for the sample)
- Sample form (short description)
- Path (where the measurement result is to be saved)
- File name (of the result)

The information about sample name and sample form is optional and will be stored in the INFO data block of the spectrum. If the measurement parameters differ from the parameters used in the loaded experiment, the experiment name is displayed in yellow. These parameters are additionally listed in the HISTORY data block of the spectra acquired.

If you accept the default settings of the measurement parameters specified on the remaining tabs, you can directly start measurement. Either click on the *Background Single Channel* or *Sample Single Channel* button. As soon as the measurement has been finished, the parameters used will automatically be stored together with the results. These parameters can be accessed by the OPUS browser pop-up menu (see chapter 2.2).

During measurement the progress is indicated by the status bar at the bottom right of the OPUS workspace. To interrupt the measurement right click on the status bar, and a menu pops up including three different options.
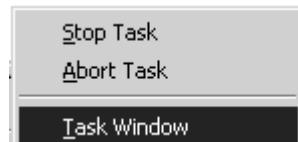
Figure 80: Pop-Up Menu to Stop Tasks

The *Stop Task* option interrupts a running measurement (a repeated measurement will be continued by the next spectrum). To completely abort a repeated measurement select the *Abort Task* option. If you click on the *Task Window* option, an additional menu pops up including the current OPUS tasks running.
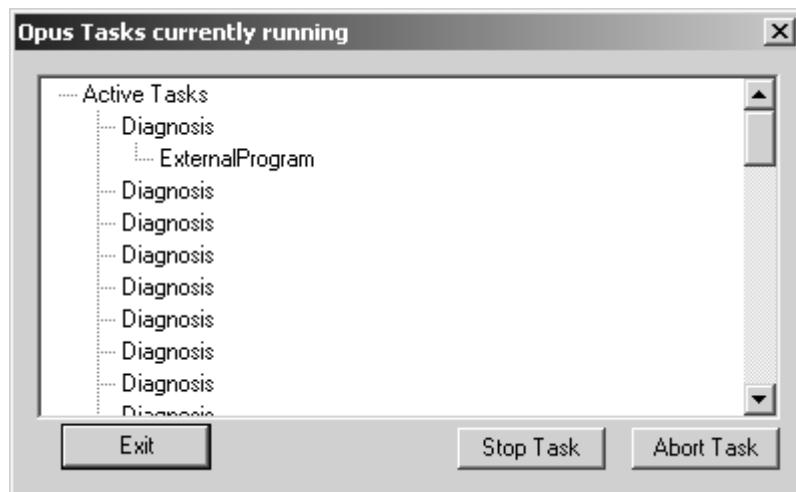
Figure 81: OPUS Task List

Select one task from the list and click on the *Stop Task* or *Abort Task* button. If the measurement has been completed, the *No Active Task* message is displayed in the status bar.

Except for emission, Raman or single-channel spectra it is always necessary to acquire a background spectrum to eliminate frequency characteristics of the source, spectrometer or sample matrix. This correction is automatically performed after the sample measurement has been completed.

7.2.3   Advanced

On the *Advanced* tab you can specify the directory path, and the data file name of the spectra to be saved. Starting with the second measurement, the data file name will be incremented, indicating the current number of measurements.

All parameters can be saved in an experiment file on the *Advanced* tab. Click on the *Save* button. The *Select Experiment File Name* dialog opens. Specify a name for the measurement experiment defined. This name can be used to re-load the experiment.

On the *Advanced* tab you   define the resolution and spectral range. Alternatively, you can determine the number of scans per spectrum, or the total time of all scans.
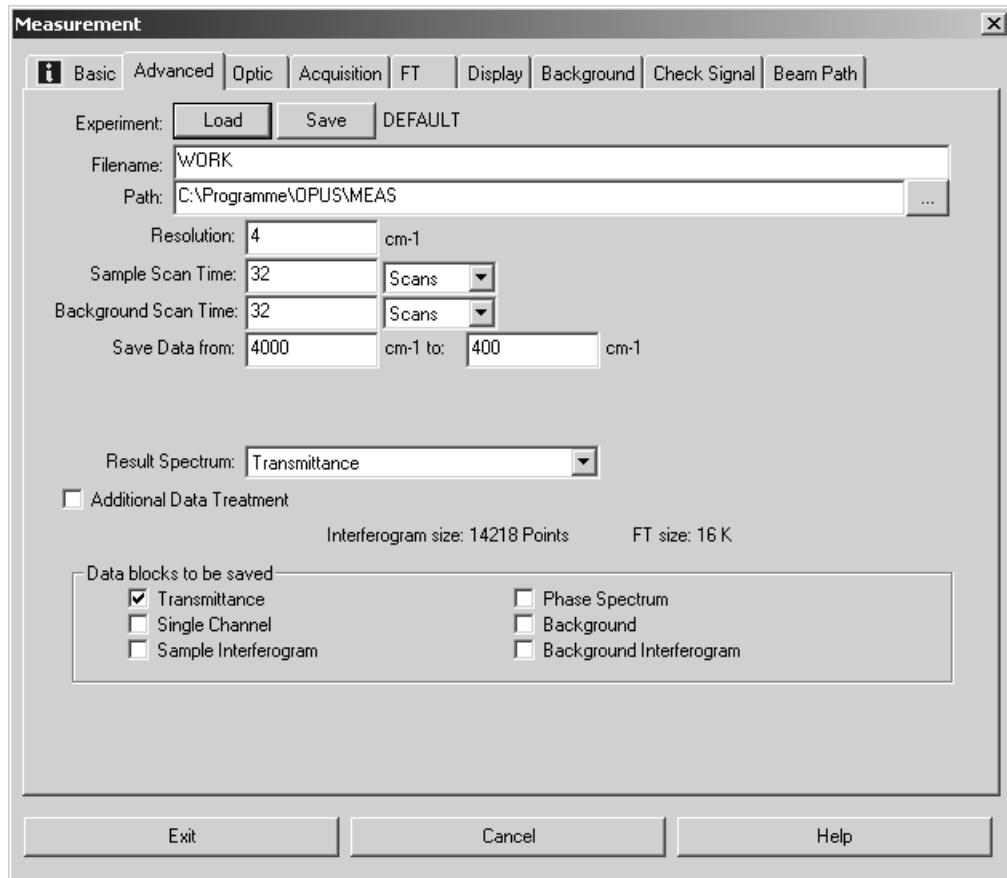
Figure 82: Measurement – Advanced tab

Do not set the resolution higher than necessary to minimize the total acquisition time. Improving the resolution, e.g. by a factor of 2, requires a four- times higher acquisition time at a constant signal-to-noise ratio of the spectrum. This is due to the fact that the signal-to-noise ratio is proportional to the square root of the acquisition time.

Possible result spectrum types have already been determined when configuring the optics. You can now select the result spectrum type from the drop-down list. In figure 82 *Transmittance* has been defined as result spectrum, and is automatically checked as first data block in the *Data blocks to be saved* group field. You can check further data blocks. A background spectrum can, of course, only be saved if it has been acquired before.

Use the *Exit* button to save the settings.

7.2.4   Optics

Depending on the optics configuration the number of entry fields displayed in figure 83 may be different.
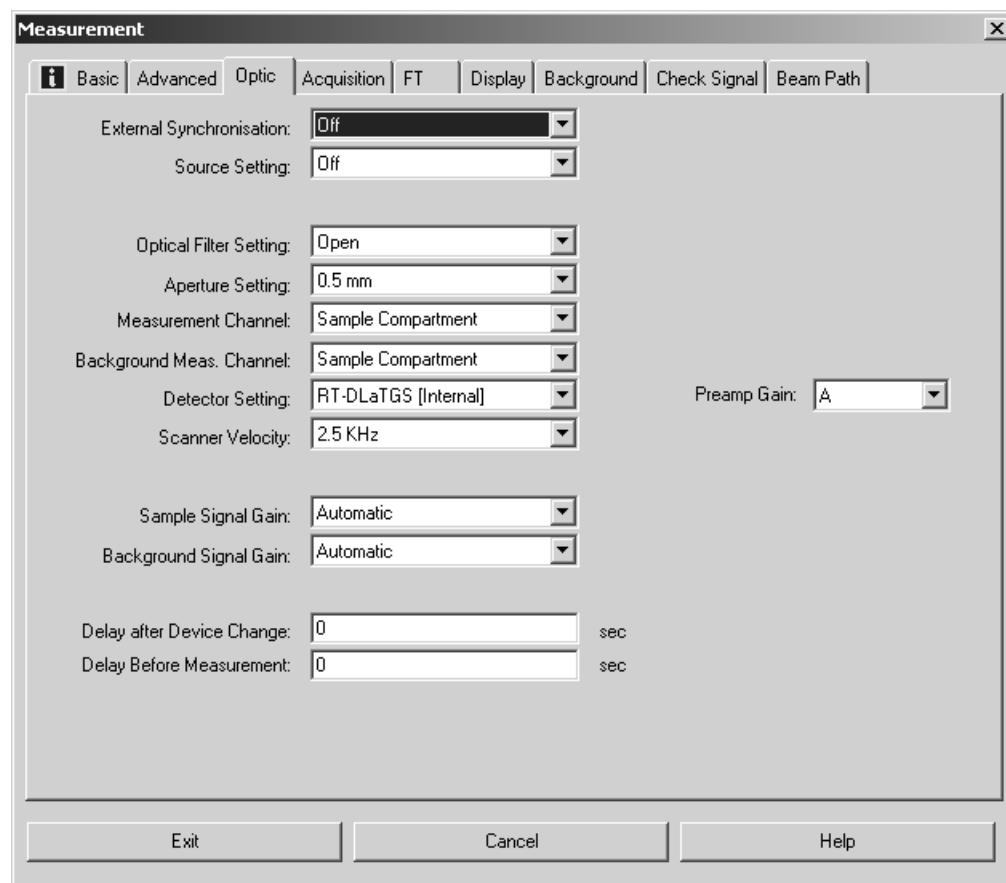
Figure 83: Measurement – Optics tab

Select an aperture setting from the *Aperture Setting* drop-down list. The aperture size defines the spectral resolution. An *A* aperture diameter causes a $\delta\sigma$ spectral peak broadening[1] at a σ wave number (provided an *F* fixed focal length of the collimated mirror in front of the interferometer is given):

$$\delta\sigma \geq \frac{A^2}{8F^2} \cdot \sigma$$

---

1. More precisely: a convolution with a delta function of width $\delta\sigma$.

Select the channel you want to use for the measurement (e.g. *Front*, *Back* or *External*). If your spectrometer is equipped with several detectors, select the detector to be used in the *Detector Setting* drop-down list.

The scanner velocity depends on the detector type installed and the current experiment. Select a slow scanner velocity (<10kHz) for photoaccoustic experiments. For DTGS detectors and photodiodes 10kHz are adequate, while you should use a higher velocity (>10kHz) if your spectrometer is equipped with MCT or InSb detectors.

We recommend to set the *Sample Signal Gain* and *Background Signal Gain* values to *Automatic*. The optimal value is automatically determined by a separate short scan before the measurement starts, to ensure that the complete dynamic ADC range will be covered.

The *Switch Gain* setting allows to amplify the interferogram by 2^N within the spectral ranges which are quite off the centerburst. This has almost the same effect as if you enhance the ADC dynamic from, e.g. 16 to $(16 + N)$ bit, which reduces digital noise. This aspect is important for data acquisition in high resolution when using a broad-band source. The window width around the centerburst can be specified in the *Window in Points* field.

You can define time intervals before a measurement start or device change. Enter the respective time intervalsin seconds into the *Delay after Device Change* or *Delay Before Measurement* entry fields. The *Delay after Device Change* option will only be performed if certain parameters, e.g. sample changer position, detector, measurement channel, have been changed to avoid problems especially in case of slow detectors (DTGS). A *Delay Before Measurement* avoids detector saturation if certain parameters (e.g. detector, measurement channel) have been changed.

7.2.5   Acquisition

Set the high and low frequency limit on the *Acquisiton* tab. The actual frequency limits will then be calculated and may deviate from the values set and are therefore displayed next to the *Wanted High* or *Low Frequency Limit* entry field on the right (see figure 84).

Restricting the sampling bandwidth reduces the amount of data and may be useful when recording high resolution spectra. However, electronic and/or optical filters have to be used to ensure that signal intensity is 0 beyond the selected frequency limits. Otherwise, the signals may be convoluted or *folded* to the selected range, and may adulterate the intensity.
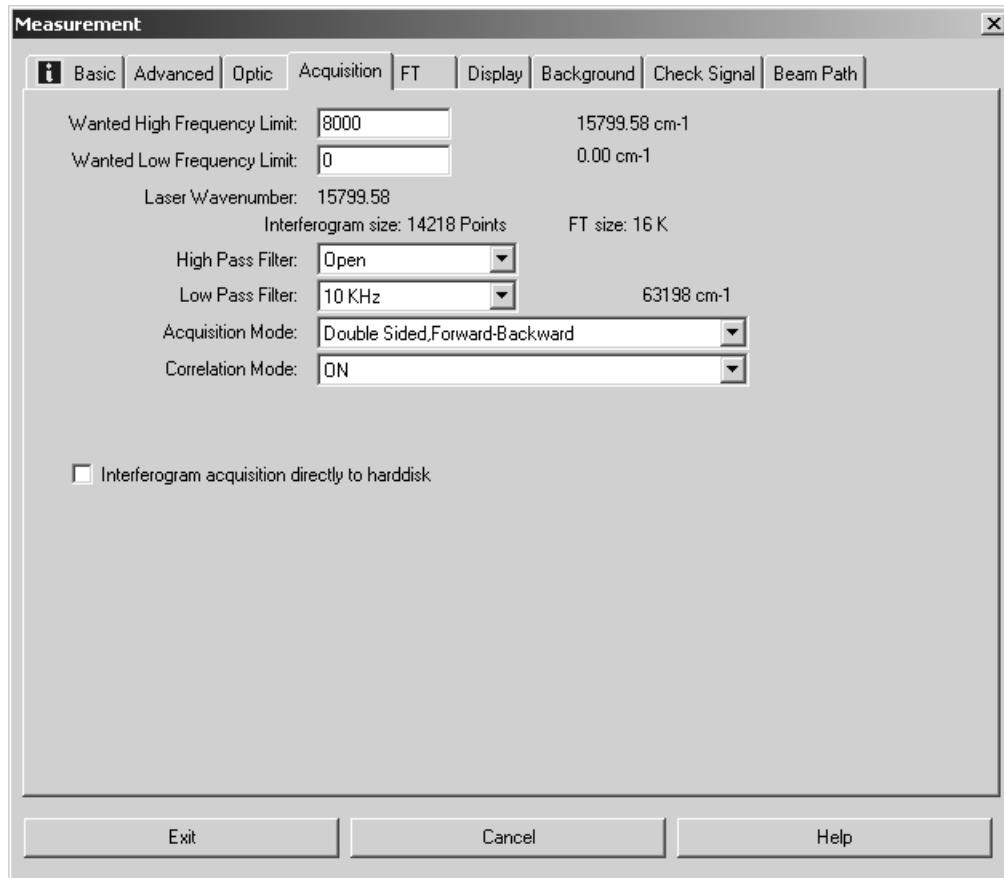
Figure 84: Measurement – Acquisition tab

Additionally, you can specify the *Low Pass Filter*, *High Pass Filter*, *Acquisition Mode* and *Correlation Mode* settings. The acquisition mode defines whether one or both sides of the interferogram is measured, and the correlation mode checks the data integrity.

As the interferometer mirror continuously moves, all frequency components of the IR spectrum are depicted in a *detector-response spectrum*. This kind of spectrum is in a lower frequency range, its bandwidth can be limited by using electronic filters.

The high pass filter limits the bandwidth within the high frequency ranges. Activate the filter by selecting *On* from the drop-down list, deactivate the filter by selecting *Open*. Note that this electronic filter is not available for all spectrometers.

Use the low pass filter to limit the bandwidth in the low frequency ranges. As the mapping of IR wave numbers to frequencies in the low frequency range is proportional to the scanner velocity *v*, the fixed cut-off frequency *f* of the filter (in Hz) corresponds to a wave number σ which depends on *v* as follows:

$$\sigma[cm^{-1}] = f[Hz]/v[cms^{-1}]$$

In case of the acquisition mode you can select between several options:

- *Single Sided*: this option only allows the measurement of one-sided interferograms, data acquisition is performed only during the forward mirror movement.
- *Double Sided*: the interferogram is measured on both sides, data acquisition is performed during the forward mirror movement. In this mode the time resolution amounts to half the value achieved in *Single Sided* mode. The signal-to-noise ratio shows an improvement of $\sqrt{2}$, and the ordinate accuracy is higher compared to the *Single Sided* mode. The *Double Sided* acquisition mode is suitable for Raman, Emission, phase correction measurements and high-resolution quantitative measurements.
- *Forward/Backward*: data acquisition is performed during the forward and backward mirror movement. Forward and backward scans are separately co-added, calculated and added. This option reduces dead time, improves the signal-to-noise ratio, but requires twice as much computation time.
- *Fast Return*: this mode offers a fast mirror retrace without data acquisition. This causes less dead time and a better signal-to-noise ratio.

Fast Return and *Forward/Backward* modes are not available for all types of spectrometers. On condition that the measurement times are identical, the signal-to-noise ratio improves in the following order:

S/N (no *Fast Return*) < S/N (*Fast Return*) < S/N (*Forward/Backward*)

The correlation mode determines whether a data integrity check is performed during data acquisition. You can select between the following options:

- *No*: data will not be checked.
- *Around Peak, Low*: is only available, if several scans are averaged. Each new interferogram is compared to the first one within a range around the centerburst. If the deviation exceeds the threshold the interferogram will be discarded. Otherwise, the interferogram will be used for averaging.
- *Around Peak, High*: same as *Around Peak Low,* but the limit is more sensitive to minor changes (e.g. caused by thermal drift in case of long-term measurements).
- *Full Igram Length*: all interferogram points are compared to each other. An interferogram is discarded if the points contain more than ten defective areas or if the number of defective points exceeds one eighth of the total number of interferogram points.

Activate the *Interferogram acquisition directly to hard disk* check box if you want to save the data acquisition results directly to hard disk.

7.2.6   FT

On the *FT* tab you define the phase resolution. Set the phase resolution in such a way that the number of *Phase Interferogram Points* amounts to at least 250.

The phase correction increases the interferogram symmetry. Phase correction is always necessary as the interferogram measured is never perfectly symmetric. For details on the phase correction method, see chapter 8.15. Select the *Phase Correction Mode* and *Apodization Function* from the respective drop-down list.

The *Zerofilling Factor* value has to be of 2^n order within the range between 1 and 512.
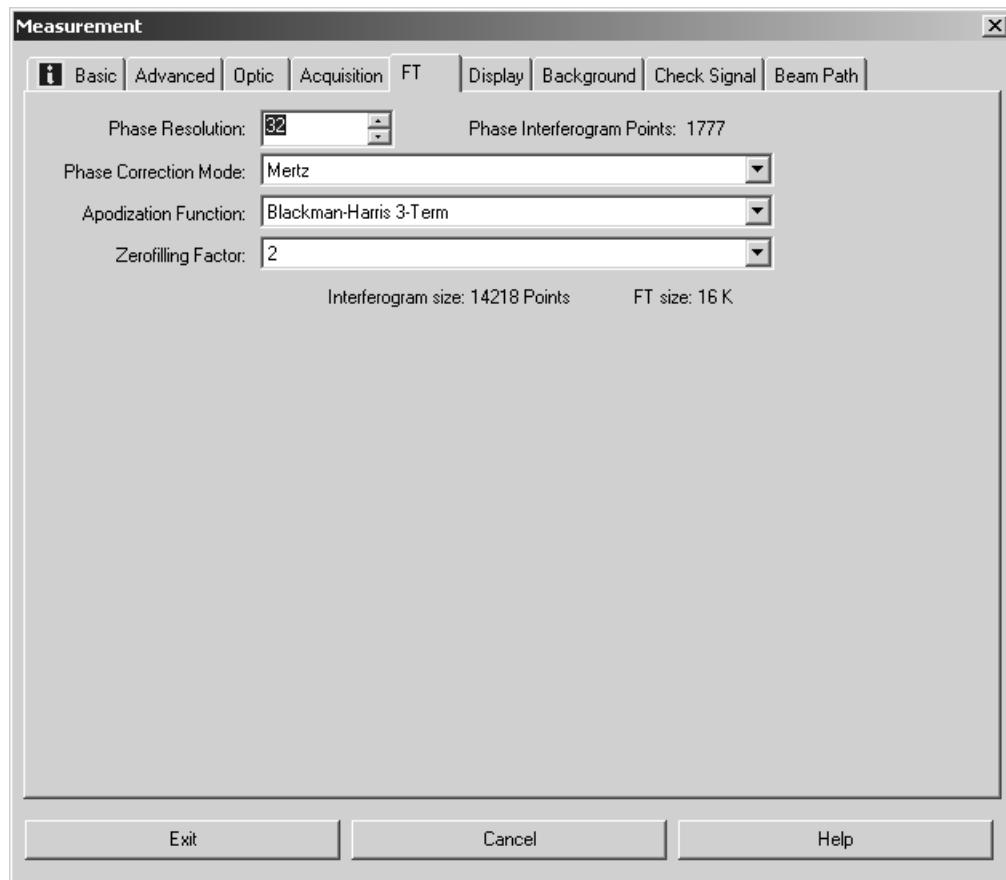
Figure 85: Measurement – FT tab

7.2.7   Display

On the *Display* tab you can define the axes settings for the spectrum display during measurement. It is possible to define upper and lower limits for the x- and y-axis.

If you activate the *Display single scans before measurement* check box, the spectrum will be calculated by single scans and displayed, before the actual data acquisition starts. The actual data acquisition is performed as soon as the operator starts measurement.

To display intermediate results during measurements, activate the *Display during measurement* check box.
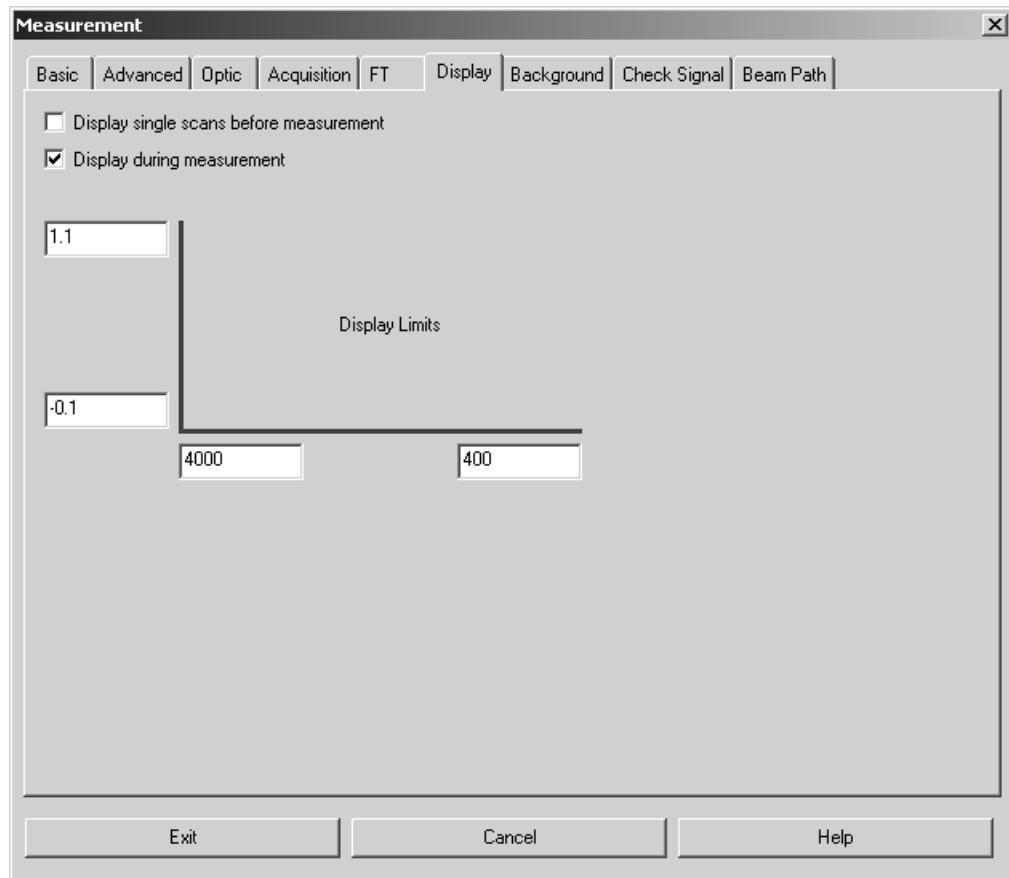
Figure 86: Measurement - Display tab

7.2.8   Background

Normally, the background spectrum remains in the AQP. Use the *Background* tab to transfer the background spectrum from the AQP to the PC and save it there. Click on the *Clear Background* button to delete the background spectrum from the AQP.

Drag & drop the saved background spectrum from the OPUS browser window or Windows Explorer into the selection field below the *Load Background* button. If you click on the *Load Background* button, the background spectrum will be transferred to the AQP and can be used for spectra calculations.

In case of MATRIX and TENSOR spectrometers the background spectrum is saved in the *OPUS.BG* file within the *OPUS* directory. When starting OPUS the last-used background spectrum, i.e. the *OPUS.BG* file, will automatically be loaded to the AQP.
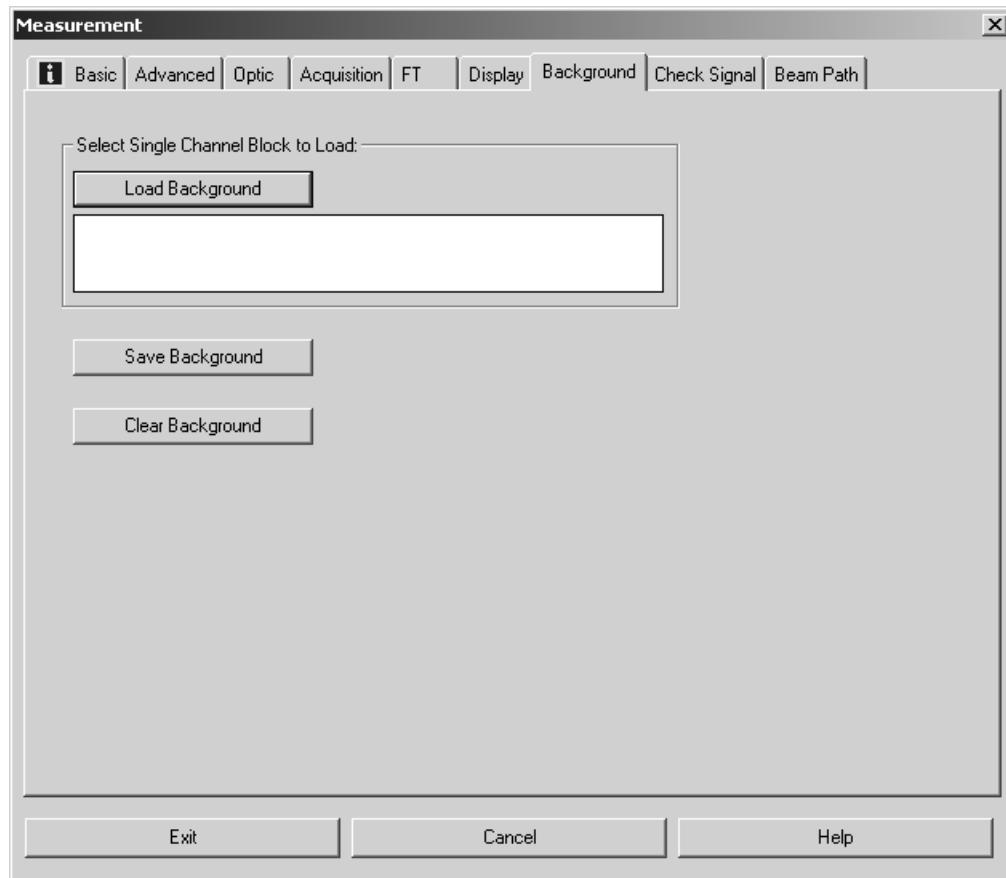
Figure 87: Measurement – Background tab

7.2.9 Check Signal

The appearance of the *Check Signal* tab depends on the spectrometer configuration. Besides the options and commands displayed in figure 88 you may have additional functions available for your system.

To determine and save the exact interferogram peak positionyou have to open the *Check Signal* tab at least once after you have installed your spectrometer. The purpose of checking the signal is to either achieve a maximum interferogram signal or optimize the shape of the single-channel spectrum.
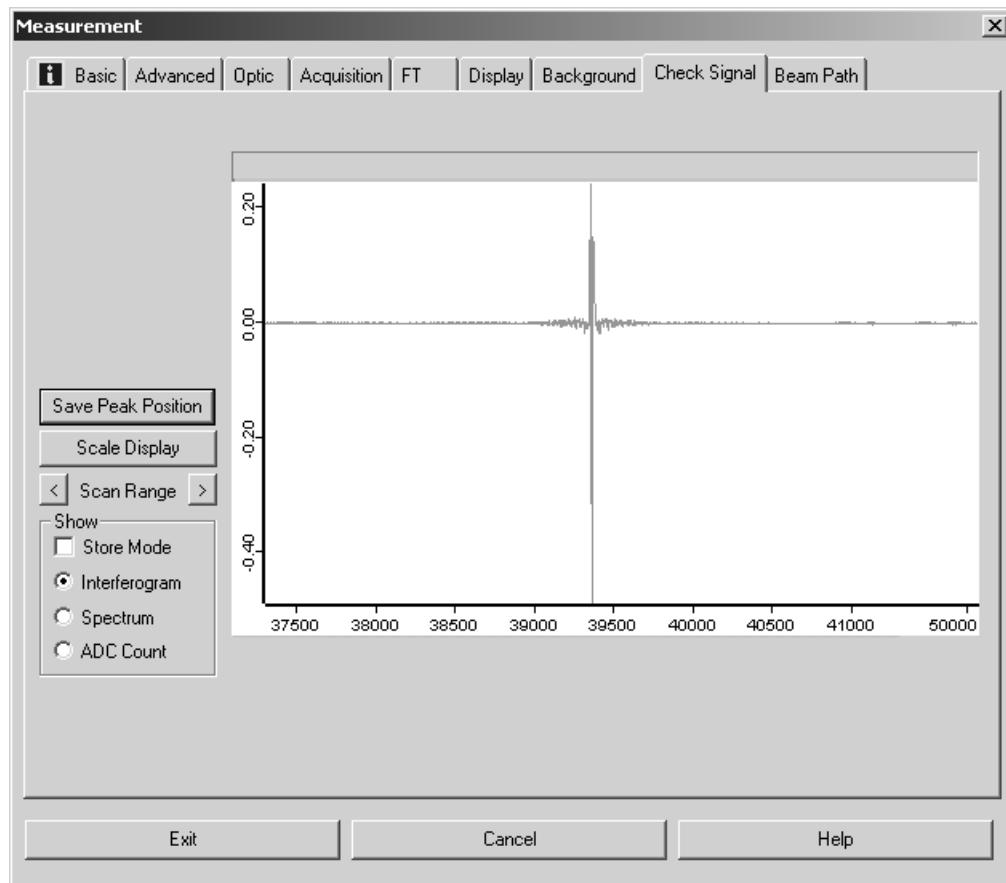
Figure 88: Measurement - Check Signal tab with interferogram

Similar to the spectrum display in the spectrum window you can also zoom in a particular section. The interferogram shown in figure 88 and 89 has been created by the AQP simulation mode. Therefore, the interferograms of your spectrometer used may be different.
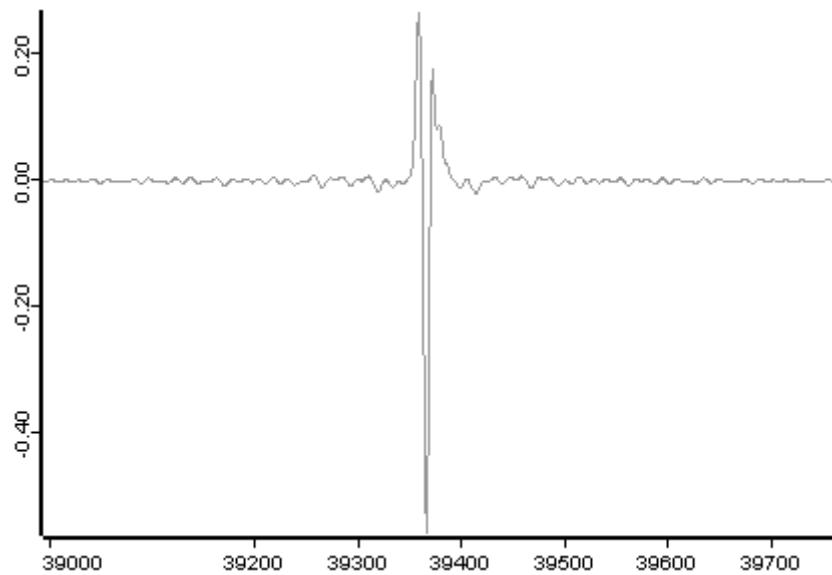
Figure 89: Interferogram zoomed-in

To undo the zooming click on the *Scale Display* button and the interferogram will be scaled on the intensity axis.

If the maximum interferogram value is not displayed, move the range by using the [<] and [>] buttons.

In the upper right corner of the interfergram plot the amplitude and zero-crossing position of the interferometer are displayed. If the peak position is constant, you can save it by clicking the *Save Peak Position* button.

To monitor the amplitude and zero-crossing position even when adjusting the interferometer from a considerable distance, check the *ADC Count* option button in the *Show* group field. The graphical display of the interferogram will be replaced by a numerical one.
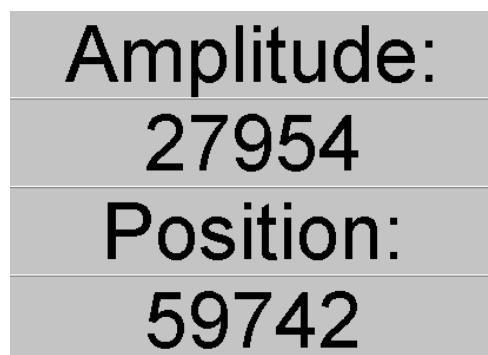
Figure 90: Numerical display of ADC count

Check the *Interferogram* option button to return to graphical display. To Fourier transform the interferogram during adjustment and have it displayed as single-channel spectrum, check the *Spectrum* option button.

Stepper Motor Adjustment

In case of spectrometers providing a software-controlled adjustment of the interferometer by using stepper motors, the motor control panel is displayed at the top on the left.

(a) Automatic alignment

(b) *Manual* fine alignment

(c) Motor display and control

(d) Restore (0,0) position of motors
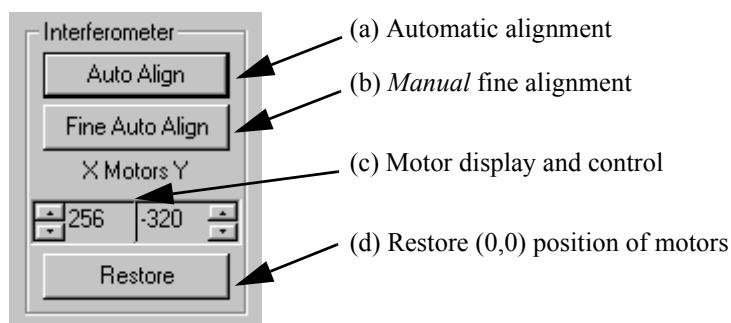
Figure 91: Menu to adjust stepper motors

The motors can be controlled manually by using the ⬍ arrow buttons. Click on the *Auto Align* button to start an automatic adjustment. Use the *Fine Auto Align* button to correct minor misalignments within the near range of the current xy-coordinates. This is especially recommended if you measure spectral regions of higher frequency (NIR to UV). The *Fine Auto Align* function produces the same result as the *Auto Align* function, however, it performs faster than *Auto Align* as it covers a smaller frequency range.

7.2.10   Beam Path

Whether the *Beam Path* tab is available or not depends on the spectrometer type. Use the *Beam Path* tab to visualize the spectrometer beam path which is based on the parameters defined on the *Optic* tab.

If you position the cursor on a beam path component, e.g. source, the component description pops up. Double click on the source component to have the beam path displayed. Figure 92 shows a TENSOR 27 beam path. Depending on the spectrometer used it is also possible to interactively change the measurement parameters (e.g. source, detector, measurement channel) on the *Beam Path* tab. Left click on one of the beam path components to activate or deactivate it. All the changes made will be automatically stored on the *Optic* tab.
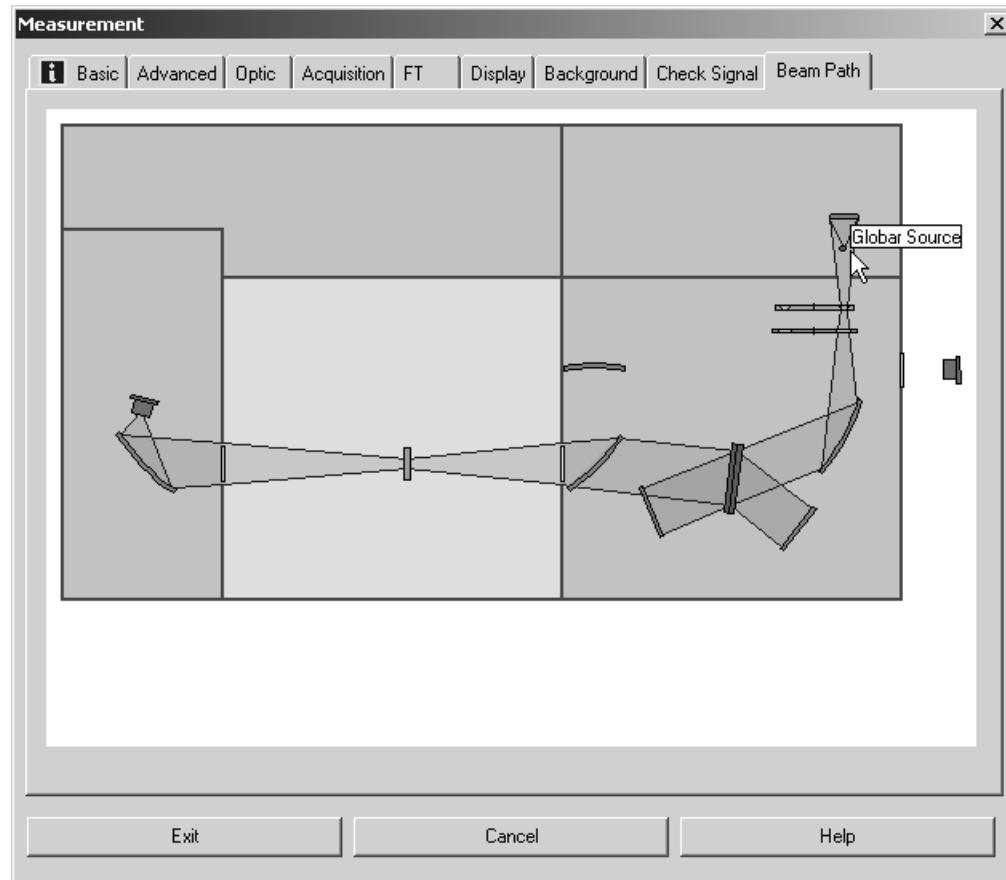
Figure 92: Measurement - Beam Path tab (Tensor 27)

7.2.11   Raman Measurements

In case of Raman measurements you can also specify the laser power on the *Basic* tab (see figure 93).
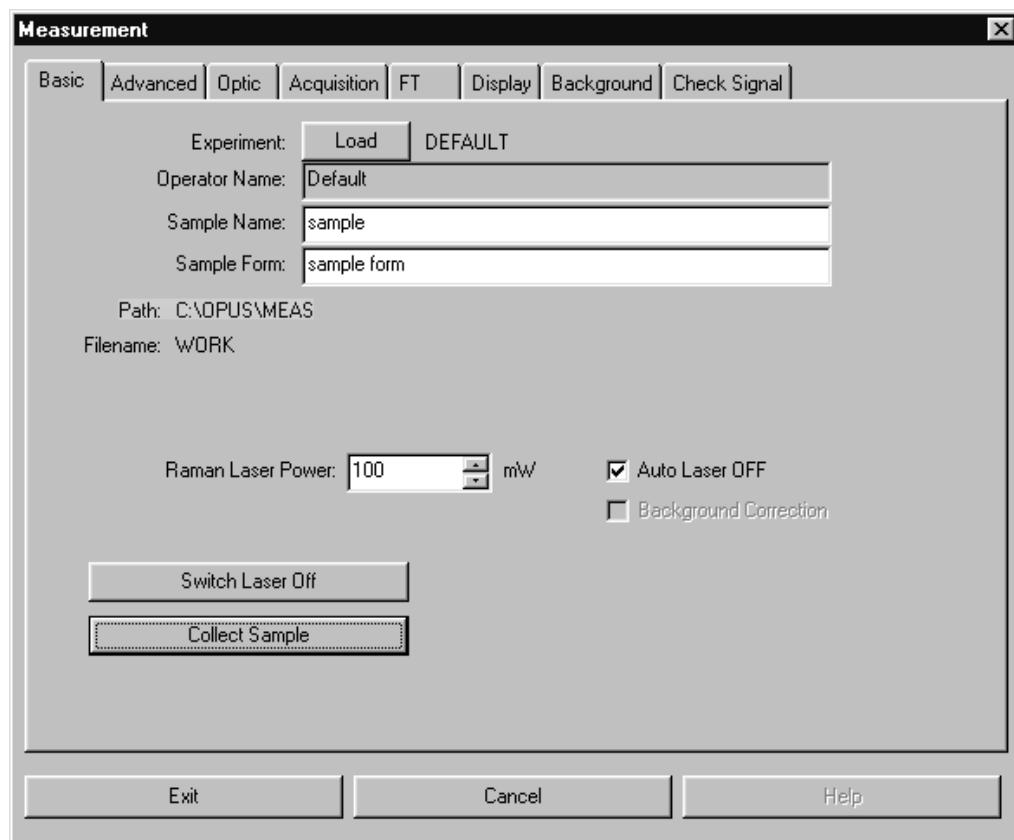
Figure 93: Raman Measurement - Basic tab

In standard configuration the laser will automatically be switched off after each measurement. For some applications, e.g. series measurements, you can deactivate this laser option. Uncheck the *Auto Laser OFF* check box.

On the *Advanced* tab the frequency range for data storage will be displayed in relation to the laser excitation frequency on a yellow background.
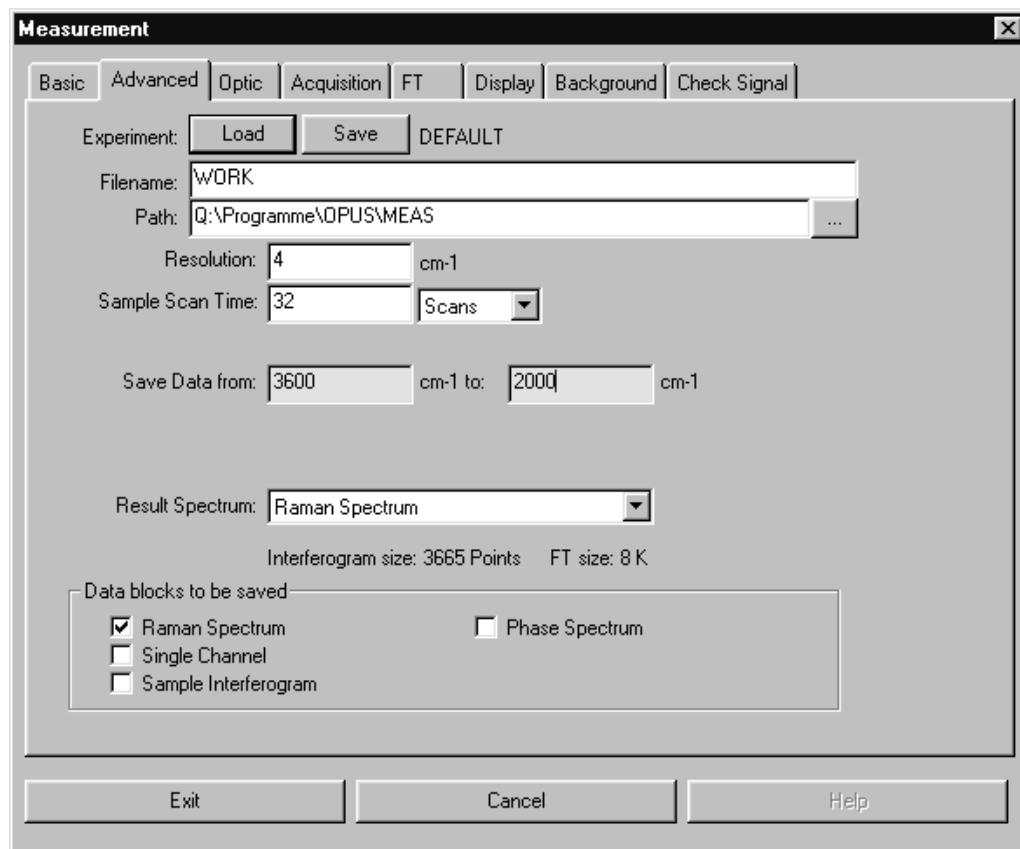
Figure 94: Raman Measurement – Advanced tab

On the *Acquisition* tab all frequencies are displayed in relation to the laser excitation energy.
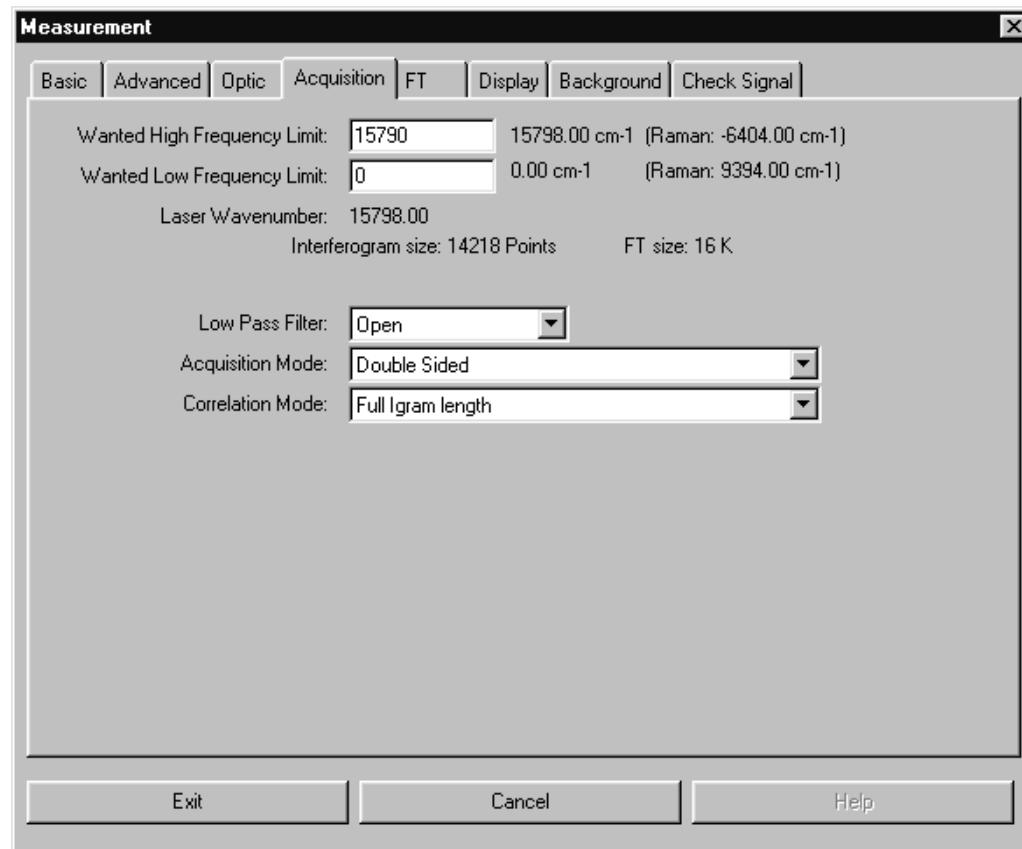
Figure 95: Raman Measurement – Acquisition tab

The laser power can be set using the slider on the *Check Signal* tab. The actual performance will be displayed.
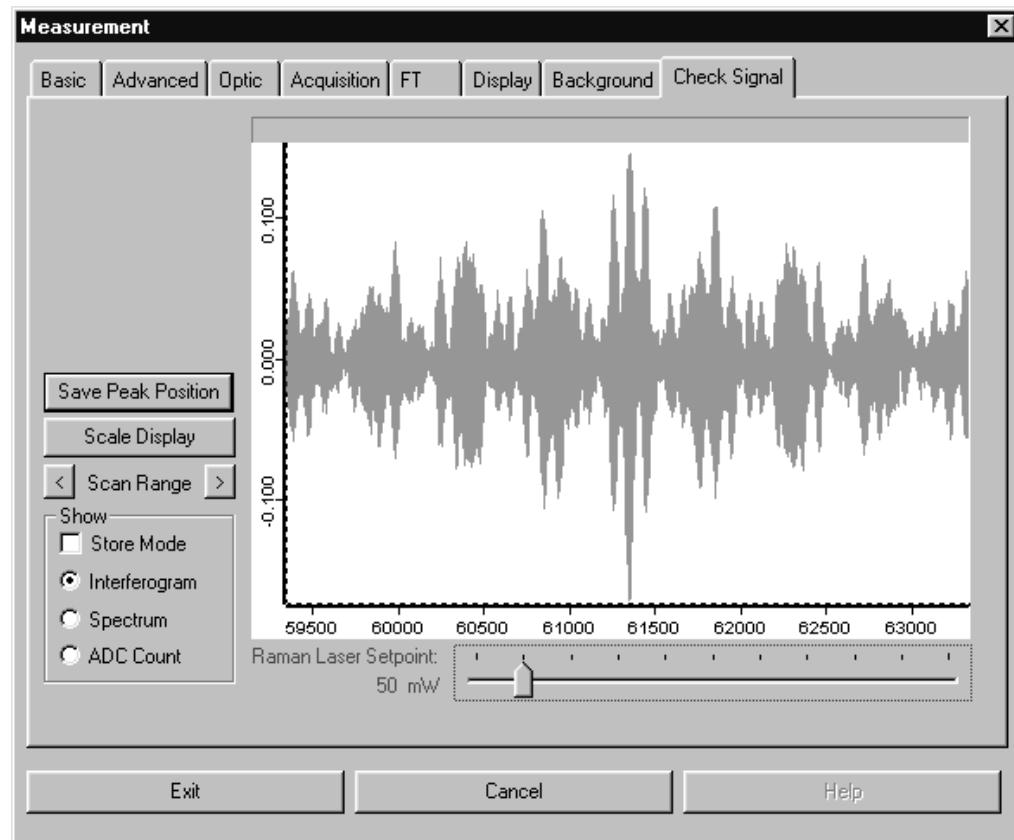
Figure 96: Raman Measurement - Check Signal tab

7.3   Repeated Measurements

The *Repeated Measurements* command allows you to define a measurement series to automate data acquisition. The *Repeated Measurements* dialog box differs from the *Measurements* dialog box only in the *Basic* tab. This tab includes two additional entry fields:

a) *Repeat the Measurement*: define the total number of measurements
b) *Delay between Measurements*: define the total number of scans and the delay between single measurements.
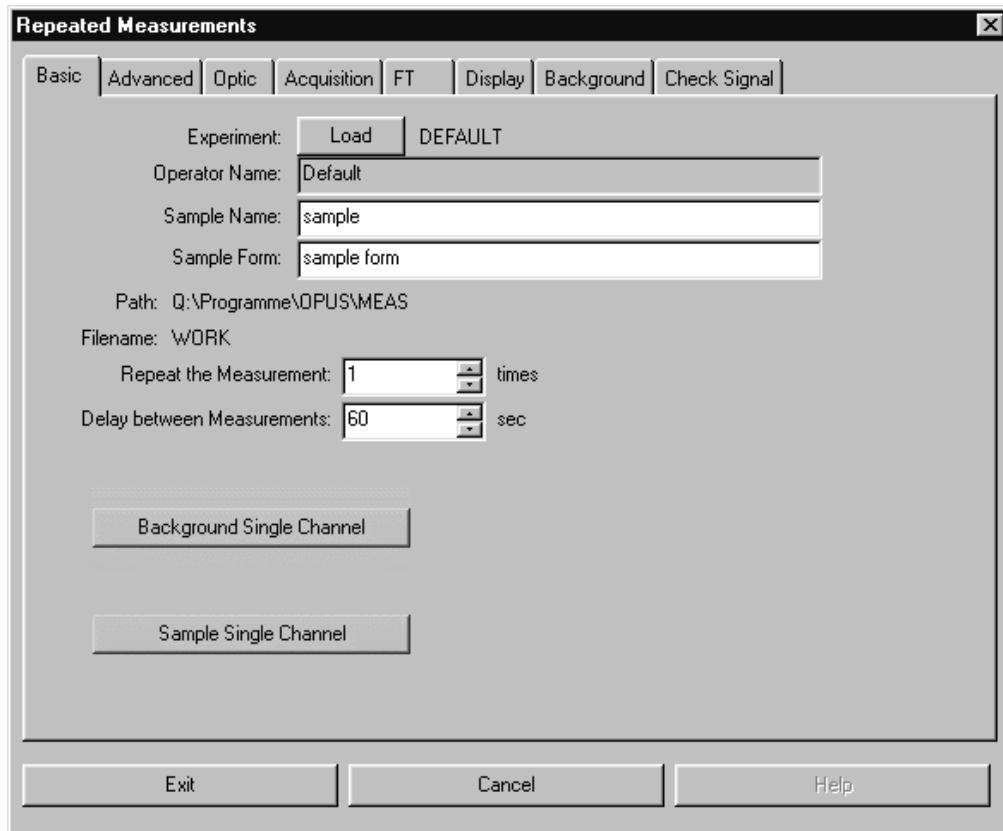
Figure 97: Repeated Measurements – Basic tab

7.4 Rapid Scan - Time Resolved Measurement

The *Rapid Scan Time Resolved Measurement* command allows you to acquire spectra in quick succession (not available for TENSOR, MATRIX, MPA, IFS125 HR or VERTEX spectrometers). Typically, time-resolved measurements (TRS) are performed to record sample changes or environmental fluctuations, to achieve an absolute time resolution (i.e. maximum possible number of measurements) or to repeat measurements with high time constant. The result of this measurement is stored in a 3D file which includes all spectra measured.

Contrary to the OPUS/CHROM software, no spectrum or chromatogram will be calculated during data acquisition. Therefore, TRS measurements do not require any additional computational power or any additional CPU capacity on your AQP board. However, the AQP has to have sufficient RAM to store all averaged interferograms. The following table lists the maximum number of interferograms per run, using a bandwidth from 0 to $7900\,\text{cm}^{-1}$ and single-sided data acquisition:

AQP Memory	Max. Number of Interfero-grams (8cm^{-1})	Max. Number of Interfero-grams (4cm^{-1})
1 MB	67	33
4 MB	480	240
16 MB	2130	1065

Basically, the *Rapid Scan Time Resolved Measurement* dialog box includes the same commands as the *Measurement* dialog box (described in chapter 7.2, ff), except for the *Method Editor* tab. Before you start a TRS measurement you have to create an experiment.
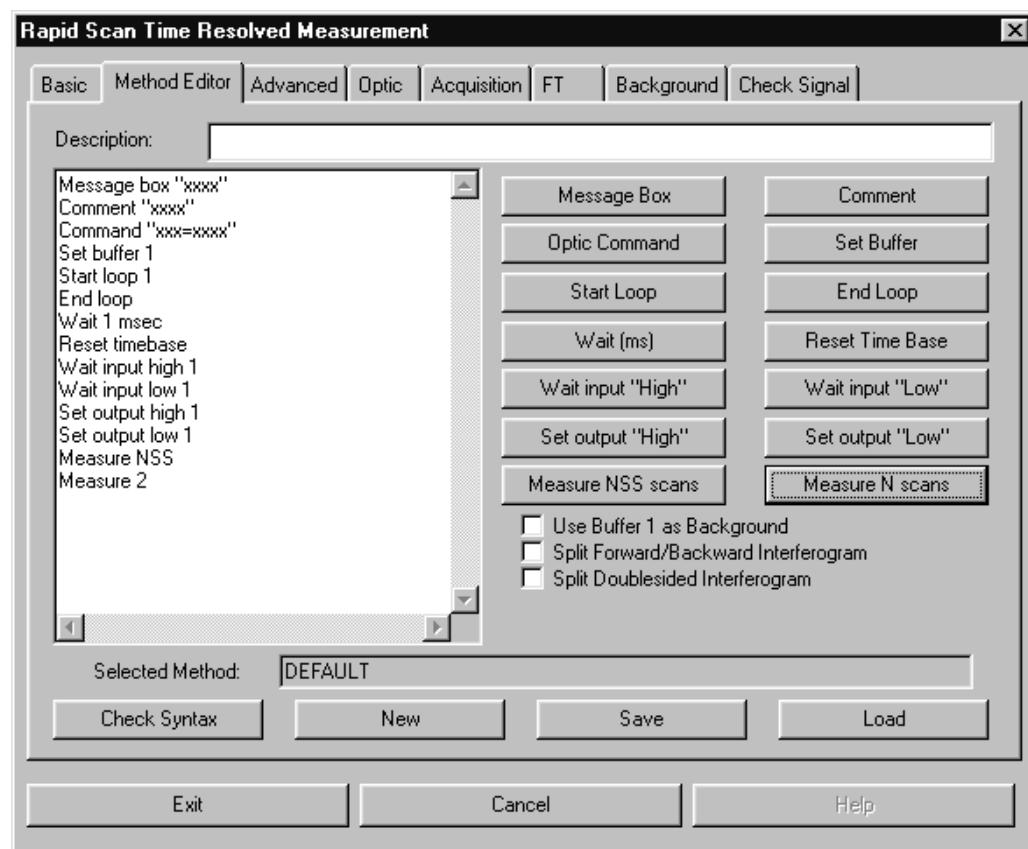
Figure 98: Rapid Scan Time Resolved Measurements – Method Editor tab

The *Method Editor* tab is used to define the timer parameters of your experiment. Time-resolved measurements are controlled by the following components:

- Measuring single scans
- Measuring several scans (average)
- Waiting for an external TTL[1] signal
- TTL signal output
- Optic commands output

---

1. Transistor-transistor-logic signal

- Message to the operator (wait for response)
- Wait times
- Start loop/end loop (repetition of a sequence)

You can directly program these components by using the respective buttons displayed in figure 98 on the right. The commands and their corresponding parameters are displayed on the left and can later be edited manually. It is also possible to exclusively perform the command input manually. In the following the commands of the different buttons will be explained.

- *Message Box*: enters the *Message box xxxx* command with *xxxx* being a wildcard which can be edited. The text edited will be displayed when running the TRS method.
- *Comment*: creates a comment line to make the method program code readable.
- *Optic Command*: allows to send text commands to the optics during run time to change certain parameter values.
- *Set Buffer*: specifies the memory area which has to be accessed. You can use the same memory area several times, i.e. you do not need to define a new memory area for repeated measurements or loops.
  Example:
  Measure 10 Scans to Buffer 5
  Writes 10 scans to buffer 5

  Buffer=1
  Start Loop=100
  Measure 1 Scan
  End Loop
  Writes 10 scans to buffer 1 to 100
- *Start Loop*: indicates that a loop starts. All commands enclosed between *Start Loop* and *End Loop* will be repeated an n-times. You can nest these loops as often as you want, provided that each *Start Loop* statement is assigned to an equivalent *End Loop* statement.
- *End Loop*: marks the end of a loop.
- *Wait (ms)*: the execution of the subsequent command will be delayed by the specified period of time (in milliseconds).
- *Reset Time Base*: the time information stored with the spectra refers to the start time of the measurement. If a *Reset Time Base* command is executed, the waiting time is reset to 0.
- *Wait Input "High"*: delays the subsequent command until the 5V TTL level is detected in the input bit specified. The following table explains the correlation between the bits and pins of the 50-pole I/O plug. The bit marked by an (s) is read by an especially fast command and should therefore be preferably used in case of extreme time resolution.

Bit Number	Pin Number Socket	Pin Number Plug
4	13	5
5	14	38
6	15	22
7 (s)	16	6

- *Wait Input "Low"*: delays the subsequent command until the 0V TTL level is detected on the input bit specified.
- *Set Output "High"*: sets the 5V TTL level to the output pin specified. The following table explains the correlation between the bits and pins of the 50-pole I/O plug. The bit marked by an (s) is read by an especially fast command and therefore should preferably be used in case of extreme time resolution.

Bit Number	Pin Number Female Connector	Pin Number Male Connector
0	5	35
1	6	19
2	7	3
3 (s)	8	36

- *Set Output "Low"*: sets the 0V TTL level to the output pin specified.
- *Measure NSS Scans*: the total number of scans that will be averaged is read from the *Measurement* dialog. The advantage is that there is no need of rewriting a new TRS method, if the same method has to be used with different numbers of scans.
- *Measure N Scans*: starts the measurement. The total number of single scans to be averaged will be displayed after the *Measure* command.

Figure 98 shows the program code generated by these buttons. Below these button there are the following three check boxes:

- *Use Buffer 1 as Background*: the background spectrum is measured during TRS measurement and used to calculate the spectra. If this check box is not activated, the background spectrum of the preceding standard measurement will be used, which is the arithmetic average of all forward and backward scans.
- *Split Forward/Backward Interferogram*: this check box can only be activated if the *Single Sided Forward/Backward* or *Double Sided Forward/Backward* option has been selected as *Acquisition Mode*. In this case a buffer is split into a forward and backward scan, and the scans are stored separately. This leads to a time resolution increased by factor 2.

- *Split Double-Sided Interferogram*: this check box can only be activated if the *Double Sided Forward/Backward, Double Sided Fast Return* or *Double Sided* option has been selected as *Acquisition Mode*. In this case a double-sided interferogram is split into two single-sided interferograms, which increases time resolution once again by factor 2.

If both check boxes, i.e. *Split Double-Sided Interferogram* and *Split Forward/ Backward Interferogram,* have been activated and the *Double Sided Forward/ Backward* option has been selected as *Acquisition* mode, 4 interferograms (spectra) are generated per buffer. This yields to the maximum possible time resolution at a given mirror velocity.

Enter a description of the method you have created into the *Description* entry field (figure 98). Use the *Save* button to store the description. To access previous methods click on the *Load* button. If you want to create a new method, click on the *New* button. After creating the method you can check the syntax programmed by using the *Check Syntax* button.

If you have defined a *Rapid Scan* measurement, start this measurement by clicking on the *Start Rapid Scan Measurement* button on the *Basic* tab. The measurement progress is displayed on the status bar. If the *Split Forward/ Backward Interferogram* mode is used, the status bar displays wice the number of scans. The *Measure 4 scans* message, e.g., produces 4 forward and 4 backward scans, i.e. a total number of 8 scans.

7.5   Interleaved Time Resolved Measurements

The electronics of several BRUKER spectrometers can generate up to 16 data points (equidistant in time) per standard interferogram data point. This can be used to analyze the kinetics of rapid processes which are completely reproducible with as many as 16 time intervals. If the time required to digitize *n* time intervals is higher than the time available between two normal interferogram data points, the time intervals can be distributed over several scans (interleave factor >1). The *Interleaved Time Resolved Measurement* function is not available for TENSOR, MATRIX, MPA, IFS 125 HR or VERTEX spectrometers.

If you select the *Interleaved Time Resolved Measurements* command, a dialog opens including tabs which are quite similar to the other measurement dialogs already described. Enter all parameters for interleaved measurements on the *Timing/Interleave* tab.
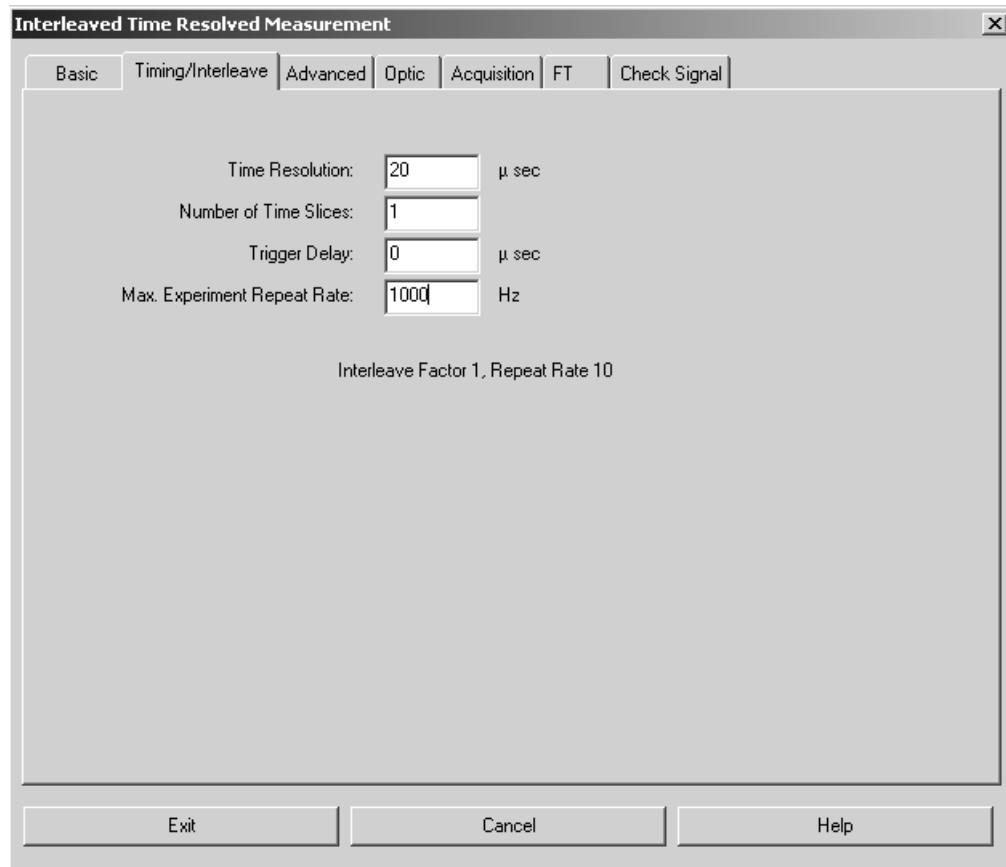
Figure 99: Interleaved Time Resolved Measurement - Timing/Interleave tab

- *Time Resolution:* Distance between two time slices in microseconds.
- *Number of Time Slices:* Number of *n* time slices which are to be measured for each normal interferogram data point. Values between 1 and 16 are possible. *n* time slices will create *n* spectra.
- *Trigger Delay:* Delay between the trigger of a normal data point and the digitalization of the first time slice in microseconds.
- *Max. Experiment Repeat Rate:* Maximum measurement repetition rate. The actual repetition rate will be below this value.

After the measurement, the data are sorted into *n* interferograms which are assigned to the respective time slices. If desired, the corresponding single-channel spectra are calculated. Similar to TRS-measurements the results are stored in a 3D data file.

7.6   Direct Command Entry

The *Direct Command Entry* command is especially used for test purposes and in case of macros. Commands sent to the optics will be logged, and also be displayed on the screen. If you click on a certain line in the entry field next to the *Send Command* button, this command line can be repeated. The answers sent by the optics are displayed in the field below.
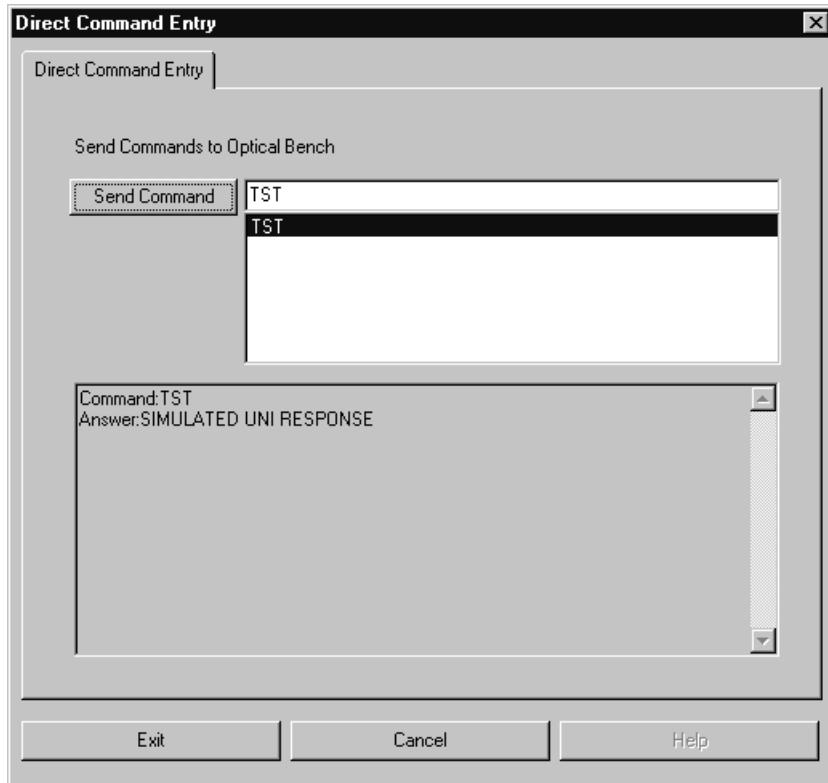
Figure 100: Direct Command Entry

7.7 Optics Diagnostic

The *Optics Diagnostic* command allows a quick check of the spectrometer components. In the *Diagnose* dialog the hardware components, e.g. source, laser, interferometer etc. are displayed in the upper line. If the test has been finished, the test result is displayed in the lower line according to the number of test channels (*IT RESULT*) defined. For details on how to define test channels refer to chapter 14.10.

A green check mark indicates that the test has been successful. The yellow *WARNING* note means that the test time has been expired. If the test has not passed, a red ERROR is displayed.

The instrument test, the so-called PQ test (Performance Qualification Test) proves that the spectrometer measures correctly in terms of routine laboratory work, and has to be performed every day.

For details on the diagnostics result log select the *Optic Setup and Service* command and click on the *Service* tab.
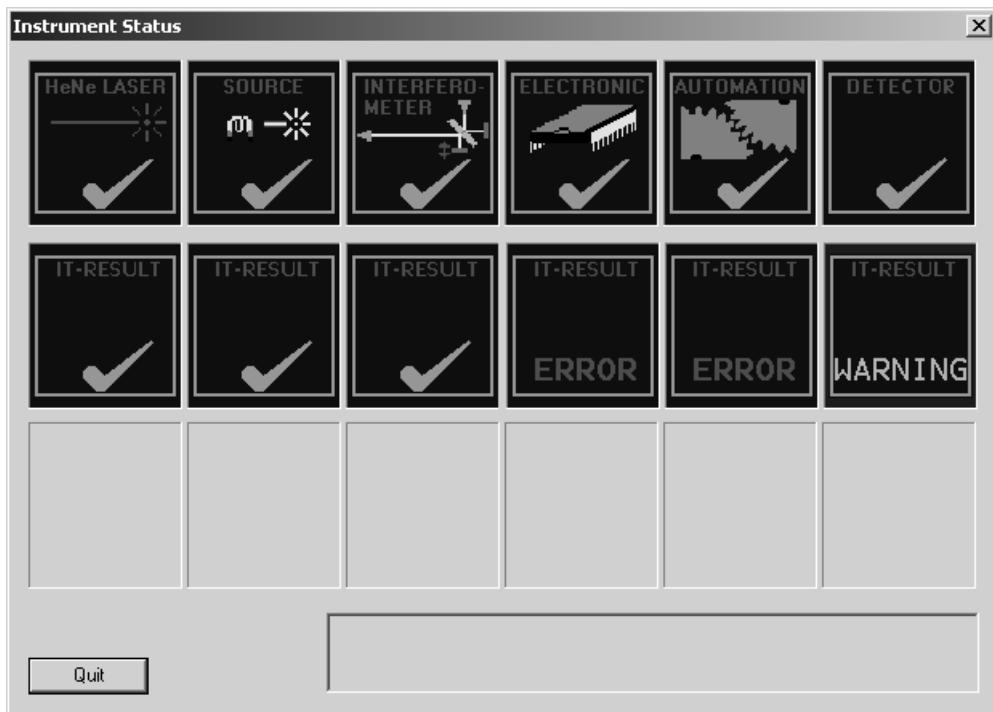
Figure 101: Optics Diagnostic - Instrument Status

7.8 Temperature Control

The *Temperature Control* command allows the operation and control of external equipment, e.g. temperature-controlled stage.
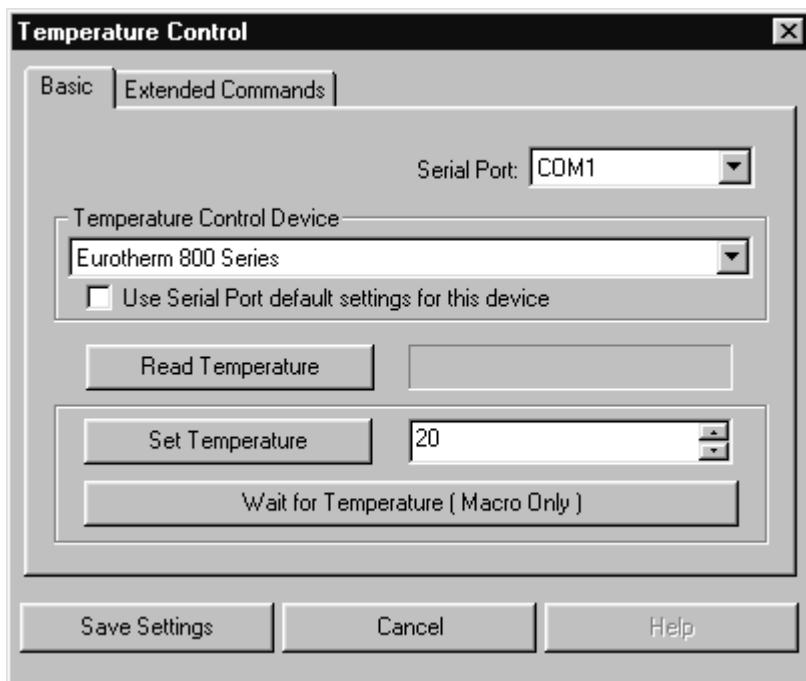
Figure 102: Temperature Control – Basic tab

Select the respective serial port which the stage is connected to from the *Serial Port* drop-down list. Specify the type of thermo-sensor in the *Temperature Control Device* drop-down list. If you activate the *Use Serial Port default settings for this device* check box, the default port parameters will be set as specified in the operating system.

To set the required temperature click on the *Set Temperature* button. The current temperature of the stage can be read by clicking on the *Read Temperature* button. If macros are used to control the temperature, click on the *Wait for Temperature (Macro Only)* button to stop the makros until the desired temperature is achieved.
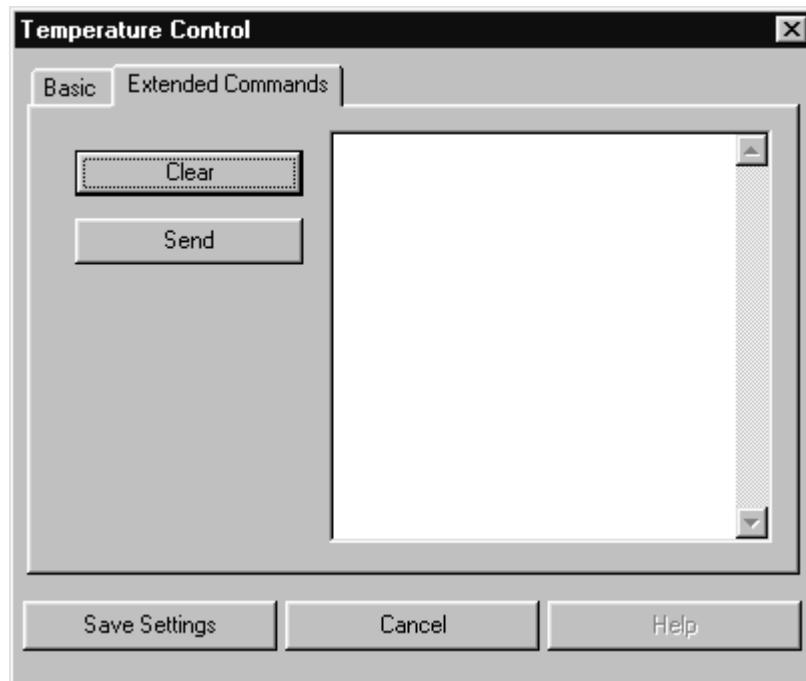
Figure 103: Temperature Control – Extended Commands tab

The *Extended Commands* tab allows command input. For details on the corresponding commands, refer to the control unit manual. The following syntax applies:

To read a command: R <command>
To write a command: W <command>

The command will only be transmitted if you press the *Send* button. *Clear* provides a blank entry field. Save your command sequence using the *Save Settings* button.

8 Manipulate

This chapter describes all OPUS data manipulation options. The term *Manipulate* involves all arithmetic methods which modify or create new spectral data of a spectrum acquired.

> ⌃ₐ Baseline Correction
> ⌇ₐ Spectrum Subtraction
> ⌖ AB <-> TR Conversion
> ⋔ Straight Line Generation
> ⊞ Spectrum Calculator
> ⋔ Cut
> ▲ Normalization
> ⌁ Make Compatible
> **CS** Convert Spectra
> ⌇⌇ Smooth
> ▲ Derivative
> ↔ Frequency Calibration
> ⃰ Raman Correction
> ▲ Black Body
> ⌇ Interferogram to Spectrum
> ⋔ Inverse FT
> Post Zerofilling
> ▲ Fourier Self-Deconvolution
> Symmetric FT
> KKT Kramers-Kronig-Transformation
> Spectrum from Interferograms
> LiM Extrapolation
> ⌀ 1/cm <-> μm, nm
> ⌁ Averaging
> ⌁ Merge Spectral Ranges
> Atmospheric Compensation
> ⊛ Straylight Correction
> — Noise Generation
> ⋀⋁ Moving mean
> ⌁ Make monotone

Figure 104: Manipulate Menu

The dialog boxes of the different *Manipulate* commands almost look like the same. Each dialog box consists of the following tabs:

- The *Select Files* tab allows to select the files to be manipulated, as well as to define the most important manipulation parameters. For details, see section 2.1.

- The *Frequency Range* tab allows to define the spectral limits of manipulation. For details on how to interactively select frequencies, see section 2.7.

As the calculation results are only temporary files (work files), you need to directly save them by using the *Save File* command of the *File* menu. If you exit OPUS without saving the work files, the manipulation data get lost. Normally, a warning pops up when you want to exit OPUS indicating the existence of data which have not yet been saved.

8.1 Baseline Correction

You can perform a baseline correction for several spectra at the same time. First, load the spectrum file(s) you want to correct by clicking on the *Load File* command in the *File* menu. Select the *Baseline Correction* command in the *Manipulate* menu. The file name will be automatically displayed in the *File(s) to Correct* selection field. If not, drag and drop the spectrum file(s) from the OPUS browser window into the respective selection field.
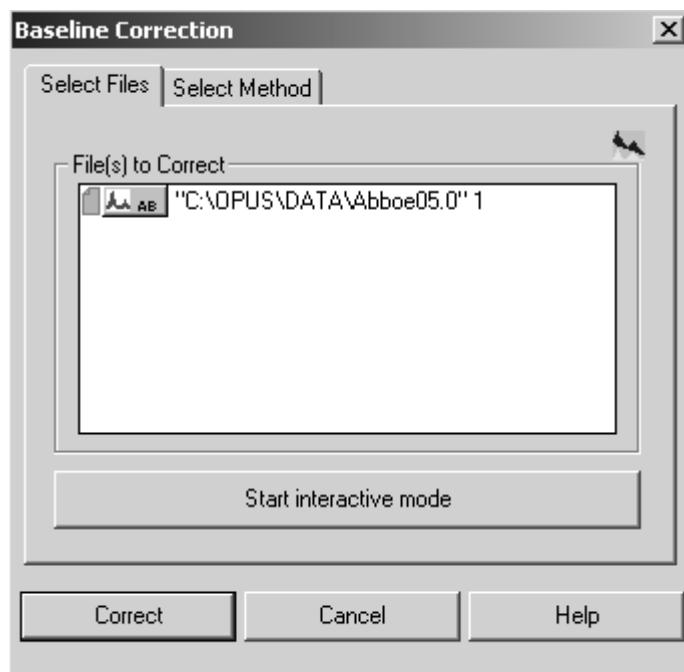
Figure 105: Baseline Correction – Select Files

You can either accept the baseline points automatically set by OPUS, or set them manually. Click on the *Start interactive mode* button. A new window opens which shows the original spectrum on top and the baseline correction at the bottom. Check the *Straight lines* or *Polynomes* option button to adjust straight lines or polynomes to the baseline.
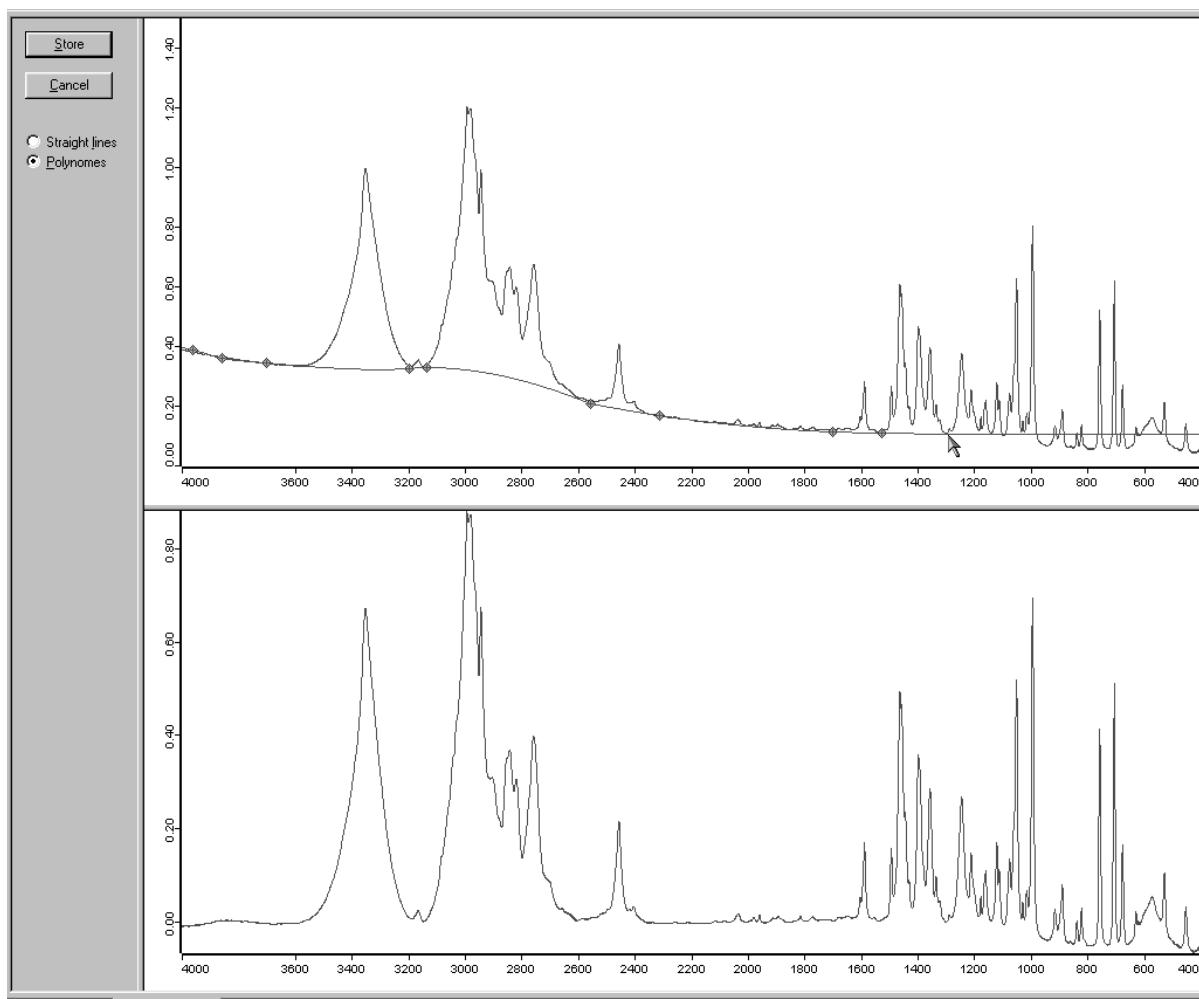
Figure 106: Baseline Correction – Interactive Mode

Double click on the original spectrum to add a baseline point. The result of this correction will be immediately displayed in the lower spectrum window. If you want to remove a baseline point, double click on this point again.

You can also zoom spectra. Right click on the original spectrum and select the *Zoom In* or *Zoom Out* command from the pop-up menu. For details, see section 2.3. Click on the *Store* button to save the correction results (figure 106).

To automatically correct the baseline of your spectrum select the *Select Method* tab (figure 105). A different dialog box opens and allows to specify the correction method, e.g. *Scattering* or *Rubberband,* and the number of baseline points. Optionally, you can exclude the spectral ranges which contain CO_2 bands (between 2400 ... 2275cm^{-1} and 680 ... 660cm^{-1}). This is only possible in case of an automatic baseline correction.
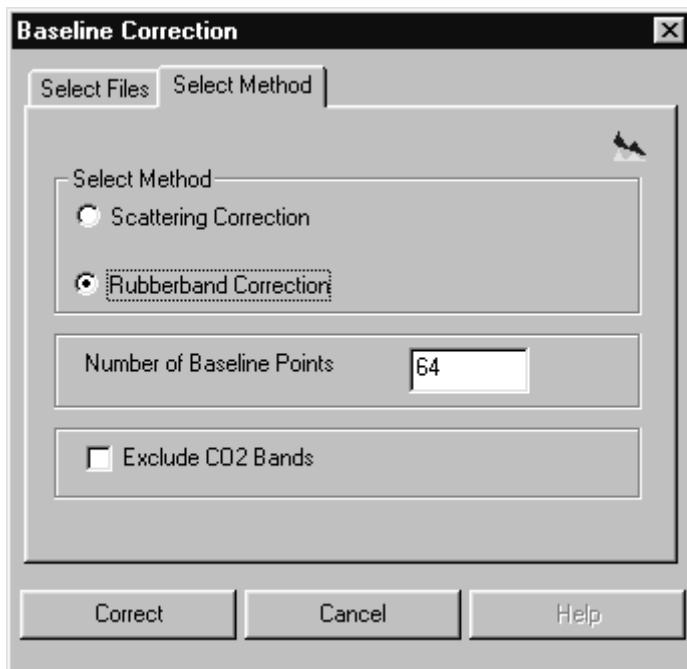
Figure 107: Baseline Correction – Select Method

Specify the number of baseline points. Enter a value between 10 and 200 (unless the frequency range selected is too small). The default value is 64. Select a correction method and start the calculation by clicking on the *Correct* button.

Both baseline correction methods divide spectra in *n* ranges (*n* being the number of baseline points) which are of equal size. In the case of absorbance spectra the minima are determined within these *n* ranges. The baseline points are connected by straight lines. From the bottom up a rubberband is stretched over this curve. Each baseline point which is not exactly on the rubberband is omitted. The rubberband serves as baseline.

If you check *Scattering Correction,* the rubberband is created in such a way that at each point the slope of the baseline must be negative for an absorbance-like spectrum (provided that the spectrum is displayed in decreasing wave numbers from left to right).

Baseline corrections can also be performed on transmittance spectra. First, maxima are determined in the transmittance spectrum and the rubberband is calculated. Then, the original spectrum is divided by the rubberband. You will get the same result if you convert the transmittance spectrum into an absorbance spectrum, perform the baseline correction and re-convert the result spectrum into a transmittance spectrum.

Figure 108 shows an original absorbance spectrum and a baseline-corrected spectrum, using the *Rubberband Correction* method and 64 baseline points.
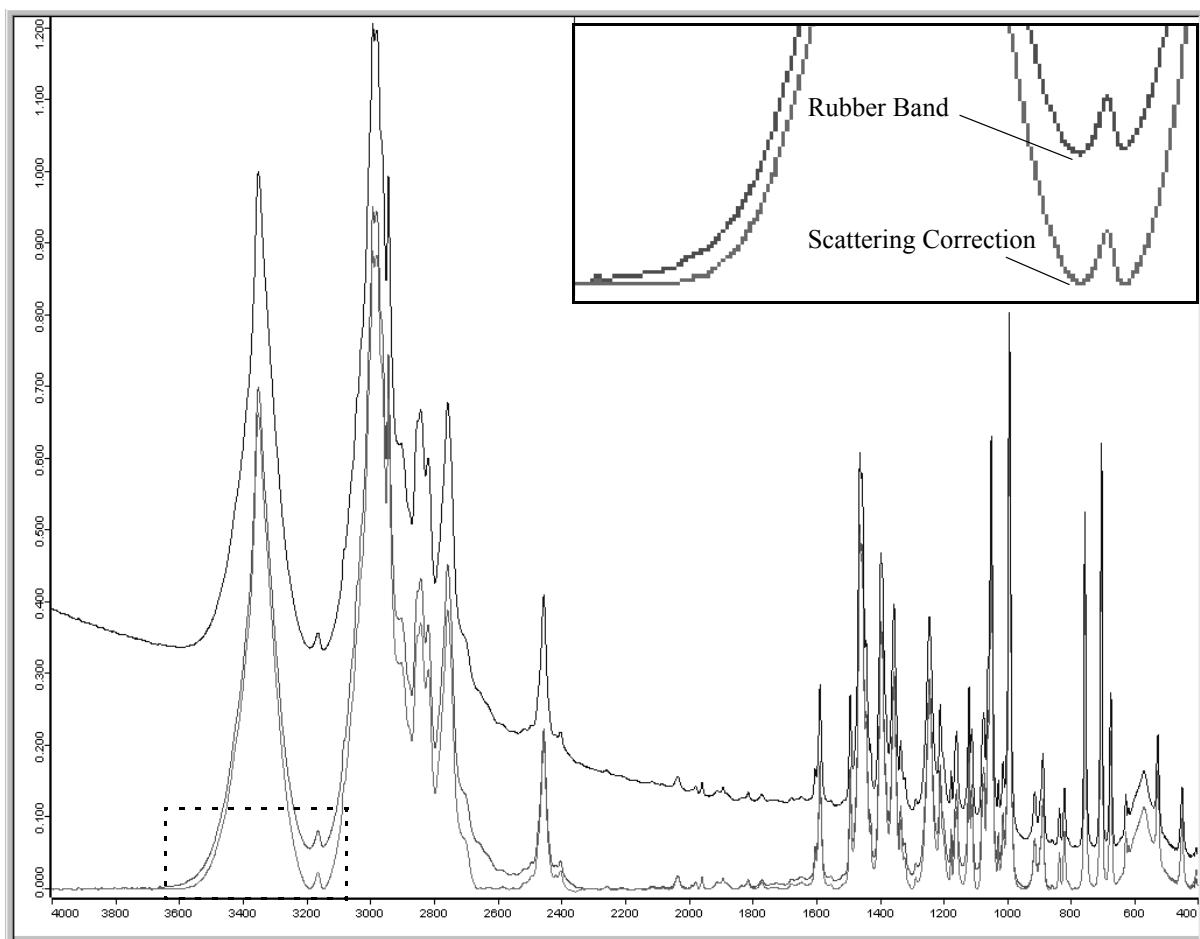
Figure 108: Spectrum prior to and after Baseline Correction

If you subtract the corrected spectrum from the original spectrum, the baseline can be determined, see figure 109.
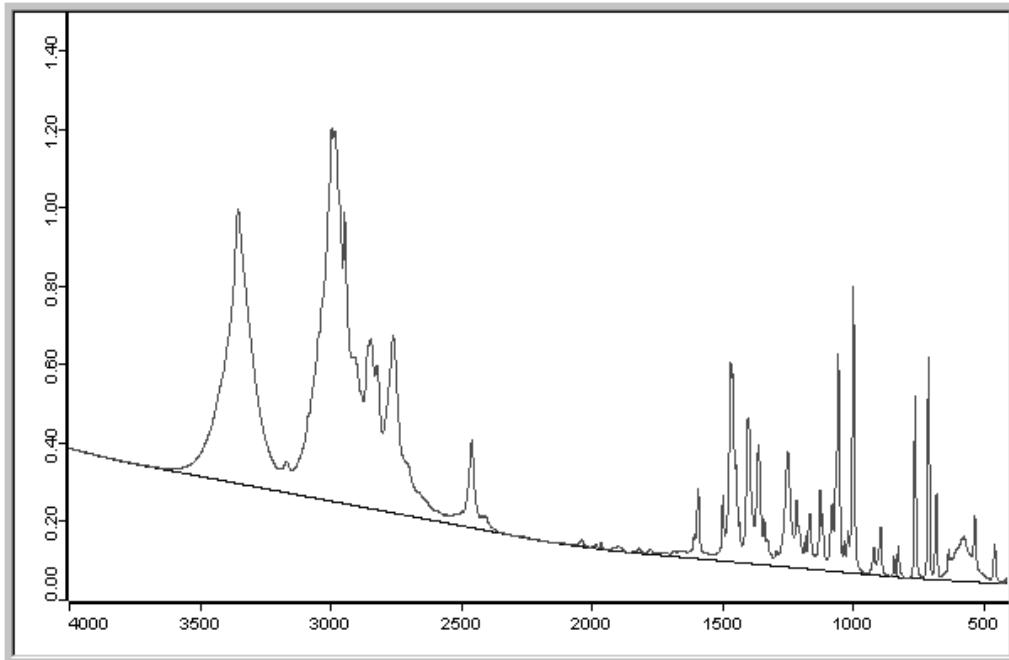
Figure 109: Original Spectrum and Rubberband Baseline

8.2   Spectrum Subtraction

This kind of calculation subtracts spectra, with one multiplication factor each, from a multi-component spectrum. An additive constant can be determined. Click on the *Spectrum Subtraction* command. Figure 110 and 111 show the *Spectrum Subtraction* dialogs:
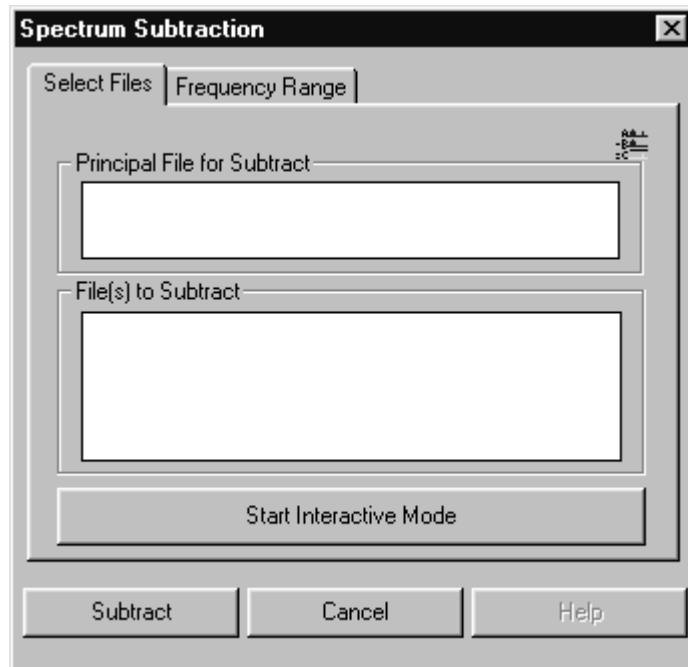
Figure 110: Spectrum Subtraction - Select Files
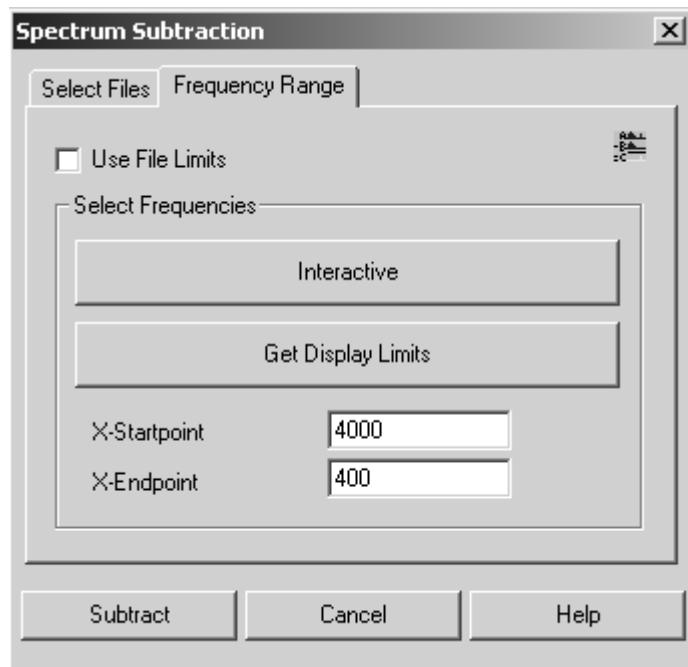
Figure 111: Spectrum Substraction - Frequency Range

The result of this calculation which can be attributed to different components is as follows:

$$\text{Result spectrum }(\nu) \quad = \quad \text{multi-component spectrum}(\nu)$$
$$- \text{ Factor1} * \text{single-component spectrum }(\nu)$$
$$- \text{ Factor2} * \text{single-component spectrum }(\nu)$$
$$...$$
$$- \text{ Offset}$$

Note: This kind of calculation is only appropriate for absorbance spectra. Transmittance spectra are automatically converted to absorbance spectra during calculation. Only if the original spectrum has been of transmittance mode, the resulting spectrum will be converted to transmittance when the subtraction has been finished.

Example:

First, generate an example spectrum using the *Spectrum Calculator* (see chapter 8.5). The spectrum has to consist of 0.7 *ABBOE12.0* spectrum parts, 1.3 *ABBOE08.0* spectrum parts and 2.3 *ABBOE05.0* spectrum parts. Save the spectrum as *CALC.6*. This spectrum should represent a generic sample consisting of an unknown amount of these three components and be analyzed by using *Spectrum Subtraction*. The automatic subtraction mode minimizes the least squares deviation in the difference spectrum.

The optimum result can only be achieved if all single components are simultaneously subtracted from one mixture spectrum. This yields to a result of almost zero.

If you click on the *Start Interactive Mode* button, the following dialog box will be displayed:
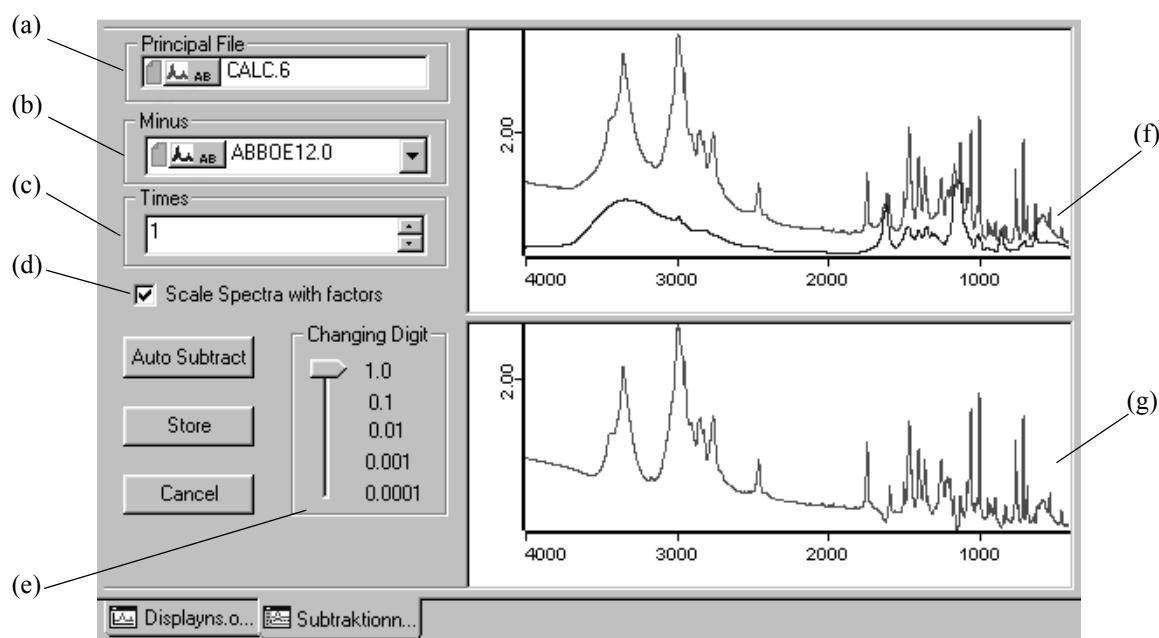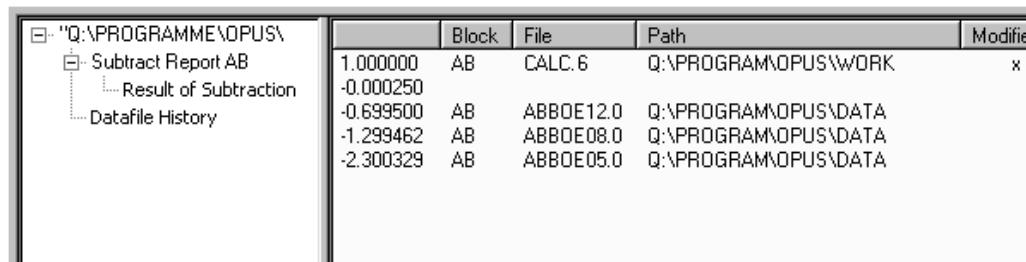
Figure 112: Interactive Spectrum Subtraction

a) Shows the name of the multi-component spectrum.

b) If you click on the drop-down list, you can select the spectra to be subtracted.

c) Depending on your spectra selection in (b), the adjusted factors are displayed. The factor value can be increased or decreased, using the control elements on the right. The value can also be entered manually. Click into the entry field and overwrite the value given.

d) If you check this option button, the displayed spectra will be scaled.

e) Use this slider to define the number of decimals which vary the components of (c).

f) This window shows both the single-component spectra and the multi-component spectrum.

g) The display is autoscaled and shows the difference between the multi-component spectrum and the weighted single-component spectra.

If you right click into the windows (f) and (g), you can zoom in specific spectral ranges using the pop-up menu. The *Auto Subtract* button would start the automatic single-component subtraction. If you click on the *Store* button, you exit this dialog box and the difference spectrum is stored as *Principal File* (a).

The numerical values used are attached to the spectrum in the form of a subtraction data block ⊞SUBTR.. This data block contains the factors used to subtract the spectra, and the result spectrum. If you right click on the subtraction data block, the *Show Report* option pops up. Select this option to open the report window:

		Block	File	Path	Modifie
⊟·· "Q:\PROGRAMME\OPUS\	1.000000	AB	CALC.6	Q:\PROGRAM\OPUS\WORK	x
⊟·· Subtract Report AB	-0.000250				
······Result of Subtraction	-0.699500	AB	ABB0E12.0	Q:\PROGRAM\OPUS\DATA	
·····Datafile History	-1.299462	AB	ABB0E08.0	Q:\PROGRAM\OPUS\DATA	
	-2.300329	AB	ABB0E05.0	Q:\PROGRAM\OPUS\DATA	

Figure 113: Spectrum Subtraction Report

The first column on the right shows the factors and the mark in the *Modified* column indicates the spectrum which the subtraction report has been attached to.

8.3   AB <-> TR Conversion

The *AB<->TR Conversion* command converts absorbance spectra to transmittance spectra and vice versa. The conversion direction can be set automatically, or individually pre-defined.
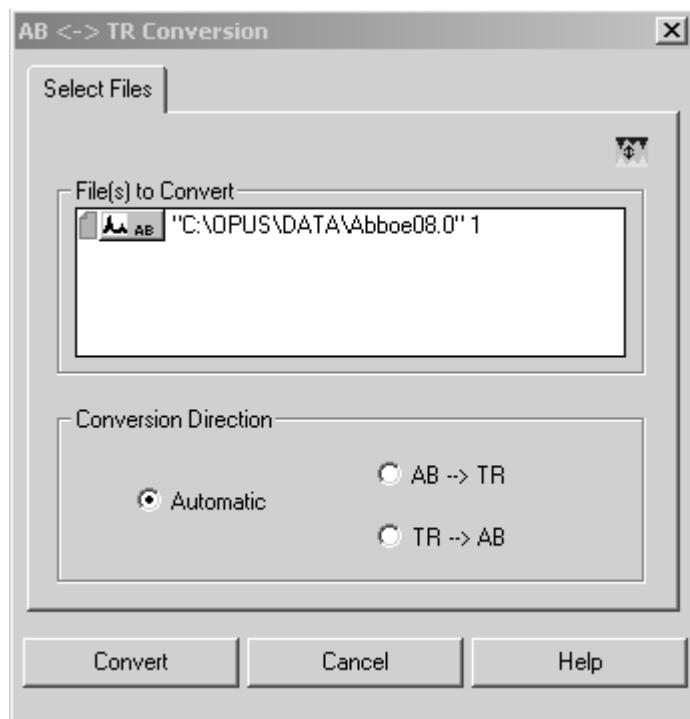
Figure 114: AB <-> TR Conversion

If you definitely determine a conversion direction, only those spectra will be converted which do not have the requested format. The option buttons in the *Conversion Direction* group field allow to create a uniform data block type for several spectra. Click on the *Convert* button to start the conversion.
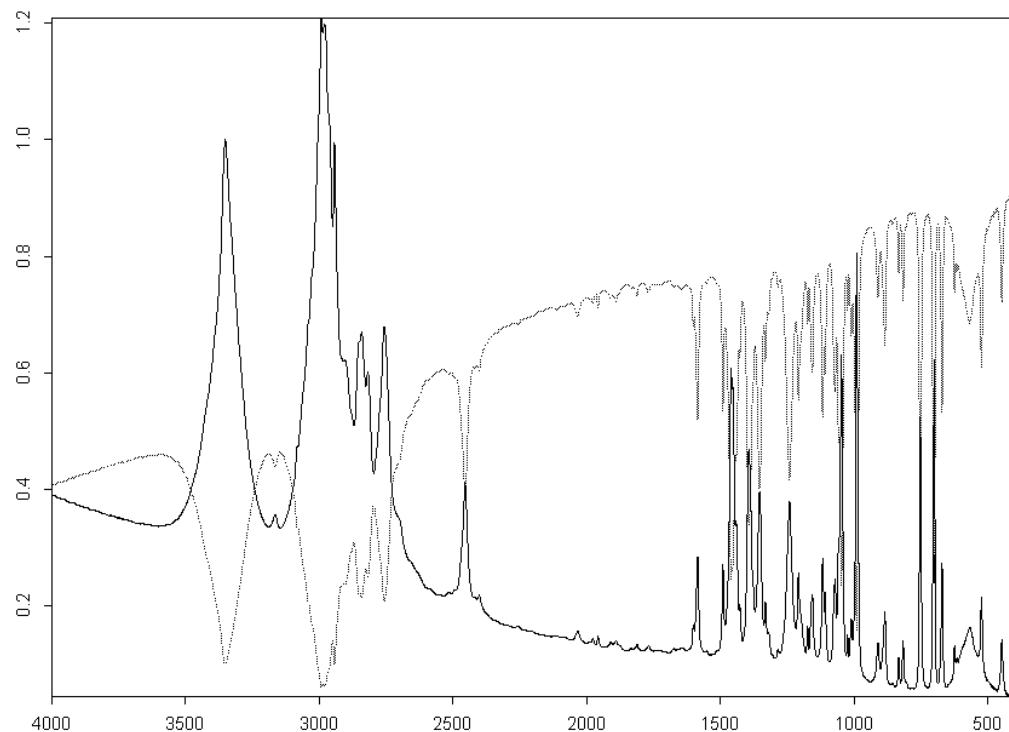
Figure 115: Converted Absorbance Spectrum into a Transmittance Spectrum

The spectrum displayed by a dotted line (figure 115) has be generated by an AB → TR conversion.

The equation required for an TR → AB conversion is:

$$AB = -\log(TR)$$

Transmittance values less than 10^{-5} are set to 5 absorbance units.

The equation required for an AB → TR conversion is:

$$TR = 10^{-AB}$$

8.4 Straight Line Generation

The *Straight Line Generation* command allows to eliminate fringe effects in the interferogram or artifacts detected in a spectrum. Select the spectrum files and define the frequency range on the *Frequency Range* tab (figure 116). You can either select the frequencies interactively, manually or accept the current frequency limits of the spectrum. When you have finished setting the frequency limits, click on the *Generate* button.
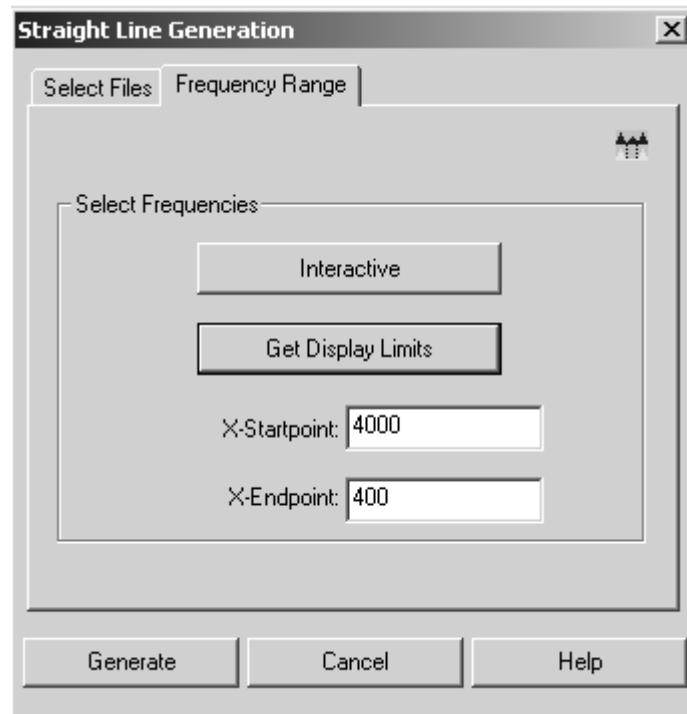
Figure 116: Straight Line Generation - Frequence Range tab

Figure 117 shows a straight line generated between 2,550 and 2,360 wave numbers, which replaces the original peak (dotted line).
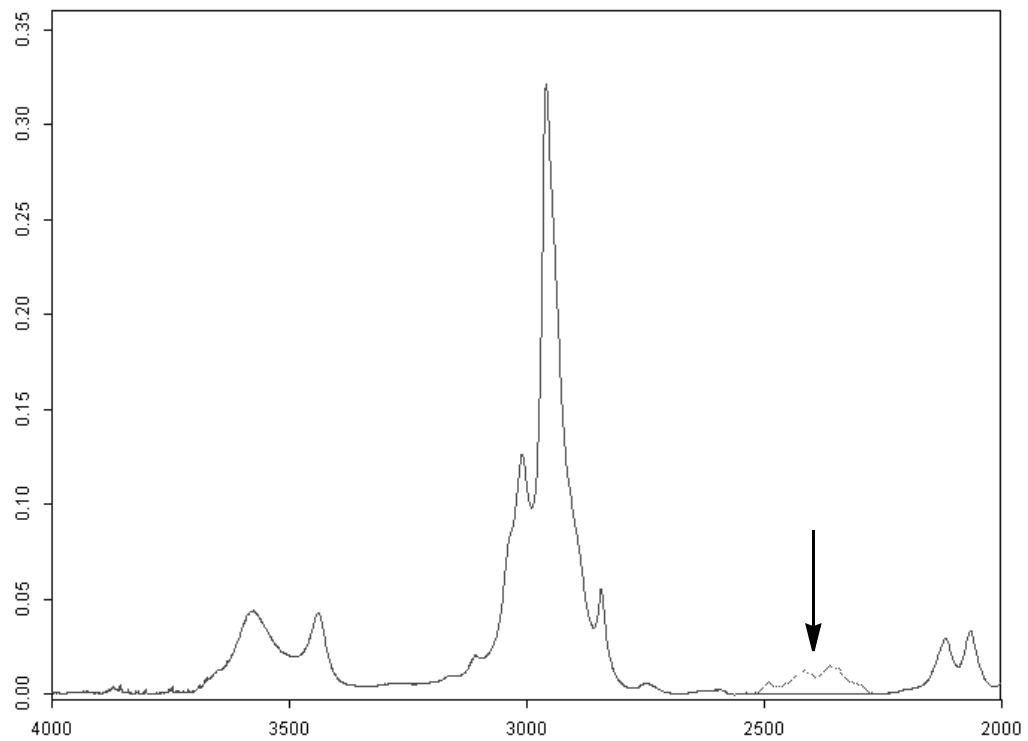
Figure 117: Spectrum Before and After Generating a Straight Line

8.5   Spectrum Calculator

The *Spectrum Calculator* is used to calculate spectra and numerical results. You can also enter algebraic terms.
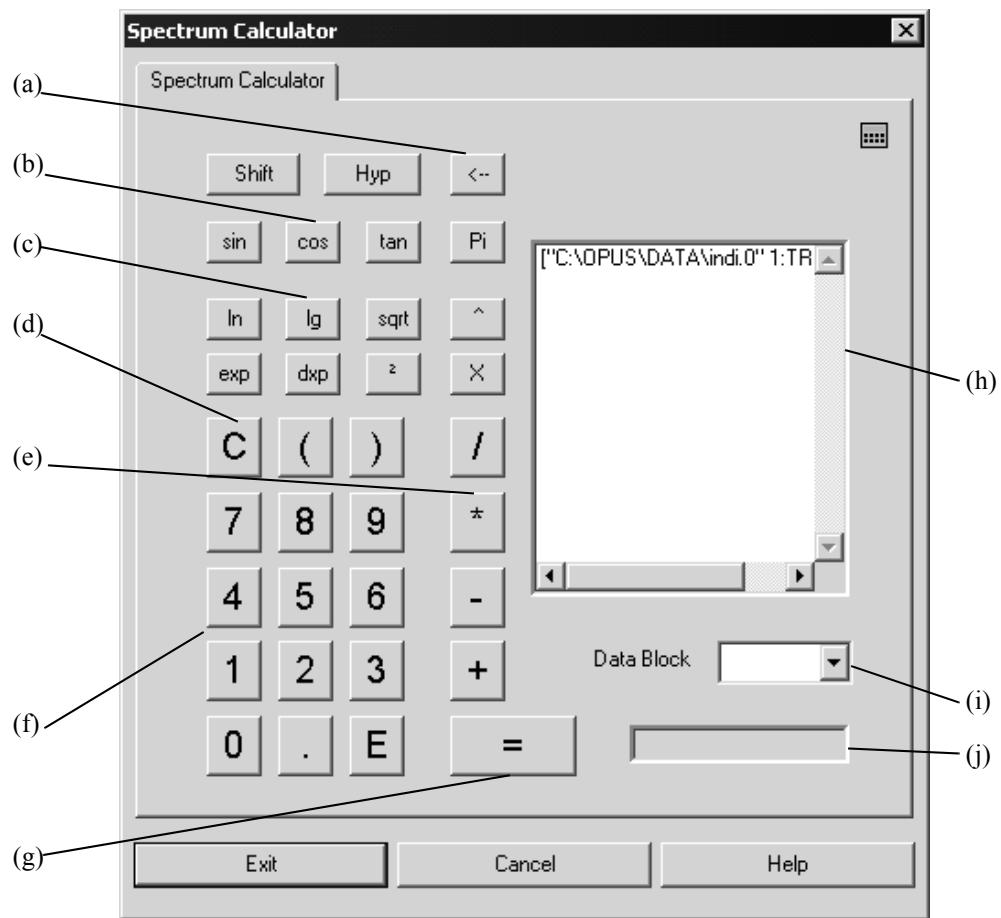
Figure 118: Spectrum Calculator

a) Use the ⟨⟨ **<--** ⟩⟩ button to delete your input.

b) These buttons provide trigonometric functions. The following functions are available if you use the *Shift* and *Hyp* button:

c) Additional mathematical functions, e.g. square function ^{2} (e.g. $3^2 = 9$) and "^", as well as π and special function **x** are made available.

 sqrt is the square root function $\sqrt{}$

 ln is the natural logarithm

 lg is the logarithm to the base 10

 exp is the exponential function *e*

 dxp takes the following entry to the power of x (i.e. 10^x)

d) *C* clears the display (h) and (i). You can use the brackets *( )* to form mathematical groups that will be calculated first.

e) The four basic arithmetic operations.

f) Numerical block which consists of the figures 0 - 9, the decimal point and exponential function *E* (e.g. 4.321E3 = 4321).

g) This button starts the calculation. The result will be displayed in the entry field (h).

h) You can drag & drop spectra from the OPUS browser window to the entry field (h). They are directly made available for mathematical calculations. You can also enter algebraic terms and numerical values into this entry field.

i) Select the result data block from the drop-down list.

j) The display field shows the calculation results or indicates ERROR in case of an incorrect entry.

You can enter figures, signs and functions either using the numerical keypad of your keyboard or clicking on the spectrum calculator keys. In the latter case inputs will always be added to the entry field (h). Delete inputs by using the ⟨-- button.

If the calculation results in a spectrum, the original spectrum file will be overwritten by the new result spectrum. This also applies to data blocks.

If two spectra are divided, a transmittance spectrum is generated in the numerator of these two spectra. The transmittance spectrum may overwrite the original spectrum.

In some cases it may be necessary to calculate frequency-dependent terms. This can be done using the x function, which represents the frequency values of the spectral data points. The term

$$\sin(x/100) + [4:TR] - [4:TR]$$

uses the group ($[4:TR] - [4:TR]$) to generate a spectrum with 0 intensity. The x function causes the frequency limits and data point (frequency) spacing to be applied. The result will be a sine wave. If you calculated $\sin(x/100) + [4:TR]$, the spectrum intensity values would be added to the sine wave.

The spectrum calculator cannot be compared with a *normal* pocket calculator. If you enter $100\sqrt{}$ into the pocket calculator you expect the result to be 10. The spectrum calculator, however, operates with algebraic formulae. Therefore, you need to enter sqrt(100).

It is also possible to use the spectrum calculator in case of 3d data. For details, see the OPUS 3D or OPUS VIDEO manual.

8.6   Cut

Use the *Cut* command to minimize the frequency range of a data file. Select the spectrum file and define the frequency range. Click on the *Cut* button to start the command. Figure 119 shows a frequency range (thicker curve line) generated by using the *Cut* command.
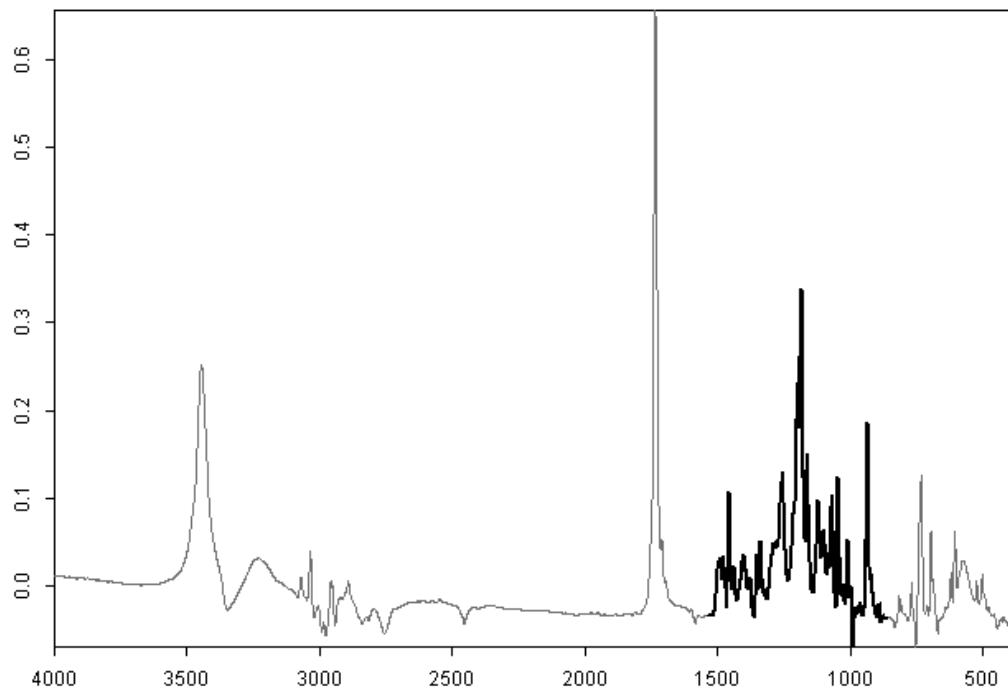
Figure 119: Original Spectrum (Thin Line) and Cut-Out Range (Thick Line)

You can also use the *Cut* command to invert the frequency limits of spectra. Select upper and lower limits which are beyond the spectral range and define them as new frequency limits in reverse order. Right click on the spectrum and select *Properties* from the pop-up menu. Invert the axes settings using the *Axes* tab. This change may not immediately appear in the spectrum window.

8.7 Normalization

The *Normalization* command allows to normalize spectra and perform offset corrections on spectra. Select the files to be normalized and click on the *Normalization* command. Three different methods are available for spectrum normalization:
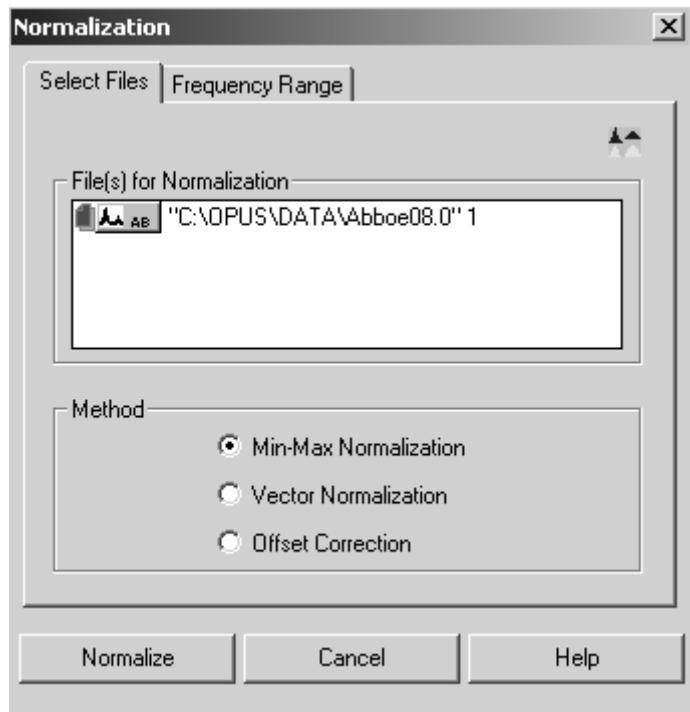
Figure 120: Normalization - Select Files tab

- **Min/Max normalization** – This method scales spectrum intensities to the effect that the minimum absorbance unit will be 0 and the maxium 2. In case of transmittance spectra the normalization is between 0 and 1.
- **Vector normalization** – This method calculates the average y-value of the spectrum. The average value is subtracted from the spectrum decreasing the mid-spectrum to y = 0. The sum of the squares of all y-values is calculated and the spectrum is divided by the square root of this sum.

  The vector norm of the result spectrum is 1: $\sum_{i=1}^{NPT} (x_i)^2 = 1$

- **Offset correction** – This method shifts spectrum intensities to the effect that the minimum absorbance unit will be 0.

8.8   Make Compatible

The *Make Compatible* command changes the data point grid of the selected files to adapt it to the *Principal File* grid. The files to be processed are manipulated to make the x-values of the spectra compatible to those of the principal file. This causes the frequency base points to be shifted. If the frequency range of a spectrum selected is larger than the range of the *Principal File*, the frequency range will be cut. Many OPUS commands make spectra automatically compatible to each other.

Figure 121: Make Compatible

There are two methods to calculate the intensities of new frequency base points. The original intensities serve as a basis.

- **Interpolation** – The method of quadratic interpolation can always be used.
- **Reduce Resolution** – The new intensities are calculated by integrating the original ones.

In case of the *Interpolation* method the curve shape is better preserved, while *Reduce Resolution* keeps the peak positions more constant.

Example:

The *Principal File* frequency limits are between 1,000 and 5,000cm^{-1}. The number of data points is 4,001 (i.e. 1cm^{-1} resolution). The frequency of the first point is 4,000.5, of the last 200.5cm^{-1}. The number of data points is 1,901 data points (2cm^{-1} resolution). The *Make Compatible* command creates a new spectrum on the basis of the original one. The first frequency point of this new spectrum is at 1,000cm^{-1} and the last one at 4,000cm^{-1}. The number of data points is 3,001 (1cm^{-1} interpolated resolution).

The x-direction (high-to-low or low-to-high) of the new spectrum always depends on the *Principal File*.

8.9   Convert Spectra

The *Convert Spectra* command performs several data conversions which mainly involve the y-axis. When selecting spectrum files for conversion certain restrictions may apply. If you try to select a spectrum which does not comply with the conversion method selected, a warning symbol will be displayed. The file name in the *File(s) to Convert* selection field on the *Select Files* tab will be red.
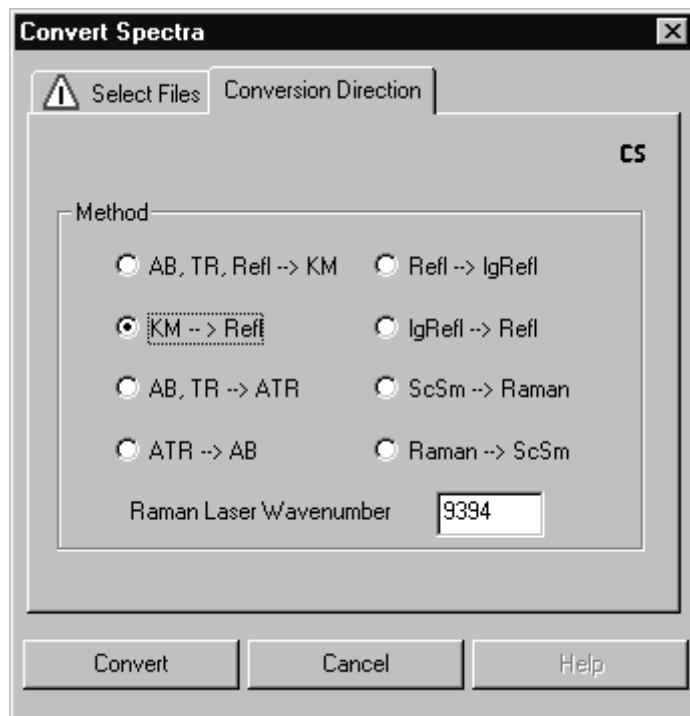
Figure 122: Convert Spectra – Mismatch of Method and Spectrum

Define the spectrum, select a conversion method and click on the *Convert* button to start the command.

8.9.1   Convert to Kubelka-Munk (KM)

The KM conversion type is appropriate for spectra which have been measured in diffuse reflectance. Compared to AB conversion the intensities are more linear to concentration. The conversion uses the following equation:

$$KM = \frac{(1 - \text{Refl})^2}{(2 \cdot \text{Refl})}$$

Rfl also means TR in this case. Absorbance spectra are first converted to transmittance spectra. The smallest value allowed for transmittance or reflectance is 0.001%. This corresponds to a Kubelka-Munk value of about 500.

8.9.2   Convert to Reflectance Spectra

The following conversion formula is applied:

$$\text{Refl} = 1 + KM - \sqrt{(2 \cdot KM + KM^2)}$$

8.9.3   Convert to ATR Spectra

The following conversion formula is applied:

$$ATR = AB \cdot \frac{X}{1000}$$

X represents the wave number. Transmittance spectra are first converted to absorbance spectra. As in case of **A**ttenuated **T**otal **R**eflection measurements the penetration depth is inversely proportional to the wave number (frequency), the spectra are normalized to a constant penetration depth.

8.9.4   Convert to Absorbance Spectra

The following conversion formula is applied:

$$AB = ATR \cdot \frac{1000}{X}$$

8.9.5   Logarithmize Reflectance Spectra

Spectra reflectance values below 0.00001 will be levelled to a lg(Refl) intensity of 5.

logRefl = -log(Refl)

8.9.6   Convert Logarithmized Reflectance Spectra

The following conversion formula is applied:

$$R = 10^{-\log(R)}$$

8.9.7 Convert Single-Channel Spectra

The start and end frequencies of a single-channel Raman spectrum will be converted using the following equations:

$$FXV(Raman) = RLW - FXV(ScSm)$$

$$LXV(Raman) = RLW - LXV(ScSm)$$

RLW stands for **R**aman **L**aser **W**ave number. This value is registered within the instrument parameter block of the Raman file created. OPUS uses the *ScSm* abbreviation to indicate a single-channel sample spectrum. *FXV* represents the starting frequency, LXV the end frequency.

8.9.8 Convert Raman Spectra

The following equation applies for the respective conversion direction selected:

$$FXV(ScSm) = RLW - FXV(Raman)$$

$$LXV(ScSm) = RLW - LXV(Raman)$$

The *RLW* parameter belongs to the instrument parameter block of the Raman spectrum.

8.9.9 Raman Laser Wave Number

This value will be used for the *ScSm* $\rightarrow$ *Raman* conversion.

8.10 Smooth

The *Smooth* command allows to smooth spectra. The smoothing is based on the Savitzky-Golay algorithm. Possible values for smoothing points are between 5 and 25. If you select a spectrum file and click on the *Smooth* command the following dialog box opens:
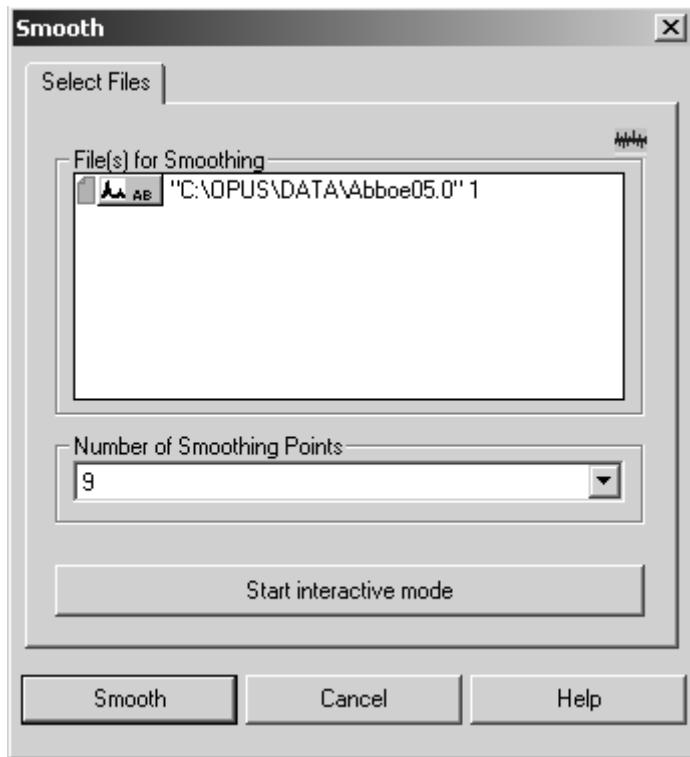
Figure 123: Smooth – Select Number of Points

Define the number of smoothing points and click on the *Smooth* button to start the command. You can also start the interactive mode. The following view is displayed:
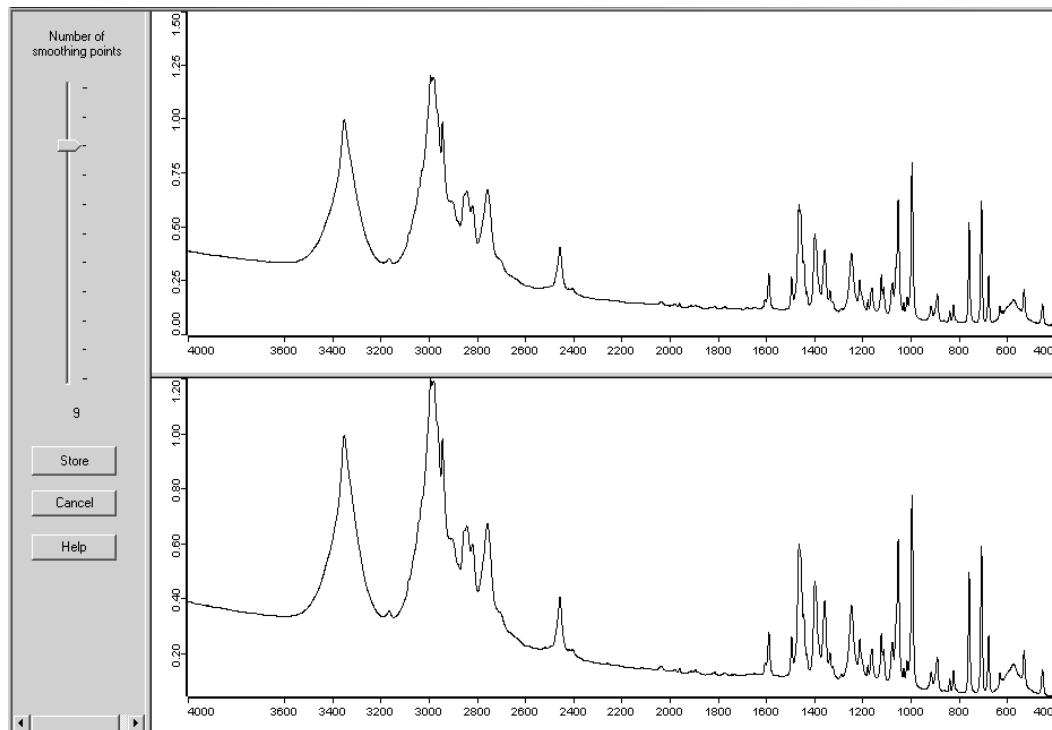
Figure 124: Interactive Smoothing

Figure 124 shows the original spectrum in the upper window and the smoothed spectrum in the lower. Use the slider to set the smoothing points interactively. The currently used number of smoothing points is shown below the slider. If you click on the *Store* button, the loaded original spectrum file will be changed. If you click on *Cancel* button, the changes made will not be stored. In both cases the view will close.

Smoothing reduces noise but also distorts signal intensities. Figure 125 directly compares the original spectrum with the smoothed one. The original spectrum band shows more pronounced peaks.
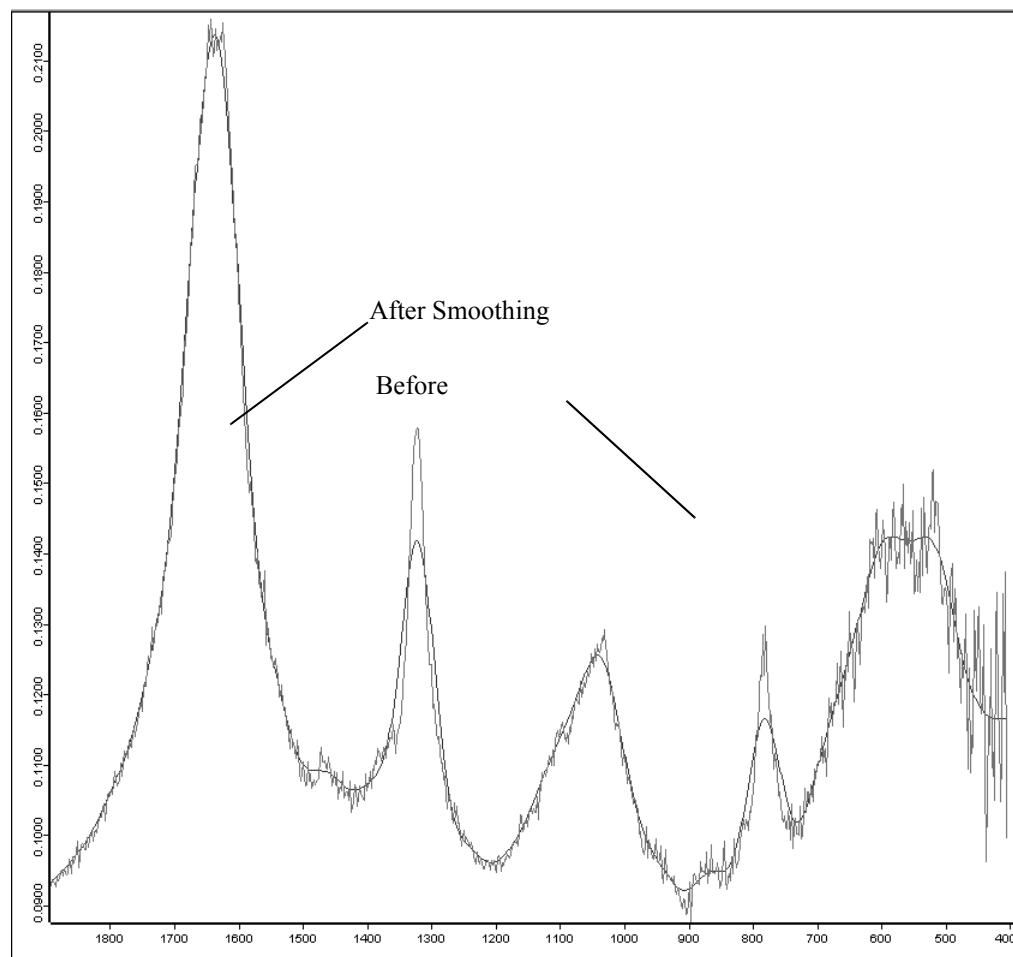
Figure 125: Smoothing Effects on a Spectrum

8.11   Derivative

The *Derivative* command calculates the first to fifth derivative of a spectrum, using the Savitzky-Golay algorithm. This algorithm allows a simultaneous smoothing of the spectrum. The smoothing effect reduces the noise generated by derivation.
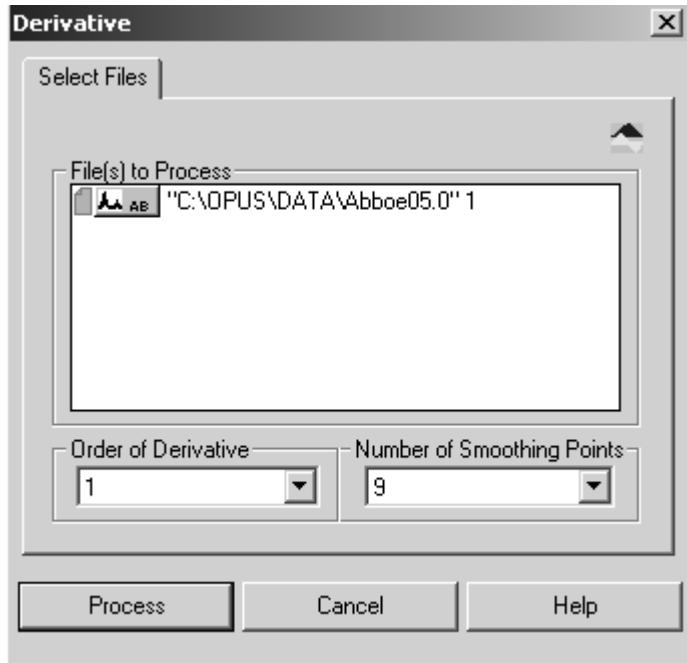
Figure 126: Derivative - Select Files tab

The minimum number of smoothing points depends on the derivative order. The higher the derivative order, the more smoothing points need to be set. You can set a maximum of 25 points.

Select a spectrum file, define the number of smoothing points and the derivative order. Click on the *Process* button to start.

As a result, a data block is generated indicating the actual derivative order of the original spectrum. If a spectrum of 1st order is subject to a 1st order derivation again, the result will be a 2nd order spectrum. The kind of derivative order is displayed in the data block of the resulting spectrum.

3rd and higher order derivations are symbolized as *n* derivation. The derivative order is stored in the parameters of the derivation data block. Right click on the spectrum file and select show parameters from the pop-up menu.

8.12 Frequency Calibration

The *Frequency Calibration* command re-calibrates the x-axis of a spectrum. You have to enter the two parameters *M* and *A*. These parameters change all ν_{old} x-values of the data points:

$$\nu_{new} = \nu_{old} \cdot M + A \qquad (or \qquad f_{new} = f_{old} \cdot M + A)$$

Select a spectrum file and click on the *Frequency Calibration* command. The following dialog box opens:
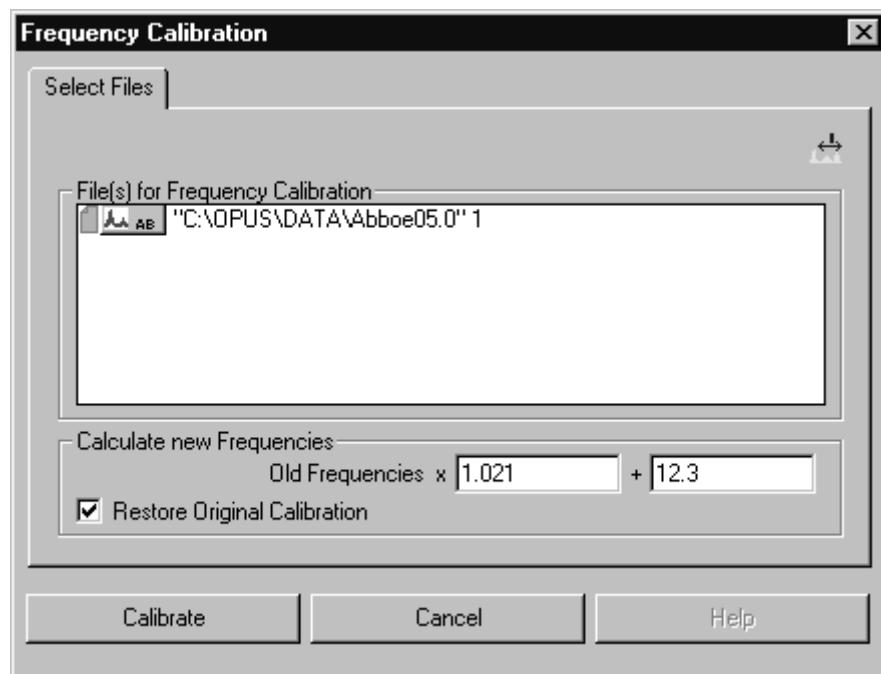
Figure 127: Frequency Calibration - Select Files

After the calibration the two parameters *M* and *A* are stored in the spectrum data block. This enables you to undo the calibration.

The original data set before the calibration looked as follows:

Figure 128: Original Set of Data Parameters

After the calibration the frequencies of the first and last data point have changed. Two additional parameters, i.e. factor M (*Mult. for Freq. Calib.)* and addend A (*Add for Freq. Calib.)* have been included in the list.

Figure 129: Set of Data Parameters after Frequency Calibration

The x-axis of a spectrum can be modified several times as follows:

$$\nu_{old,1} = \nu_{old} \cdot M_1 + A_1$$

and later by

$$\nu_{new,2} = \nu_{new,1} \cdot M_2 + A_2$$

For the first run select the parameters M_1 and A_1, and for the second the parameters M_2 and A_2. The parameter list displays the parameters M_{total} and A_{total}, which represent the total change compared to the original calibration:

$$\nu_{new,1} = \nu_{old} \cdot M_1 + A_1$$

$$\nu_{new,2} = \nu_{new,1} \cdot M_2 + A_2$$

$$\nu_{new,2} = \nu_{old} \cdot M_{total} + A_{total}$$

$$\Rightarrow (\nu_{old} \cdot M_1 + A_1) \cdot M_2 + A_2 = \nu_{old} \cdot M_{total} + A_{total}$$

$$\Rightarrow M_{total} = M_1 \cdot M_2$$

$$A_{total} = A_1 \cdot M_2 + A_2$$

You can undo these changes all at once.

8.13 Raman Correction

The special features of the optics and the frequency dependent scattering that occur in Raman spectra can almost be eliminated by using the *Raman Correction* command. To undo the Raman Correction, click on the ↻ symbol on the toolbar.

Select a spectrum file, only Raman spectra, and click on the *Raman Correction* command.
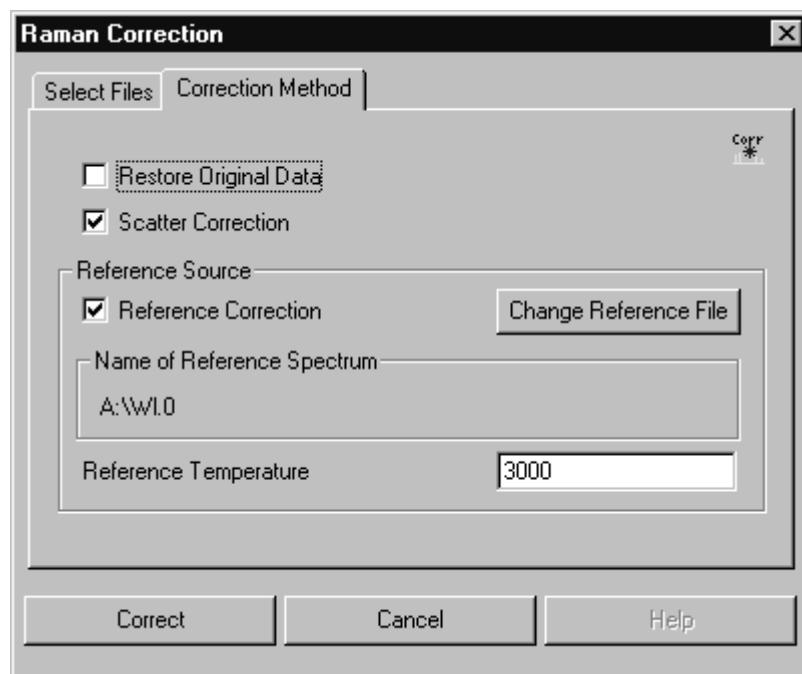
Figure 130: Raman Correction - Correction Method

The *Correction Method* tab allows to define the correction method and the reference spectrum which is to be used as well as the temperature. If you check the *Reference Correction* option, you correct the influence which the optics has on the spectrometer. This requires a current spectrum of the reference lamp installed in the sample compartment. The spectrum should not be older than two weeks to reflect the ageing of the lamp.

The correction spectrum (almost similar to the one acquired by *Black Body* can be selected if you click on the *Change Reference File* button. If the sample spectrum and the reference lamp spectrum do not match in your data point grid, click on the *Make Compatible* command of the *Manipulate* menu. *Scatter Correction* corrects the dependence between scattered radiation and excitation frequency.

Click on the *Correct* button to start the correction. The correction parameters are stored in the *Instrument parameters* list:

Figure 131: Raman Correction Flags

Thus, it is avoided that the same correction is used several times. Ensure that the Raman laser wave number and the source temperature have not changed just before performing the correction.

8.13.1 Raman Correction Theory

Rayleigh's υ^4-law relates the scattering as a function of the wave number. This effect increases with the spectral distance of the line of interest to the wave number of the Raman laser. In case of *Scatter Correction* the Raman spectrum is multiplied point by point using:

$$\left(\frac{\upsilon_{Laser}}{\upsilon} \right)^4$$

In case of the *Reference Correction* the point-to-point multiplication for the Raman spectrum to be corrected will be as follows:

$$\frac{(\text{Black Body Spectrum})(\text{Raman Spectrum})}{(\text{Reference Spectrum})}$$

8.14 Black Body

The *Black Body* command calculates the emission spectrum of a black body. The frequency range and data point grid used to calculate the curve are both based on a reference spectrum. This also applies to the units of the x-axis (frequency or wave number).

The black body (light source) temperature will be indicated in Kelvin. It is stored as TMP parameter together with the calculated distribution. Optionally, the energy distribution or flux density of the photons (depending on the frequency or wave number) can be calculated.

In case of Raman spectra the x-axis is displaced so that the Raman laser signal is at 0 wave numbers and the Stokes spectrum range includes positive wave numbers. The Raman laser wavelength is determined by the *RLW* parameter of the spectrum measured, and can be manually set to 9394cm^{-1}.
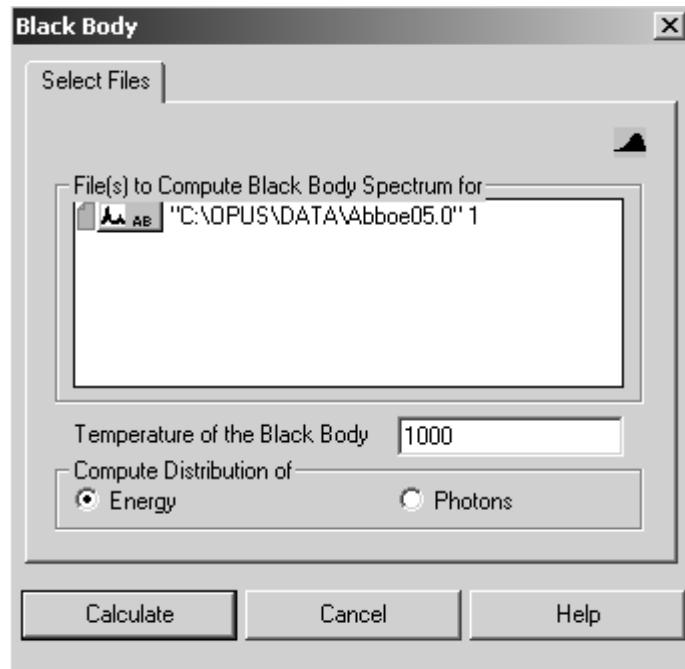
Figure 132: Black Body

Select a spectrum file and indicate the temperature of the black body. Activate the respective option button for the type of distribution and click on the *Calculate* button to start the calculation.

8.14.1   Black Body Theory

The radiative properties of a black body are only determined by its temperature. This enables an approximation of the true light source spectrum, assuming that a single-channel spectrum of the light source is available. Figure 133 shows the radiation spectrum of a black body at a temperature of 1000K.
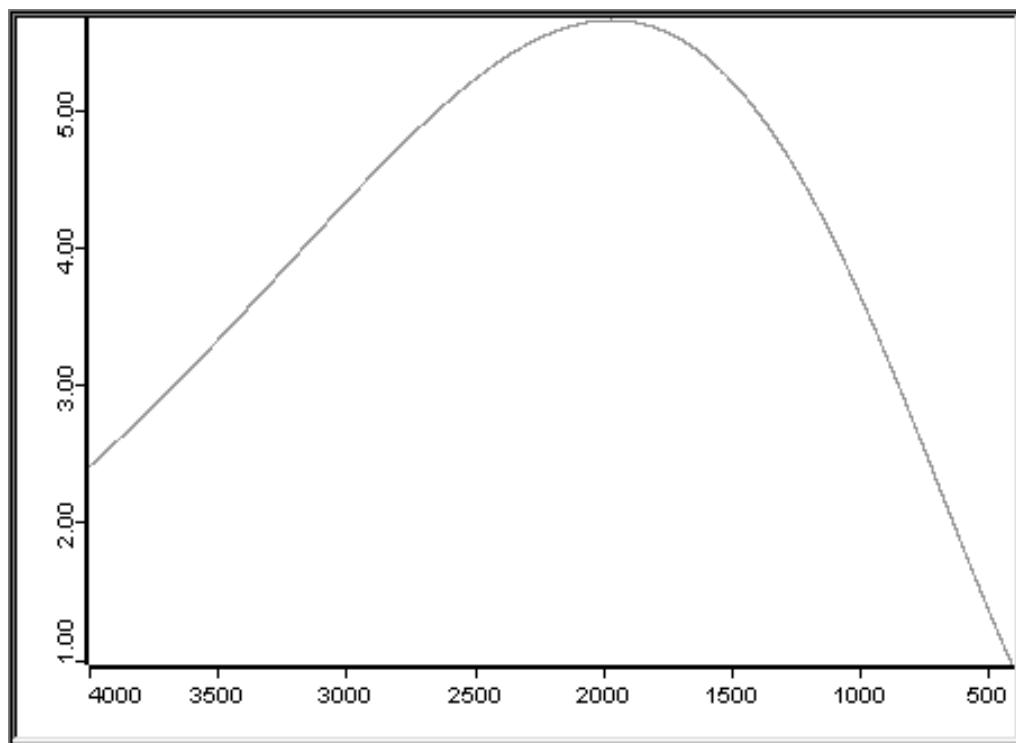
Figure 133: Radiation emitted by a black body at 1000K

The energy and photon flux of a black body is determined by:

Energy per wave number:
$$y = \frac{2 \times 10^{8} hc^2 v^3}{e^{\left(\frac{100 v h c}{kT}\right)} - 1}$$

Photon flux per wave number:
$$y = \frac{2 \times 10^{-15} c v^2}{e^{\left(\frac{100 v h c}{kT}\right)} - 1}$$

where:

T = Temperature [K]
c = $2.99792458 \cdot 10^8$ [ms^{-1}]
h = $6.626176 \cdot 10^{-34}$ [m^{2}kgs^{-1}]
k = $1.380662 \cdot 10^{-23}$ [m^{2}kgs^{-2}K^{-1}]
v = Wave number [cm^{-1}]

8.15   Interferogram to Spectrum

The *Interferogram to Spectrum* command converts an interferogram into a spectrum and performs the same operations which immediately run after AQP data acquisition:

- Apodization
- Phase computation
- Zerofilling
- Fourier Transformation of the interferogram
- Phase correction

This allows to repeat spectra calculation after measurement, using different parameter settings for apodization, zerofilling and phase correction.

The original data files have to be interferograms. You specify these data files on the *Select Files* tab. The frequency range of these files has to be between the upper and lower folding limit parameters used during measurement.

In addition to the spectrum calculated, which is always a single-channel spectrum, you can also save the phase and power spectrum on the *Store* tab. The latter two spectra are calculated by the double-sided known part of the interferogram, using the phase resolution setting.
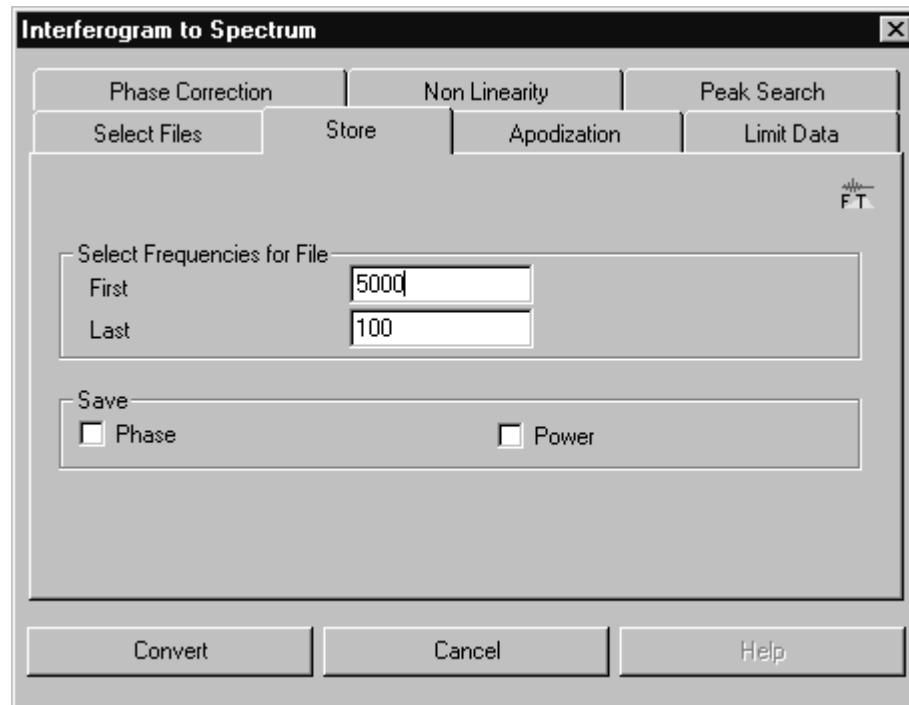
Figure 134: Interferogram to Spectrum – Store tab

Use the *Apodization* tab to select the apodization function and zerofilling factor. Due to the finite mirror travel, the interferogram is only recorded up to a certain point (i.e. a finite resolution). This leads to artificial side lobes on spectral lines, the natural width of which is smaller than or comparable with the measured resolution. By multiplying the interferogram by an apodization function, these side lobes can be suppressed, however at the expense of line broadening.
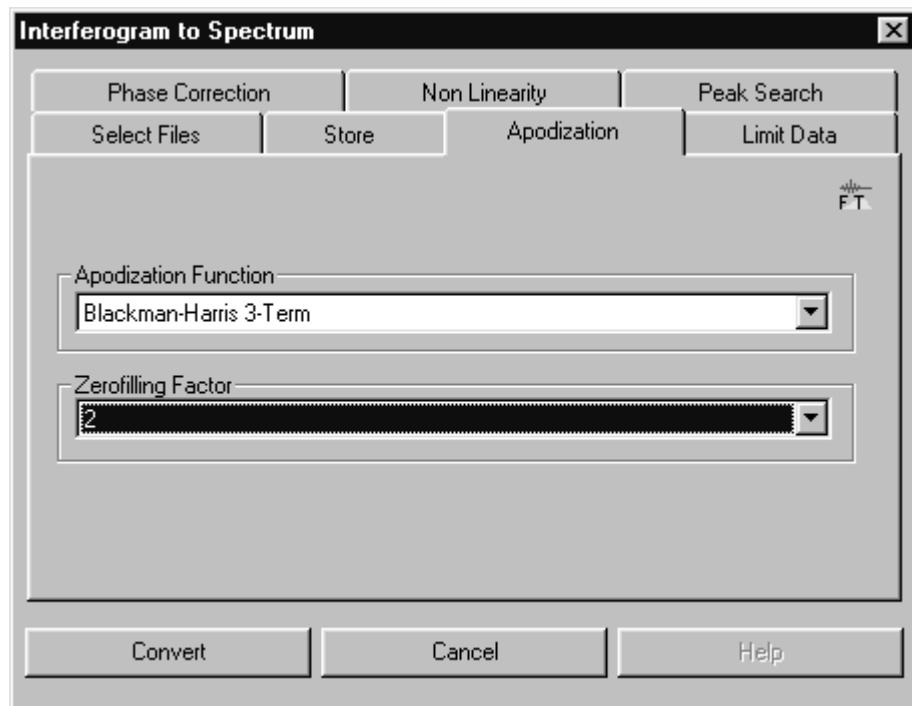
Figure 135: Interferogram to Spectrum – Apodization tab

A detailed description of the apodization function would go beyond the scope of this manual. In case of standard measurements in liquid or solid phases the *Blackman-Harris-3-term* is recommended. To obtain the highest resolution, you either select no (*Boxcar*) or at best a weak apodization function (*Norton-Beer, Weak*).

Zerofilling means adding zeros to both ends of the interferogram before performing Fourier transformation. This increases the number of data points in the spectrum, which is equivalent to an interpolation. The number of data points can be increased by zerofilling using the factors selected (e.g. 2, 4, 8,..., 512).

In case of a zerofilling factor of 1 zeros are added up to the next power of two. If the number of data points has already been a power of two, no zeros will be added.

Single-sided interferograms require a minimum zerofilling factor of 2. In case of double-sided interferograms, the zerofilling factor can be halved in comparison to single-sided interferograms. By increasing the number of data points in the spectrum the depiction improves by sharper lines (a mere cosmetic

effect). However, an n-fold zerofilling requires an n-fold computing time and n-fold storage space (depending on the computing method).

Select the *Limit Data* tab to define the resolution.
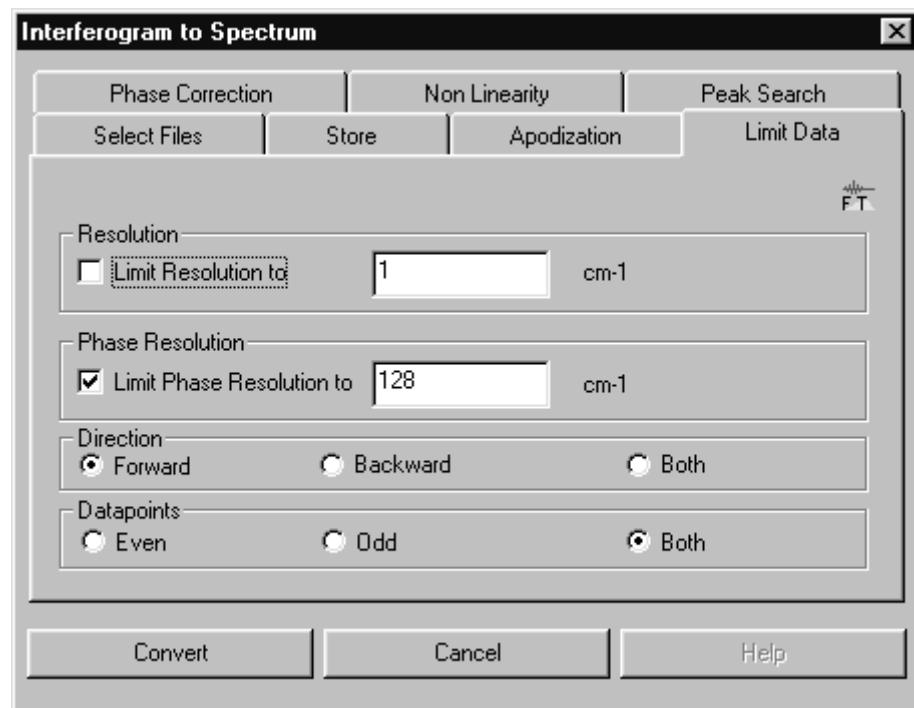
Figure 136: Interferogram to Spectrum – Limit Data tab

If you activate the *Limit Resolution to* check box, you can vary the resolution by entering a value which is greater than or at least equal to the value used during measurement. In this case only a fraction of the measured interferogram is used for computation.

In the *Phase Resolution* group field you specify how precise the phase has to be determined. Generally, you should enter the same value as being used for the measurement. The value is limited by the length of the double-sided part of interferogram.

In case of interferograms recorded in forward/backward mode you can specify which direction(s) of mirror travel have to be evaluated during transformation. If both mirror travels should be evaluated, the forward and backward scans will be transformed separately, phase corrected and averaged.

If data have been recorded in multiplex mode, the interferogram contains alternating data from two analog-to-digital converters (ADCs). The *Even* and *Odd* option allow the data from both ADCs to be evaluated separately. There is no such option in case of backward scans. Therefore, record multiplex measurements only by using the *Forward* mode.

If you activate the *Even* option button, the intensity values I_0, I_2 ... of the first ADC will be transformed. If you activate the *Odd* option button, the intensity values I_1, I_3 ... of the second ADC will be transformed.

The phase correction can be compared with an interferogram symmetrizing, which is always necessary due to the asymmetry of any measured interferogram. Click on the *Phase Correction* tab.
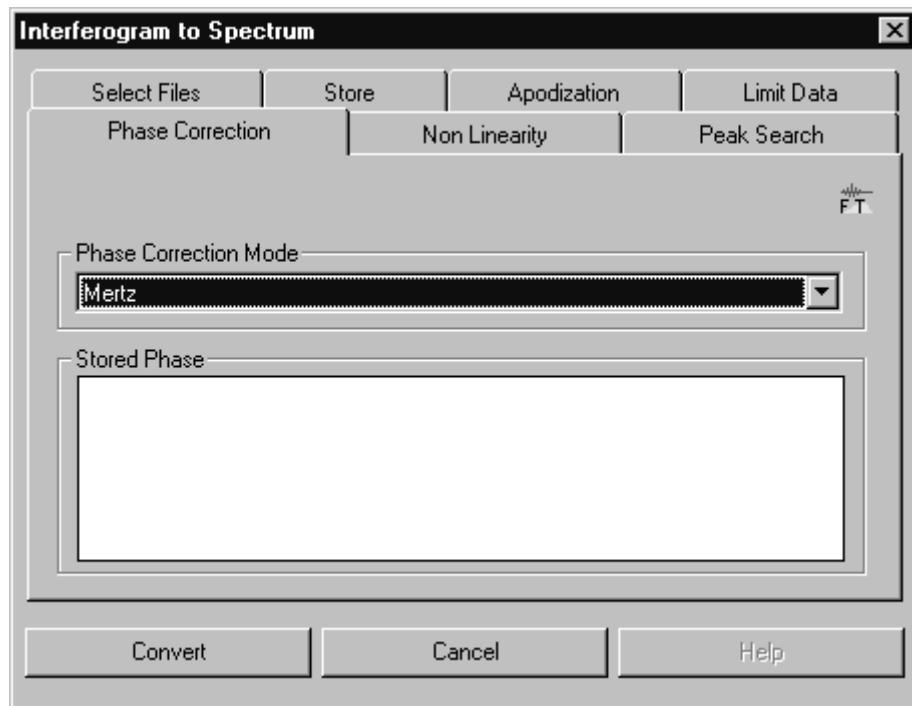
Figure 137: Interferogram to Spectrum – Phase Correction tab

Several phase correction modes are available:

- *Mertz*: this is the standard procedure for phase correction.
- *Mertz Signed***:** modified Mertz function which is used if the single-channel spectrum is expected to contain negative contributions.
- *Power Spectrum*: this can be used instead of Mertz or Foreman, **but only for double-sided interferograms**, if the spectrum includes wide ranges of low light intensity (total absorption, Raman, emission). Disadvantage: up to $\sqrt{2}$ more noise compared with Mertz or Forman.
- *Mertz/Stored Phase***:** like Mertz, whereas the phase is not re-calculated but based on previously existing data which have been calculated by using the regular Mertz method. This method can be useful, if the single-channel spectrum includes less-defined ranges (i.e. an undefined phase), which frequently occurs in case of emission measurements. Furthermore, it can also be useful if the spectra are expected to contain negative contributions. In this case, the phase stored should derive from a spectrum with absolute positive values.

- *No/Save Complex Data***:** the data will not be phase corrected but Fourier transformed in complex form and stored as real and imaginary parts.
- *Forman*: a method mathematically equivalent to Mertz, offers a slightly higher precision at the cost of higher computational costs.
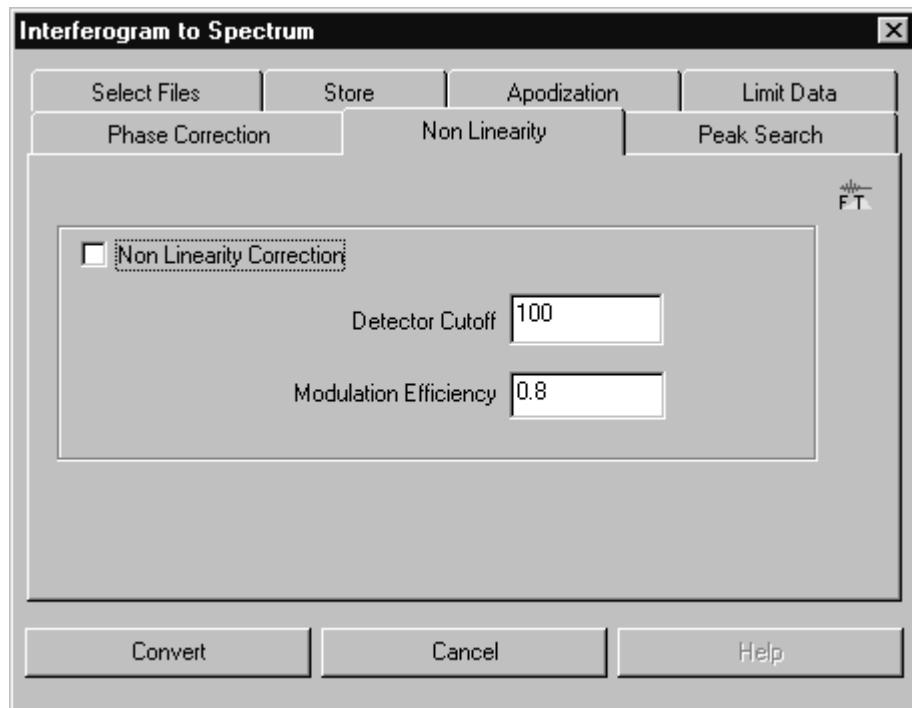
Figure 138: Interferogram to Spectrum - Non-linearity tab

In a single-channel spectrum there should be no signal below the absorption edge of the detector. The non-linear detector response causes the signal to be non-zero below this edge. The non-linearity of the detector can be calculated from the ratio of the intensity of these artifacts and the total energy flow in the detector. As soon as the non-linearity is known a corrected spectrum can be calculated showing less artifacts. As a rule, the interferograms stored will not be modified. The non-linearity correction only effects the spectra.

To ensure a successful non-linearity correction the following conditions have to be fulfilled:

- The spectrum must be recorded from 0^{cm-1} up to the maximum wave number at which the detector can send a signal.
- Electronic filters must not be used. Spectra have to undergo a broad-band recording to avoid aliasing.
- The *Phase resolution* FT parameter should be set to result in at least 500 phase interferogram points. Too low a phase resolution results in an inaccurate non-linearity correction.

After phase correction the non-linearity correction coefficients are calculated, using all the data points of the single-channel spectrum.

The modulation efficiency causes an additional multiplicative correction of the entire spectrum. It can be set either to the correct value (typically between 0.7 and 1.0), or to 1.0 if the correct value is unknown. If you use a preamplifier which reverses the signal polarity, the value of the detection limit has to be multiplied by -1.

Use the *Peak Search* tab to select the position of the zero path difference (ZPD):
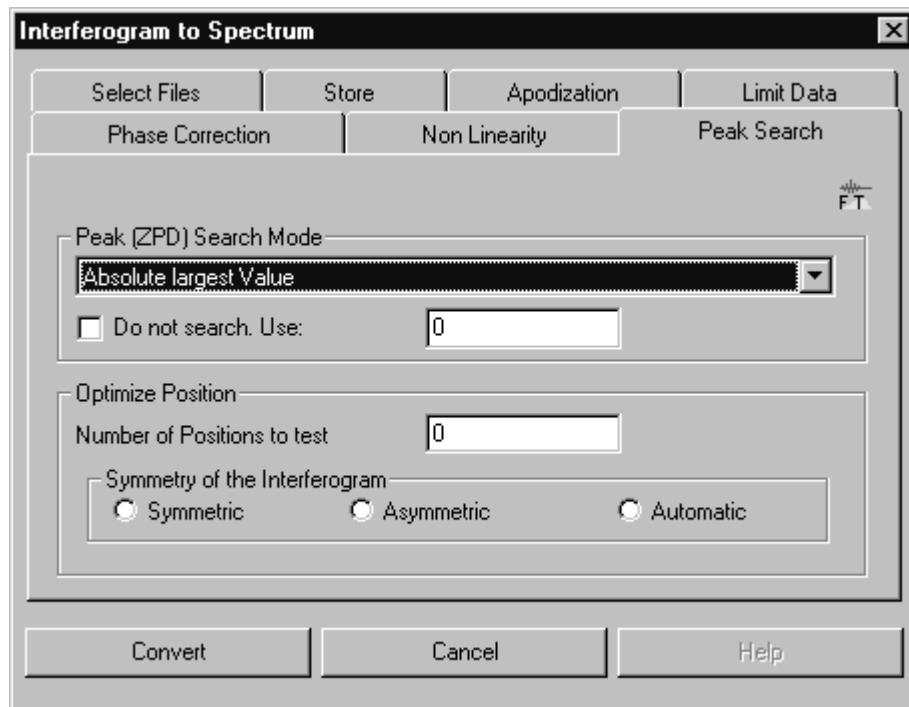
Figure 139: Interferogram to Spectrum - Peak Search tab

- *Absolute largest value* searches the peak with the highest absolute intensity.
- *Maximum* searches the highest peak with the largest positive value.
- *Minimum* searches the lowest peak, if known that the peak has a negative intensity.
- *Mid between Min./Max.* calculates a value between the minimum and maximum limit.
- *No peak search* uses the position saved in the interferogram. If this value is known, it can be entered manually.
- *Mid between largest two* searches the peak between the two largest values.
- *Take from stored phase* uses the value calculated for the phase stored.

The position of the peak can be influenced by considering additional data points apart from the range evaluated by one of the algorithms mentioned before. Each position will be tested for its symmetry or asymmetry. The position with the highest symmetry will be defined as ZPD. Check the respective option button in the *Symmetry of the Interferogram* group field.

8.16   Inverse FT

The *Inverse FT* command transforms a spectrum into an interferogram, and can be used for all types of spectra.
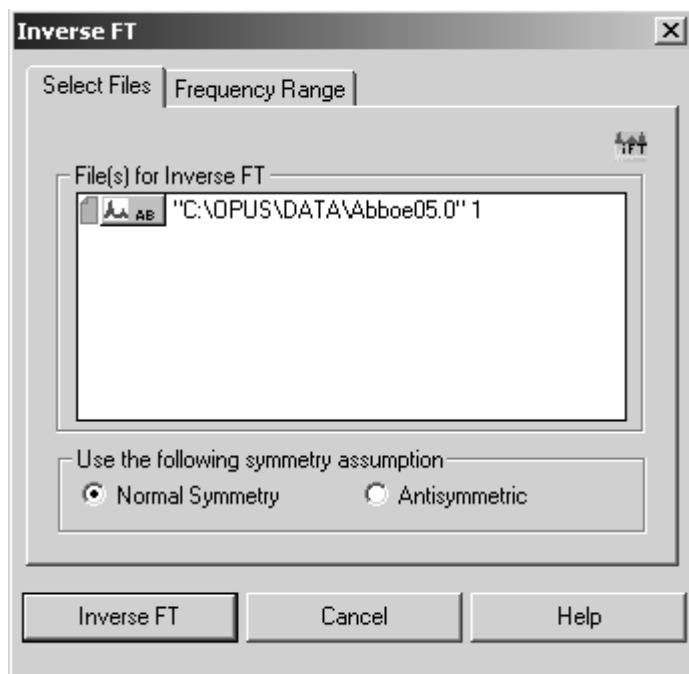
Figure 140: Inverse FT

You have to specify whether the spectral data are part of a symmetric or antisymmetric interferogram. Generally, you activate the *Normal Symmetry* option button, as antisymmetric interferograms only occur in special cases, e.g. complex spectra. Interferograms symetrically generated only contain values on the positive side of the x axis. Therefore, in case of Fourier transformation you have to define how these values have to be completed on the negative side.

Select the spectrum file and frequency range as usual and specify the symmetry. Start the procedure by clicking on the *Inverse FT* button.

8.17   Post Zerofilling

The aim of post zerofilling is to increase the digital resolution of a spectrum, i.e. to create more data points per wave number. This is especially useful for the peak picking in case of high-resolution spectra, as the result will be smoother spectra plots. When calculating spectra a zerofilling is performed by indicating the Zerofilling factor. This kind of zerofilling increases the digital resolution of spectra within the entire spectral range. The advantage of post zerofilling is that only the spectral range of interest will be interpolated, which allows to save storage space.
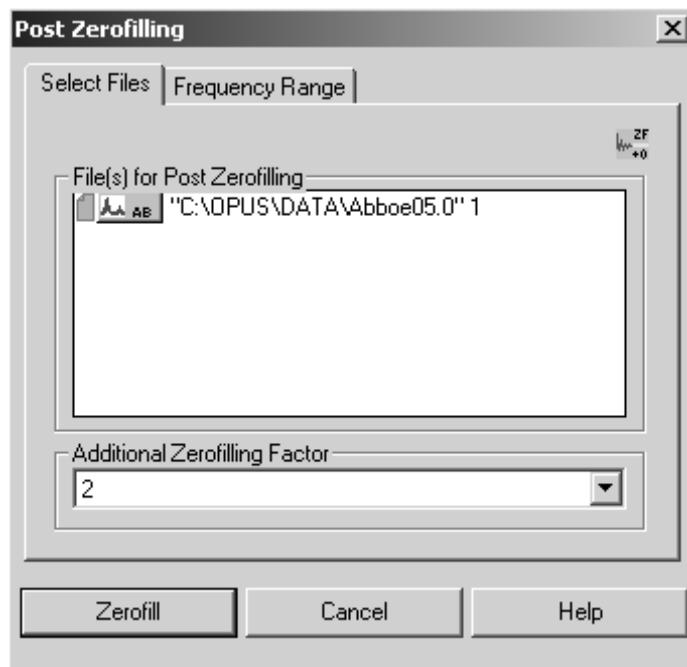
Figure 141: Post Zerofilling - Select Files tab

Specify the *Additional Zerofilling Factor*. The possible values range from 1 to 512.

Example 1

A spectrum with a digital resolution of 8cm^{-1} is post zerofilled by an additional zerofilling factor of 2. The digital resolution after the interpolation is 4cm^{-1}.

Example 2

A spectrum with a digital resolution of 8cm^{-1} is post zerofilled by an additional zerofilling factor of 8. The digital resolution after the interpolation is 1cm^{-1}.

In both cases the digital resolution has been 8cm^{-1}. To avoid artifacts allow at least 50 more data points on each side of the desired interval. This frequency range must also contain meaningful spectral information.

If you click on the *Zerofill* button (figure 141), the spectra file(s) selected will be interpolated using the *Additional Zerofilling Factor* specified.

Figure 142 exemplifies a post zerofilling factor of 4. The interpolated curve definitely includes more (quadruple) data points as the original data.
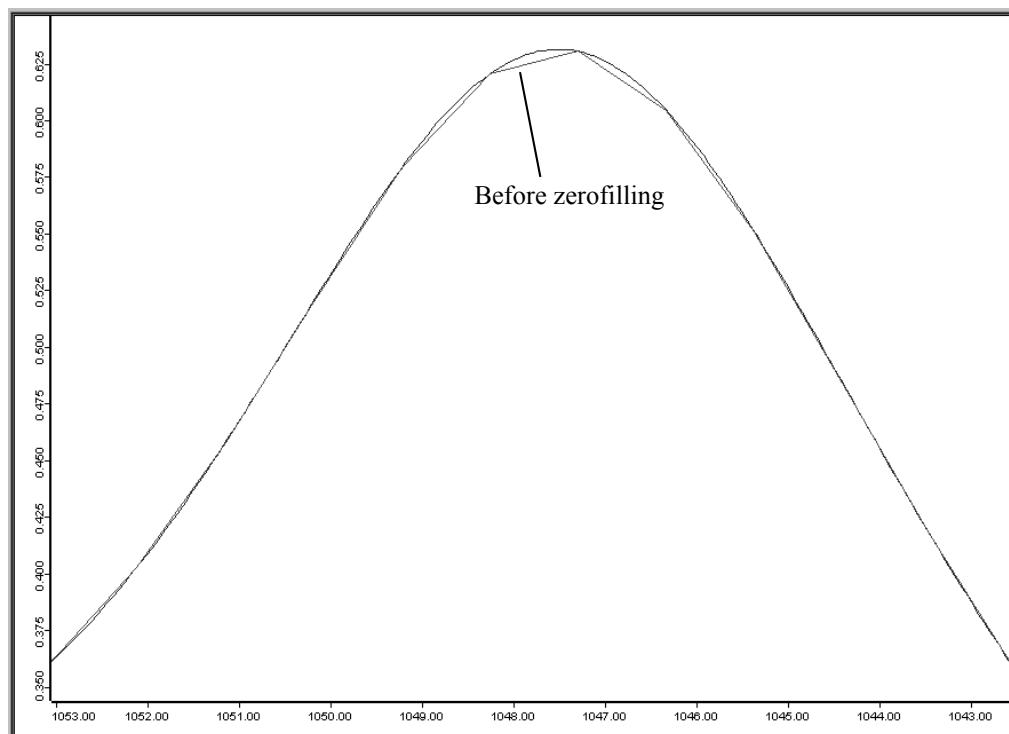
Figure 142: Digital resolution before and after post zerofilling

8.18   Fourier Self-Deconvolution

The aim of Fourier Self-Deconvolution is to enhance the apparent resolution of a spectrum, or to decrease the line width. Spectral ranges comprising broad and overlapping lines can thus be separated into sharp single lines. **The Fourier Self-Deconvolution is only useful in case of lines which are substantially broader than the spectral resolution.**

Select the respective spectra file(s) on the *Select Files* tab. On the *Adjust Parameter* tab you have to define the line shape. Check either the *Gaussian* or *Lorentzian* option button. The appropriate line shape type depends on the line-broadening procedure. In case of doubt it is recommended to assume a Lorentzian shape.

Specify a deconvolution and noise reduction factor, or alternatively define a factor for the band width and resolution enhancement. The effect will be the same. Start the self-deconvolution by clicking on the *Deconvolute* button.
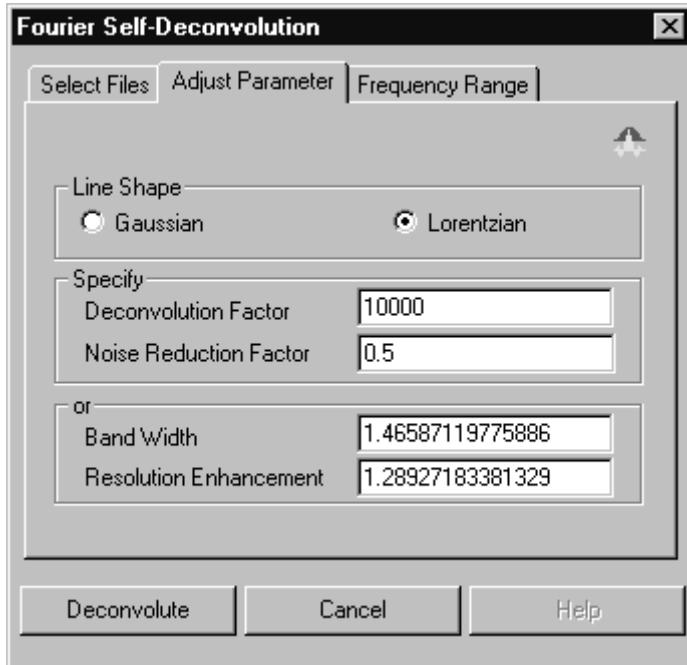
Figure 143: Fourier Self-Deconvolution

8.18.1   Fourier Self-Deconvolution Theory

The Fourier Self-Deconvolution (FSD) assumes that the spectrum to be measured consists of well-resolved lines which have been convoluted (broadened) by the same type of line-broadening function (LBF). If the shape and width of the LBF are known, its effect can be arithmetically excluded from the spectrum. It is recommended to perform this arithmetic exclusion on the basis of the interferogram as in this case the deconvolution is equivalent to a simple interferogram division caused by the LBF Fourier transformation.

In general, the deconvolution corresponds to a multiplication of the interferogram I(x) using the exp(a*x) deconvolution function for Lorentzian and exp(a*x*x) for Gaussian shapes, which intensifies the interferogram edges. The deconvolution factor is the maximum value of these functions at the end of the interferogram.

The amplification of the interferogram caused by self-deconvolution also amplifies both the signal and noise. However, especially on the interferogram edges the signal-to-noise ratio is worse than at the centerburst. To avoid the increase of noise, a Blackman-Harris apodization is simultaneously performed such that the interferogram is multiplied by the result of an ascending deconvolution function and a descending apodization function. The apodization function value is 1.0 at the beginning and 0 at the end of the interferogram. Between these two limits the value exhibits a maximum.

Deconvolution factors of 100, 1000 and 5000 correspond to a maximum amplification of 3.4, 12.8, and 40 in case of Lorentzian shapes, and 1.06, 3.2 and 16 in case of Gaussian shapes. If you work with Lorentzian shapes it is

recommended to increase the deconvolution factor in the order 50, 100, 1000, 5000, and to stop if the resultant spectrum shows artificial oscillations.

The noise reduction factor should range from 0.0 to 1.0. It is the fraction of the interferogram, which apodization function has been decayed to 0 and thus used for evaluation. A value of 1.0 corresponds to the full interferogram length. It is recommend to start with a value of 0.5 (half interferogram length). If the spectrum has been calculated using a zero filling factor >2, a start value of 1/ (zerofilling factor) is recommended to reduce noise.

Figure 144 shows a spectrum before and after a deconvolution, using the parameters shown in figure 143. The intensity at the maximum of a deconvoluted spectrum line is usually higher, in relation to its edges, than of an original spectrum. However, the peak ratios are not changed. The deconvoluted spectrum always depicts the higher maxima.
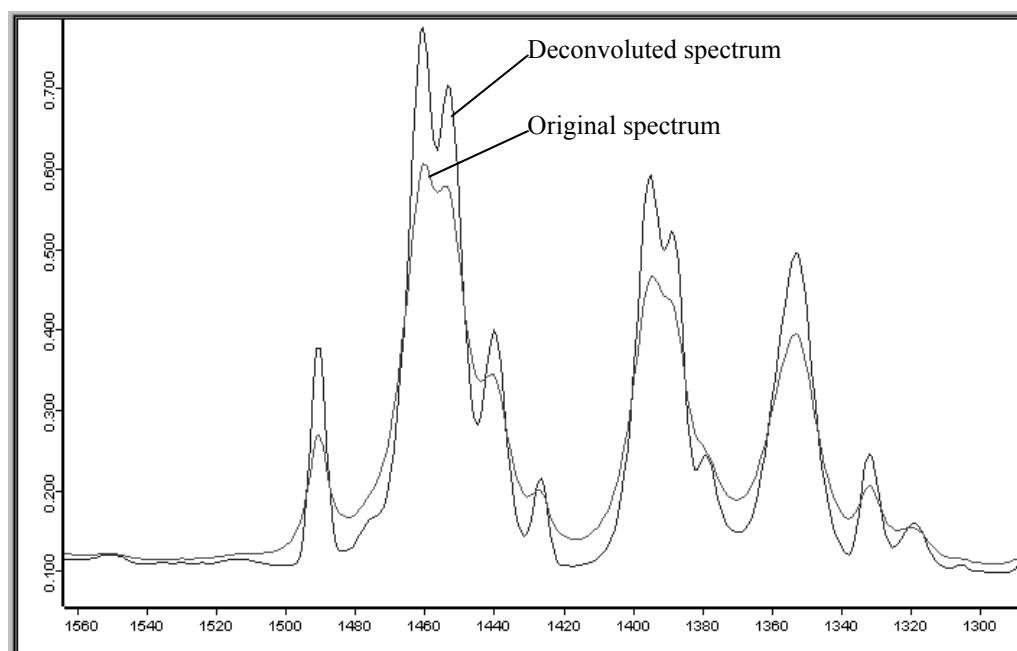
Figure 144: Spectrum before and after Fourier Self-Deconvolution

8.19   Symmetric FT

Symmetric Fourier Transformation is used if a phase correction is not necessary, e.g. if the interferogram has been generated by inverse Fourier Transformation, or does only include one half of a scan, relative to the highest maximum.
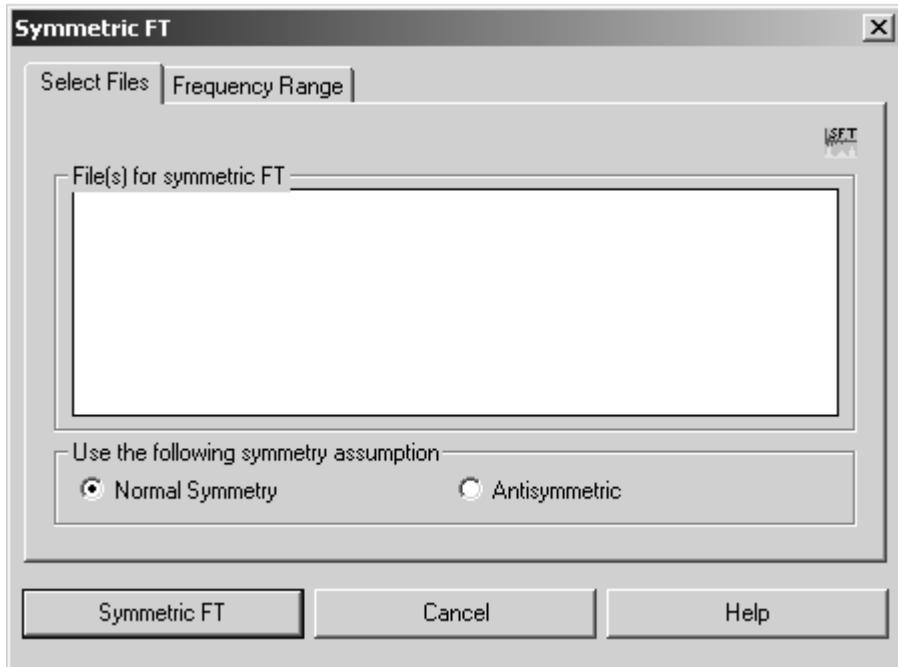
Figure 145: Symmetric FT - Select Files tab

Define the symmetry assumption on the *Select Files* tab. Generally, you check the *Normal Symmetry* option button. If, however, the interferogram has been generated by inverse Fourier transformation using the antisymmetric function, check the *Antisymmetric* option button.

Select the frequencies on the *Frequency Range* tab and start the transformation by clicking on the *Symmetric FT* button. The result will be a single-channel spectrum. In case of an antisymmetric transformation only the positive part of the single-channel spectrum will be saved.

8.20   Kramers-Kronig Transformation

The *Kramers-Kronig Transformation* command extracts from a sample reflectance spectrum either the complex refractive index, complex dielectric constant, an absorption spectrum or the phase change of the IR beam due to reflection. This requires the following conditions:

- The sample has to consist of a pure, homogeneous material (neither mixtures, layered systems nor powders).
- The beam has to be measured in specular (not diffuse) reflection at nearly normal incidence (e.g. 10° unit).
- The sample must be thick enough ("half-space") to ensure that no light returns from the inner sample to the sample surface (e.g. after reflection on one back edge). Especially, multiple reflections and interferences have to be avoided. If the sample is not thick enough to absorb all radiation, roughen the backside to prevent possible reflection.

- The spectral cut-off has to fall in a moderately flat and unstructured range. It must not be interrupted among significant structures.
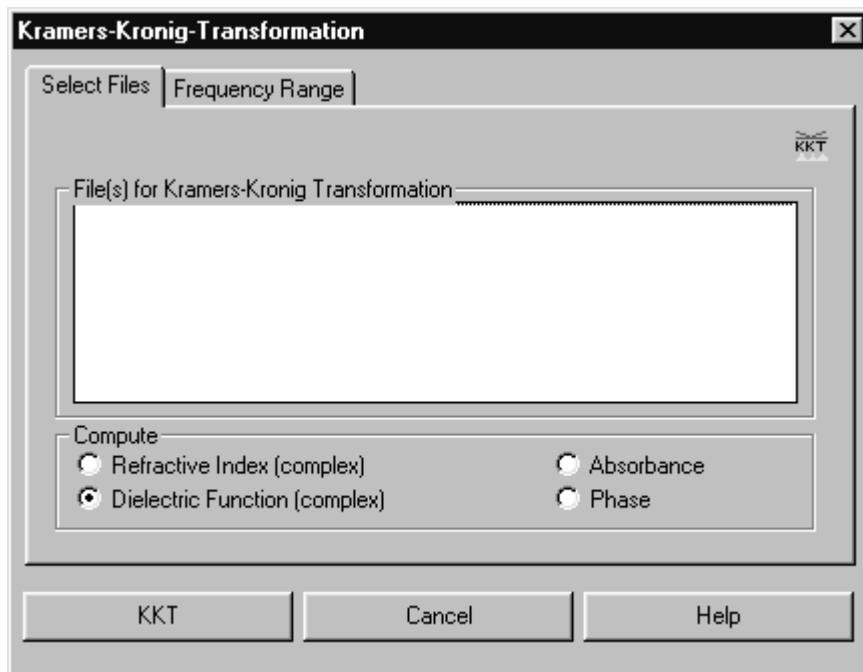
Figure 146: Kramers-Kronig Transformation - Select Files tab

On the *Select Files* tab you select the spectra to be processed and specify the desired result function. You can either calculate the *Refractive Index (complex)*, *Dielectric Function (complex)*, *Absorbance* or *Phase* spectrum. In case of the first two options the result file includes two data blocks: the real and imaginary part of the functions (indicated by "R" or "I" in the file symbol).

If an absorbance spectrum is calculated, it only includes pure absorption contributions, but no reflection losses. To be able to compare the absorbance spectrum directly with a transmission spectrum, you have to consider the reflection losses at both boundaries of the sample layer by adding the correction -2lg (1-[*Input - Reflectance spectrum*] using the OPUS spectrum calculator.

8.20.1 Kramers-Kronig-Transformation Theory

The real and imaginary parts of complex physical quantities describing the interaction between radiation and sample, e.g. the complex refractive index $n = n + ik$, dielectric constant $\varepsilon = \varepsilon' + i\varepsilon''$ and the logarithm of the amplitude-reflectivity $\ln(re^{i\phi}) = \ln(r) + i\phi$), depend on each other due to the causality principle. The two parts can be transformed into each other by the so-called Kramers-Kronig Transformation (KKT). OPUS uses this to first calculate the phase rotation angle $\phi(v)$ (a function of the wave number v) from the measured reflectance spectrum $R(v) = r^2(v)$ of an optically thick sample using KKT. Then, the reflectivity of the air/sample edge (vertical incidence) is calculated from $r(v)$ and $\phi(v)$ using the Fresnel equation:

$$\Gamma(\nu)e^{i\phi(\nu)} = [n(\nu) - 1]/[n(\nu) + 1]$$

The real and the imaginary parts of the refractive index are calculated as follows:

$$n(\nu) = [1 - R(\nu)]/[1 + R(\nu) - 2R^{1/2}(\nu)\cos(\phi(\nu))]$$
$$\kappa(\nu) = 2R^{1/2}(\nu)\sin(\phi(\nu))/[1 + R(\nu) - 2R^{1/2}(\nu)\cos(\phi(\nu))]$$

If desired, the dielectric function is calculated:

$$\varepsilon' = n^2 - \kappa^2$$
$$\varepsilon'' = 2n\kappa$$

From the imaginary part of the refractive index, the so-called absorption index $\kappa(\nu)$, the absorptivity $A(\nu)$ of a layer with a thickness d can be calculated by:

$$A(\nu) = \log(e)2\pi\nu d\kappa(\nu)$$

In principle, KKT enables to determine all important optical sample properties on the basis of <u>one</u> single measurement (reflectance spectrum $R(\nu)$).

> **Note:** A separate description on how to use the KKT and some exemplary spectra are available on request.

8.21   Spectrum from Interferograms

The *Spectrum from Interferograms* command can be used to create a spectrum by comparing a sample interferogram with a reference interferogram. The result spectrum can either be displayed in absorption or transmission.
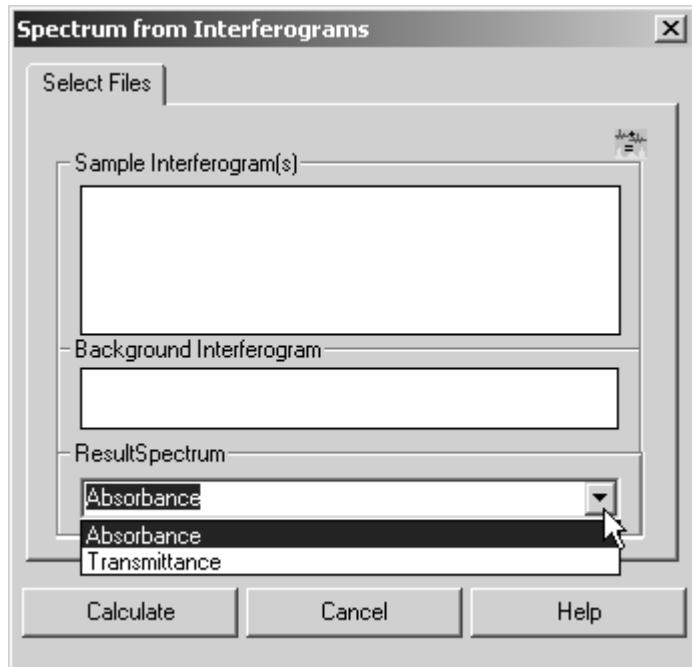
Figure 147: Spectrum from Interferograms - Select Files tab

Drag & drop the sample and background interferogram into the corresponding selection field. Note that the interferogram files include the parameters set during measurement. Select the respective result spectrum format from the drop-down list and start the calculation by clicking on the *Calculate* button.

8.22 Extrapolation

You can extrapolate reflectance spectra to 0cm^{-1} or to an upper frequency limit selectable by the user. The previous wave number ranges are used without being modified. In case of extrapolation to 0cm^{-1} it is distinguished between insulators and semiconductors. OPUS interprets the sample as semiconductor if the input for $R\,(0\text{cm}^{-1})$ is *1*.

Select the spectrum and the frequency range as usual. Specify a limit for R at the *At infinity* and *At 0* entry field. Start the calculation by clicking on the *Extrapolate* button.
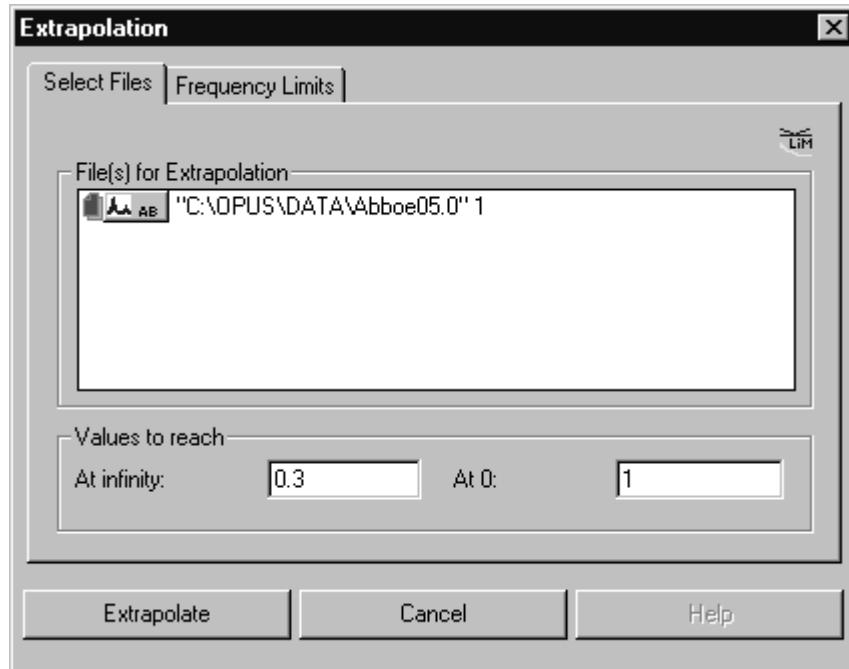
Figure 148: Extrapolation

8.22.1   Extrapolation to 0cm^{-1}

The R_0 and i_1 parameters are used for the extrapolation to 0cm^{-1}. R_0 can be any value between 0 and 1. i_1 represents the inner limit of the wave number interval which the approximate function for the extrapolation has to fit to. The beginning of the original spectrum will be automatically selected as the second limit i_2. If in case of i_1 a wave number smaller than the lower wave number of the original spectrum has been specified (i.e. no overlapping range), i_1 will be set to include two data points to fit the function.
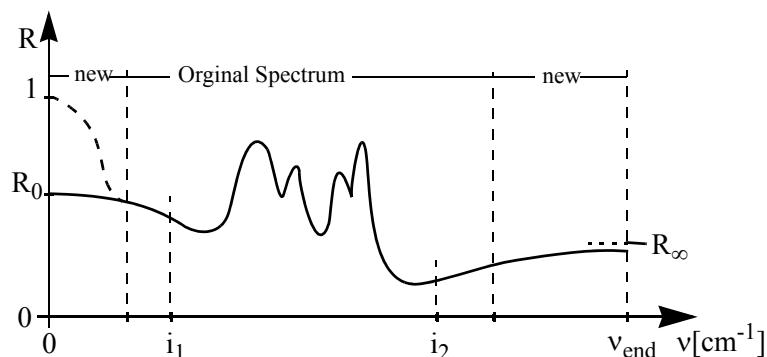
Figure 149: Parameters used for extrapolation

8.22.1.1 Theory of extrapolating n to 0cm⁻¹ in case of semiconductors

The approximation function is:

$$\Phi_4 = 1 - a_4\sqrt{\nu} + \frac{a_4^2}{2}\nu + a_5\nu^{1.5}$$

As $R(s) = \Phi(s)$ has already been specified (s being wave number of the spectrum beginning), the a_5 coefficient can be eliminated:

$$R(s) = 1 - a_4\sqrt{s} + \frac{a_4^2}{2}s + a_5\nu^{1.5}$$

$$a_5 = \frac{R(s) - 1 + a_4\sqrt{s} - \frac{a_4^2}{2}s}{s^{1.5}}$$

The remaining function is:

$$\Phi_4 = 1 - a_4\sqrt{\nu} + \frac{a_4^2}{2}\nu + \left(R(s) - 1 + a_4\sqrt{s} - \frac{a_4^2}{2}s\right)\left(\frac{\nu}{s}\right)^{1.5}$$

Now, specify a_4 in a way that the sum of all error squares within the overlapping area can be minimized.

8.22.1.2 Theory of extrapolating n to 0cm⁻¹ in case of insulators

The approximation function is:

$$\Phi_1 = R(0) + a_1\nu^2 + a_2\nu^4$$

As $R(s) = \Phi(s)$ has already been specified (s being the wave number of the spectrum beginning), the a_2 coefficient can be eliminated:

$$R(s) = R(0) + a_1 s^2 + a_2 s^4$$

$$a_2 = \frac{R(s) - R(0) - a_1 s^2}{s^4}$$

The remaining function is:

$$\Phi_1 = R(0) + a_1\nu^2 + (R(s) - R(0) - a_1 s^2)\left(\frac{\nu}{s}\right)^4$$

Now, specify a_1 in a way that the sum of all error squares within the overlapping area can be minimized.

8.22.2 Extrapolation to ∞ (infinity)

The R_∞, i_1 and v_{end} parameters are used for extrapolating to ∞. R_∞ and i_2 are equivalent to R_0 or i_1 used in case of extrapolating to 0cm^{-1}. v_{end} represents the wave number up to which the extrapolation has to be performed.

8.22.2.1 Approximation for extrapolating n to ∞

The approximation function is:

$$\Phi_3 \,=\, R(\infty) + \frac{a_1}{v^2} + \frac{a_2}{v^4}$$

As $R(s) \,=\, \Phi(t)$ has already been specified (t being the wave number of the spectrum end), the a_2 coefficient can be eliminated:

$$R(t) \,=\, R(\infty) + \frac{a_1}{t^2} + \frac{a_2}{t^4}$$

$$a_2 \,=\, \left(R(t) - R(\infty) - \frac{a_1}{t^2} \right) t^4$$

The remaining function is:

$$\Phi_3 \,=\, R(\infty) + a_1 v^2 + \left(R(t) - R(\infty) - \frac{a_1}{t^2} \right) \left(\frac{t}{v} \right)^4$$

8.23   1/cm <-> µm, nm

The *1/cm <-> µm, nm* command changes the x-axis (abscissa) unit of a spectrum. Wave numbers can be converted into micrometer and nanometer, or vice versa. Load the spectrum file and drag and drop it from the OPUS browser window to the *File(s) to Convert* selection field. Define the conversion direction by using the *Conversion Direction* drop-down list on the right.
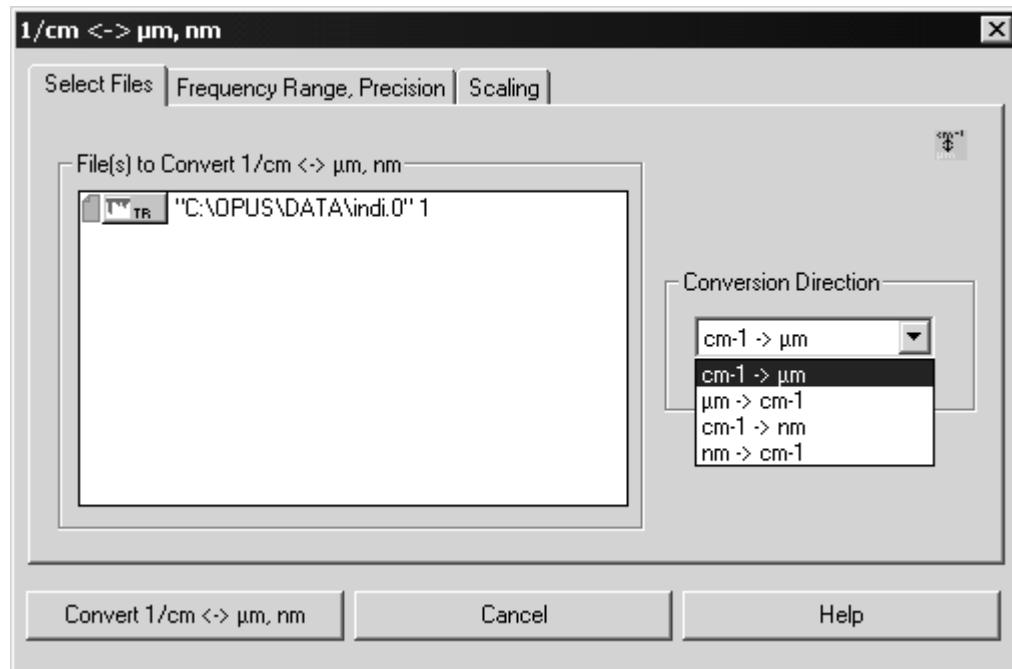
Figure 150: 1/cm <-> µm, nm – Select Files tab

On the *Frequency Range, Precision* tab you can individually define the frequency range or use it from the original spectrum.
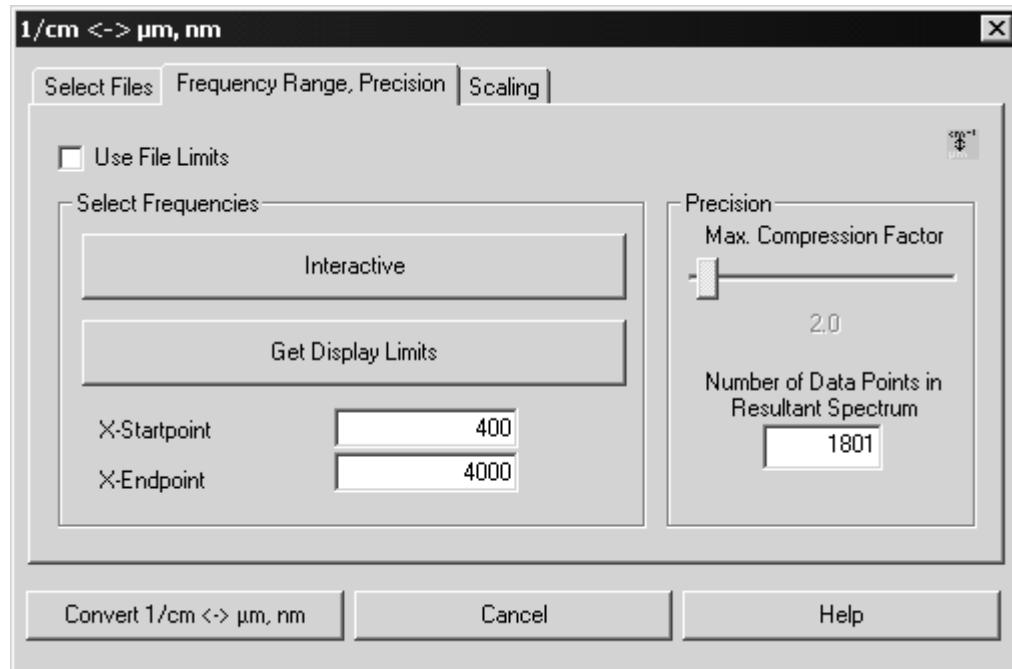
Figure 151: 1/cm <-> µm, nm – Frequency Range, Precision tab

The maximal compression factor (MCF) can be specified by using the slider in the *Precision* group field. In case of fixed frequency limits define the number of data points in the result spectrum. If, however, the frequency limits of each input spectrum are used, the interpolation is determined by the MCF.
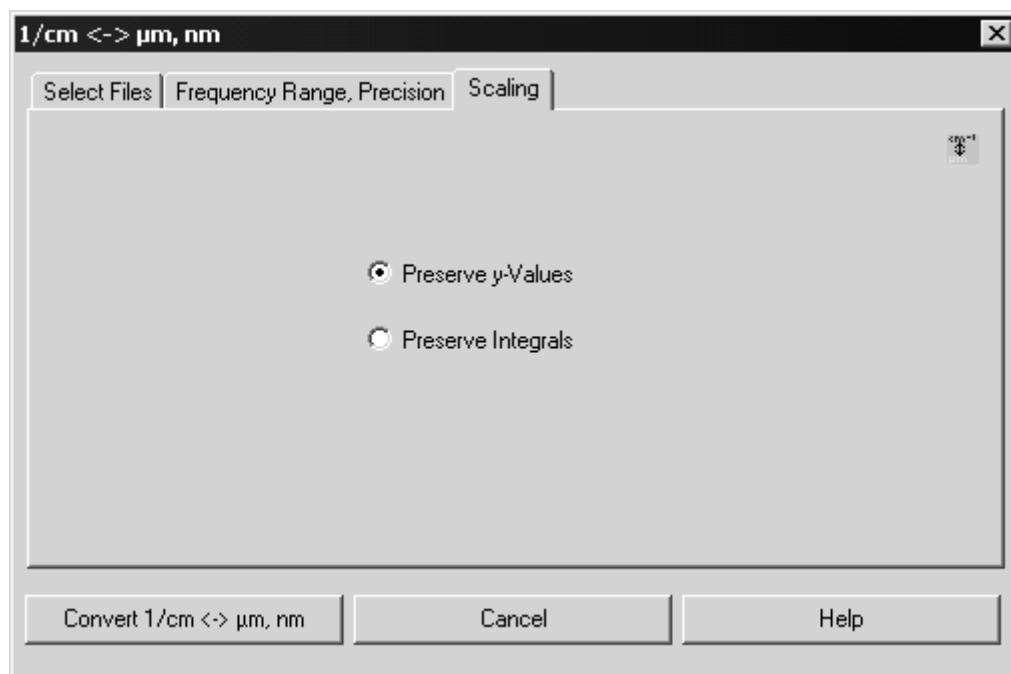
Figure 152: 1/cm <-> μm, nm – Scaling tab

On the *Scaling* tab you define the scaling of intensities. If you check the *Preserve y-Values* option button, the intensities will generally not be changed. Only interpolation effects play a more or less important role. The spectrum appearance does not change, with the x-axis being substantially distorted.

If you check the *Preserve Integrals* option button, the y-values are multiplied by a frequency or wavelength-dependent factor (proportional to $1/x^2$). This preserves the integrals, provided the original spectrum and the new spectrum both use equivalent integral limits.

Frequency Conversion Theory:

The connection between wave number [cm^{-1}] and wavelength [μm] is based on the following formula:

Wavelength [μm] x wave number [cm^{-1}] = 10000.

Each wave number can be converted into a wave length. Digitally recorded spectra have no continuous data, but discrete data points. OPUS saves these equidistant data points, e.g. two data points per wave number. After the conversion, however, the data points are no longer equidistant.

Wave number [cm^{-1}]	Wavelength [μm]	Difference [μm]
400	25.00	
		1.19
420	23.81	
		1.08
440	22.73	
		0.99
460	21.74	
		0.91
480	20.83	
		0.83
500	20.00	

Since OPUS always saves spectra as a set of equidistant data points only, an interpolation must be performed after the abscissa conversion.

The interpolation type for frequencies (or wavelenghts) is determined by the MCF or the number of resulting data points. The minimum number of data points for the micron spectrum created is equivalent to the number of data points found in the cm^{-1} spectrum. The MCF defines the conversion properties in the high frequency end of the wave number spectrum which is converted to the low wavelength end of the micron spectrum.

If, e.g., a factor of 5 is selected, 5 frequency intervals are converted to 1 wavelength interval (distance between each data point), which causes the loss of spectral information. The ratios get better if lower wave numbers (higher wavelengths) are selected.

The MCF can vary between 0.5 and 50. However, the new spectrum has never fewer data points than the original spectrum. Therefore, it may occur that the number of data points, e.g. starting from a factor of 20, remain unchanged.

In case of a small MCF the number of data points of the new spectrum may become quite large. This depends on the upper and lower frequency limits as well as on the distance of data points in the original spectrum. By reconverting the new spectrum and comparing it with the original one it can be verified whether the factor selected has been reasonable.

The upper left spectrum in figure 153 shows the original data scaled in wave numbers. On the right it has been converted to wavelengths, with the intensities remaining unchanged. In the lower left spectrum the intensities have been converted without changing the integrals. The lower right spectrum shows the original spectrum (B) which has been converted from wave numbers to wavelengths and reconverted for comparison. Spectrum (A) uses an MCF of 1, spectrum (C) an MCF of 15. The number of data points in (A) is about ten times higher than in (C), and comes very close to the original data.
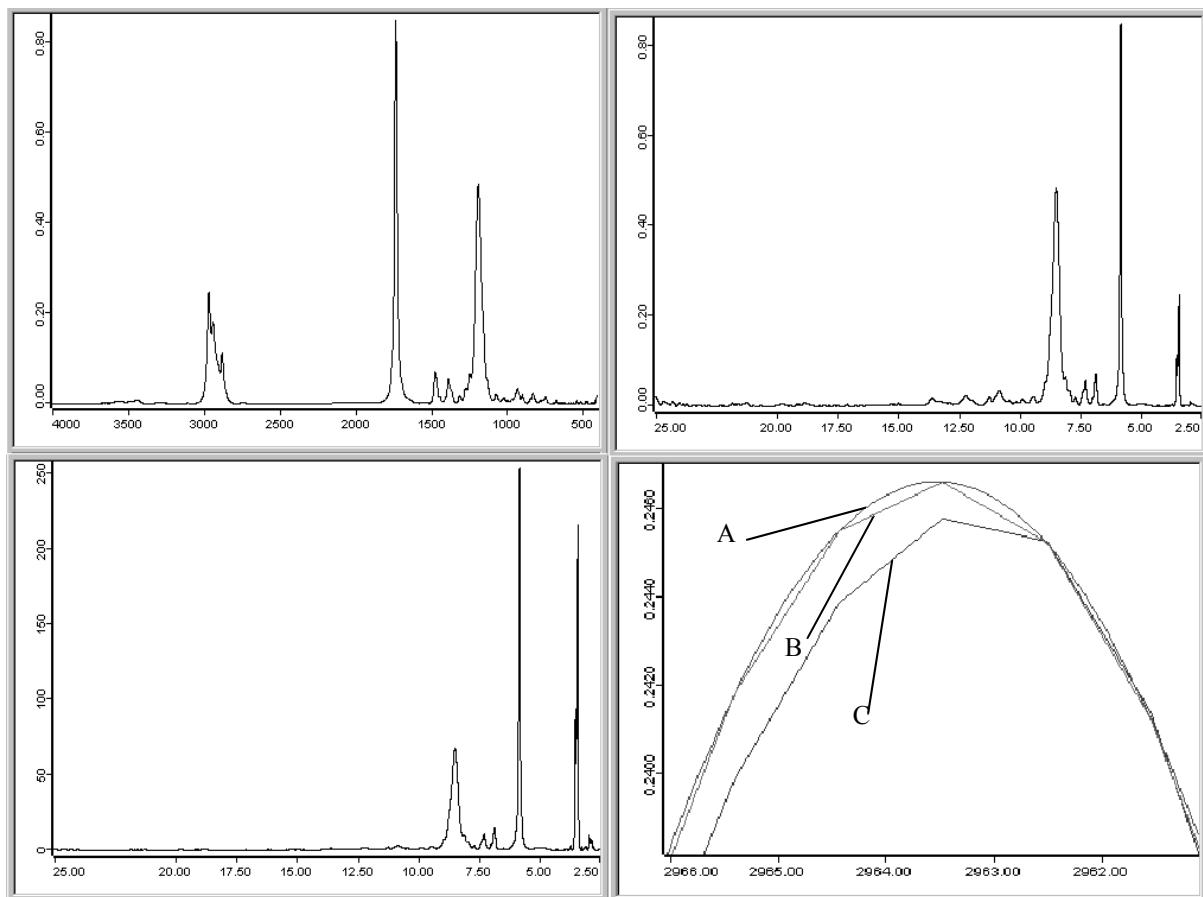
Figure 153: Original data and converted spectra after abscissa conversion

8.24   Averaging

The *Averaging* command generates a new spectrum from a set of original spectra of the same type. The intensities of this new spectrum are calculated by averaging the intensities of the original spectra.
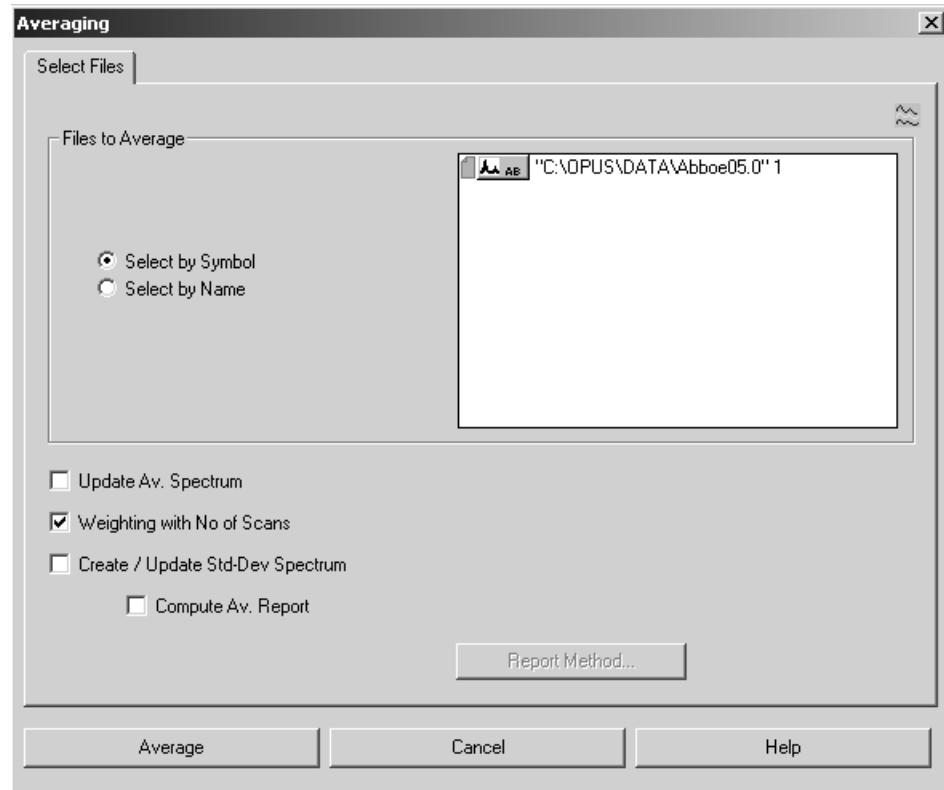
Figure 154: Averaging - Select Files tab (select by symbol)

The *Files to Average* group field provides two different options to select the respective data file. Check the *Select by Symbol* option button if you want to select the file by Drag & Drop from the OPUS browser window into the respective selection field.

Check the *Select by Name* option if you want to select the file by specifying its path and data block. In this case the dialog looks different (figure 155).
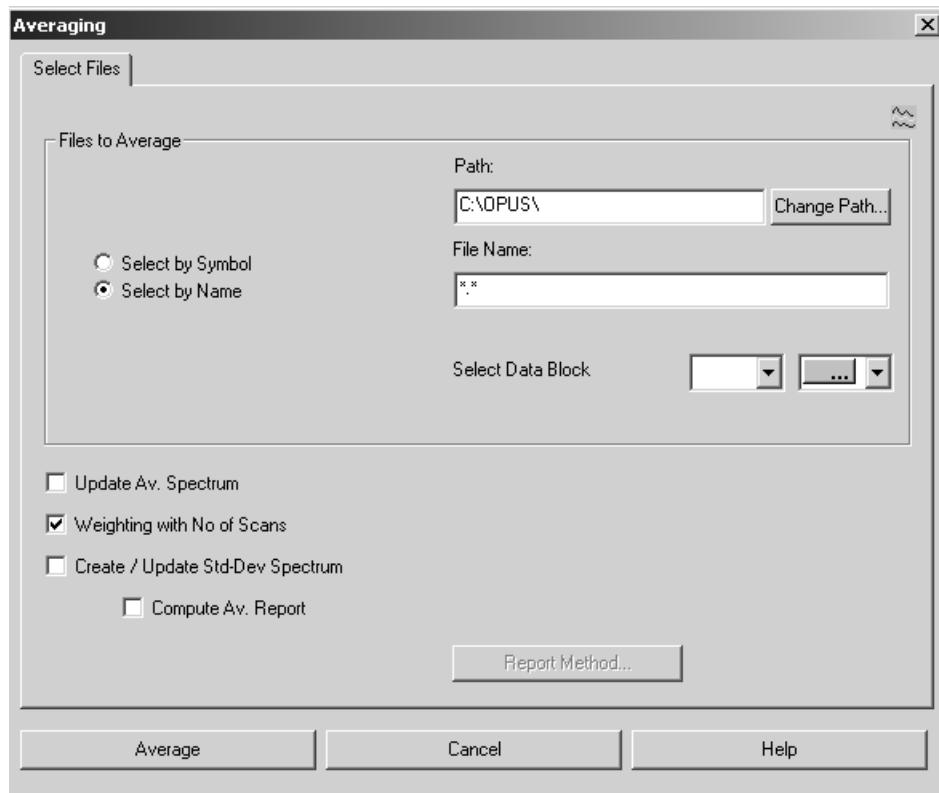
Figure 155: Averaging - Select Files tab (select by name)

The average spectrum calculated includes the largest wavelength range which is common to all original spectra.

Activate the *Update Av. Spectrum* check box to save the average spectrum on your hard disk. An additional entry field will be displayed next to this check box function in which you have to enter the name of the file to be saved. If a file with the same file name already exists, it will automatically be added to the set of spectra to be averaged and overwritten by the result file.

To weight spectra files proportional to their number of scans measured for each file before the average spectrum will be calculated, activate the *Weighting with No of Scans* check box.

Calculate the standard deviation of single-spectra intensities from the average spectrum intensities by activating the *Create/Update Std.-Dev. Spectrum* check box. An additional entry field will be displayed next to this check box function in which you have to enter the name of the file to be saved.

The *Compute Av. Report* check box function performs an identity comparison between the original set of spectra and the average spectrum. This will result in an average report which includes information on the single spectra used to create the average spectrum. The report also outlines the deviation of each single spectrum from the average spectrum, and the frequency range and averaging method selected.

The single-spectra deviation is indicated in multiples of the standard deviation to make the detection of outliers easier.

Click on the *Report Method...* button to select the respective kind of method used to calculate the spectral distance.

8.24.1   Averaging Theory

Averaging means to calculate the arithmetic mean of $\bar{y}$ identity values included in *n* original spectra:

$$\bar{y} = \frac{\sum\limits_{i=1}^{n} y_i}{n}$$

The σ standard deviation is:

$$\sigma = \sqrt{\frac{\sum\limits_{i=1}^{n} (y_i - \bar{y})^2}{n-1}}$$

When comparing standard deviation spectra, calculated with and without weighting the number of scans, the results will slightly differ even if the number of scans is the same for all original spectra. The reason is that the sum of *1* to *n* in the above equation is not divided by *n,* but *n-1*. As *n* does not represent the number of spectra but the number of scans when weighting, the results will differ by a constant factor. This factor approaches 1 the more the number of single spectra increases.

8.25   Merge Spectral Ranges

Several spectra of the same type (e.g. transmittance spectra) can be merged to a new spectrum. Any gap in the frequency region is filled by a straight line.

If the original spectra overlap within one or more frequency ranges, linear weighting is performed to avoid a step. If the frequency range of one spectrum is completely overlapped by a second one (i.e. one spectrum is obsolete), a warning message pops up and stops the merging. The parameter set of the first spectrum on the list of spectra to be merged is used as result spectrum.

To merge spectra, drag them from the OPUS browser window into the *File(s) to Merge Spectra Ranges* entry field on the *Select Files* tab. Click on the *Merge* button.
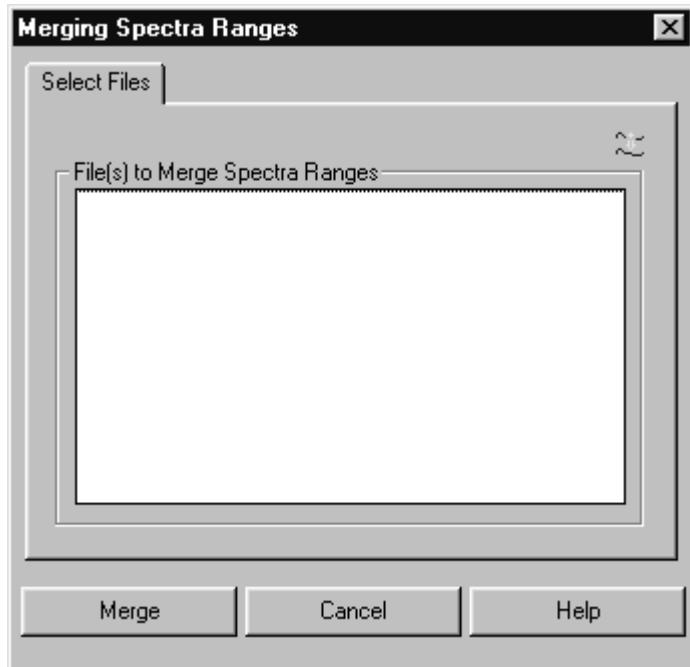
Figure 156: Merging Spectra Ranges
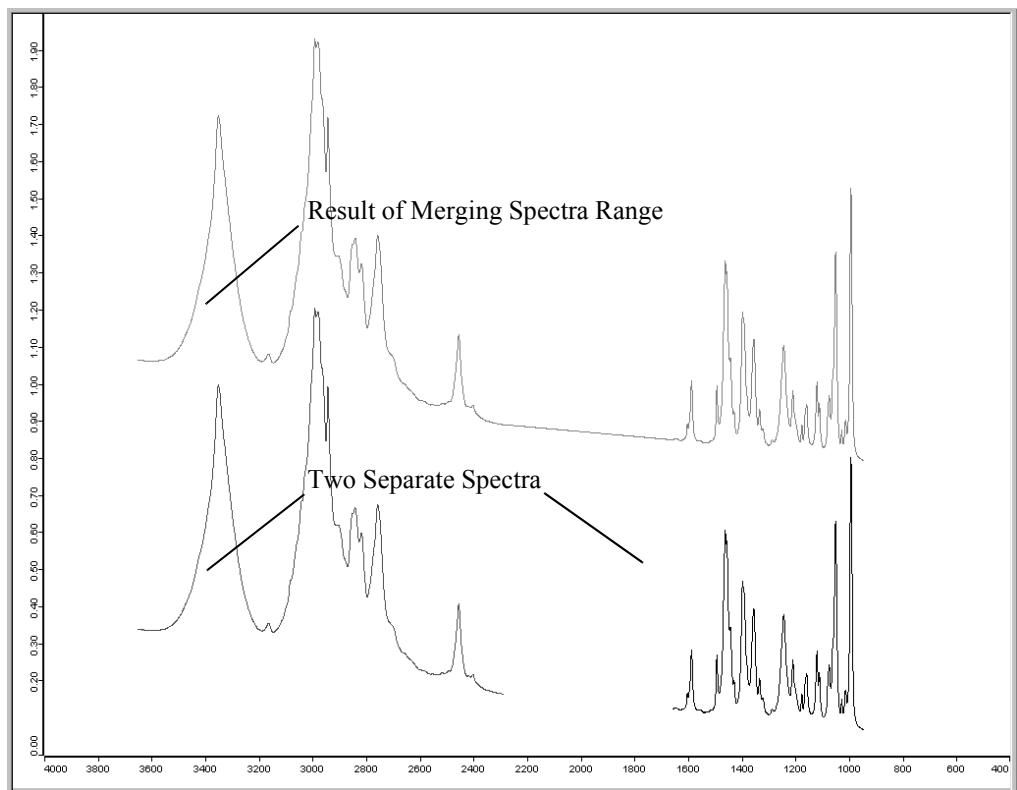
Figure 157: Original and merged spectra

8.26   Atmospheric Compensation

The *Atmospheric Compensation* command eliminates disturbing H_2O and/or CO_2 bands in ratio spectra. These bands arise due to different H_2O/CO_2 vapor concentrations in the beam path if you measure reference or sample spectra, respectively.

To perform *Atmospheric Compensation* a single-channel reference spectrum and single-channel sample spectrum are analyzed and transformed into a ratio spectrum without any (or hardly any) H_2O and/or CO_2 bands.

If you select the *Atmospheric Compensation* command the following dialog box opens:
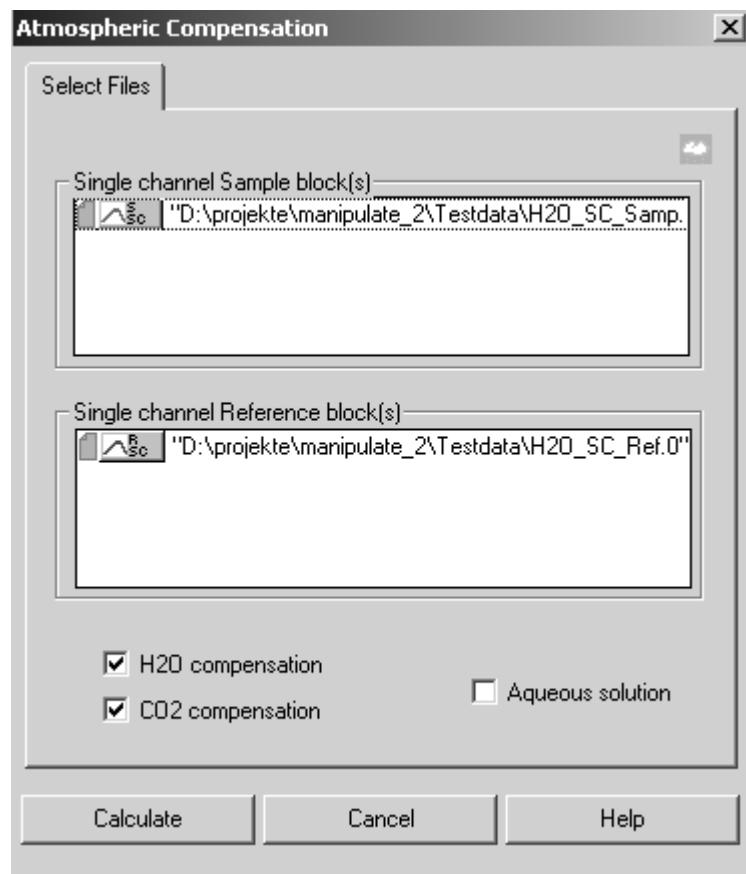
Figure 158: Atmospheric Compensation - Select Files tab

8.26.1   Select Files

The *Atmospheric Compensation* command requires two single-channel spectra to calculate one compensated ratio spectrum. Drag the single-channel sample spectrum into the *Single-channel Sample block(s)* field, and the single-channel reference spectrum into the *Single-channel Reference block(s)* field.

If you want to compensate several spectra simultaneously, the two single-channel spectra which belong together have to be uniquely defined. To do so, you have two possibilities which are described in the following:

8.26.1.1 Single-channel sample and single-channel reference spectrum in one file

If the single-channel sample and single-channel reference data block are stored in one file, select the desired file and drag and drop it into the respective selection fields on the *Select Files* tab. Only the correct data block type will be accepted (see figure 158).

If you have selected several files, a data block for each file selected will be displayed in both selection fields.

8.26.1.2 Single-channel sample and single-channel reference spectrum in different files

If the single-channel sample and single-channel reference data block are stored in different files, select the single-channel reference spectrum and drag and drop it into the *Single-channel Reference block(s)* field. Select the single-channel sample spectra and drag and drop them into the *Single-channel Sample block(s)* field.

If you want to compensate several sample spectra simultaneously, which belong to one single-reference spectrum, drag and drop all single-channel sample spectra in the upper selection field and the single-channel reference spectrum in the lower selection field, see figure 159.
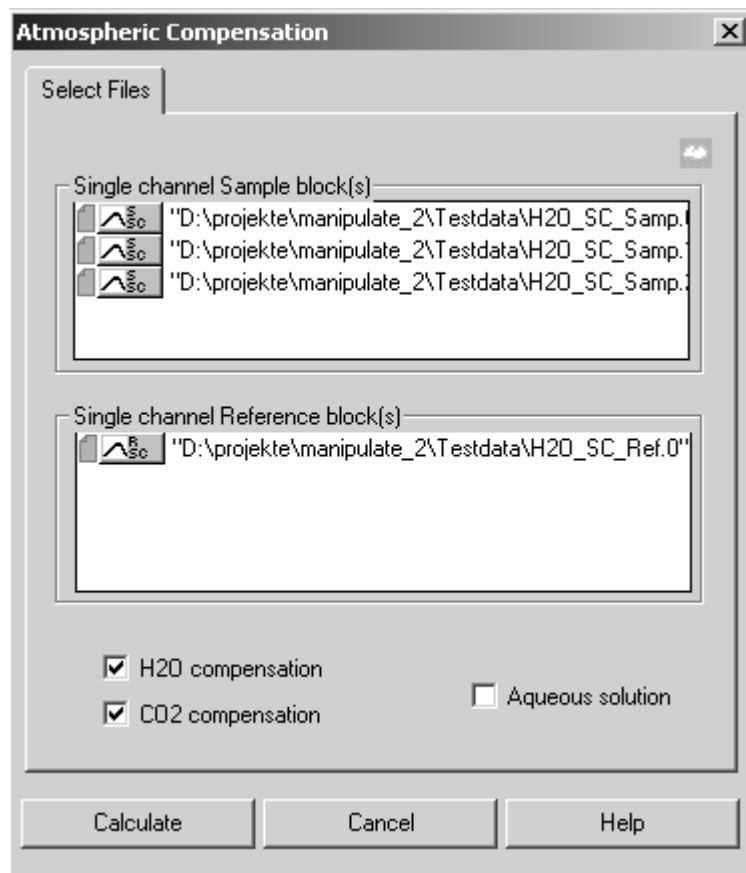
Figure 159: Atmospheric Compensation - Single-Channel Spectra in Different Files

8.26.2   H$_2$O/CO$_2$ Compensation

You can define the atmospheric gas you want to be compensated. If you deactivate both compensation check boxes on the left side (see figure 159), you will get an uncompensated transmission spectrum, i.e. the ratio between a single-channel sample spectrum and a single-channel reference spectrum.

Activate the *Aqueous solution* check box if your measurement sample is an aqueous solution (e.g. proteins in water). A different compensating algorithm optimized for aqueous solutions will be used for calculation.

8.26.3   Calculate

Click on the *Calculate* button to start the *Atmospheric Compensation* command. For each single-channel sample block the appropriate ratio block will be calculated and added to the original spectrum file.

If a ratio data block already exists, it will be overwritten by the calculated ratio data block and the original data will be replaced. Figure 160 shows *Atmospheric Compensation* effects.
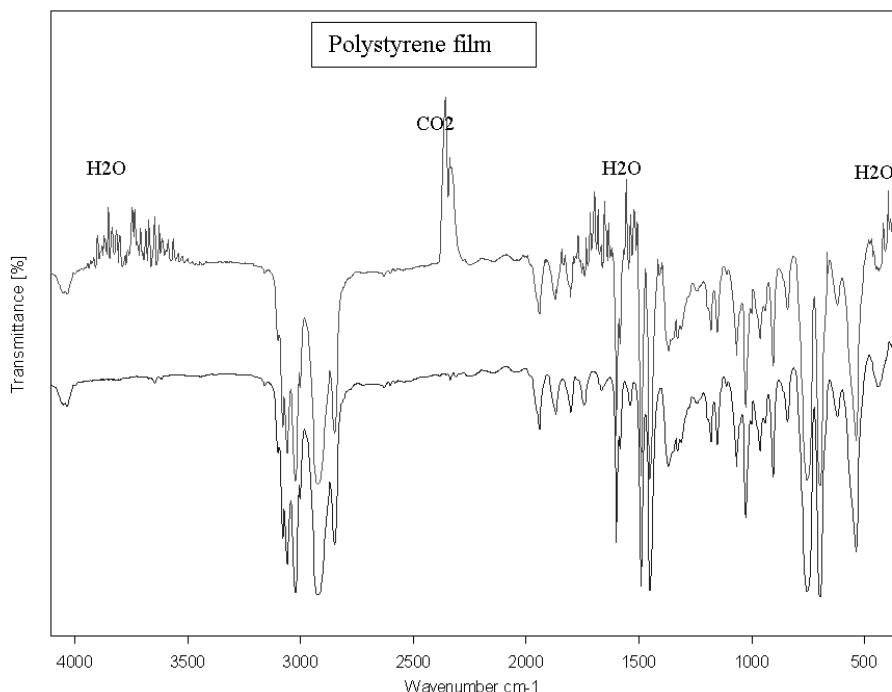
Figure 160: Atmospheric compensation effects

The upper curve is the transmission spectrum of a polystyrene film. H_2O and CO_2 bands can be clearly seen in several wave number ranges. The lower curve is the result of atmospheric compensation. Disturbing absorption lines of H_2O and CO_2 have nearly been eliminated.

8.26.4   Requirements

- Single-channel spectra have to include wave number ranges starting from 3600 to $4000cm^{-1}$ for H_2O compensation, and 2300 to $2400cm^{-1}$ for CO_2 compensation.

- Sample absorption within these wave number ranges will result in poorer quality with regard to compensation.

- The sample and reference spectrum have to be acquired using the same spectrometer resolution. Different zero-filling factors are possible.

- The spectrum should not end at a wave number which shows strong absorption of atmospheric gases. To get a similar H_2O compensation (see figure 161), the lower wave number limit **must not** be around $1700cm^{-1}$.

- For compensation in aqueous solutions the spectrum has to include wave number ranges of $2300-2400cm^{-1}$ and $1800-1900 \ cm^{-1}$ for both CO_2 and H_2O.

- These wave number ranges must be free of sample absorption bands.

8.26.5 Limits

The *Atmospheric Compensation* command uses physical models to estimate the amount of atmospheric gases in the single-channel spectra and therefore compensates disturbing H_2O and/or CO_2 bands. *Atmospheric Compensation* is a kind of data manipulation and has to be used with due care.

8.26.6 Atmospheric Compensation as part of the measurement process

If you want to use *Atmospheric Compensation* to manipulate spectra immediately after the measurement process, you have to perform the following steps:

1) Select the *Advanced Measurement* command in the *Measure* menu and set the parameters for your experiment. Click on the *Advanced* tab.

2) Activate the *Single Channel* and *Background* check boxes in the *Data blocks to be saved* option field.

3) Check *Additional Data Treatment* and click on the [...] button.

4) The following window pops up:

Select Function for additional treatment from OPUS Menus and Icons, or click here to Abort

5) Select *Atmospheric Compensation* from the *Manipulate* menu. The *Atmospheric Compensation* dialog box opens.
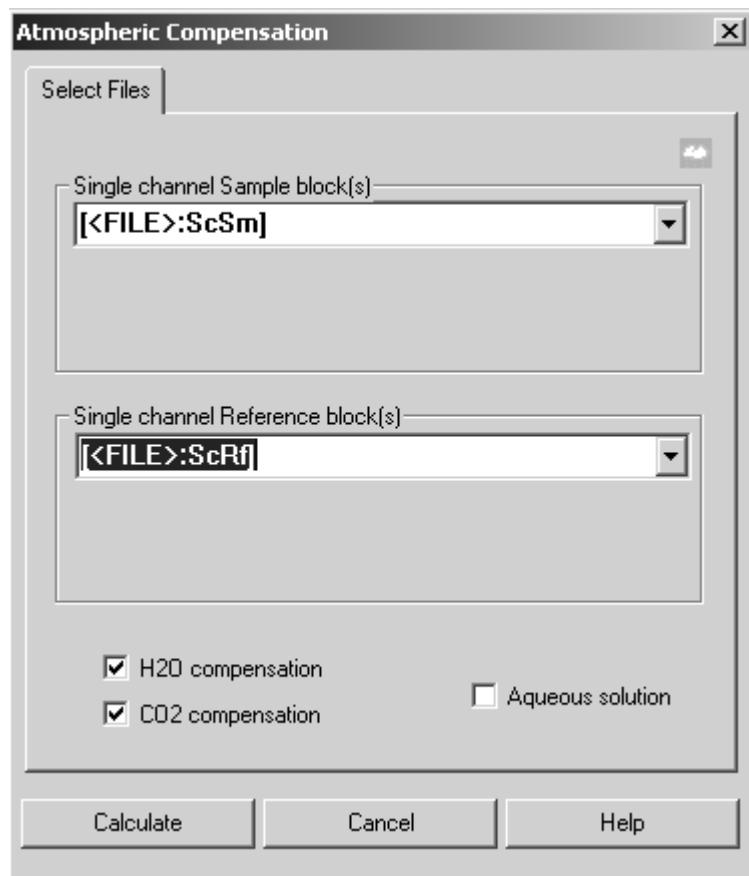
Figure 161: Atmospheric Compensation - Select Files

6) Select *[<FILE>:ScSm]* from the *Single channel Sample block(s)* drop-down list and *[<FILE>:ScRf]* from the *Single channel Reference block(s)* drop-down list. Activate the different check boxes, if required.

7) Click on the *Calculate* button.

The *Additional Data Treatment* option on the *Advanced* tab of your *Measurement* dialog has to be similar to figure 162. If the sample measurement has been successful, *Atmospheric Compensation* will be performed immediately after the measurement.
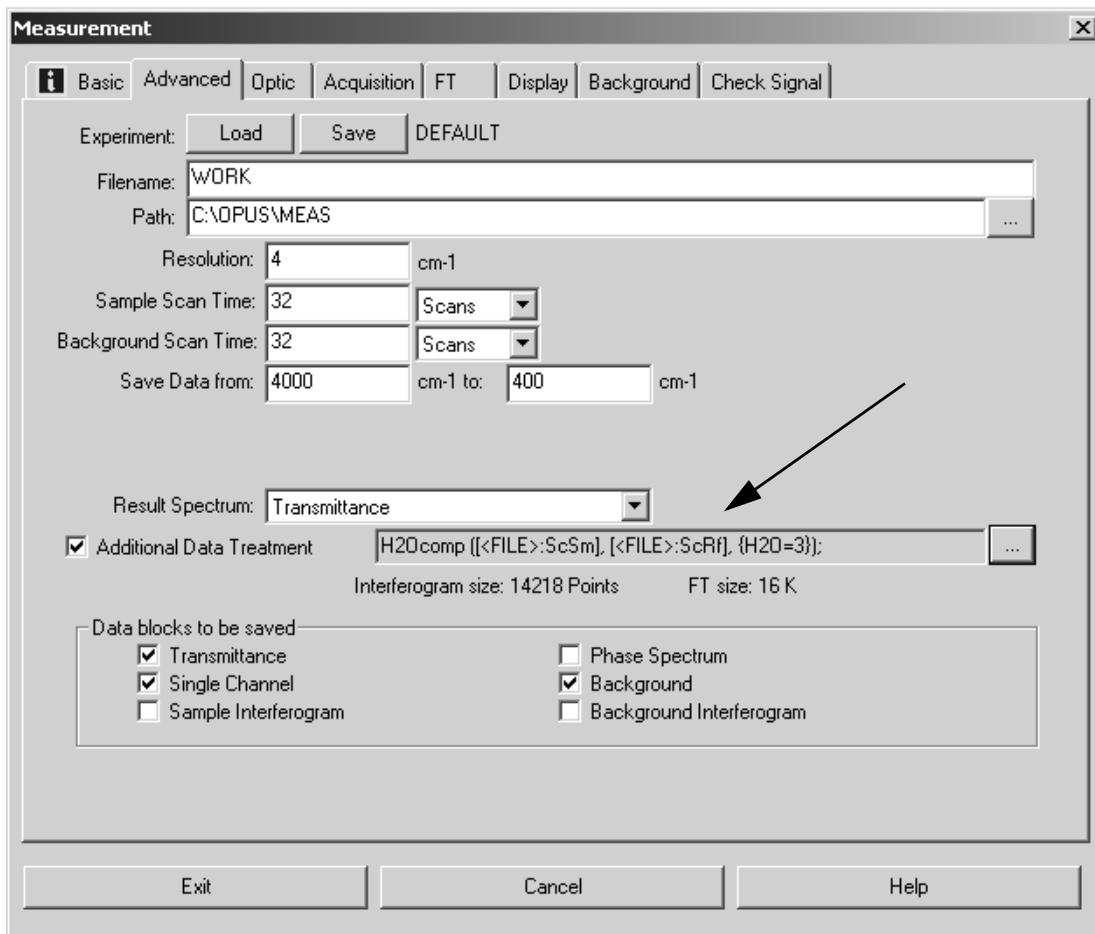
Figure 162: Measurement - Activated Post-Measurement Manipulation

8.27   Straylight Correction

The *Straylight Correction* command allows to correct two phenomena which normally occur in case of diffuse reflection measurements:

1) Diffuse reflection of the measurement light at the window, mainly due to scratches and contaminations.

2) Multiple reflections between sample and window, which lead to increased absorption.

The *Straylight Correction* eliminates these errors of ratio spectra (i.e. transmission, absorbance, Kubelka-Munk, reflection) partly by intrinsic correction spectra and partly by using mathematical algorithms. The result will again be a ratio spectrum.

If you select the *Straylight Correction* command the following dialog box opens:
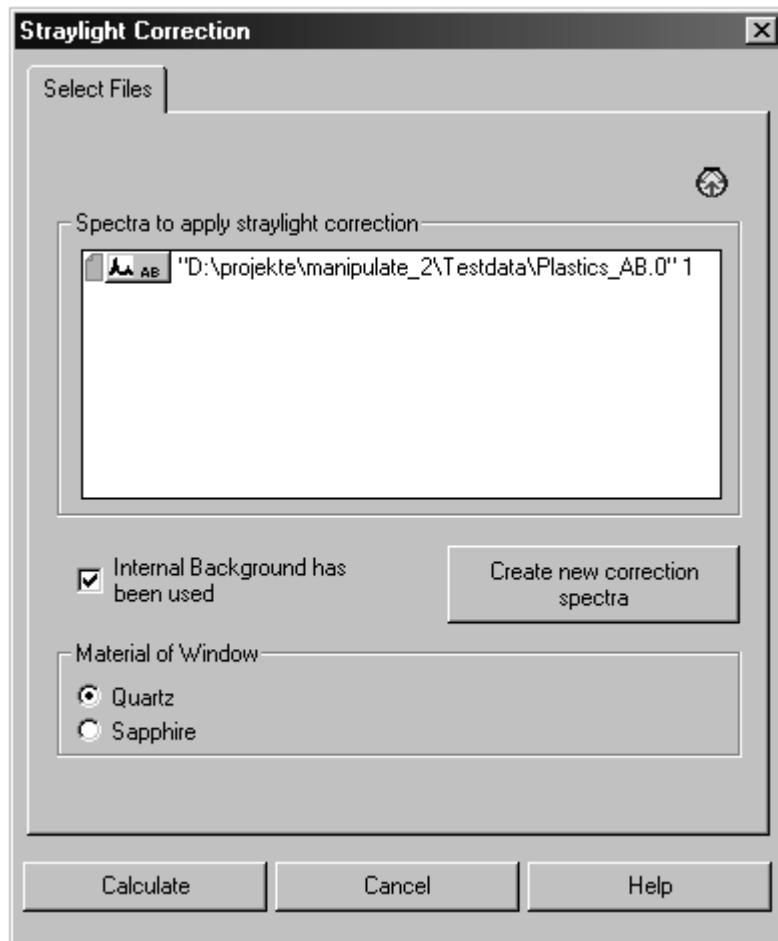
Figure 163: Straylight Correction - Select Files

8.27.1 Select Files

Drag and drop the desired spectra files from the OPUS browser window into the *Spectra to apply straylight correction* field. Only ratio blocks, e.g. absorbance, transmittance, Kubelka-Munk, reflectance or log-reflectance will be accepted.

8.27.2 Internal Background

Activate or deactivate the *Internal background was used* check box to specify whether your reflection measurement has been performed by an internal or external background. *External* means that you have used your own standard, e.g. a gold stamp or certified Labsphere standard during background measurement. *Internal* means that you have used built-in features of the Ulbricht sphere to determine the background spectra (i.e. *Sphere Background-Channel* in case of an MPA spectrometer).

8.27.3 Window Material

The correction of multiple reflections depends on the refraction index of the window material. To specify the window material used, activate either the *Quartz* or *Sapphire* check box. In most cases quartz has been used as standard window material. MPA and MATRIX spectrometers, e.g. are always delivered with quartz windows. Some Vector and TENSOR spectrometers are supplied with sapphire windows. If you are not quite sure about the material of your spectrometer window, contact your Bruker Service.

8.27.4 Calculate

Click on the *Calculate* button to start *Straylight Correction*. The ratio spectrum will be calculated for each ratio block which is displayed in the *Spectra to apply straylight correction* field. The ratio block data will be overwritten by the calculation result.

The correction algorithm considers the following effects:

1) Straylight effects caused by diffuse reflection of the incoming light at the measurement window. These effects will be corrected by calculating a corrected ratio spectrum:

$$TM_{corrected} = \frac{TM - Stray}{Extref - Stray}$$ If *TM* has been recorded using an internal background.

$$TM_{corrected} = \frac{TM - Stray/Extref}{1 - Stray/Extref}$$ If *TM* has been recorded using an external background (nearly 100%).

TM is the original transmission spectrum, $TM_{corrected}$ the resulting spectrum. *Stray* stands for transmission spectrum of a measurement performed without sample (open channel). *Extref* is the ratio between the single-channel spectra of the external reference and single-channel spectra of the internal reference.

2) Multiple reflections between the measurement window and sample: After the first diffuse reflection of the light at the sample, a fraction of this light can be reflected again both at the window and the sample. This leads to incorrect measurement results, especially in case of a mid-range sample absorbance ratio (30-70%). This effect is compensated by multiplying the transmission spectrum by the following factor:

$$\frac{1+c}{1+TM \cdot c}$$ where $c = R \cdot \left(1 + (1-R)^2\right)$

TM is the original transmission spectrum and *R* is the reflection coefficient of the window material.

3) The ratio spectrum may have different values when using an internal background instead of an external standard.

The difference between internal and external background is the portion of light reflected directly at the measurement window. This part of light leaves the Ulbricht sphere by the input. This effect is taken into account by a correction spectra which quantifies this background difference.

Figure 164 shows straylight correction effects.
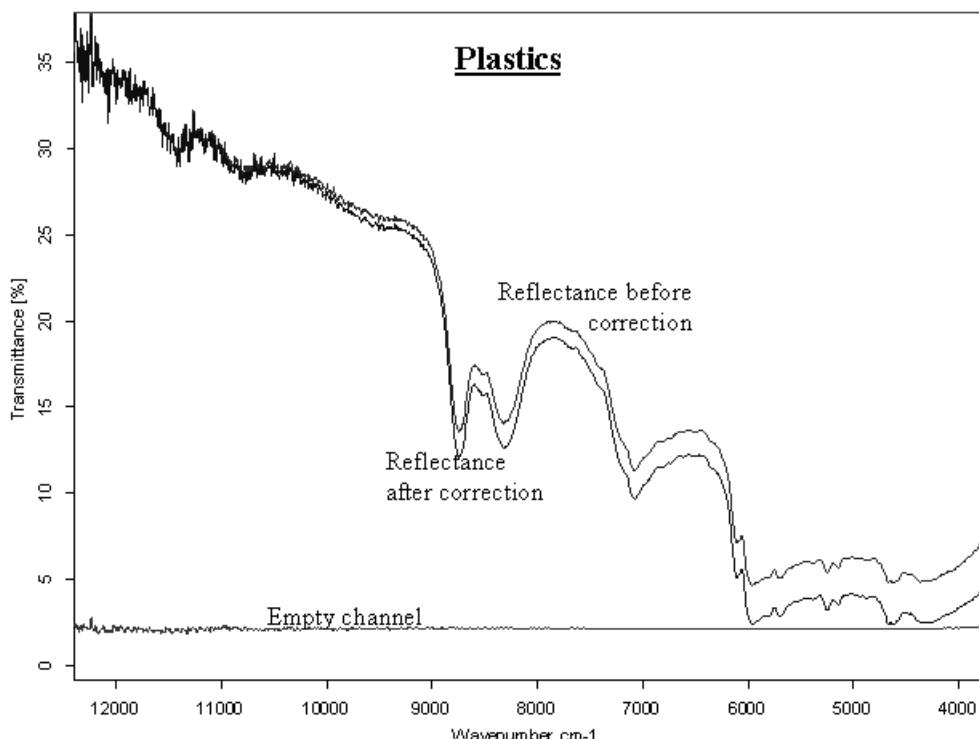
Figure 164: Straylight correction effects

8.27.5   Create new correction spectra

Each OPUS release includes a set of correction spectra which can be used for straylight correction. It is, however, important that these spectra reproduce the properties of your spectrometer. Therefore, it is recommended to create your individual set of correction spectra before using the OPUS *Straylight Correction* command. Correction spectra should be created regularly (e.g. each month).

To proceed successfully you need a standard material, e.g. gold standard or certified Labsphere standard (99%). Even if no standard is available it is still possible to create new correction spectra but not reasonable, because you may obtain correction spectra which are even worse than the OPUS default spectra. The correction algorithm assumes that the standard used has a diffuse reflection

of about 100% within a wave number range of 15,000 to 3,000cm^{-1}.

To create new correction spectra, click on the *Create new correction spectra* button. A new dialog opens. Follow the on-screen instructions. If you have finished, the new correction spectra will be automatically stored on hard disk.

The *Straylight Correction* command always uses the latest correction spectra measured.

When running the *New correction spectra* script three different single-channel spectra are measured:

- SCintBG: Single-channel measurement of internal background
- SCextBG: Single-channel measurement of external background
- SCStray: Single-channel measurement without sample

   Note: If you use an MPA spectrometer, two additional single-channel spectra will be measured for the *External Transmission* channel.

The following ratio spectra are calculated from the three different single-channel spectra:

- ExtRef: SCextBG/SCintBG
- Stray: SCStray/SCintBG

The ratio spectra are stored by the *ExternalReference_macro.0* and *EmptyChannel_macro.0* file name in the *(OPUS-Dir)\StrayCorr* directory.

   Note: If you use an MPA spectrometer, two additional spectra will be created which have the extension *_micro.*
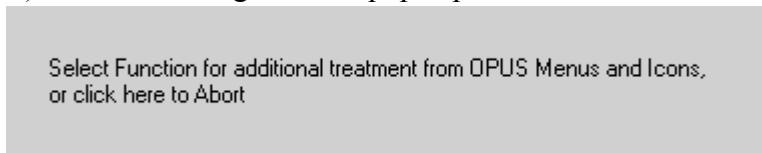
The *ExtRef* and *Stray* single-channel spectra are used to perform straylight correction on the spectra measured.

8.27.6   Using straylight correction as part of the measurement process

If you want to use *Straylight Correction* to manipulate spectra immediately after the measurement process, you have to perform the following steps:

1) Select the *Advanced Measurement* command in the *Measure* menu and set the parameters for your experiment. Click on the *Advanced* tab.

2) Use the *Result Spectrum* drop-down list to define the result spectrum type. This type has to be one of the following: transmittance, absorbance, Kubelka-Munk, reflectance or log reflectance. Activate the appropriate check box in the *Data blocks to be saved* option field.

3) Check *Additional Data Treatment* and click on the [···] button.

4) The following window pops up:

Select Function for additional treatment from OPUS Menus and Icons, or click here to Abort

5) Select *Straylight Correction* from the *Manipulate* menu. The *Straylight Correction* dialog box opens.
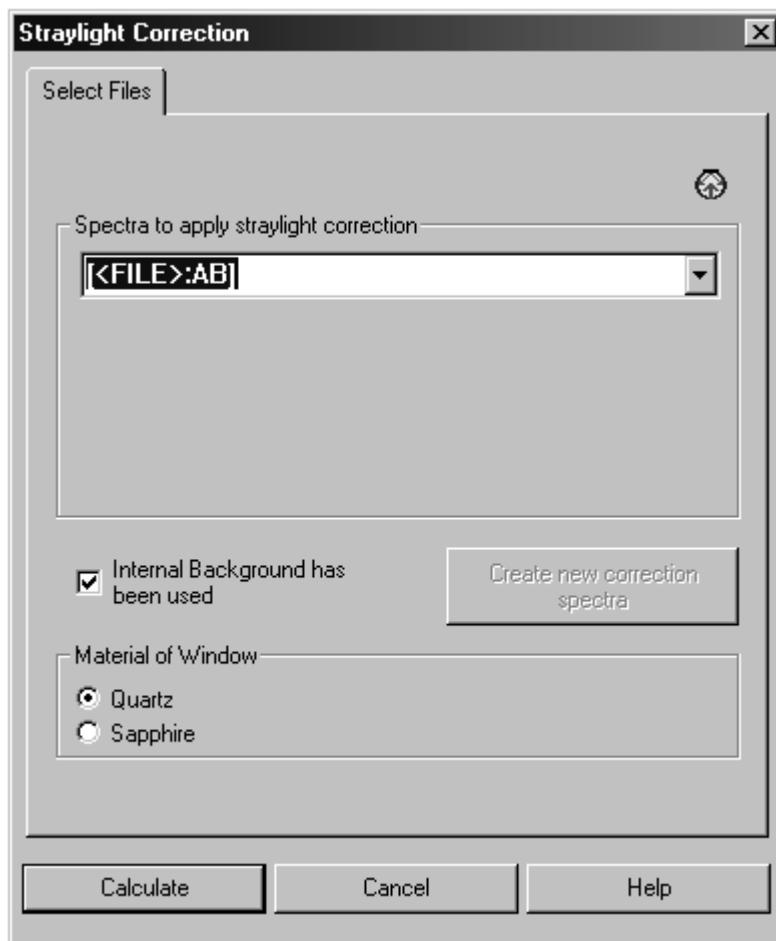
Figure 165: Straylight Correction - Select Files

6) Select the result spectrum, e.g. [<FILE>:TR] from the *Spectra to apply straylight correction* drop-down list. Activate the check box and radio buttons, if required.

7) Click on the *Calculate* button.

The *Advanced* tab of your *Measurement* dialog may be similar to figure 166. If the sample measurement has been successful, additional spectra manipulation, e.g. *Straylight Correction* will be performed immediately.
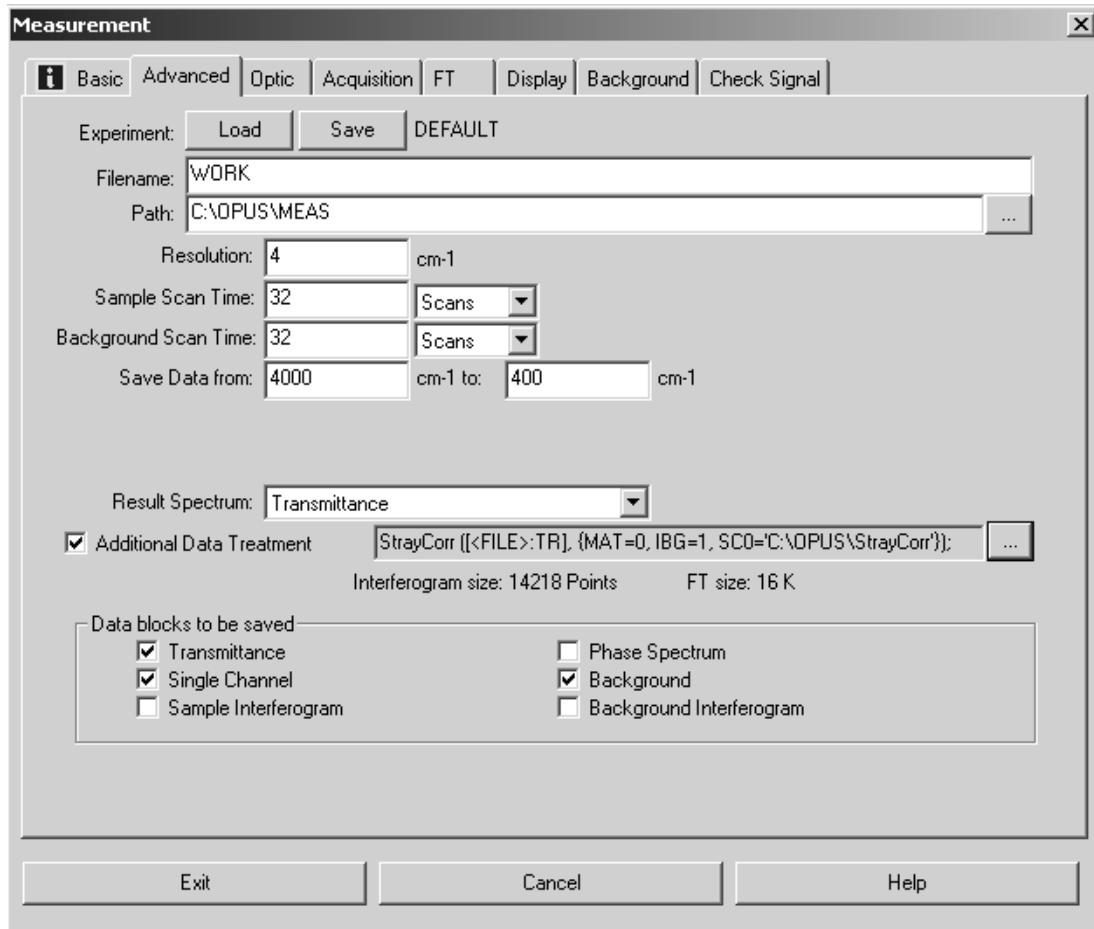
Figure 166: Measurement with Activated Post-Measurement Manipulation

8.28   Noise Generation

The *Noise Generation* command adds artificial noise to a spectrum. It adds random positive or negative numbers to the spectrum values. Select a spectrum file and click on the *Noise Generation* command. The following dialog box opens:
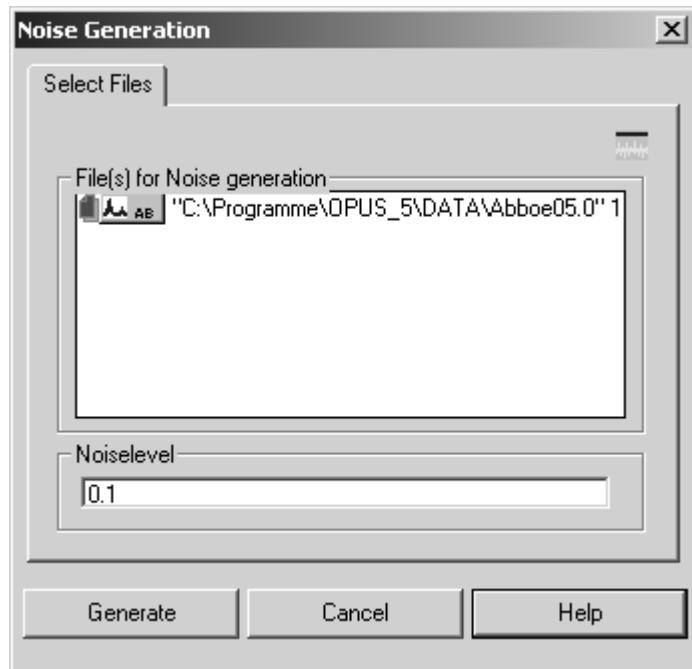
Figure 167: Noise Generation - Select Files

In the *Noise level* entry field you enter the maximum value by which the spectral values will be changed. Click on *Generate* to start this kind of manipulation.

8.29   Moving Mean

Moving Mean performs some kind of smoothing on a spectrum. Select a file and click on the *Moving Mean* command. The following dialog box opens:
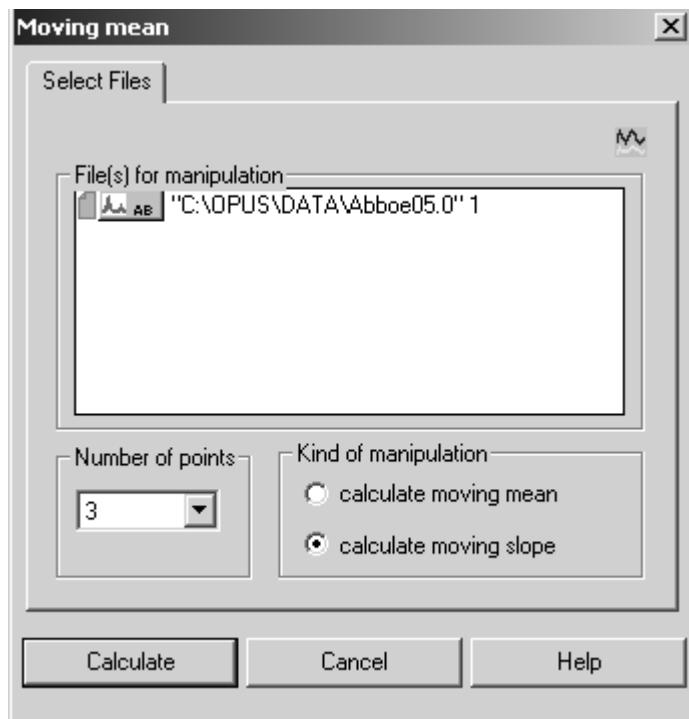
Figure 168: Moving Mean - Select Files

Two different types of manipulation are possible. In both methods the *Number of points* parameter always represents the number of subsequent spectrum points. These spectrum points are used for the calculation to be able to create new spectrum values.

If you check *Calculate moving mean*, spectrum values being next to each other are averaged over and replaced by their mean value. If you check *Calculate moving slope*, the first and the last point of a sequence of data points are used to calculate a straight line between these two data points. The spectrum values between these two data points are replaced by values which are on the straight line. These steps are repeated using the next sequence of data points. The number of data points are defined in the *Number of points* entry field.

Click on the *Calculate* button to start this manipulation command.

8.30   Make Monotone

Depending on the options selected and the spectrum curve shape, the *Make Monotone* command allows to correct a trace or spectrum such that the resulting curve increases or decreases in a monotonic manner. Select a file and click on the *Make Monotone* command. The following dialog box opens:
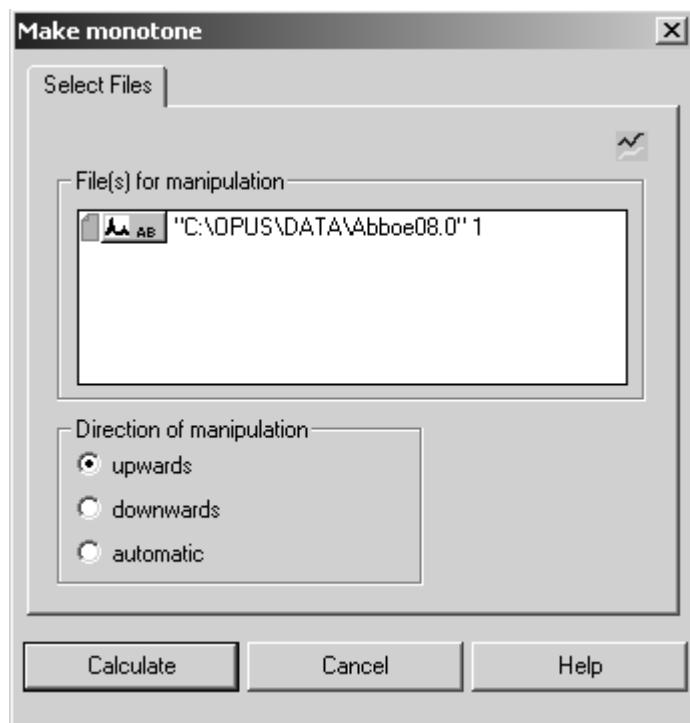
Figure 169: Make Monotone - Select Files

You can select between three manipulation directions. If you check *Upwards*, the spectrum values will be changed to the effect that the resulting spectrum values increase in a monotonic way. If you check *Downwards*, the resulting spectrum values will decrease in a monotonic way. Activating the *Automatic* option automatically determines whether the resulting curve increases or decreases, considering two data points at the boundary of the wave number interval.

9   Evaluate

The command included in the *Evaluate* menu primarily intend to calculate results from existing spectra. This could be a quantitative data analysis, peak identification or a library search. These calculations do not alter the spectrum files.
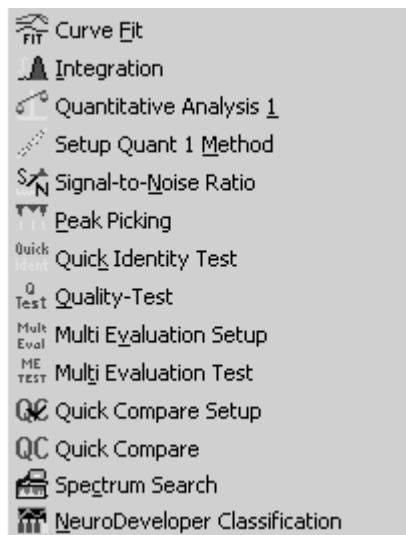
Figure 170: Evaluate Menu

9.1   Curve Fit

The *Curve Fit* command allows to calculate single components in a system of overlapping bands. A model consisting of an estimated number of bands and a baseline should be generated before the fitting calculation is started.

The model can be set up interactively on the display and is optimized during the calculation. As the result of this calculation highly depends on the model selected, make sure that the model is reasonable from the chemical point of view.

Setup Model

Select the *Curve Fit* command and a dialog box opens which you use to specify spectrum to be fitted, and the frequency range.
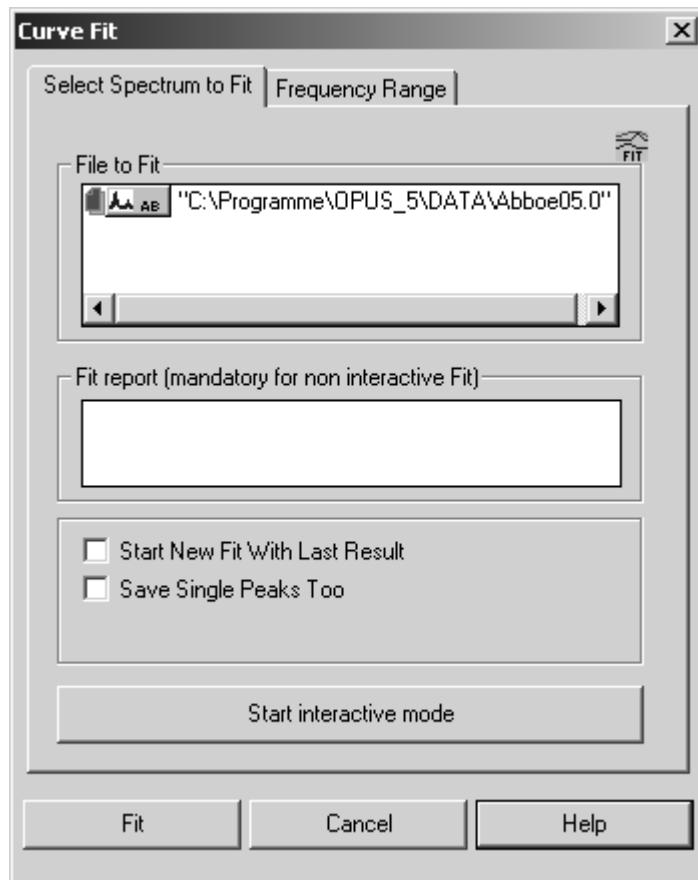
Figure 171: Curve Fit - Select Spectrum

Drag & drop the spectrum to be fitted from the OPUS browser window into the *File to Fit* selection field on the *Select Spectrum to Fit* tab. Make sure that the spectrum is of absorbance type and baseline corrected.

If you activate the *Save Single peaks Too* check box, every fitted peak will be stored as a separate file. You can also start a new fit using the last result.

On the *Frequency Range* tab you define the frequency range of the spectrum you want to fit. If you click on the *Interactive* button, a new window opens which allows to define the area to fit interactively. To take the limits from the respective display window click on the *Get Display Limits* button. Activate the *Use File Limits* check box if you want to take the original frequency range of the file. The previous two options will then be disabled.

Once a suitable model has been found (see next paragraphs), it can be applied to other spectra of the same kind, there is no need to set up a new model for each spectrum. The spectra to be analyzed must always be defined in the *File to Fit* selection field. The Fit Report block (🔳) of the already fitted spectrum will then be dragged into the *Fit Report* selection box. Click on the *Fit* button to start the *Curve Fit* procedure of all spectra with the method selected.
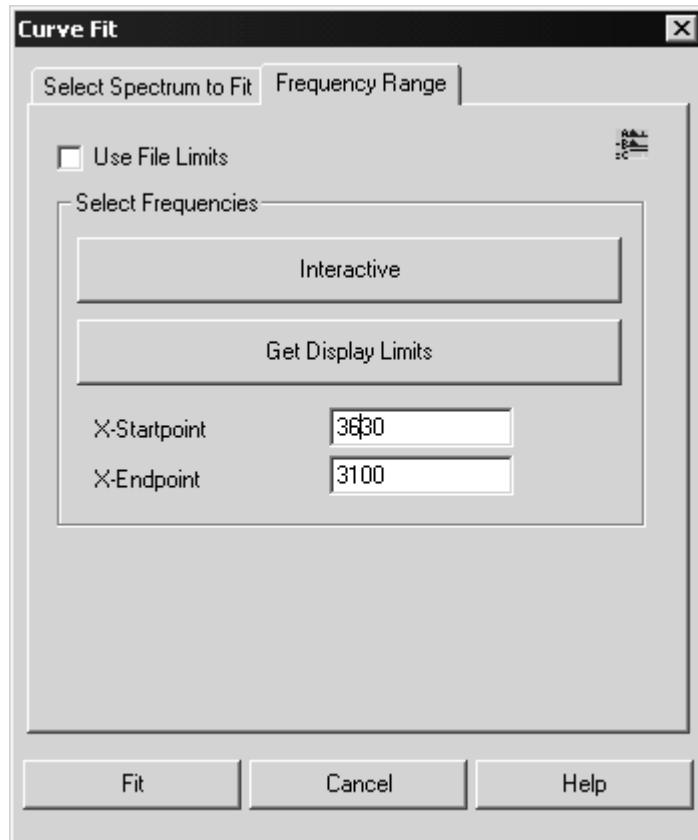
Figure 172: Curve Fit - Frequency Range

To perform a curve fit you first have to create a fit method first. Click on the *Start Interactive Mode* button on the *Select Spectrum to Fit* tab and the spectrum you selected will be opened in the curve fit setup window (see figure 173).

In the upper window, the spectrum to be fitted is displayed, whereas in the bottom window the difference between the original spectrum and the fitted spectrum is shown. As there was no fitting carried out at this point, both windows show the same spectrum.

You can create a curve fit model by moving the cursor into the top window. The mouse pointer will change from an arrow to an ADD symbol ($\overset{\frown}{\text{ADD}}$). By clicking onto the peak, a curve will appear close to the selected peak. Each left click will generate a new curve. The intensity of the curve corresponds to the cursor position. The generated curves will appear in red.
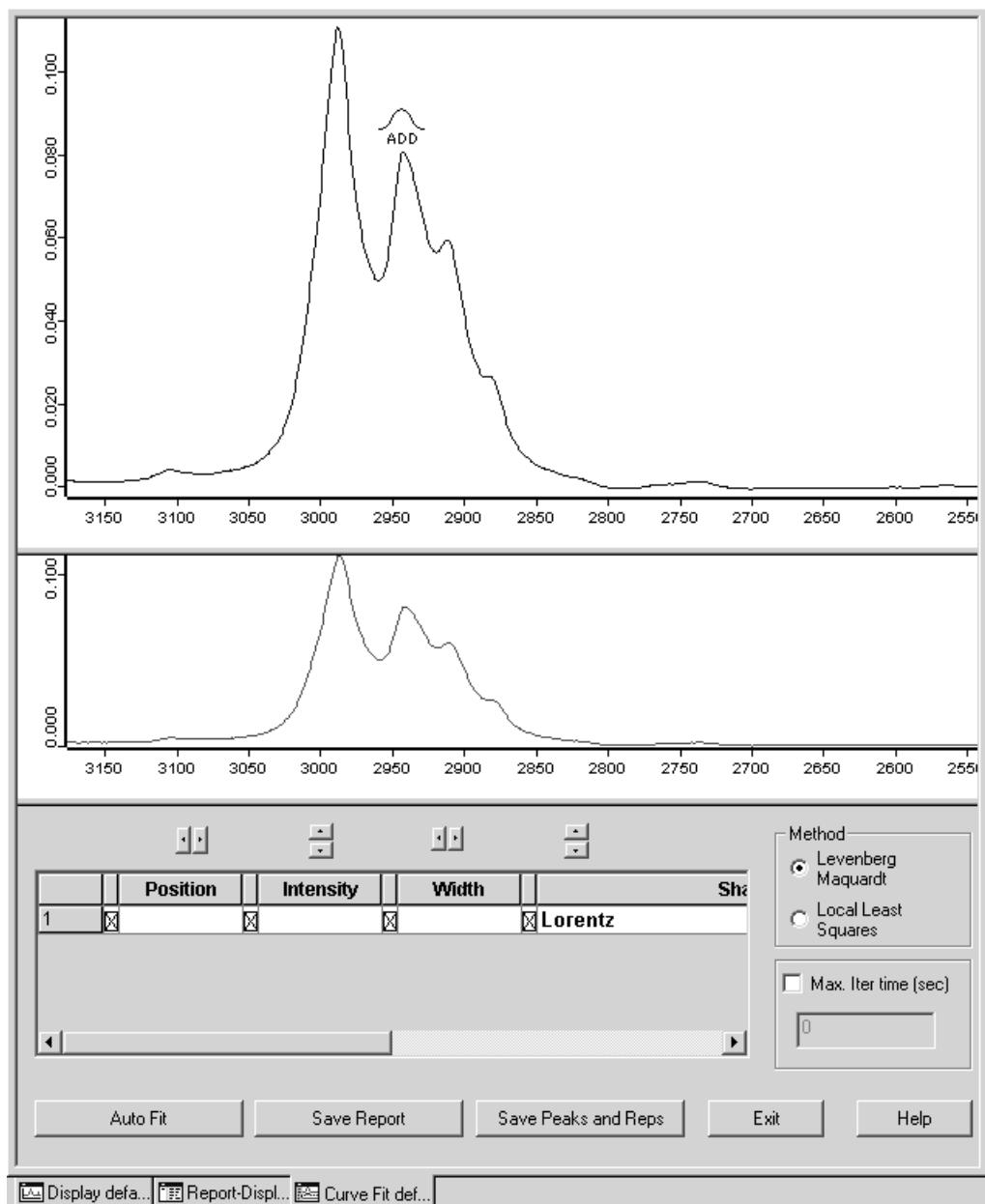
Figure 173: Curve Fit Window before Fit

When the cursor is positioned close to the top of the peak, the MOVE symbol ($_{MOVE}^{\oplus}$) is displayed. You can now move the curve by clicking and dragging it to the desired position.

To change the width of the peak, position the cursor slightly below the top of the curve. The WIDTH symbol ( ) will appear. By clicking and dragging to the left, the curve will become wider, whereas dragging to the right makes the curve narrower.
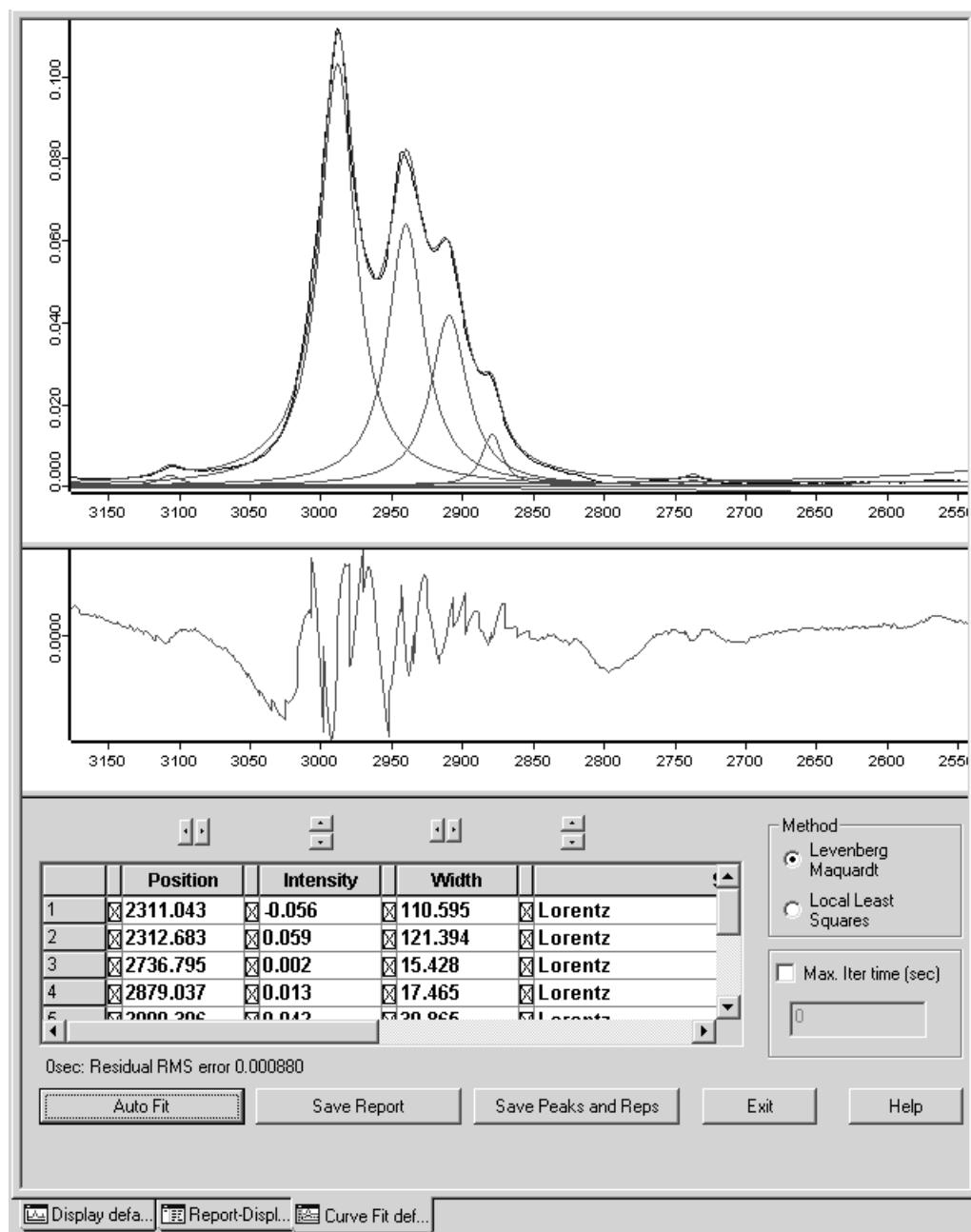
Figure 174: Curve Fit Window after Fit

Peak Parameters

In the bottom half of the window, various parameters can be edited. *Position*, *Intensity* and *Width* can here be manipulated more precisely than with the cursor. To change the values of a curve, it must be selected first by clicking onto the respective field. Than the values can be directly typed in or changed with the respective arrow key above the field.

Peak Shape

Several different options exist for the peak shape. The default setting is *Lorentz*, i.e. a pure Lorentzian curve. A single click on the upper arrow key switches immediately to a pure *Gaussian* function. The next click on the same arrow sets the peak to *Baseline*. If, beginning again with the Lorentz type, the down arrow is clicked on instead, the peak shape changes to *100%Lorentz + Gauss*. In principle the peak shape simulated is also a pure Lorentzian function but it represents the special case of a mixture of Lorentzian and Gaussian functions. Repeated clicking, on the down arrow manually decreases the Lorentz function percentage. This type of manipulation is typically left to be performed by OPUS.

Baseline

In some cases it may be necessary to use a *Baseline* in addition to the peaks. A baseline is always a straight line defined by a reference point and a slope. The baseline can be defined by the operator or calculated by OPUS. The parameter *Width* is replaced by *Slope* in the peak list. Baseline parameters can be set interactively with the mouse or directly in the peak table.

The parameters of the baseline are automatically modified only if the *Levenberg-Marquardt* algorithm is used. If the *Local Least Squares* algorithm is selected, the parameters are set manually.

Peak List

Each peak is shown in one line of the peak list including all peak parameters. The lines with non-selected peaks are green and the currently selected peak is marked in violet. The peaks in the list are always sorted by peak position. Algorithm

Two different algorithms are available for the optimization of the model:

- Levenberg-Marquardt
- Local Least Squares

The algorithm can be selected before starting the calculation but can also be changed during the calculation. The algorithm principles are described below.

Status Line

The status line is activated after starting the calculation. It shows the iteration time and the error of the fit.

Example: 12 sec: Residual RMS error 0.009109

The smaller the error value the smaller the deviation between measured and calculated curve.

Message: * Bad Fitting Model! *

Sometimes an additional message *Bad Fitting Model!** is displayed in the status line. This message is displayed if the program was not able to fit one or more peaks. These peaks are found at the left or right end of the frequency range and usually have very small intensities. These bands needs to be deleted before the calculation is continued. To delete a band, click on its band number (left row) to select the band and press *Delete* on your keyboard.

Max Iter. Time (sec)

The maximum iteration time for *Auto Fit* in seconds is specified in this field.

Auto Fit

The *Auto Fit* button is used to start the calculation. After clicking on this button the calculation begins and the button text changes to *Stop*. During the iteration the newly calculated peaks are shown on the display in real time. The calculation can be interrupted at any time by clicking on the button. To restart, click the button again.

Autoscale

At any time, the standard display functions can be used to zoom, expand or roll the contents of the display. To return to the original frequency and intensity limits click on the *Autoscale* button.

Save Report

Select the *Save Report* button to save the current report. The resulting sum-spectrum is stored as a temporary work file. This fit report can be used for the curve fit of new spectra.

Save Peaks and Reps

In addition to the previously described functions for the *Safe Report* button, the fit report is added to the original spectrum.

Theoretical Background

Two different algorithms are used for the curve fit:

- Levenberg-Marquardt
- Local Least Squares

Both algorithms are based on the least squares method. The difference between the original and the calculated curve are kept as small as possible. The fitting model is described by: $Y_G = y(x;S)$

Y_G	Measured data
y	Model
x	Frequency
S	Set of curve parameters

Levenberg-Marquardt Algorithm

The quadratic equation for the deviation between measured and calculated curve is: $\chi^2(S) = \sum_{i=1}^{N} [Y_G - y(x;S)]^2$

χ^2	Quadratic deviation
N	Number of points

The function is minimized by iteration. The gradient of the function χ^2 is calculated for the current set of peak parameters. The gradient is then used to determine a new set of parameters S.

Some additional restrictions have also been implemented to make the calculation more effective:

- All peaks must lie within the specified frequency range.
- The width of a peak must not be greater than the specified frequency range.
- Peak intensities must be positive.
- The contribution of Lorentz- and Gauss functions for mixtures must lie within the range 0% to 100%.
- The sum of both parts must always be 100%.

Local Least Squares Algorithm

The *Local Least Squares* algorithm performs an independent fit for each individual peak. The calculation is thereby restricted to the range around the peak maximum. This dramatically reduces the amount of data required for the calculation, enhancing the speed compared to the *Levenberg-Marquardt* method. Some loss of precision vs. the *Levenberg-Marquardt* method occurs.

The *Local Least Squares* algorithm has some conditions:

- The parameters for the baseline are taken from the model, not calculated.
- The peak parameters are always variable, none of them can be fixed.

The given model can be looked at as an area in a *n*-dimensional space with *n* being the total number of peak parameters. In most cases this area has one absolute minimum and several local minima. The quality of the calculation depends on the quality of the selected model, i.e. does the calculation find the absolute minimum or does it orbit in the vicinity of the local minima. The latter case can be detected by a relatively large error and an visually obvious poor fit. In case of a poor fit, start again with a new optimized model.

Criteria for the selection of an algorithm

The *Levenberg-Marquardt* algorithm in most cases gives a better fit compared to the *Local Least Squares* algorithm, but needs significantly more calculation time. If the number of points in the selected region and the number of peaks in the model is small the *Levenberg-Marquardt* algorithm can be used immediately.

If the amount of data is large or many peaks need to be fitted, start with the *Local Least Squares* algorithm which converges very quickly. As soon as the variation of the error becomes small, switch to the *Levenberg-Marquardt* algorithm for the final fit.

9.2   Integration

This *Integration* command allows the integration of peaks as well as the calculation of peak heights. There are 18 different integration modes available. Click on the *Integration* command to open the following dialog:
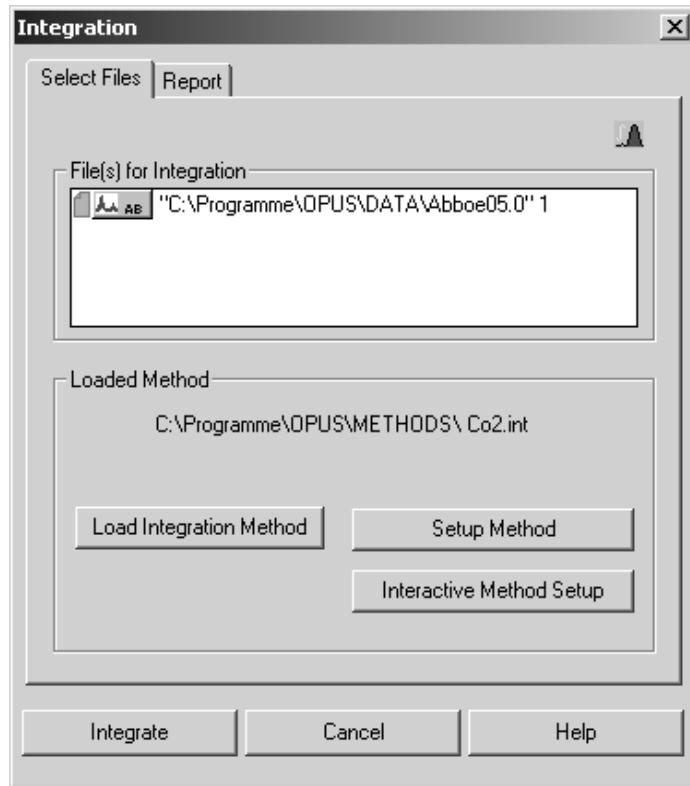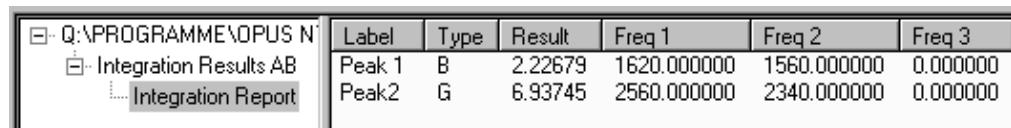
Figure 175: Integration - Select Files tab

Drag & drop the file(s) to be integrated from the OPUS browser window into the *File(s) for Integration* selection field. Before you can start an integration you have to load a method previously created, or set up a new one.

The integration method includes the integration type and the frequency ranges to be considered to integrate spectra. Integration methods have the extension *.INT* and can be stored separately. The integration method previously loaded will be displayed by default in the *Loaded Method* group field, unless you load a different method or create a new one. If no integration method has been loaded, the text reads *No Integration Method loaded*.

To load a method click on the *Load Integration Method* button and select the respective method from the dialog that opens. When creating a new integration method, you can define an integration method for each peak of interest, also see 9.2.1.

The integration result is stored in the INTEG data block (![INTEG]). Right click on this data block and select the *Show Report* option from the pop-up menu. The report displayed includes the frequency limits as well as the integration method used.

Figure 176: Integration Report

The integration report displayed in figure 176 is based on an absorption spectrum (AB) and includes two bands (peak 1 and peak 2) which have been integrated by mode A (also see 9.2.1). In case of this mode the result will be an integral which is indicated by the *Result* column. Mode A requires 2 frequencies per area, indicated in the *Freq 1* and *Freq 2* columns.

If the same spectrum is integrated a second time, e.g. by using a different method, you can select between three different options available to store the report. Click on the *Report* tab.
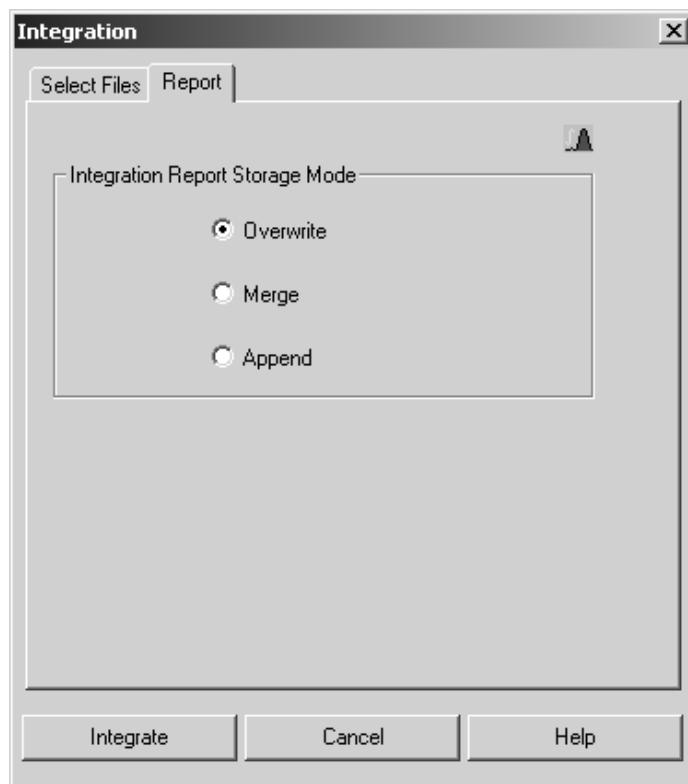
Figure 177: Integration – Report tab

- The *Overwrite* option button is activated by default. By means of this option you can replace an existing integration report.
- If you activate the *Merge* option button, you add the results to an existing report.
- If you activate the *Append* option button, a new single report will be created and appended to the existing file.

Figure 178: Appending a new integration report to an existing one

9.2.1   Set up Method

An integration method specifies the frequencies for one or more areas which are to be integrated. Click on the *Setup Method* button of the *Integration* dialog to create a new method.
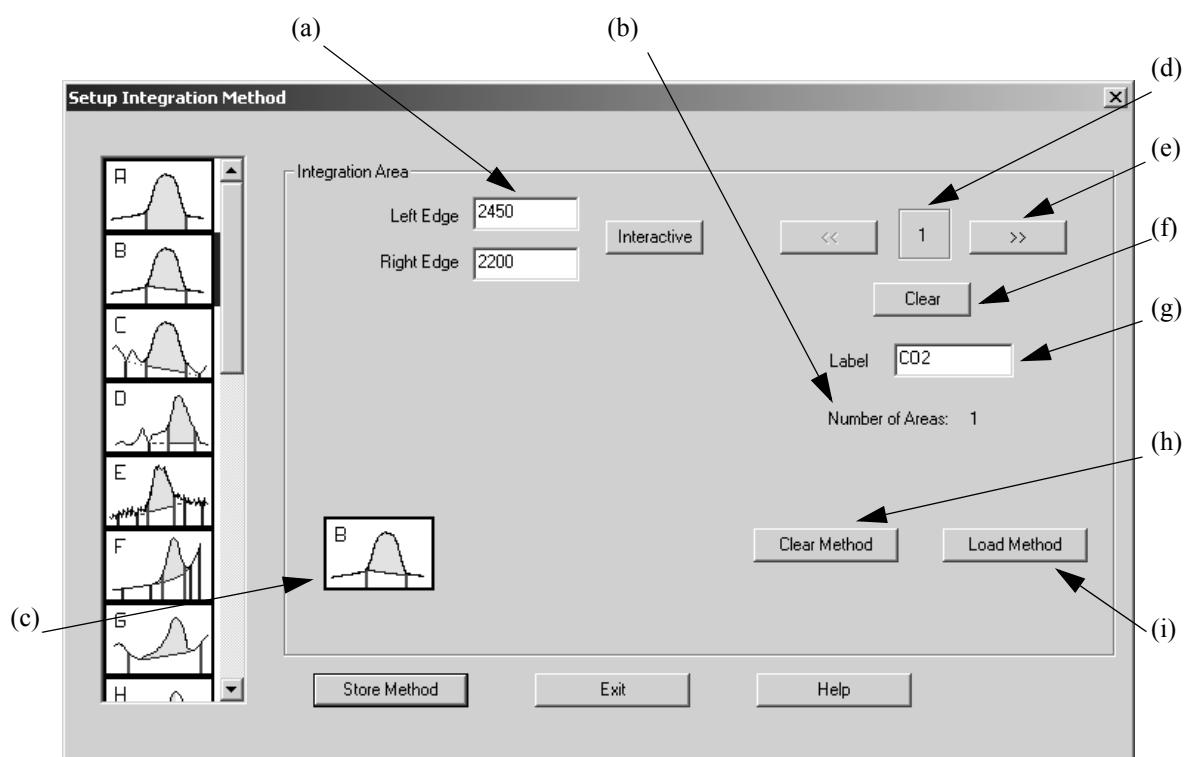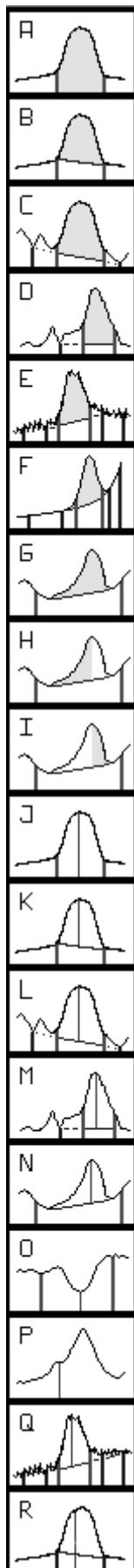

Figure 179: Integration Method Setup

a) Determines the left and right edge used to perform an integration or search an extremum. If you click on the *Interactive* button, you can set the limits interactively.

b) Shows the total number of integration areas.

c) Shows the integration mode used for the current area.

d) Shows the number of the current integration region.

e) Use the forward and backwards buttons (>>) to switch between the integration areas.

f) If you click on the *Clear* button, you can delete limits, baseline points and the label of the area defined by (d), as well as undo the integration mode selected.

g) Shows the label of the current area.

h) If you click on the *Clear Method* button, all areas with the relevant information will be deleted. Before you create a new method click on this button to delete possible default settings caused by the previously loaded integration method.

i) Click on the *Load Method* button if, e.g. you want to add new areas to an existing method, or to edit methods which have been previously created.

Note: Save possible changes by clicking on the *Store Method* button before you exit this dialog. If you fail to do so, the changes will be discarded.

A) The integration will be performed between the band, abscissa and the frequency limits defined.

B) A straight line is drawn between the peaks of the two frequency limits defined. The area above this line will be integrated.

C) The baseline is determined by the first and second baseline point. The area within the band will be integrated.

D) The baseline is horizontal and determined by the baseline point defined.

E) To eliminate noise the average peak values between the 1st and 2nd as well as the 3rd and 4th baseline point are averaged. These average values form the baseline in combination with the abscissa of the 2nd and 3rd baseline point.

F) The baseline is determined by a least square fit of a parabola to the data points between the 1st and 2nd, and between the 3rd and the 4th baseline point.

G) Looks for the highest peak between the left and right edge, and for the minima on the left and right of this highest peak. The baseline connect these minima.

H) Integrates from the maximum to the left minimum.

I) Integrates from the maximum to the right frequency minimum.

J) Highest absolute peak intensity

K) Peak intensity relative to the local baseline

L) Peak intensity relative to the baseline, same as D

M) Peak intensity relative to the horizontal baseline

N) Peak intensity relative to the baseline defined by the minima

O) Minimum between the frequency limits

P) Intensity at the specified frequency

Q) Peak intensity relative to the baseline, same as E

R) Peak intensity at a given frequency

Figure 180: Integration Modes

9.2.2 Interactive Method Setup

To interactively set up a new method first load a spectrum file and click on the *Interactive Method Setup* button of the *Integration* dialog.
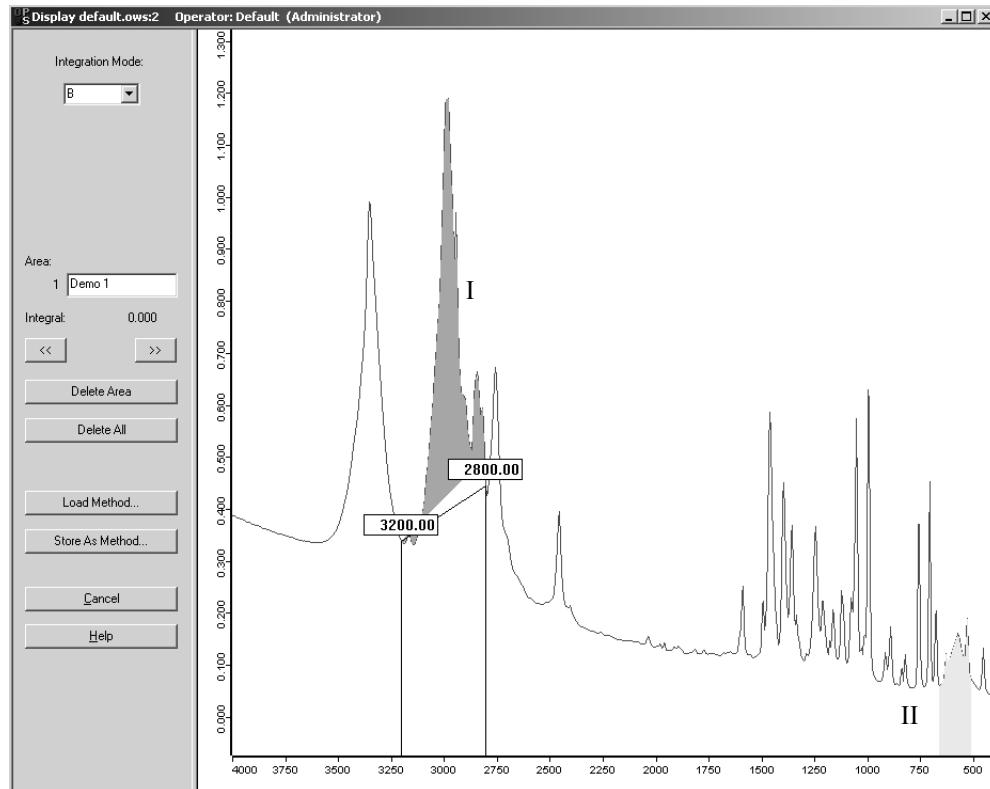

Figure 181: Integration - Interactive Method Setup

The integration modes *A* and *B* (see chapter 9.2.1) are available to interactively set up an integration method. Select either one of them by the *Integration Mode* drop-down list. For integration mode B a straight line (baseline) is drawn between the intensity values of the frequency limits specified. The area above this line will be integrated. In case of integration mode *A* the integration will be performed using zero as baseline.

The limits are exactly defined by the frequency range set. There will be no minimum. To set new baseline points click on a certain band position, press the left mouse button and draw the line. The frequency limits will always be indicated by the exact wave number (see figure 181). A black help line additionally indicates this value on the abscissa.

To change between the different integration areas use the forward (>>) and backward (<<) arrow buttons. Each integration area is defined by a certain name displayed in the *Area* selection field. The number next to this selection field indicates the order in which the integration areas have been defined. The activated integration area is displayed in red (I in figure 181), non-activated areas are displayed in light red (II in figure 181).

To move an integration area you first have to select it. If you position the cursor on the area edge, it will change into ↔. Now, move the area to the position desired.

If you want to delete an area, select it and click on the *Delete Area* button. To delete all areas click on the *Delete All* button.

You can also load a method and apply it to the current integration mode, or define new areas and store them as integration method.

9.3 Quantitative Analysis 1

Quant 1 is the software algorithm used to determine component concentration values for unknown samples. To quantify the components of a multicomponent sample, calibration measurements are required.

Quant 1 is only suited for spectra with well separated peaks. In case of peak overlap the use of Quant 2 is recommended.

9.3.1 Setup QUANT 1 Method

Several samples are necessary for calibration. These calibration samples should contain each component of interest in various concentrations. Furthermore, the concentrations have to be known, i.e. were determined by a different analytical method. Using these calibration samples their spectra can be correlated with the compound concentration.

Each component is assigned to exactly one peak in the spectrum; there are 17 different possibilities (different baselines, intensity or area) to evaluate a peak. Finally, a calibration function (linear, quadratic or polynomial) is fitted to the data obtained from the calibration samples, and this function is then used to determine the concentrations of the unknown sample.

IR spectra are usually depicted as absorption spectra. Ideally, for weakly absorbing compounds, a linear correlation between the concentration and the absorption is to be expected (Beer's law).

A wizard will guide you through the setup of a Quant 1 calibration. Each step will be performed on a separate tab of the dialog. Using the arrows you can flip through the pages.

On the first tab a short overview of the necessary steps is given. You can also load and edit an existing method; this can also be a method created with OPUS-OS/2. In the following we will generate a new method:
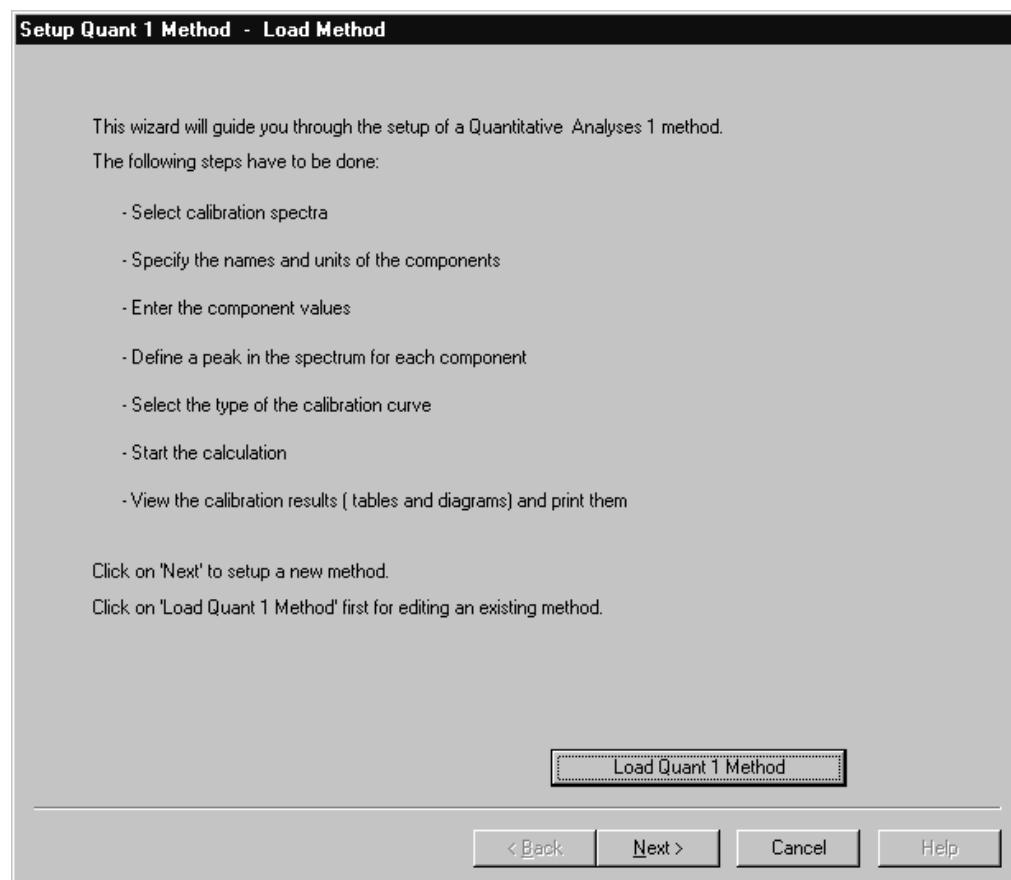
Figure 182: Setup Quant 1

Switch to the next page. Here you can enter the name of the components and their units. Start by clicking on the *Add Component* button.
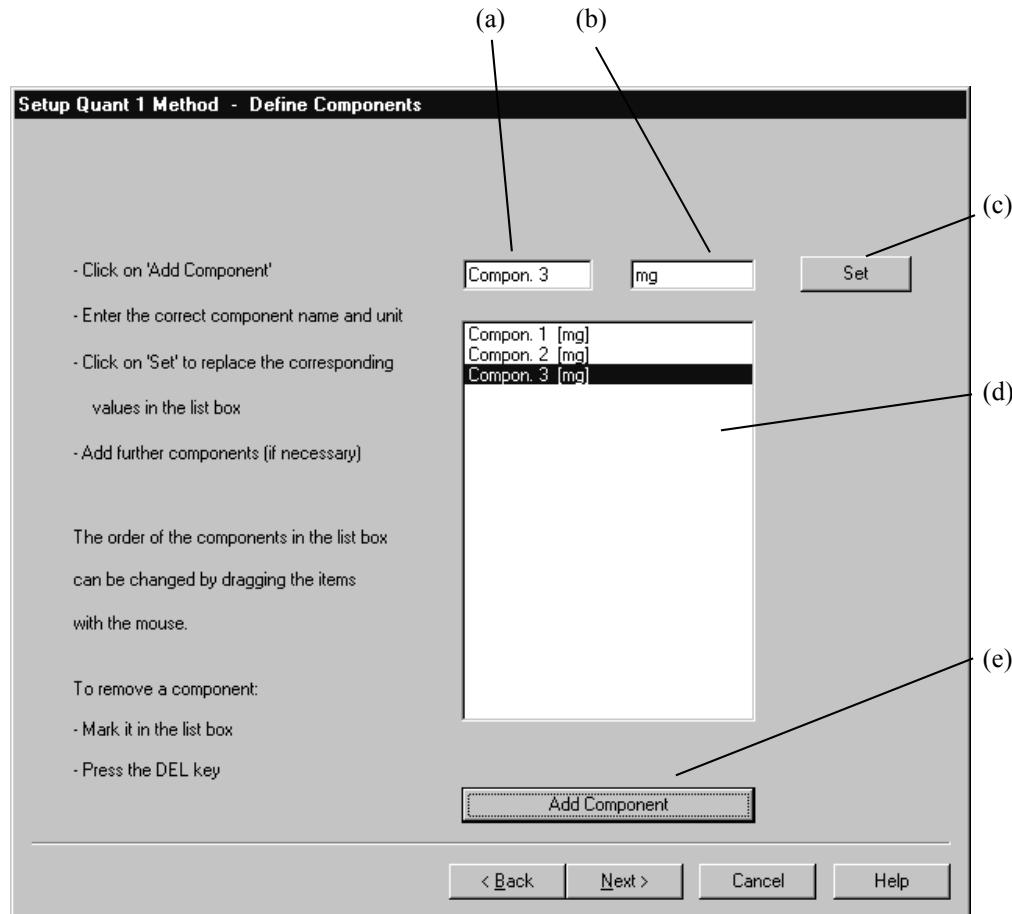
Figure 183: Define Components

The default name of the first component and the unit *mg* appears in the entry fields (a) and (b). If you like, choose a name representative of the compounds you use and save it using button (c). To include additional compounds use *Add Component* (e); list (d) displays all components and weights. To remove a component, select it with the mouse and press the delete key on your keyboard.

On the next page you load the calibration spectra and enter the value of each component for each sample of the calibration set (mg). The example includes 10 spectra and two components.

Figure 184: Component List – Component Value Input

Using the *Add Spectra* button you can include spectra in the list. Navigate to the directory holding the spectra by clicking on *Change Path*. If you want to exclude a spectrum do so by selecting the spectrum and press *Remove Selected Spectra*. You can also print this table for your records by means of the *Print* button.

Previously, you have defined the number of components, their name and value for each sample. Now, you have to define one isolated peak for each component, whose peak height or integral is to be used for calibration.
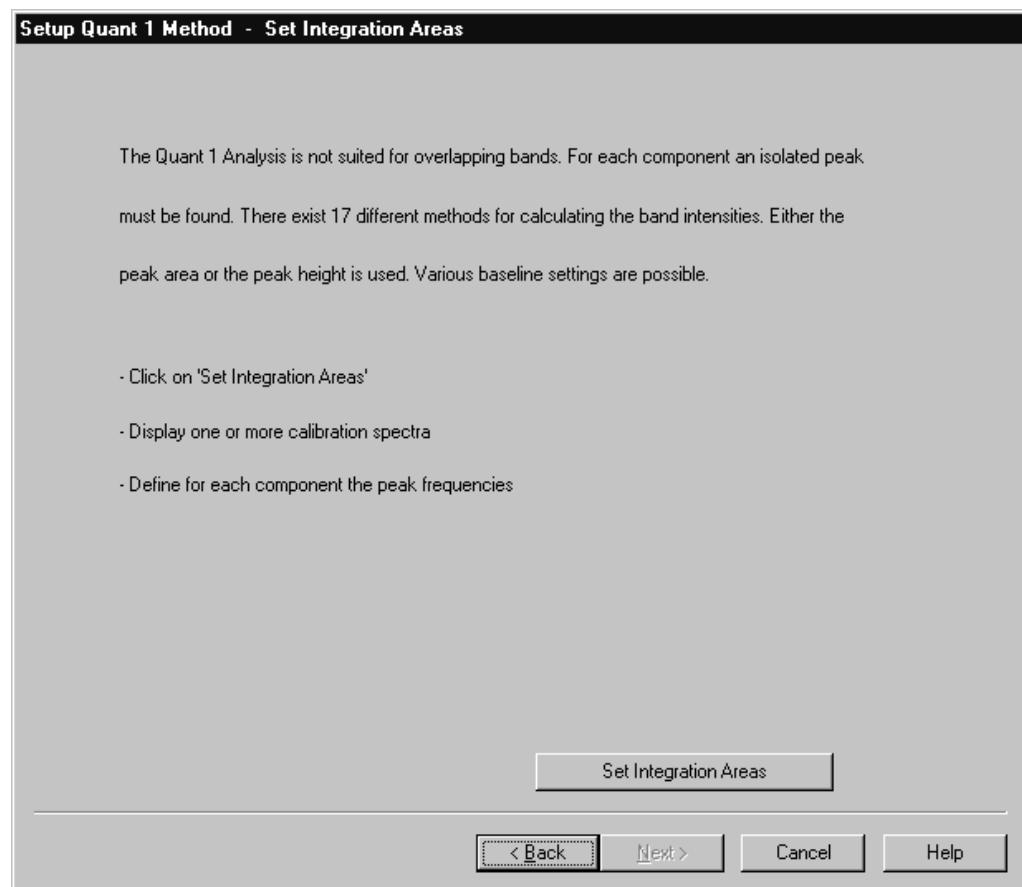
Figure 185: Setup Integration Method

Click on the *Set Integration Areas* button and select an appropriate method as well as the frequency limits as described in the integration chapter of this manual.
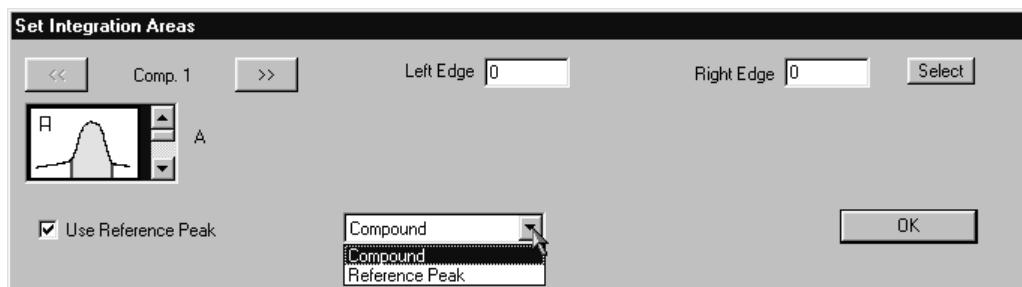
Figure 186: Defining the Integration Method

In addition, you have the possibility to define a reference peak by placing a mark in the *Use Reference Peak* check box. Select an integration method and frequency region for this peak as you would for any other peak. Be sure to indicate *Reference Peak* in the drop-down list. This reference peak will be used to normalize the spectrum.

As the final step you must define the type of calibration function you would like to fit to your calibration set. While a linear function is suitable for samples which obey Beer's law, deviations can be taken into account by choosing a quadratic or cubic function.
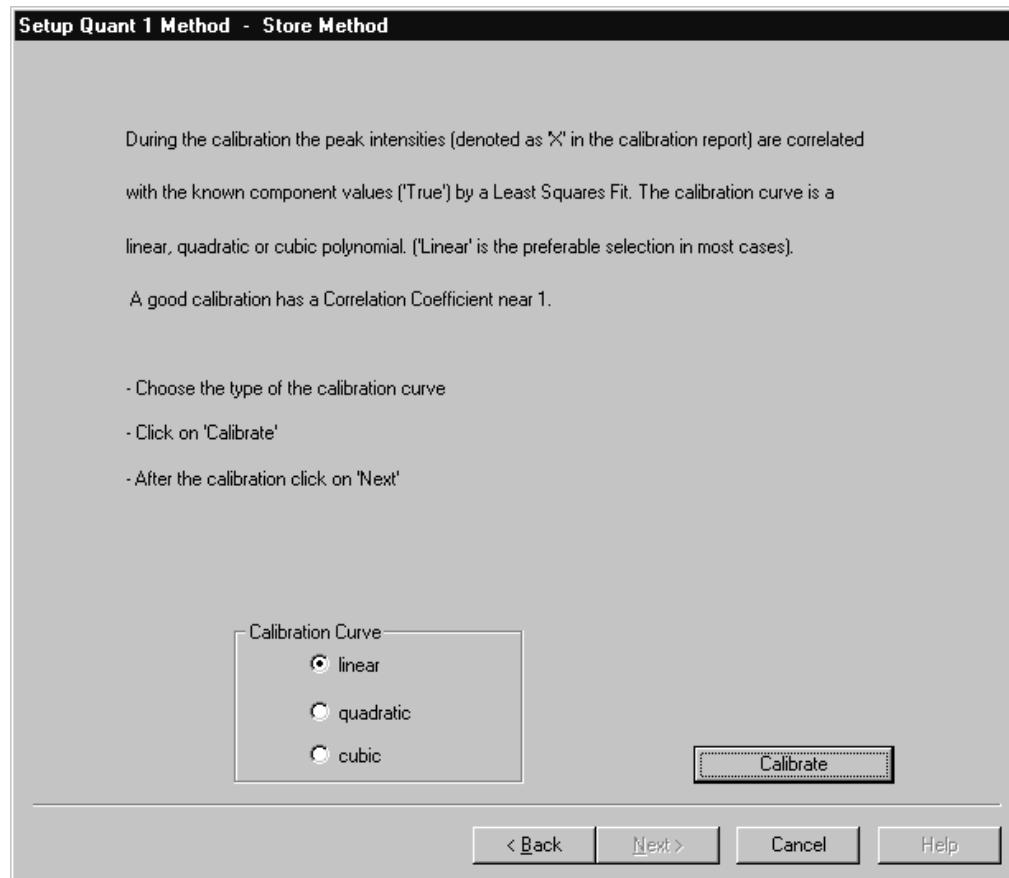
Figure 187: Choose Calibration a Method

After you have set up your Quant 1 method you will be asked to save the method to disk. Usually, Quant methods will be saved in the "Quant" subdirectory of the OPUS folder. Then the computation of the calibration function starts. Depending on the number of calibration spectra, this may take up to a few seconds or longer.

Click on *Next* to display the results of the calibration. Each component has its own tab. The first column lists the file names of the calibration set. The true value (i.e. the known amount of the substance) and the value calculated by the fit are given in the next two columns. The difference between these values, the error of the calculated value and the peak size "X" calculated from the spectra are also shown.

	Filename	True	Fit	Differ	Error (%)	X
1	ST100.0	4.5	4.505	-0.004836	-0.107	101.6
2	ST101.0	1	0.9861	0.01389	1.39	22.72
3	ST102.0	2.4	2.406	-0.00573	-0.239	54.56
4	ST103.0	3.6	3.595	0.005131	0.143	81.23
5	ST104.0	2.5	2.492	0.008003	0.32	56.5
6	ST105.0	1.6	1.618	-0.01807	-1.13	36.89
7	ST106.0	0.6	0.593	0.006991	1.17	13.9
8	ST107.0	1.6	1.601	-0.0006851	-0.0428	36.5
9	ST108.0	3.5	3.495	0.004988	0.143	78.99
10	ST109.0	1.9	1.906	-0.005542	-0.292	43.34
11	ST110.0	3.9	3.897	0.002584	0.0663	88.02
12	ST111.0	3.6	3.61	-0.01025	-0.285	81.58
13	ST112.0	4.2	4.189	0.01146	0.273	94.55
14	ST113.0	2.7	2.693	0.007015	0.26	61
15	ST114.0	1.8	1.809	-0.00939	-0.522	41.19
16	ST115.0	1.4	1.399	0.0006697	0.0478	31.99
17	ST116.0	2.6	2.626	-0.02574	-0.99	59.5
18	ST117.0	0.6	0.592	0.00797	1.33	13.88
19	ST118.0	2.5	2.489	0.01095	0.438	56.43
20	ST119.0	3	2.992	0.007709	0.257	67.72
21	ST120.0	1.2	1.207	-0.007047	-0.587	27.68
22	ST121.0	0.9	0.9001	-8.126E-005	-0.00903	20.79

Figure 188: Calibration Results

You can switch between the result pages for each component using the arrow button. Toggle between the tabular view and a report view of the results by selecting the *Calibration Report* check box. The report view will give you a printable version of the report. Clicking on *Next* will get a graph of the calibration result. The graph allows one to easily recognize data with poor correlations (for example incorrect values caused by typographical errors during data entry).
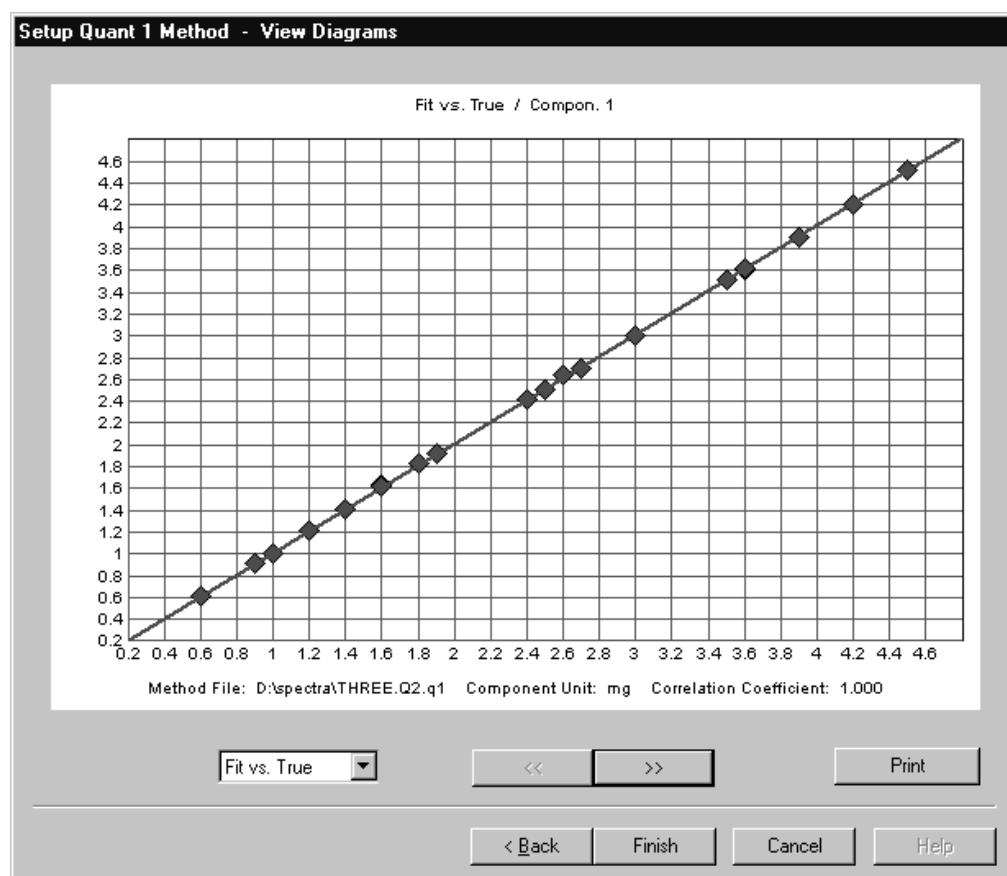
Figure 189: Graphic Display of Calibration Results – Fit vs. True

Below the graphics, The method file, the correlation coefficient and the calibration equation are stated.

Using the pull-down menu at the bottom of the graph you can switch between different representations of the calibration result: "Fit vs True" displays the values obtained by the fit against the known (true) values of the component. Other options are "Difference vs. True" or "True vs. X".
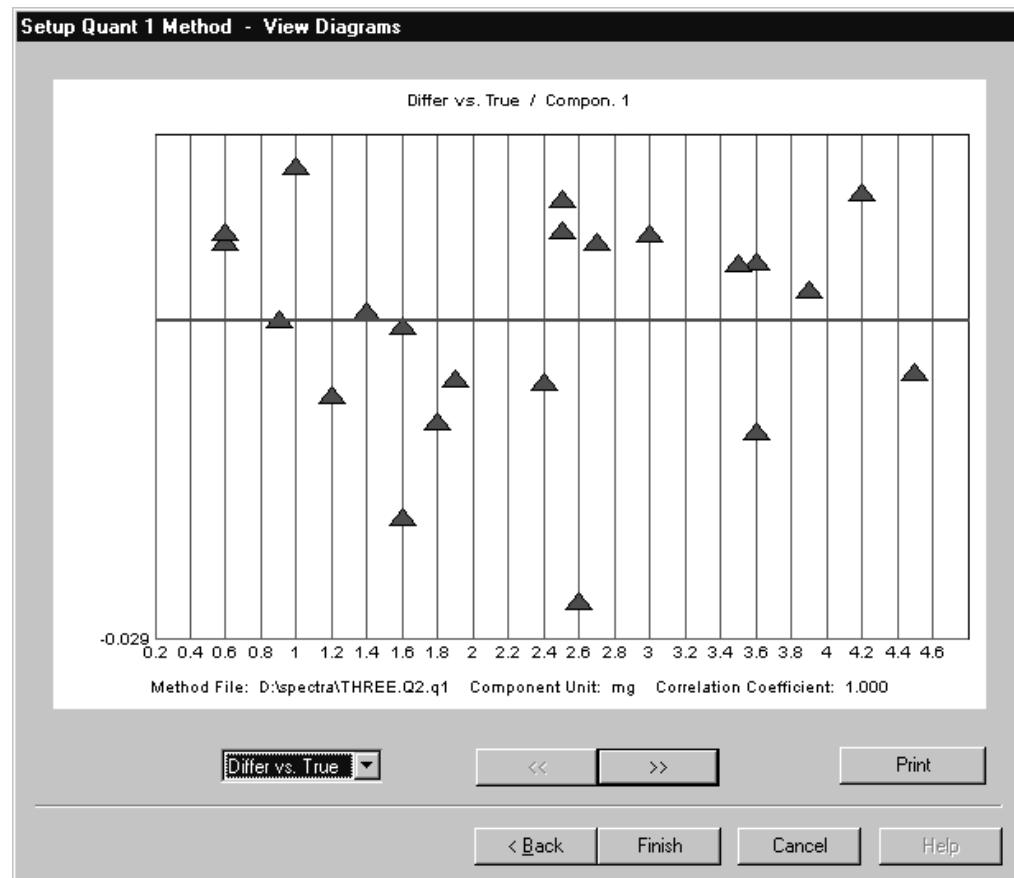
Figure 190: Graphic Display of Calibration Results – Difference vs. True
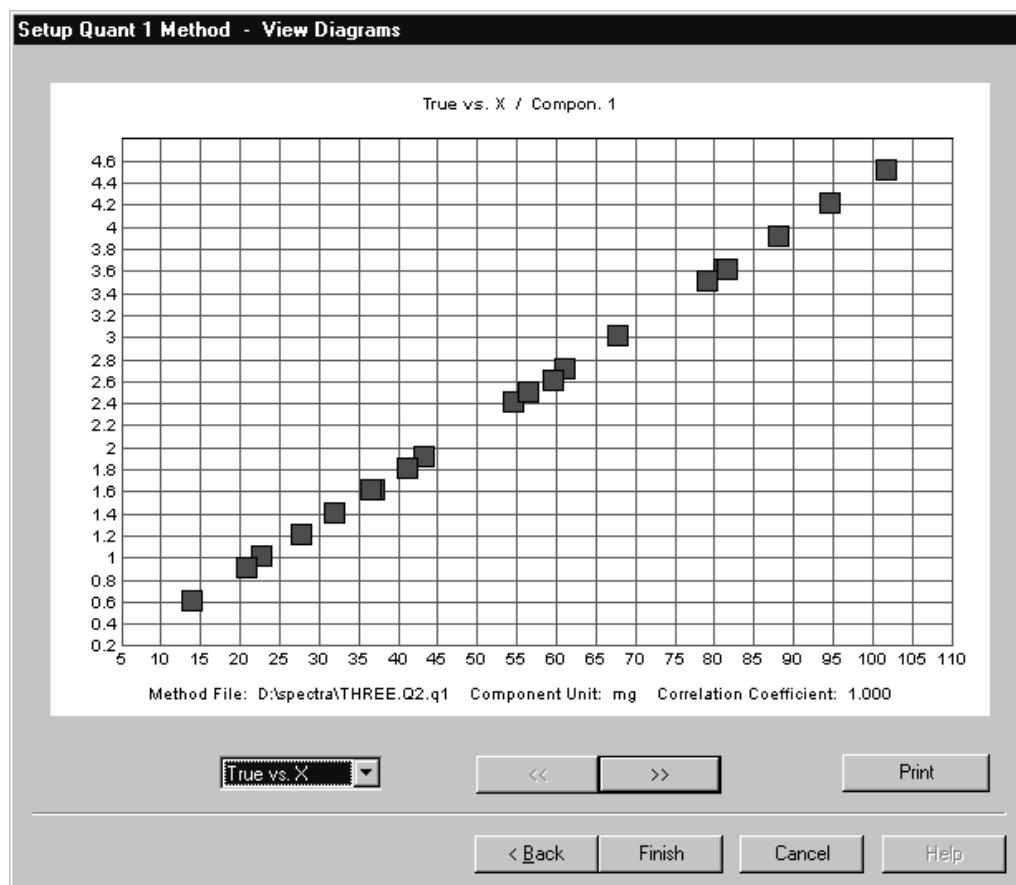
Figure 191: Graphic Display of Calibration Results – True vs X

You can print the results, the figures as well as the data tables, using the *Print* button. A report of the results including the calibration equation is stored together with the method file. Exit the program by clicking on *Finish*.

9.3.2 Quantitative Analysis 1

After you have created a calibration set you can now start to analyze your samples. Keep in mind that the concentration of the samples should fall within the concentration interval covered by the calibration set. Furthermore, the spectrum of the unknown sample must be acquired using the same parameters as for the spectra of the calibration set.
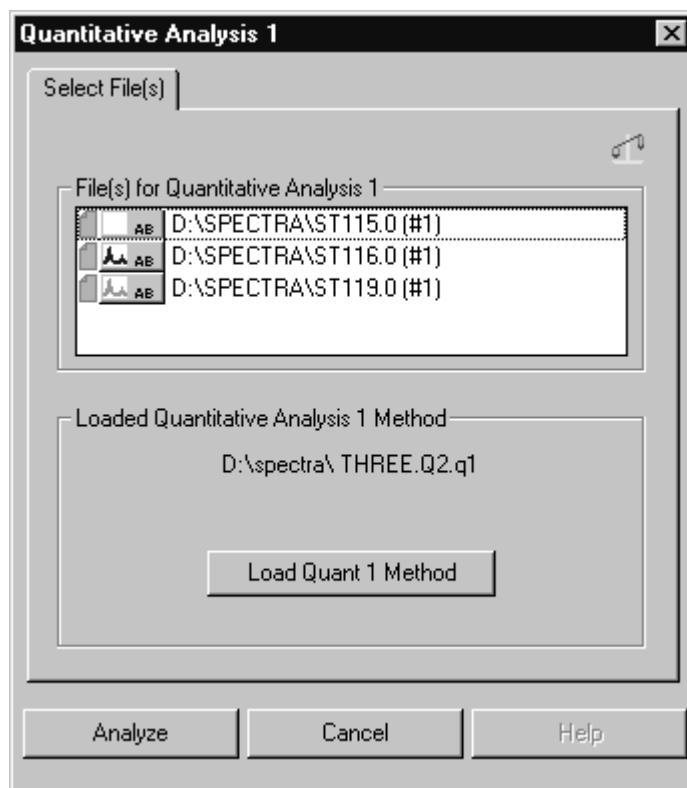
Figure 192: Quantitative Analysis
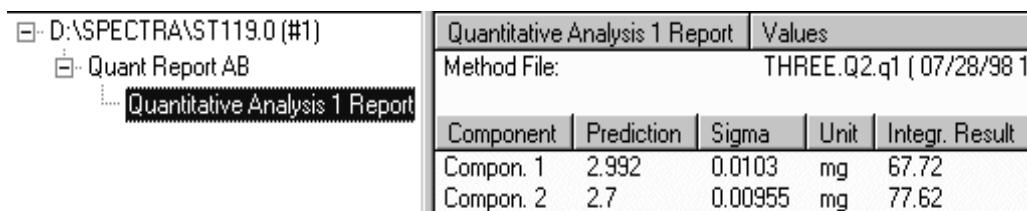
Select the spectra you wish to analyze and load the appropriate Quant 1 method. If a method had been created or loaded before, it will automatically be available for the analysis.

Click on *Analyze* to start the analysis. The result will be saved in a Quant 1 data block together with the analyzed spectrum and the spectra will be marked as modified in the browser.

Figure 193: Quant Info Block

Like every other report, you can read Quant reports by opening a report window. Open the header of the report by right-clicking on the report window. The header contains the name of the Quant method used for the analysis and the date the method was created. The report lists the component names, their predicted concentration together with their units, the correlation coefficient sigma and the results of the peak integration.

Figure 194: Quant 1 Report

You can apply more than one Quant method to analyze a spectrum; the resulting reports are saved in the same report data block. They appear as entries in the tree of the report window. Switch between reports by clicking on the report name of the tree.

Theory:

The functions used for the calibration will be saved in the calibration record as Y = f(X); where the Y are the values obtained by the fit and X is the peak size obtained from the spectra. Sigma is a parameter representing the difference between predicted and true value. Keep in mind that the *true* values are also prone to statistical errors, depending on how carefully they have been determined. An indication for the quality of the calibration is the correlation coefficient r:

$$r = \frac{\sum((Z_i - Z_m)(Y_i - Y_m))}{\sqrt{\sum(Z_i - Z_m)^2 \sum(Y_i - Y_m)^2}}$$

Here, Z stands for the true concentrations of the components, while m is the respective average value. The correlation coefficient should be close to 1.0.

The error in analyzing samples of unknown concentration can be estimated by σ. There is an approximately 68% probability that the concentration of the unknown sample falls within an interval of the predicted value plus or minus σ:

$$\sigma = \sqrt{\frac{1}{M-f}\sum(Z_i - Y_i)^2}$$

M: number of calibration samples
f: degree of freedom (linear 2, quadratic 3, cubic 4)
Z: true concentration
Y: predicted concentration

9.4 Signal-to-Noise Ratio

This command calculates the Signal-to-Noise ratio (SNR) of a spectrum over a given spectral range. The results may be stored with the spectrum.

Two S/N values are calculated: RMS (Root Mean Square) and PP (Peak to Peak). In both cases a function is fitted to the spectrum in the region of interest. This command is either a straight line or (optionally) a quadratic parabola. This curve defines the (nominal) signal. RMS is calculated as the root of the mean square of deviations (i. e., the standard deviation). PP noise is the peak to peak excursions (maximum - minimum) in the y-direction.

Some spectra types (e. g. Absorption, Emission) have base lines near zero. Specifying a Signal-to-Noise ratio makes no sense in these cases.

The (mean) nominal signal is divided by the newly calculated noise values and yields the SNR. The result for the PP SNR is always smaller ("worse") than that for the RMS value.
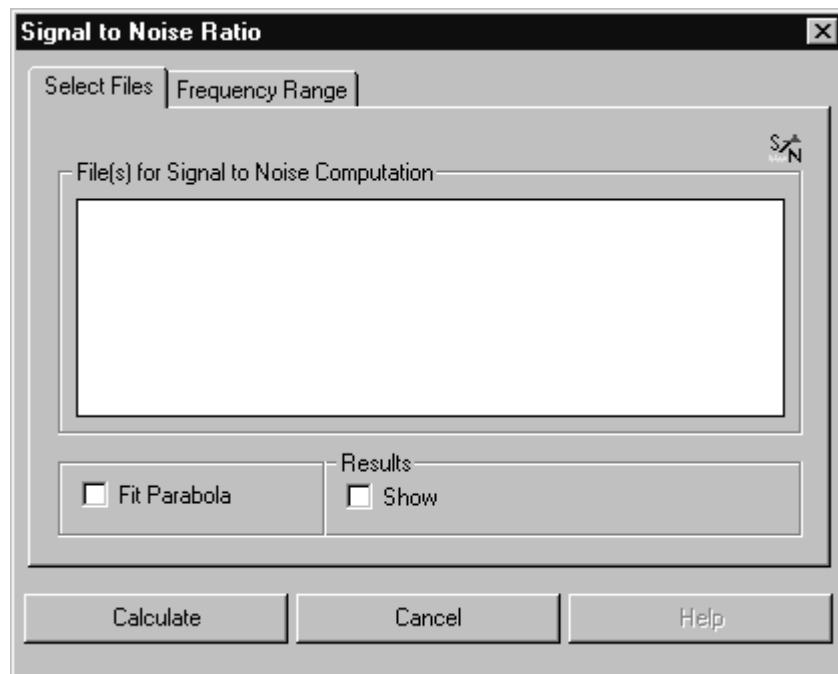
Figure 195: Signal-To-Noise Ratio

You can choose the parabolic fit function by checking the *Fit Parabola* box, otherwise a linear function is automatically fit to the data. Click on *Show* to display the results of the fit. If desired, you can save the fit in combination with the spectrum.
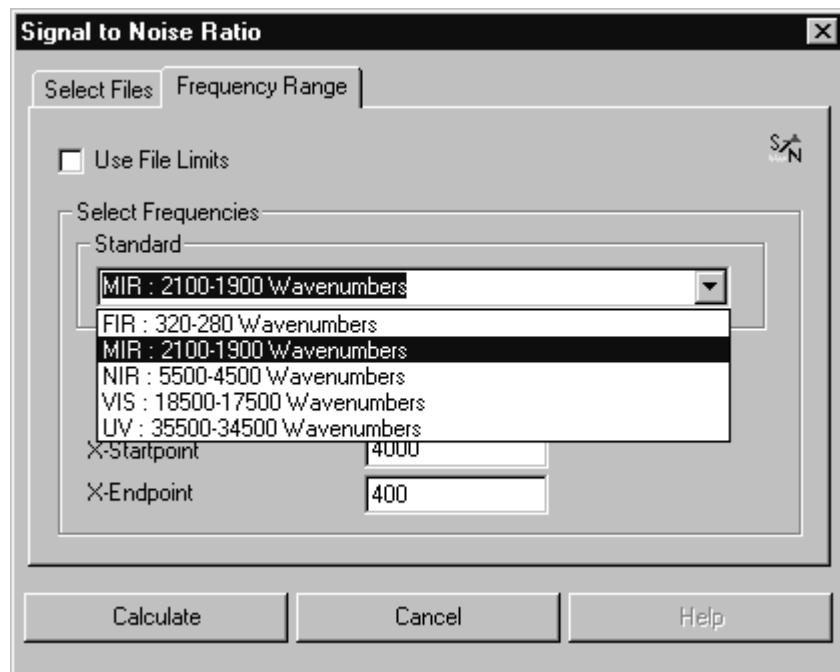
Figure 196: Select a Frequency Range from the Pull-down Menu

The frequency range is entered on the second tab; in addition to manual input, pre-defined spectral ranges are provided.
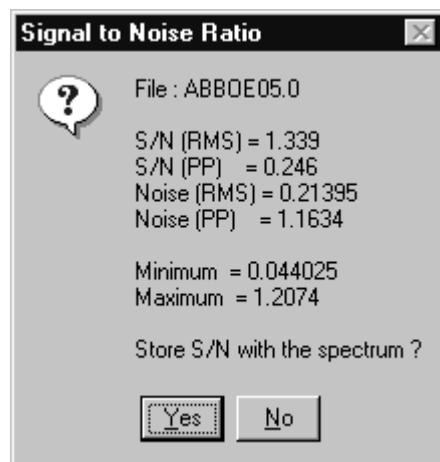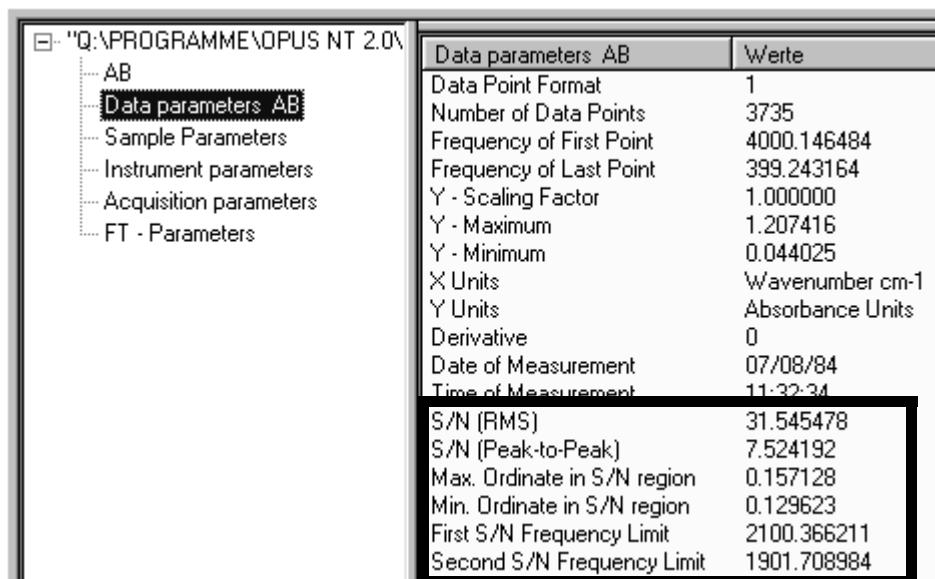
Figure 197: Signal To Noise Evaluation

Minimum and *Maximum* gives the extrema of the ordinate values over the evaluated range. To locate the results of a SNR calculation, open a new report window by right-clicking on the "Display" icon in the Browser. Drop the file of interest into the report window and open the "Data Parameters AB" branch (alternatively, right-click directly on the file name and choose *Show Parameters*).

Figure 198: Report Window Showing Data Parameters AB Branch

9.5   Peak Picking

The *Peak Picking* command helps you to identify peaks in spectra. The command offers high flexibility and allows to adjust and fine tune the search parameters.

Select the *Peak Picking* command and drag & drop the spectra from the OPUS browser window into the *File(s) to peak picking* selection field. Define the frequency range by clicking on the *Frequency Range* tab. Specify the *Sensitivity* on the *Select Files* tab, which is the most important parameter for the identification.
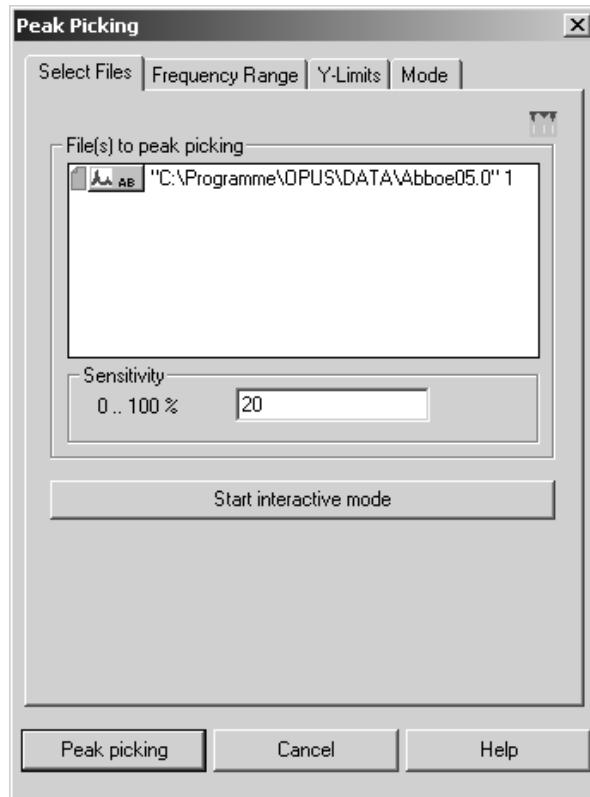
Figure 199: Peak Picking – Select Files tab

To work in interactive mode click on the *Start interactive mode* button. According to the threshold value set by the slider the number of identified peaks changes (see figure 200).
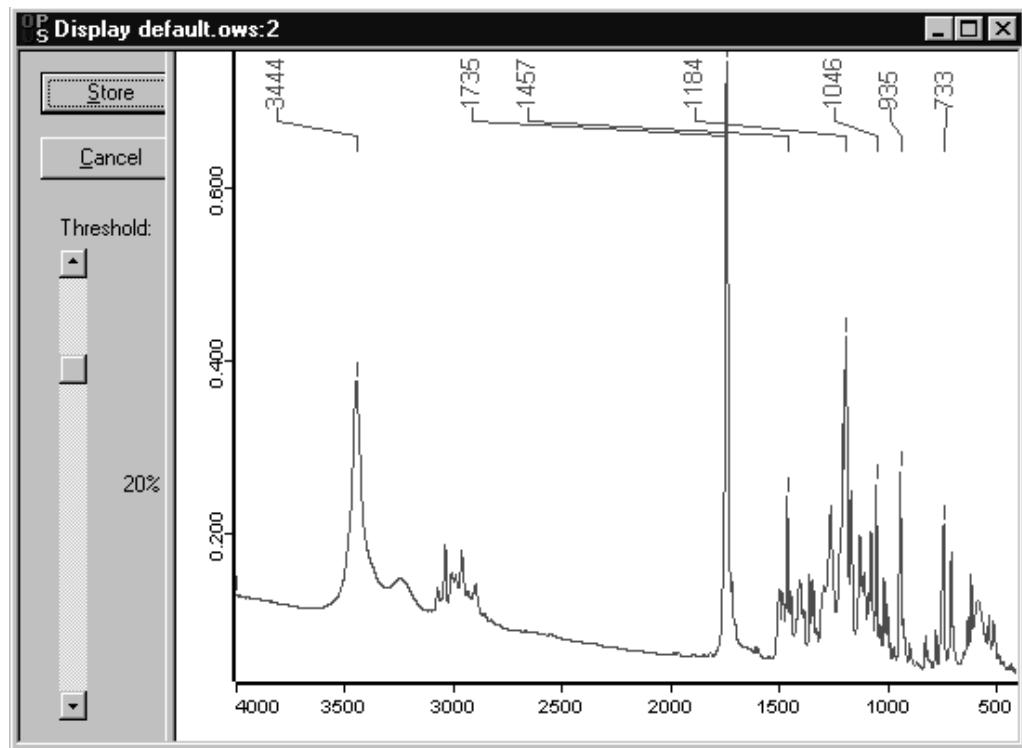
Figure 200: Peak Picking – Interactive Mode

In some applications very small bands may be neglected, and in other cases high-intensity peaks are normal and thus the low-intensity peaks may be crucial. Therefore, specify the intensity range to be considered for the peak picking on the *Y-limits* tab.
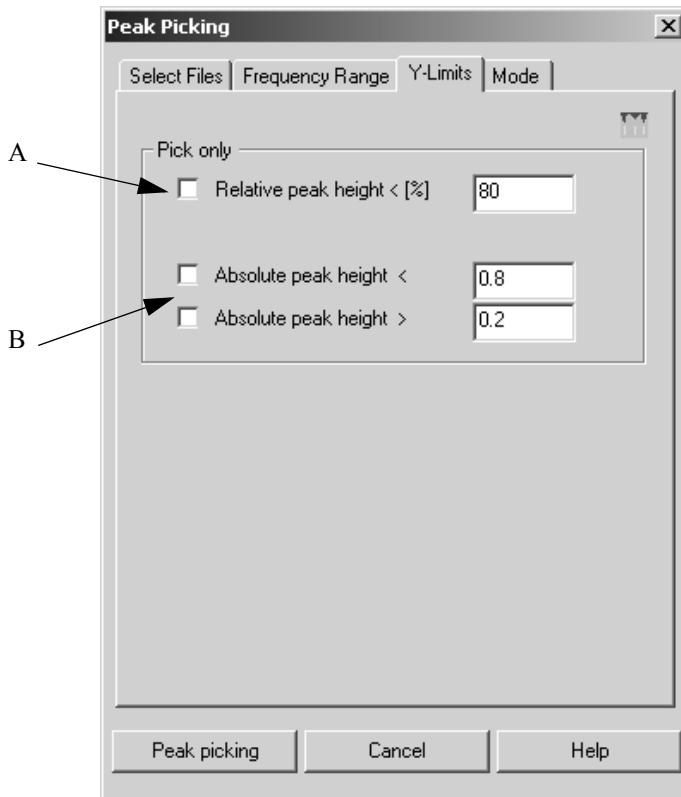
Figure 201: Peak Picking – Y-Limits

The relative peak height (A in figure 201) allows to define a maximum peak intensity in relation to the surroundings of the peak and the baseline. It is also possible to define an absolute peak height in absorption units, i.e. to specify the limits as absolute absorption values (B in figure 201).

In case of absorbance spectra usually the maxima are of interest, whereas for transmittance or reflectance spectra the minima are the important features. This can be accounted for by selecting the appropriate peak picking mode on the *Mode* tab. The *Automatic* mode uses the spectrum type information stored in the data block to determine if maxima or minima are picked.

Not very often (e.g. when subtracting photoacoustic spectra) is it necessary to specify whether the algorithm should pick for minima (i.e. transmittance spectra) or maxima (i.e. absorbance spectra).
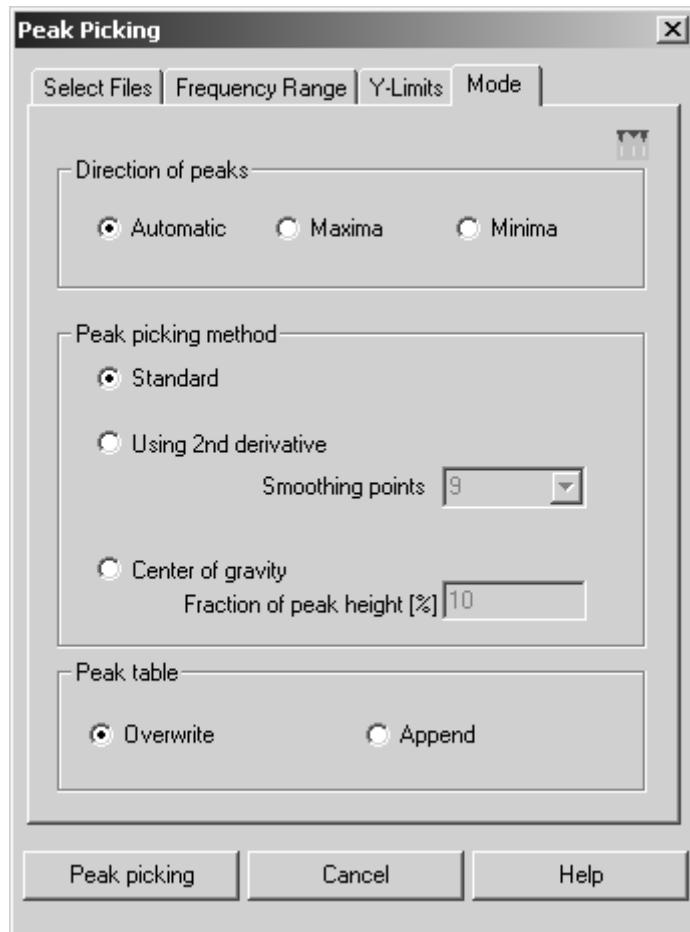
Figure 202: Peak Picking – Mode tab

To be independent of the baseline, the second derivative algorithm is typically used, since the first derivative does not isolate peaks sufficiently well in case of weak shoulders. The Savitzky-Golay algorithm is actually used to obtain the derivative.

The number of smoothing points used can be adjusted to suppress the effect of noise. As a rule of thumb, the number of smoothing points should not be greater than the full width at half maximum of the smallest peak of interest. This value is ignored when using the standard method.

An additional peak picking method is the calculation of the center of gravity. This algorithm calculates, from a certain fraction of peak height, the centroid of an area. The position of this centroid determines the peak position. Specify which portion of band area (in %) has to be considered to calculate the gravity, in the *Fraction of peak height* entry field. You can only enter integers between 1 and 99.

The center of gravity method yields the same results in case of symmetric bands. In case of antisymmetric bands the band position is moved towards the broader edge. This interacts with the size of the peak height used for the

calculation. If the fraction of peak height is too small, the band will not be listed on band list. Too small a fraction of peak height would decrease the number of measuring points, used to calculate the band position, to less than 3.

The band position is calculated as follows:

Based on the band maximum Y_{max}, X_{max}, which is usually not the maximum of the measuring values, the measuring points are consecutively numbered to the left and right. The numbering starts from 0 for both sides, while the y- value of each measuring point must be greater than $Y_i \geq Y_{max} - (Y_{max} - Y_{min}) \cdot Fraction$, with Y_i being the measurement values, and the *Fraction* term being the percentage value defined for the peak height. This yields to the following sums:

$$SumY = \sum_{i=0} (Y_{right}(i) - Y_{Fraction}) + \sum_{i=0} (Y_{left}(i) - Y_{Fraction})$$

$$SumYX = \sum_{i=0} (Y_{right}(i) - Y_{Fraction}) \cdot (i + 0,5) - \sum_{i=0} (Y_{left}(i) - Y_{Fraction}) \cdot (i + 0,5)$$

Thus, the band position yields

$$PeakPos_{COG} = [x_{max}] + 0,5 + \frac{SumYX}{SumY}$$

whereas $[x_{max}]$ represents the next smaller integer of the x-value for the band maximum.

The band position in wave number units is:

$PeakPos_{COG}(v) = PeakPos_{COG} \cdot \Delta v + v_{min}$ and Δv being the wave number distance between two measuring points and v_{min} being wave number of the first data point.
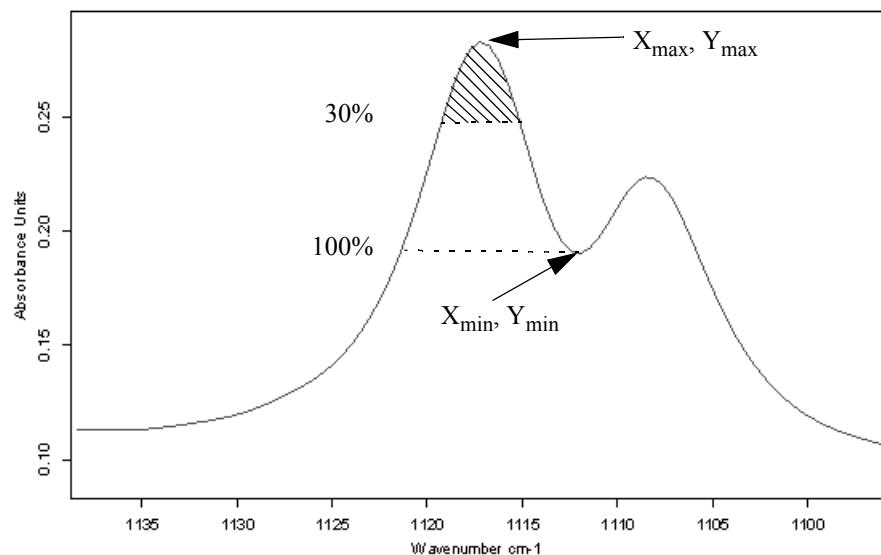
Figure 203: Band edge

If you use the *Peak Picking* command on a spectrum that already has a peak table appended, you can either overwrite the previous table by the new one, or append the new table to the existing one.

Theory:

The standard method is used for peaks with small or no overlap in spectra of low or average spectral resolution (0.5cm^{-1} or above).

The x-position is the x-value of the interpolated maximum or minimum, with intensity being the y-value of this point. To determine the relative intensity an internal local baseline between two lateral minima (or maxima) is drawn. The relative intensity is then the y-axis distance between this baseline and the maximum (or minimum).
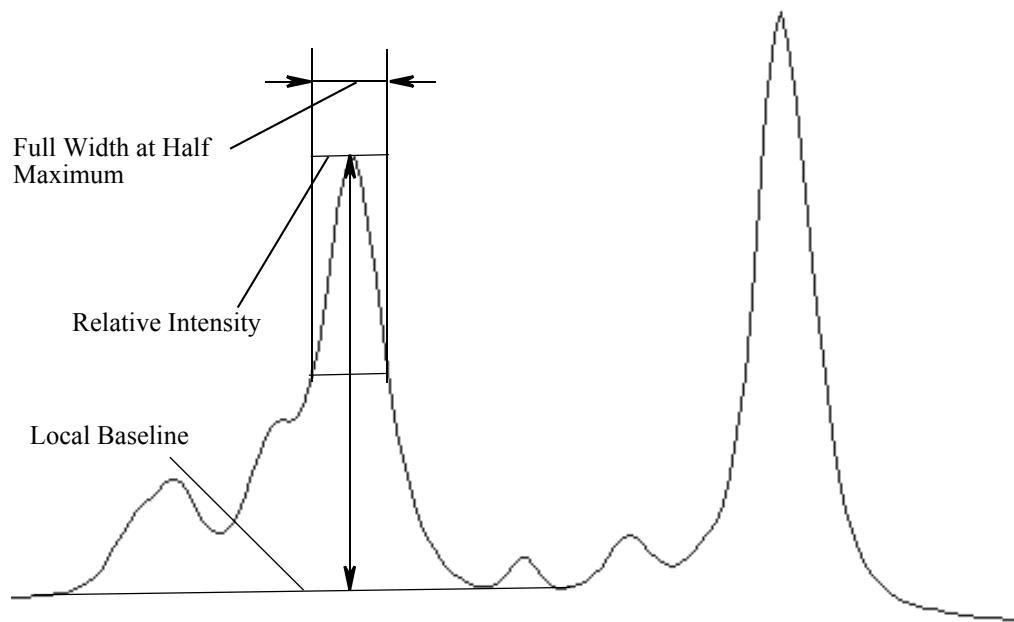
Figure 204: Spectrum with Line width, Relative Intensity and Baseline Indicated

The lateral extremes are determined by going outwards from the x-position of the line, until another line at least as strong is found (or the end of the spectrum is reached). The lowest point in this interval is then used as a lateral minimum (or maximum).

To find the line width, a line parallel to the local baseline is drawn which intersects the middle of a vertical line connecting the maximum (or minimum) of the band and the local baseline.

Peaks will be included in the peak pick table if their relative intensity falls within the interval defined on the *Y-Limits* tab. This interval was normalized such that the difference between maxima and minima corresponds to 100%. The definition of the upper limit is optional and can be used to mask, for example, large water bands.
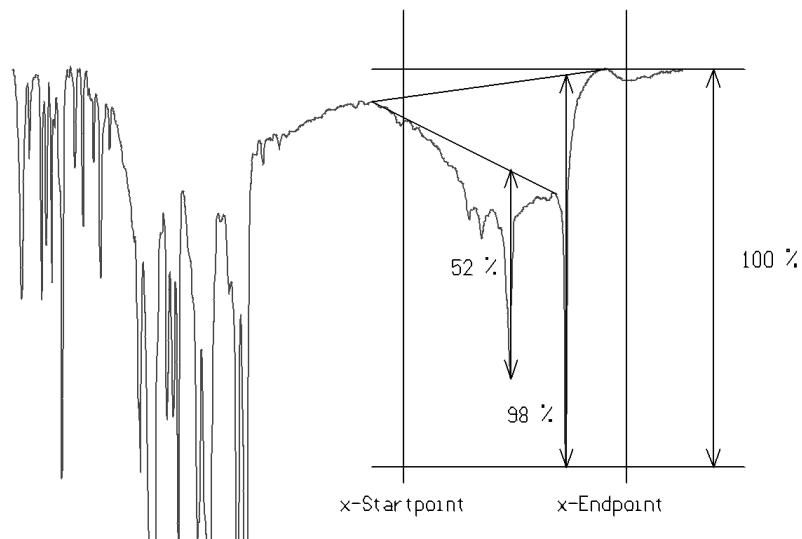
Figure 205: Calculation with Baseline Reference

The peak search using the second derivative method is recommended for high resolution spectra only.
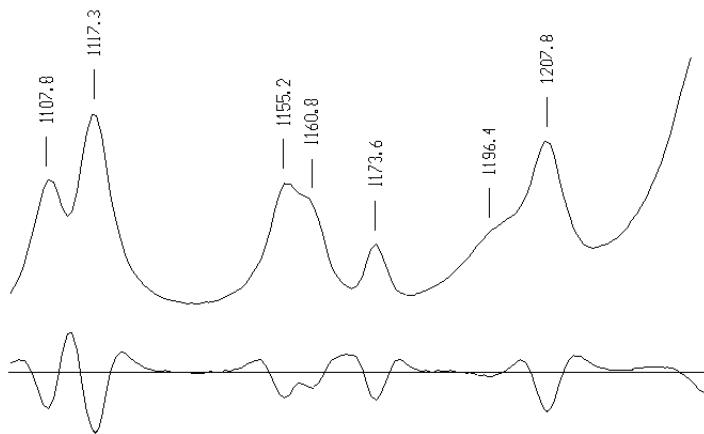

Figure 206: Absorption Spectrum and Second Derivative

The x-positions are the x-values of the minima (or maxima) of the smoothed, second derivative spectrum. This is particularly useful for seriously overlapping bands because in this case an extremity of the spectrum is frequently not shifted with respect to the true band position. Weak shoulders can also be recognized using the second derivative method.

In order to calculate the relative intensities and the width of the peak, the zero-points and the minima of the second derivative are computed. These points are significant for the peaks that make up the envelope:

$[\nu_{-1}, 0]$ (zero-point)

$[\nu_0, I''_0]$ (minimum)

$[\nu_1, 0]$ (zero-point)

In figure 207 two Lorentzian curves are superimposed. The zero-points and the minima of both signals are almost identical (both for the derivatives of the isolated signals as well as for their superposition). The maxima of the overlapped signals are shifted and therefore misleading.

If a strong signal overlaps a weak signal, a maximum could be found where a zero-point should be. If a maximum is found prior to a zero-point, during the search for a minimum of the second derivative, the position of the maximum has to be used instead. This points to the limitations of the method.

Apparent Peak Positions

True Peak Positions

Apparent Peak Positions

True Peak Positions
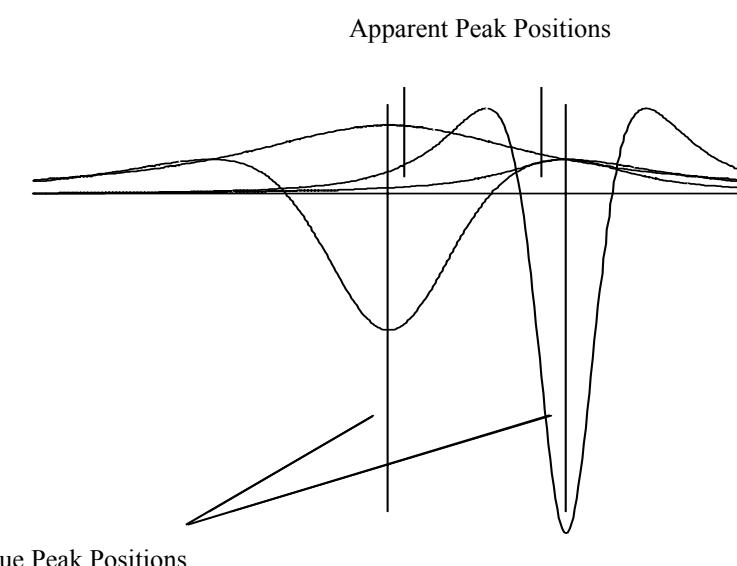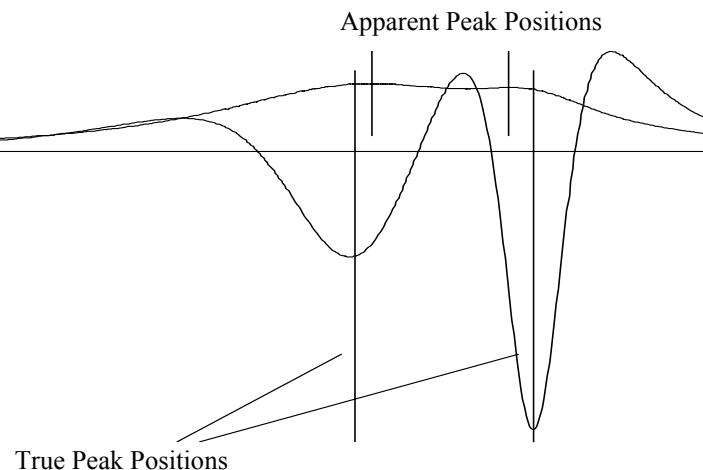
Figure 207: Apparent and True Peak Position

To access the Peak Table, right-click on the Peak Pick report block and select the *Show Peak List* command from the pop-up menu. A table created using the standard method for low resolution spectra and relative intensities of higher than 10% (accuracy to 4 decimal points) could look like the following:

	Peak Picking	Values	
⊟·"E:\PROGRAMME\OPUS 2.0	Method:	Standard	
⊟·Peak Table AB	Searched for minima:	No	
┊···Peak Picking	Number of peaks:	19	
	Sensitivity > [%]:	10.000000	
	From:	4000.146484	
	to:	399.243164	
	Peaks > [abs.]:	0.000000	
	Peaks < [%]:	0.000000	
	Peaks < [abs.]:	0.000000	

Wavenumber	Abs. Intensity	Rel. Intensity	Width	Found if Threshold <	Shoulder
3350.199	1.001	0.666	87.012	57.068497	0
2991.063	1.208	0.891	45.614	75.167953	0
2941.990	0.995	0.148	7.942	12.581351	0
2840.313	0.670	0.192	49.294	13.778638	0
2755.903	0.679	0.259	32.663	21.586529	0
2453.723	0.411	0.201	20.498	16.598145	0
1585.035	0.286	0.168	10.258	14.209115	0
1459.848	0.609	0.495	20.159	42.362061	0
1394.194	0.470	0.331	15.972	28.272161	0

Figure 208: Result of a Peak Search

9.6   Quick Identity Test

The Quick Identity Test offers a user friendly method to judge the similarity of two spectra. This method requires a reference spectrum of the substance of interest. The test determines the Euclidean distance between the test and reference spectrum.
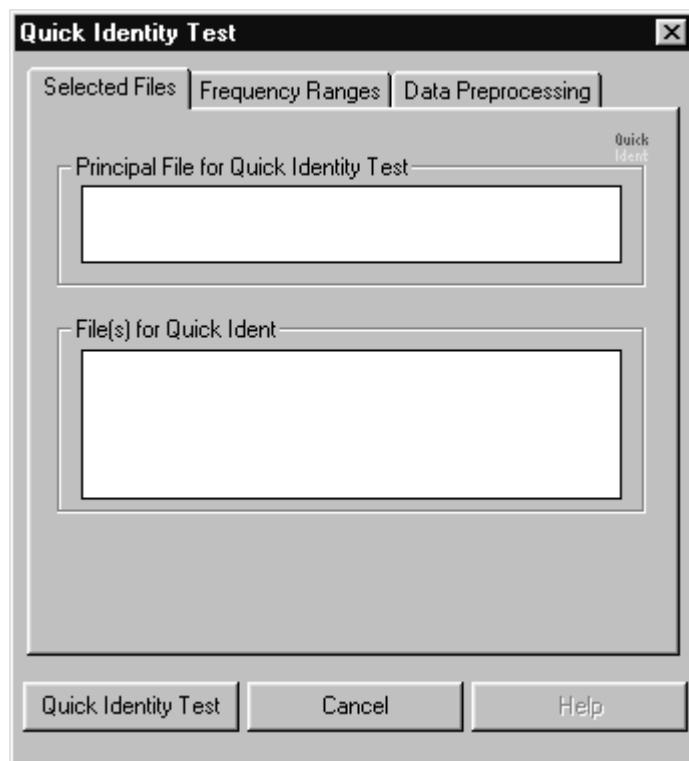
Figure 209: Quick Identity Test – Selected Files

Enter the reference spectrum in the field *Principal File for Quick Identity Test,* and the files to be tested in the field *Files for Quick Ident*.

You can define several frequency regions on the *Frequency Ranges* tab. The data of the regions indicated will be compared, only. You can also compare the frequency range common to all spectra by activating the *Use File Limits* check box. Switch between regions by using the arrow key. Delete a region by clicking on the *Clear* button.
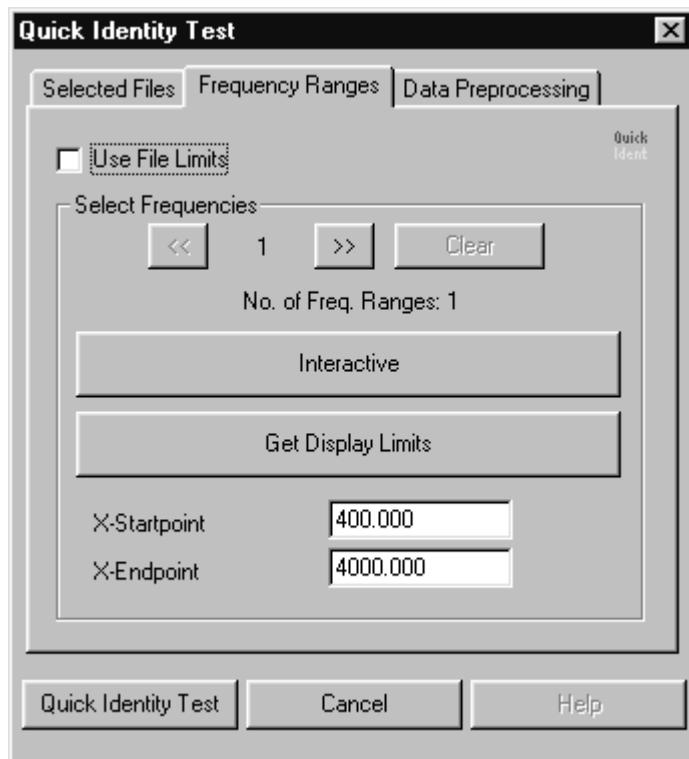
Figure 210: Quick Identity Test – Frequency Ranges

Select a data preprocessing method, the derivative or the vector normalization. A vector normalization causes the Euclidean distance to fall within an interval of 0 and 2.

On the third tab you can define the data preprocessing method. It is possible to perform a spectrum derivative and vector normalization. The latter has to be selected to be able to set the scale level of the spectral distances to a value range between 0 and 2.
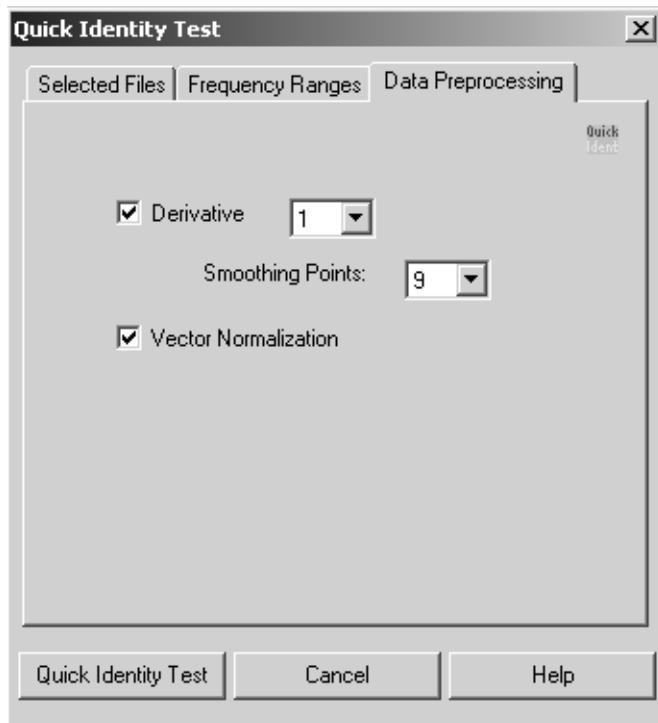
Figure 211: Quick Identity Test - Data Preprocessing

A report block will be appended to every spectrum which was compared to the reference spectrum. This *Report of Correlation Search* lists the spectrum name and sample name (as taken from the spectrum parameter block), the number of the spectrum, the *Hit Quality* and the file name. The hit quality should preferably be a small number, with zero being an absolute match.

In addition, a new file *QIDNT.0* will be created that summarizes the reports of all test spectra. The report headers of this report are identical with the headers of the respective test spectra reports.

Figure 212: Quick Identity Test Report

The report is structured similar to an OPUS/IDENT report. In this report you can vary between several parameters which are defined in the Quick Identity Test.

The following information is important when using the Quick Identity Test:

- **Method file**
  File name of the method used for the test
- **Expected Reference**
  The principal file used
- **Vector normalized spectra**
  Indicates that vector normalization has been was used.
- **X-Ranges**
  Number of frequency ranges.
- **Order of Internal Derivation**
  Specifies the order of the derivative used
- **Smoothing Points for Internal Derivation**
  Specifies the number of smoothing points

9.7   Quality-Test

The quality assessment of spectra measured using the *Quality-Test* command is an integral part of spectral analysis and should always be carried out before the actual evaluation.

This test assesses the quality of spectra measured with regard to absorbance values, signal-to-noise ratio and intensity of the water vapor lines. Spectra that exceed certain limit values should not be considered for analysis.

Select the *Quality-Test* command from the *Evaluate* menu. The following dialog box (see figure 213) opens:
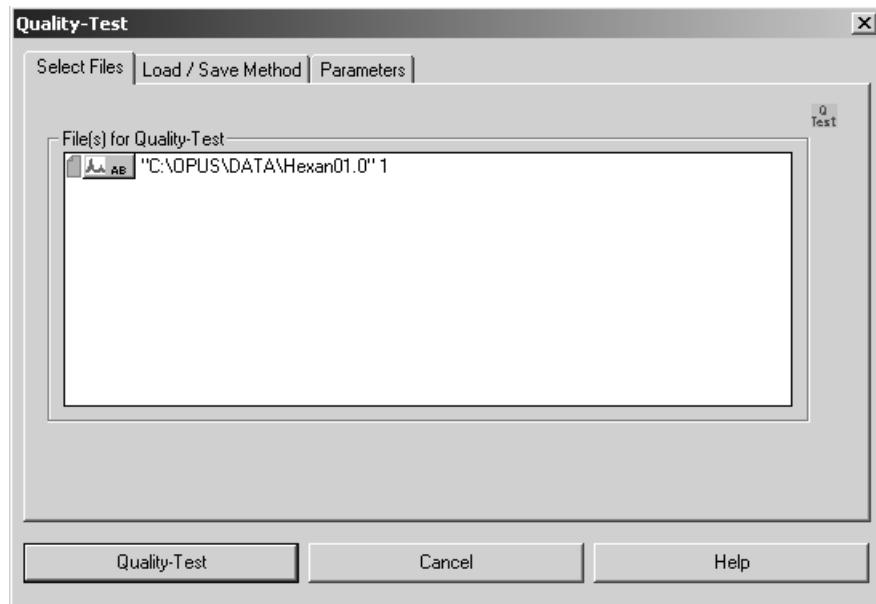
Figure 213: Quality Test - Select Files

The *Select Files* tab includes the spectrum to be tested. You can drag and drop the file icon from the browser window into the *File(s) for Quality-Test* field. Note that the spectrum to be evaluated needs to be an absorbance spectrum.

Click on the *Quality-Test* button to perform the test using the parameters of the method currently loaded. To load or save a method, click on the *Load/Save Method* tab of the *Quality-Test* dialog box.
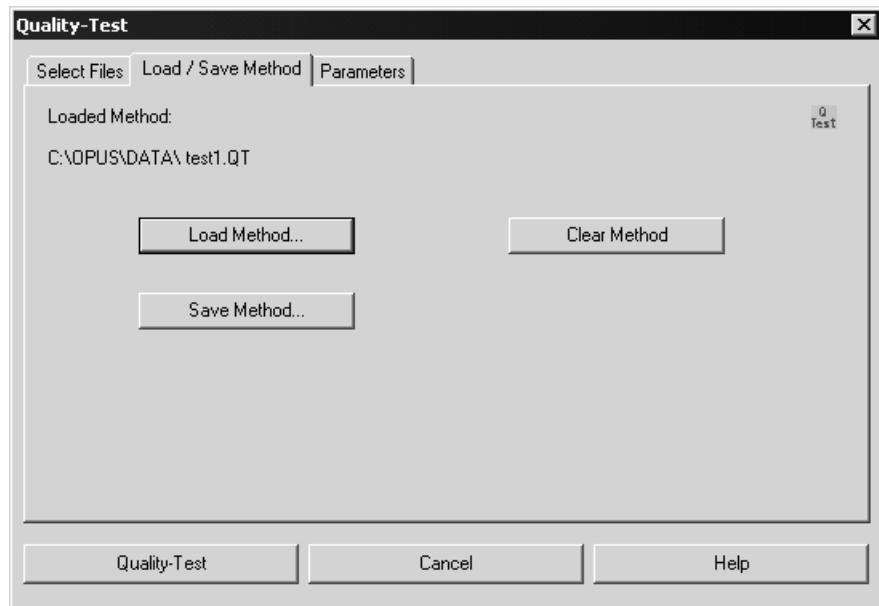
Figure 214: Quality Test - Load/Save Method

The quality test results are stored in the *Quality-Test Report* data block (☐QTEST)
which is added to the evaluated spectral file. Double click on the *QTEST* block
in the OPUS browser window to open the *Quality-Test Report* window. Figure
215 shows an example of a *Quality-Test Report*.

Figure 215: Quality Test Report

The first line of the report indicates the test result. A value of *1* means *passed*,
whereas *0* means *failed*. Do not use spectra that failed for further analysis. The
second line includes the file path of the test method used. The lower window
shows all parameters and their limit values (min. and max.) as well as their
measured values. These parameters can be defined if you click on the
Parameters tab.
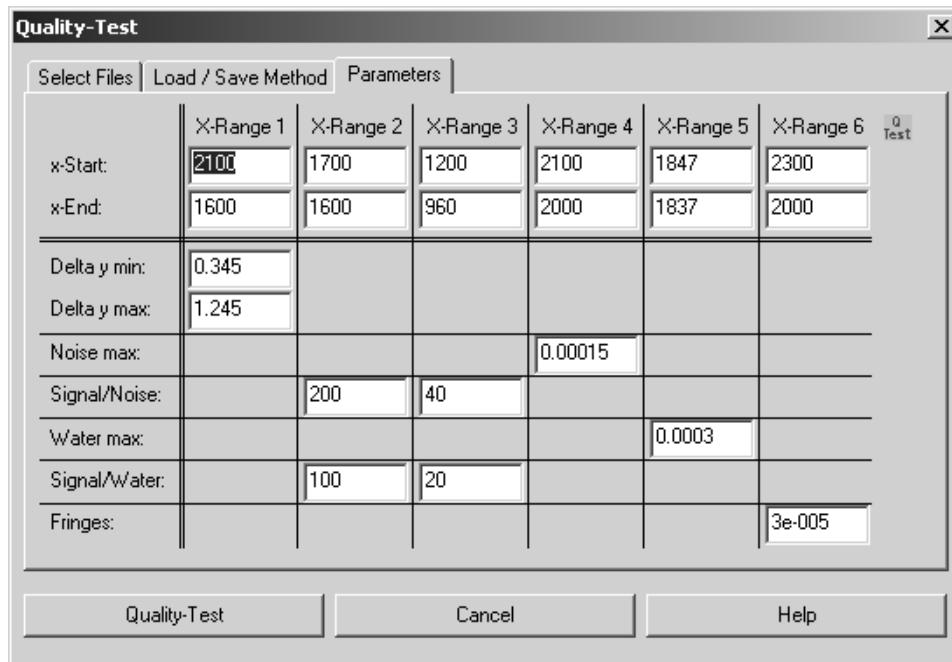
Figure 216: Quality Test - Parameters

Parameters

Some parameters and their limit values are explained in the following:

x-Range 1

The range defined in the first column (2100 - 1600cm^{-1}) calculates the maximum and minimum absorbance values of the original spectrum ([AB] data block). The difference between these two values has to be higher than the one indicated in the *Delta y min* entry field and lower than the limit defined in the *Delta y max* entry field (0.345 to 1.245 absorbance units).

x-Range 2

The range defined has to represent a characteristic band of the sample (Amide I at 1700 - 1600cm^{-1}). The first derivative is calculated and the maximum and minimum absorbance values are determined. The difference between these two values results in S_1, a parameter which approximately corresponds to the intensity of the band defined.

S_1 is used to calculate the signal-to-noise ratio, i.e. S_1 is divided by the noise determined from the first derivative within a spectral range which shows no absorbance bands (as defined in the x-Range 4). The minimum S_1/Noise-ratio value is indicated in the *Signal/Noise* entry field (value: 200).

S_1 is also divided by the water vapor signal determined in the x-Range 5. The minimum S_1/WaterVapor-ratio value is indicated in the *Signal/Water* entry field (value: 100).

x-Range 3

The range defined has to represent a second characteristic sample band (sugar-ring vibration at 960 - 1260cm^{-1}). The first derivative is calculated and the maximum and minimum values are determined. The difference between these two values results in S_2, a parameter which approximately corresponds to the intensity of the band defined.

S_2 is used to calculate the signal-to-noise ratio, i.e. S_2 is divided by the noise determined within a spectral range which shows no absorbance bands (as defined in x-Range 4). The minimum *S_2/Noise-ratio* value is indicated in the *Signal/Noise* entry field (value: 40).

S_2 is also divided by the water vapor signal determined in the x-Range 5. The minimum *S_2/WaterVapor-ratio* value is indicated in the *Signal/Water* entry field (value: 20).

x-Range 4

The spectrum noise is calculated within a spectral range that shows no absorbance bands of the sample (range: 2000 - 2100cm^{-1}).

In this range the first derivative is calculated and the maximum and minimum values are determined. The difference between these two values is termed noise and should not exceed the maximum value defined in the *Noise max* entry field (value: 0.00015, i.e. 1.5×10^{-4}).

x-Range 5

The water vapor intensity is calculated in a spectral range which indicates strong water vapor absorbance but no sample absorbance (range: 1847 - 1837cm^{-1}). The first derivative is calculated and the maximum and minimum values are determined within the range defined. The difference between these two values causes this strong water absorbance. The value should not exceed the maximum value defined in the *Water max* entry field (value: 0.0003).

x-Range 6

The frequency range is determined if the spectrum shows interferences (fringes). The defined frequency range has to be free of any sample absorbance (range: 2200 - 2000cm^{-1}). The maximal difference between the highest and lowest value of the first derivative is defined in the *Fringes* table line (value: 5×10^{-5}).

9.8   Multi Evaluation

The *Multi Evaluation* function is the automated evaluation of NIR spectra for qualitative or quantitative analysis. It combines IDENT, QUANT and conformity test methods with the results being displayed in one single report.

The advantage of multi evaluation is, e.g., if you want to identify an unknown product, you can first perform an IDENT analysis. Based on the results obtained you can continue with a QUANT analysis. Sometimes it is advisable to perform a preliminary test to see whether the product to be used for a quantitative analysis has been measured at all. The combination of an IDENT analysis and conformity test may similarly be appropriate.

Multi evaluation parameters are stored in a special method file with the extension *.ME*. Before you can start a multi evaluation you have to create a multi evaluation method. If you want to edit the multi evaluation path of this method, make sure that you have the right to change parameters. To verify the user rights select the *User Settings* command in the *Setup* menu, and click on the *21CFR11 Rights* tab. For further details, see chapter 14.10.

9.8.1   Multi Evaluation Setup

To start the multi evaluation analysis you have to set up a method or load a method which has been previously created. Click on the *Multi Evaluation Setup* command to open the following dialog:
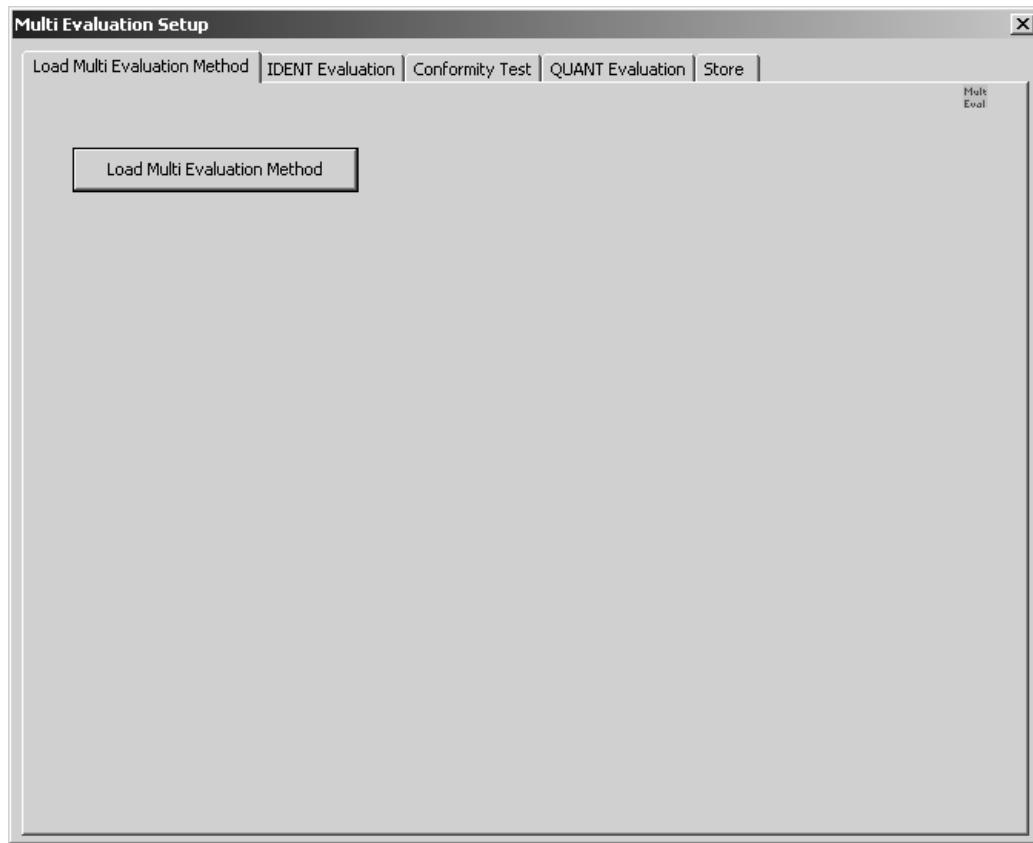
Figure 217: Multi Evaluation Setup - Load Method tab

To load an existing method click on the *Load Multi Evaluation Method* button and select the particular method from the dialog that opens.

Depending on the kind of evaluation you want to perform on the original spectrum or spectra set up a new method by means of the other evaluation option tabs available. The evaluation options correlate with each other, i.e. the sequence of product analysis shall be as follows:

1) IDENT (no further test)
2) IDENT → Conformity Test
3) IDENT → Conformity Test → QUANT
4) IDENT → QUANT
5) Conformity Test → (no further test)
6) Conformity Test → QUANT
7) QUANT (no further test)

The sequences 2 and 4 allow to identify the product in a first step by using the *No Reference defined* IDENT test option.

If you use the *IDENT Evaluation* with several substance groups, and the multi evaluation test result shows that some of these groups may apply to the product to be evaluated, any further test would not be reasonable. This result, however,

will only be generated if the basic IDENT library had not been validated properly and overlappings had not been eliminated either.

Otherwise, if only one substance group applies, you can continue by performing the *Conformity Test* and/or *QUANT Evaluation*. This test depends on the substance group selected for the *IDENT Evaluation*.

It is also possible to perform the multi evaluation analysis by the *Conformity Test* only. If one conformity test method turns out to be successful, you can continue with the *QUANT Evaluation*.

As soon as you close the *Multi Evaluation Setup* command without saving the changes made the following dialog pops up:
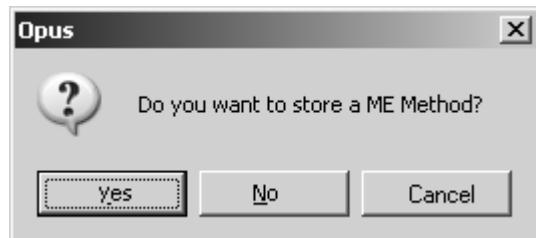
Figure 218: Multi Evaluation Setup - Pop-up dialog

This dialog pops up even if you have not made any changes on the method at all, but clicked on one of the *IDENT*, *Conformity* Test or *QUANT* Multi Evaluation tabs.

9.8.1.1   IDENT Evaluation
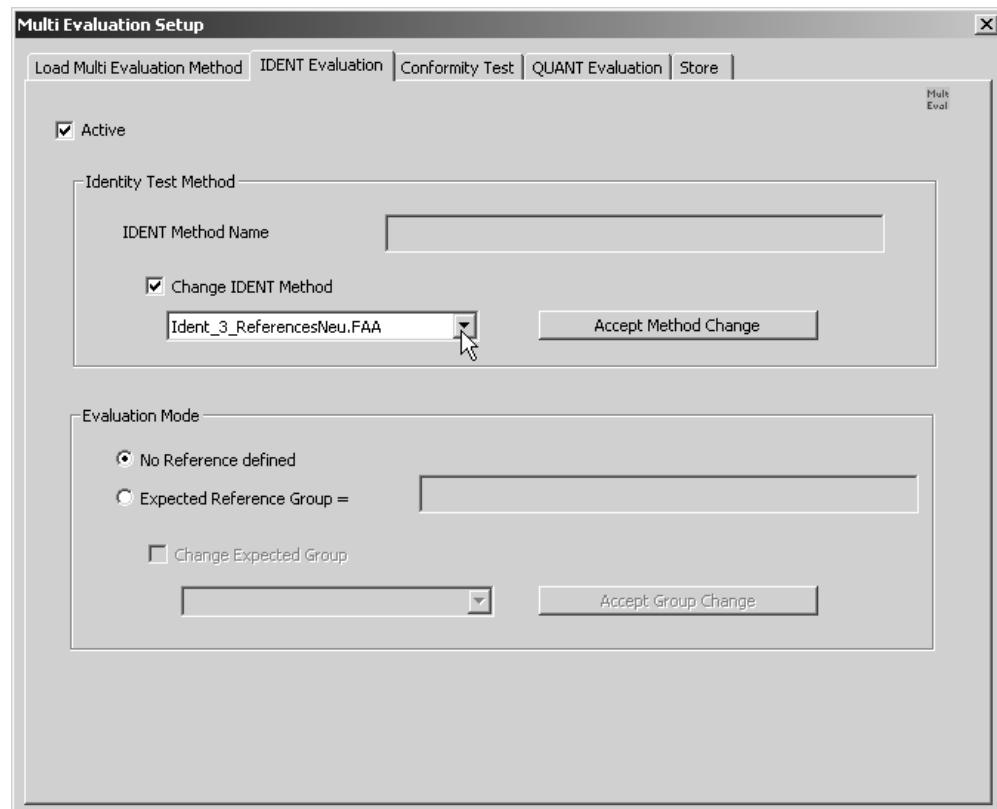
Figure 219: Multi Evaluation Setup - IDENT Evaluation tab

The *Active* check box is deactivated by default and thus all functions and controls are disabled and grayed. Activate the *Active* check box. If you activate the *Change IDENT Method* check box, you can select the appropriate IDENT method from the drop-down list.

Note: All IDENT, Conformity Test and QUANT methods used for multi evaluation have first to be copied to the sub-directories of the multi evaluation root directory. The following default setting applies:

...\OPUS\MultiEvaluation
                    \Conformity Test Method
                    \IDENT Method
                    \QUANT Method

These paths will be created in OPUS not until the *Multi Evaluation Setup* command has been selected for the very first time.

Confirm the choice by clicking on the *Accept Method Change* button. The name of the IDENT method file with the extension *.FAA* will be displayed in the upper selection field (see A in figure 220).
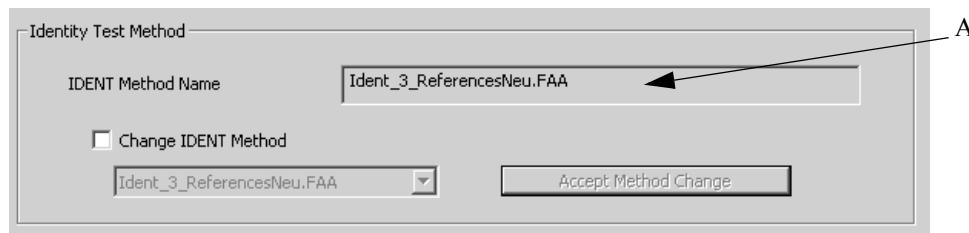
Figure 220: Identity Test Method group field

The *Change IDENT Method* check box and the drop-down list will be deactivated again.

For the IDENT analysis two alternative evaluation modes are available. The mode *No Reference Defined* (see figure 219) works without a pre-defined reference spectrum and allows the complete analysis of all substances. This, however, requires the substances to be part of <u>one</u> validated IDENT library, and further evaluation methods, e.g. QUANT, to be assigned properly.

To work with an expected reference group check the *Expected Reference Group* option button. The reference group previously selected will always be set as default. To change the reference group activate the *Change Expected Group* check box and select the particular group from the drop-down list. This list includes all groups of the current IDENT library.
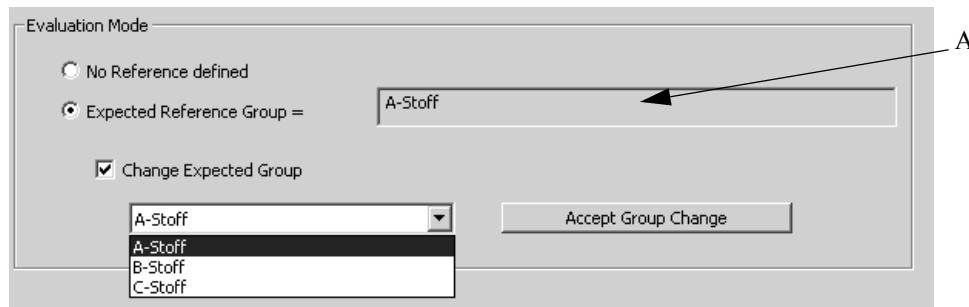
Figure 221: Evaluation Mode group field

Confirm the choice by clicking on the *Accept Group Change* button. The name of the reference group selected will be displayed in the upper selection field (A in figure 221), and the *Change Expected Group* check box and the drop-down list will be deactivated again.

All the settings made on the *Conformity Test* and *QUANT Evaluation* tab correlate with the expected reference defined.

9.8.1.2 Conformity Test
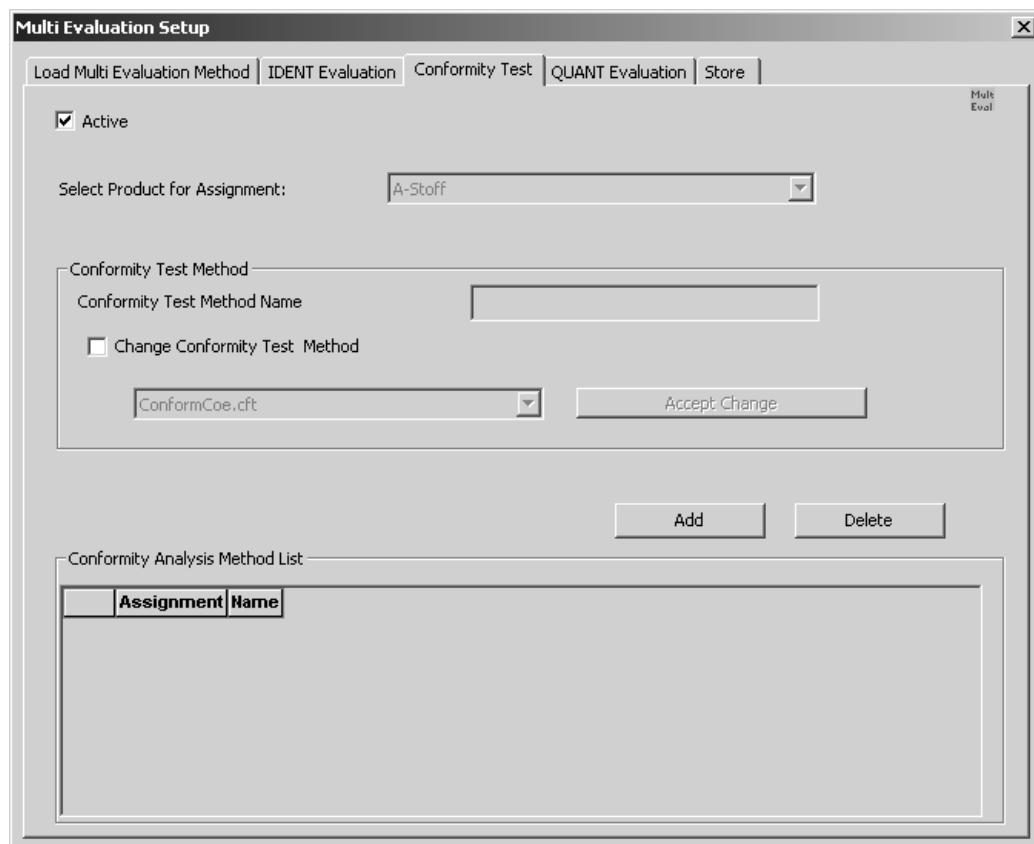
Figure 222: Multi Evaluation Setup - Conformity Test tab

Activate the *Active* check box. If you have defined an expected reference group on the *IDENT Evaluation* tab, the upper drop-down list includes the name of the reference group defined and will be deactivated. If no reference group has been defined, the drop-down list will be activated and you can select a particular group of the IDENT library (see figure 223).
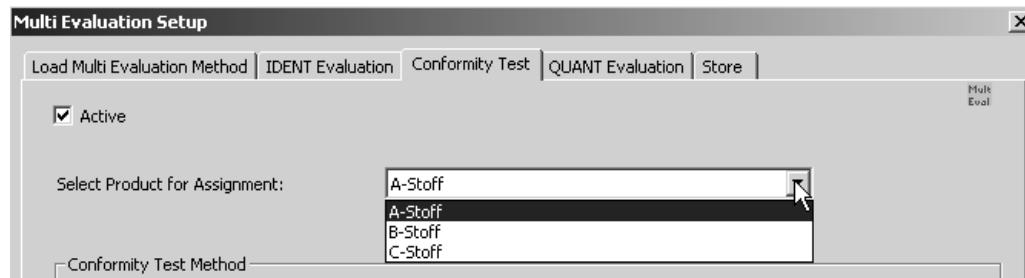
Figure 223: Select Product for Assignment

Assign an individual conformity test method to the selected IDENT library group. Activate the *Change Conformity Test Method* check box and select the appropriate method from the drop-down list. Confirm the choice by clicking on the *Accept Change* button (see figure 224).
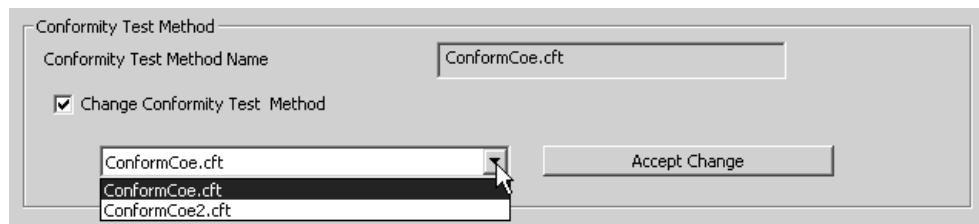
Figure 224: Select Conformity Test Method

If the settings are made, click on the *Add* button (see figure 225). A table will be displayed including the assignments made, and the name of the conformity test method. To remove a particular assignment from the list, select the corresponding line and click on the *Delete* button.

Figure 225: Method List of Conformity Test

9.8.1.3   QUANT Evaluation
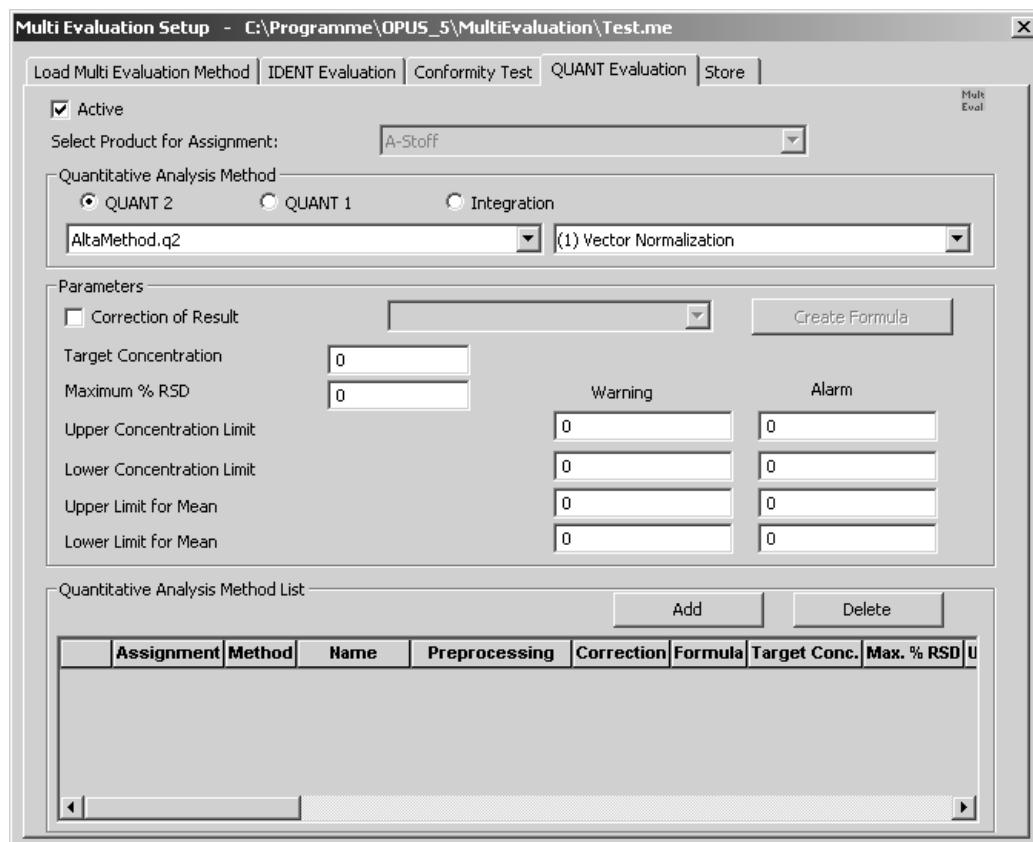
Figure 226: Multi Evaluation Setup - QUANT Evaluation tab

Activate the *Active* check box. If you have defined an expected reference group on the *IDENT Evaluation* tab, the upper drop-down list includes the name of the reference group and will be deactivated. If no reference group has been defined, the drop-down list will be activated and you can select a particular group of the IDENT library.

Assign an individual QUANT or INTEGRATION method to the selected IDENT library group. Activate one of the *Quantitative Analysis Method* option buttons and select the appropriate method from the drop-down list.
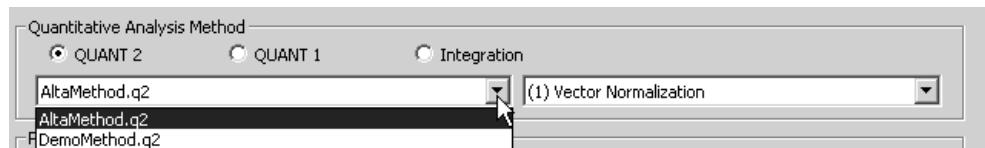
Figure 227: Quantitative Analysis Methods

In case of QUANT 1 and INTEGRATION you can also select between different data preprocessing methods. The methods include *Vector Normalization*, *1st* and *2nd Derivative* and combinations of both methods. Frequently, the *Vector*

Normalization method is used to preprocess data. In many cases, however, you even get better results if you select *1st* or *2nd Derivative*. For further details on the preprocessing methods, see chapter 8.

In the *Parameters* group field you can specify additional values which are set to 0 by default.
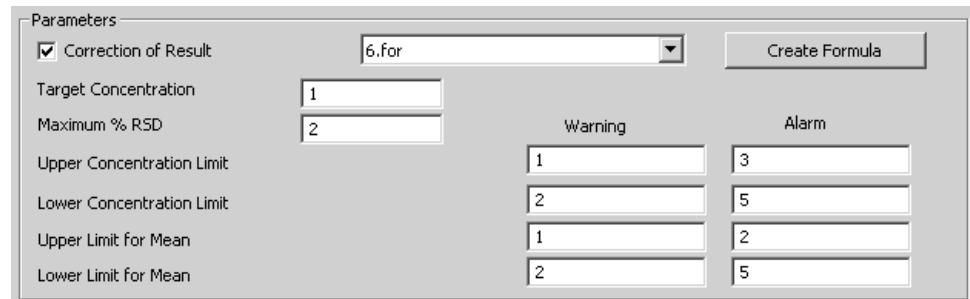
Figure 228: Parameters group field

Activate the *Correction of Result* check box and apply a formula from the drop-down list. If you want to create a new formula for the correction of analysis results, click on the *Create Formula* button. The following dialog pops up:
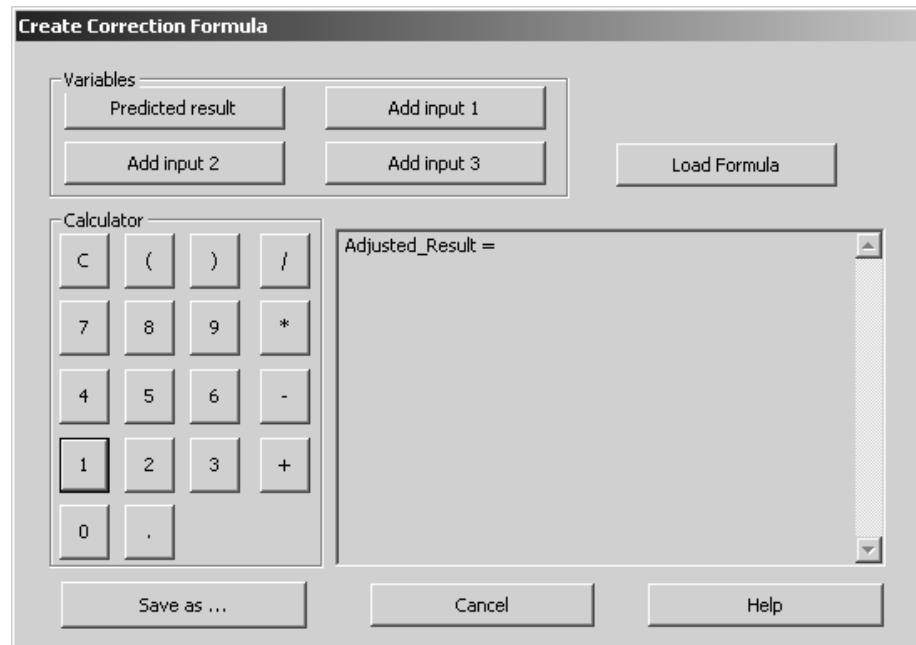
Figure 229: Correction Formula Calculator

By means of the *Load Formula* button you can load an existing formula with the file extension *.for. The string code begins with the *Adjusted_Result =* term, and you can add up to 4 different variables:

- 1 variable for the result predicted by the method
- 3 variables for input values which can be set during spectra evaluation

If you click on the *Add input...* button(s) or *Predicted result* button or on one of the figure buttons, the string code will be continued according to the entries made.

Example: Adjusted_Result = Predicted_Result * 3.01/Add_input 1 * Add_input 2/5.2

Always use the *Calculator* block which includes brackets, decimal point and the four basic arithmetic operations. To save the new formula click on the *Save as...* button. Make sure that you use a valid formula which does not produce any arithmetic error.

No recommendations can be made for the values to be entered for *Target Concentration* or the highest allowable standard deviation in case of several analysis (*Maximum% RSD*). The optimum value has to be determined empirically.

Depending on the test result warning and alarm values can be set in case of the concentration and average value limit. As soon as the warning value defined will be exceeded, a warning is given and informs you where the error has occurred. If all parameters have been set, click on the *Add* button to have the method list displayed. The warning and alarm values will be set to 0 again.

Quantitative Analysis Method List | | | | | Add | | Delete | |

	Assignment	Method	Name	Preprocessing	Correction	Formula	Target Conc.	Ma:
1	A-Stoff	0	AltaMethod.q2	No Spectral Data Preprocessing	1	6.for	1	2
2	A-Stoff	1	Quant1 .q1	No Spectral Data Preprocessing	1	6.for	1	2
3	A-Stoff	2	Co2.int	No Spectral Data Preprocessing	1	6.for	1	2

Figure 230: Quantitative Analysis Method List

The analysis method list includes all the parameters set. The figure displayed in the *Method* column refers to the method selected, i.e.:

0 = QUANT 2
1 = QUANT 1
2 = INTEGRATION

To remove a particular assignment from the list, select the corresponding line and click on the *Delete* button.

9.8.1.4   Store Method

Figure 231: Load Multi Evaluation Setup - Store tab

To finish the multi evaluation setup procedure click on the *Store Method* button. The method will be stored in the OPUS *MultiEvaluation* directory whose root path can be defined in the *Setup* menu by means of the *User Settings* command, provided you have the necessary user rights. For the *MultiEvaluation* directory the default root path will always be the currently used local OPUS directory.

9.9   Multi Evaluation Test

Start the multi evaluation by clicking on the *Multi Evaluation Test* command. The following dialog opens:
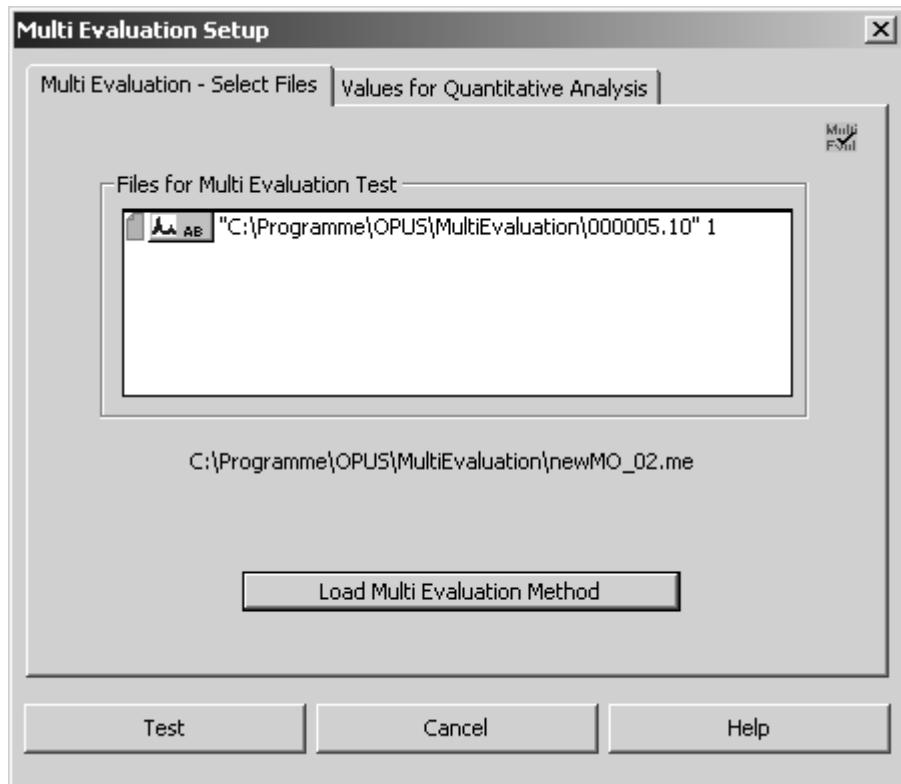
Figure 232: Multi Evaluation Test - Select Files tab

Drag & drop the file(s) to be tested from the OPUS browser window into the *File(s) for Multi Evaluation Test* selection field.

Click on the *Load Multi Evaluation Method* button and load the particular method. Normally, the path of the method previously used is displayed above this button.

The *Values for Quantitative Analysis* tab displays the three input variables defined by means of the formula calculator (see figure 233).
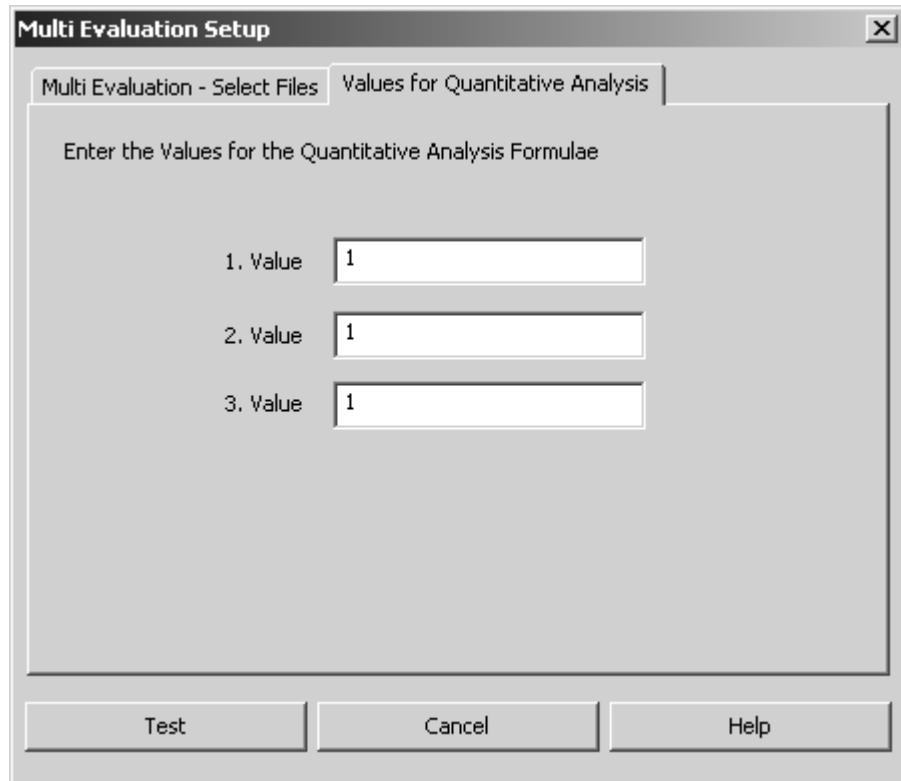
Figure 233: Multi Evaluation Test - Values for Quantitative Analysis tab

Start the multi evaluation analysis and click on the *Test* button. Each step performed during multi evaluation will be indicated by the status bar. The multi evaluation results are stored in an *ME* data block ([ME]) and displayed in a special report (see figure 234).

Figure 234: Multi Evaluation Report

The multi evaluation test report contains the test name and path as well as the results of the different method tests, e.g. QUANT, IDENT or Conformity Test (A in figure 234). The Multi Evaluation final test status is indicated by either ERROR, REGULAR, UNCHECKED, WARNING or ALARM (B in figure 234).

If, e.g., in the QUANT evaluation method the upper and lower concentration limit defined for warning or alarm differs, the final result is checked against these limits.

The concentration limits are not taken into account if all concentration limits are set to 0 (default setting). If they are not evaluated, the status is reported as UNCHECKED unless an ERROR occurs. Any ALARM supersedes a WARNING. An error occurs if, e.g., a data block type does not correspond to a method.

If the assignments made on the *Conformity Test* tab correspond to the ones made on the *QUANT Evaluation* tab, the evaluation will be performed. Otherwise, the evaluation will not performed.

9.10   Quick Compare

The *Quick Compare* function is an easy quality control tool which can be used for MIR spectra. Loaded spectra are compared with one reference spectrum or all spectra files of a directory, and a correlation coefficient (see chapter 9.10.2) is calculated. To perform the *Quick Compare* function you have to use spectrum files which include either an *AB* (absorption) or *TR* (transmission) data block.

Quick Compare parameters are stored in a special method file with the extension *.QCM* (Quick Compare Method). To create such a *QCM* method file use the *Quick Compare Setup* command. If you want to edit a *QCM* method file, make sure that you have OPUS administrator rights. For further details on this subject, refer to section 14.10.

9.10.1 Quick Compare Setup

Before you can start Quick Compare you have to set up a method or load a method previously created. Click on the *Quick Compare Setup* command to open the following dialog:
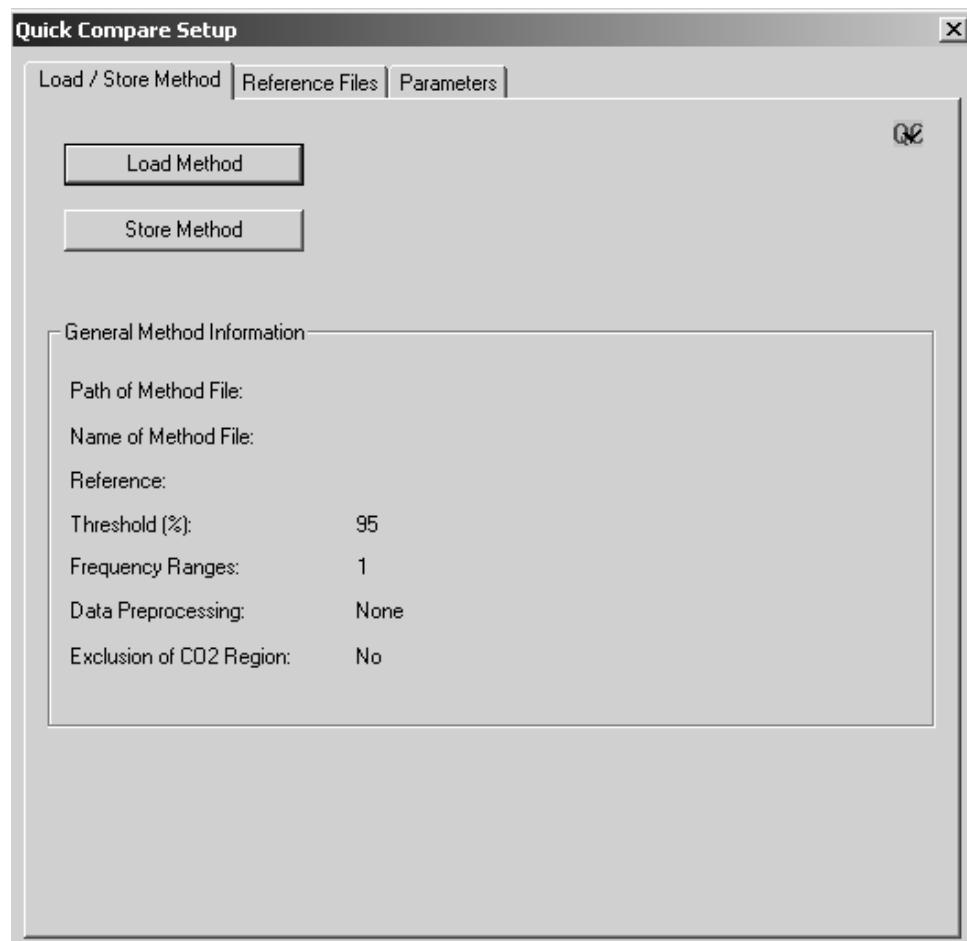
Figure 235: Quick Compare Setup - Load/Store Method

To load an existing method click on the *Load Method* button. The *General Method Information* group field includes information on the method, e.g. path and method file name, threshold, data preprocessing etc. As the *Use File Limit* check box on the *Parameters* tab is checked by default, the frequency range value will be set to 1.

To select the reference file(s), click on the *Reference Files* tab.
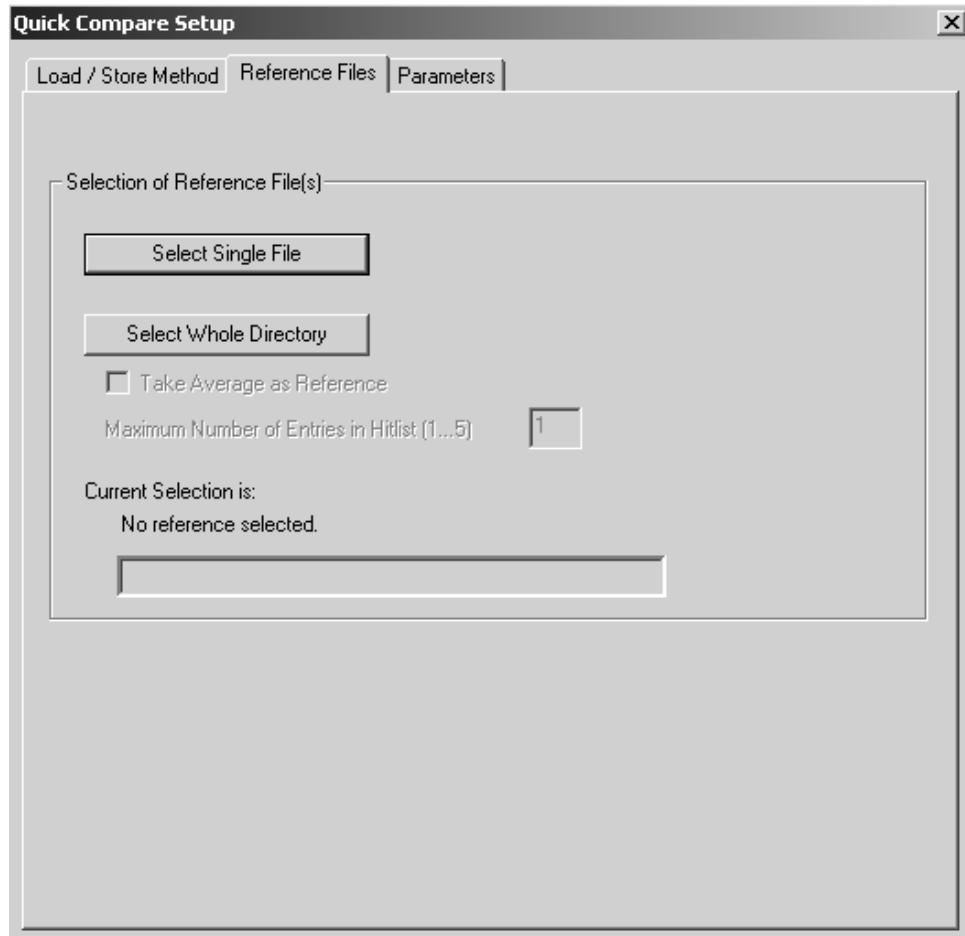
Figure 236: Quick Compare Setup - Reference Files

You can either select one single spectrum file or all spectra files of a complete directory. Click on the *Select Single File* or *Select Whole Directory* button. In either case a dialog opens which you use to select the correct OPUS spectrum file(s).

The current selection will be displayed in the file selection field on the bottom of the *Reference Files* tab. It is also possible to drag & drop a spectrum file from the OPUS browser window to the file selection field.

If you have selected a complete directory, the *Take Average as Reference* check box will be enabled. If you activate this check box, an average reference spectrum will be calculated from all spectra stored in the directory selected. To perform the comparison with all reference files, define the maximum number of entries to be included in the hit list. Up to 5 entries are possible.

To set up additional *Quick Compare* parameters click on the *Parameters* tab.
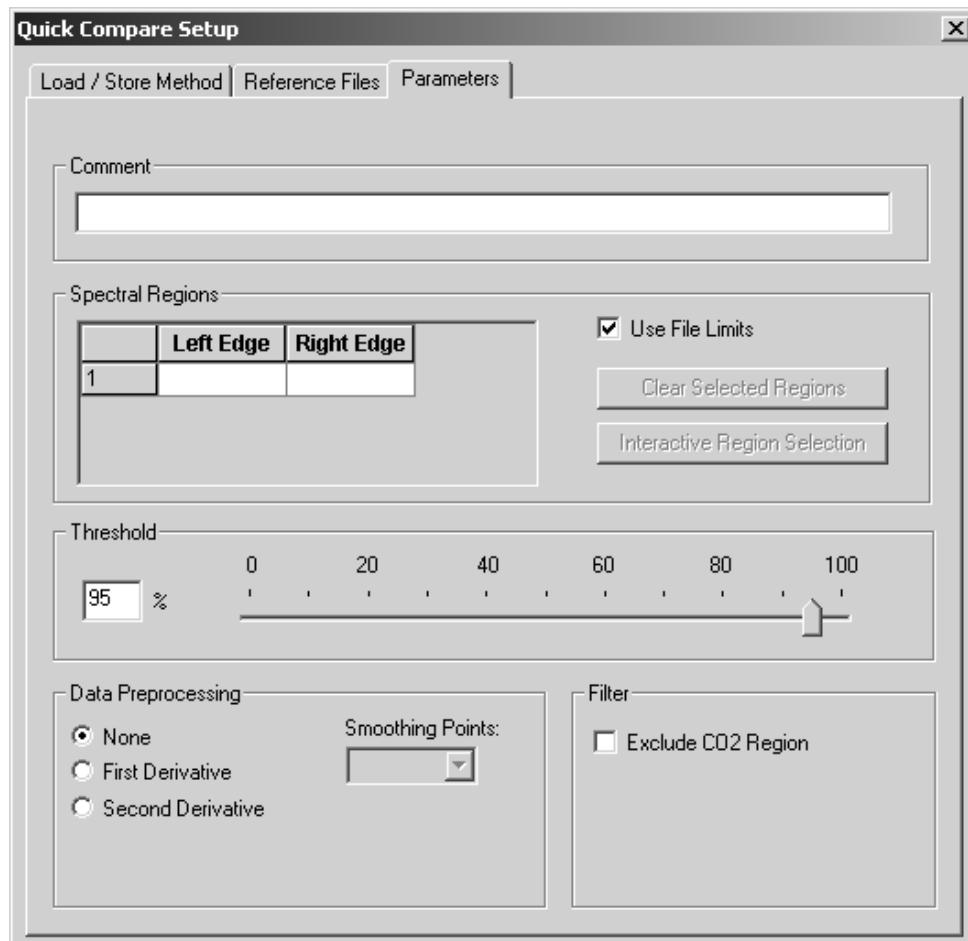
Figure 237: Quick Compare Setup - Parameters

The *Comment* entry field can be used to enter any kind of text, e.g. details about the method created such as *Two spectral regions, No data preprocessing* etc.

As the *Use File Limit* check box is activated by default, the wave number range is based on the first, and possibly only, reference spectrum. If you deactivate this check box, the *Interactive Regions Selection* and *Clear Selected Regions* buttons as well as the *Spectral Regions* table will be enabled.

To select the spectral regions you can either type in the limits manually into the *Spectral Regions* table or select them interactively. In the latter case click on the *Interactive Region Selection* button. Move the borders of the frequency region accordingly, or right click into the frequency region and select one of the options from the pop-up menu.

If you want to delete one or more spectral region(s), select the respective line(s) on the *Spectral Regions* table and click on the *Clear Selected Regions* button. To delete the spectral regions when working in interactive mode right click on the region and delete it by the *Remove* pop-up menu.

Use the slider to determine the threshold which influences the *Quick Compare* result. If the result is OK, the correlation coefficient is greater than the threshold selected. The result is not OK if the correlation coefficient is less than the threshold selected. You can also enter the exact threshold value between 0 and 100%, manually into the corresponding entry field.

Optionally, you can select between three different data preprocessing methods. If you check the *First* or *Second Derivative* option button, the *Smoothing Point* selection box will be enabled. The optimal number of smoothing points set for the specific preprocessing methods has to be determined empirically.

The *Exclude CO₂ Region* check box allows to exclude CO_2 bands from the calculation. If you activate this check box, the wave number regions of 660 to 680cm^{-1} and 2,275 to $2,400\text{cm}^{-1}$ are excluded when calculating the correlation coefficient (see chapter 9.10.2).

If you have set all parameters, return to the *Load/Store Method* tab and click on the *Store Method* button to store the new method. This button is only enabled if you have specified a reference file and a wave number range.

9.10.2 Quick Compare Theory

The comparison between sample and reference spectrum will be performed by calculating the correlation coefficient.

The correlation coefficient *r* of the two functions $y_1(k)$ and $y_2(k)$ is calculated as ratio from the covariance and product of the two standard deviations σ_{y_1} and σ_{y_2}:

$$r = \frac{Cov(y_1(k), y_2(k))}{\sigma_{y_1} \cdot \sigma_{y_2}}$$

The value of *r* ranges between -1 (inverted spectra) and +1 (identical spectra). This correlation coefficient *r* will be calculated into a percentage and reflects the similarity of the two spectra. The $-1 \le r < 0$ range is mapped to 0%, and the $0 < r \le 1$ range is mapped linearly to 0% ...100%.

9.10.3 Quick Compare

Start the comparison by clicking on the *Quick Compare* command. The following dialog opens:
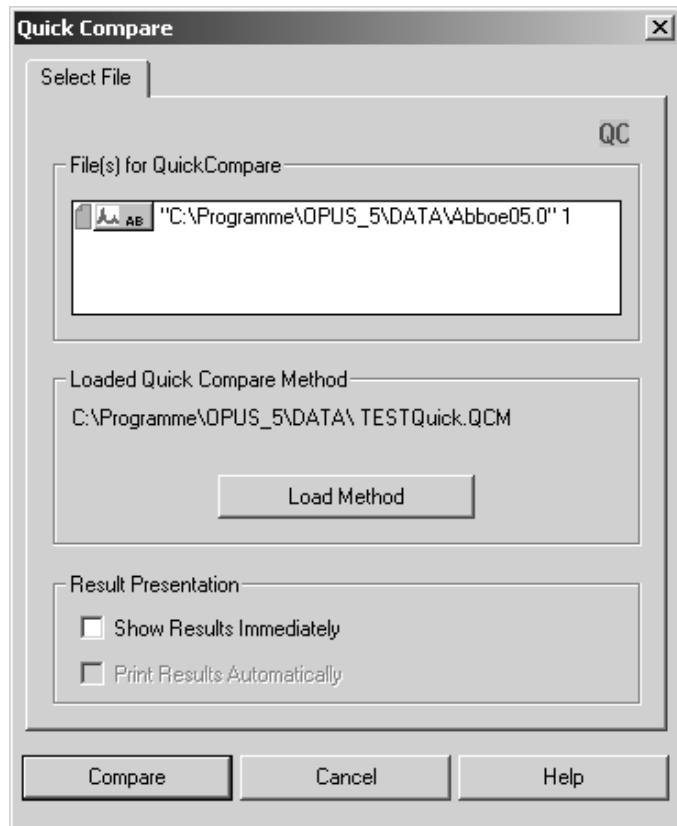
Figure 238: Quick Compare - Select File

Drag & drop the file(s) to be compared from the OPUS browser window into the *File(s) for Quick Compare* selection field. Make sure that the data blocks for the sample and reference files are of the same spectra type, i.e. AB (absorption) or TR (transmission). Besides, the wave number range of the sample spectrum has to be at least as large as the range defined for the reference spectra. You can also load 3D files as sample files to perform a Quick Compare. However, 3D files cannot be loaded as reference files.

Click on the *Load Method* button and load the particular method. Normally, the path of the method previously used is always displayed above the *Load Method* button.

The settings in the *Result Presentation* group field will be stored as OPUS parameters and are set by default if you start the *Quick Compare* command the next time. The same applies to the method selected. If you activate the *Show Results Immediately* check box and click on the *Compare* button, the *Quick Compare* results will be displayed in the *QC Results-Display*, see figure 239 et seq.

In case of 3D-files the *Show Results Immediately* and *Print Results Automatically* check boxes will be disabled. The *Quick Compare* results in case of 3D-files will be stored in a TRC data block ( ) of the sample file and displayed in a specific report view.
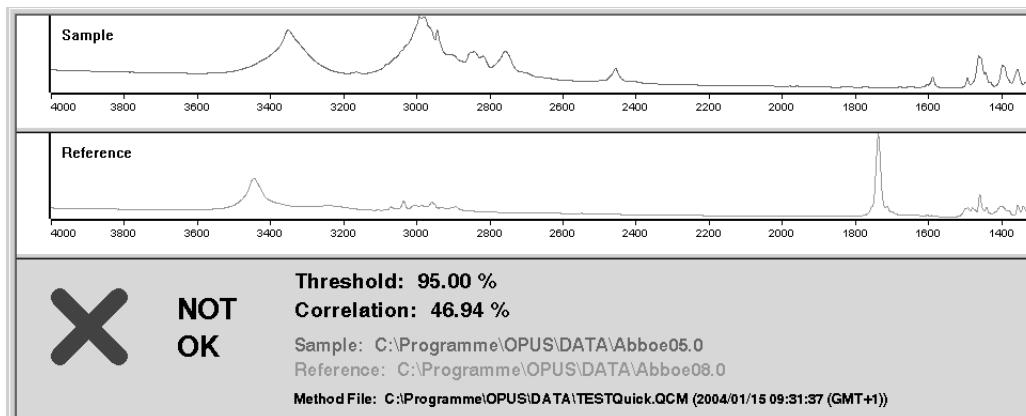
Figure 239: QC Results-Display - Result Not OK

The *QC Results-Display* consists of a sample and reference spectrum window. In the lower part of the display the *Quick Compare* result is indicated. A red cross and the description *NOT OK* would indicate that the comparison has failed. In this case the correlation value calculated is less than the threshold value defined in the method. A green check mark and the description *OK* would indicate that the comparison has passed. In this case the correlation value calculated is greater than the threshold value defined in the method.
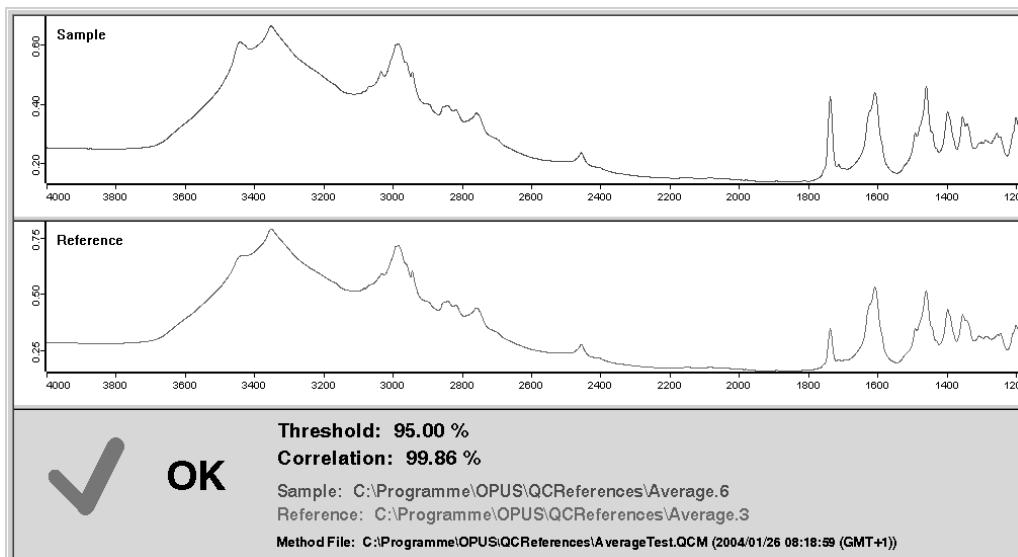
Figure 240: QC Results-Display - Result OK

Figure 240 shows a *QC Results-Display* which was based on a Quick Compare between a sample spectrum and several single spectra files of a complete directory.
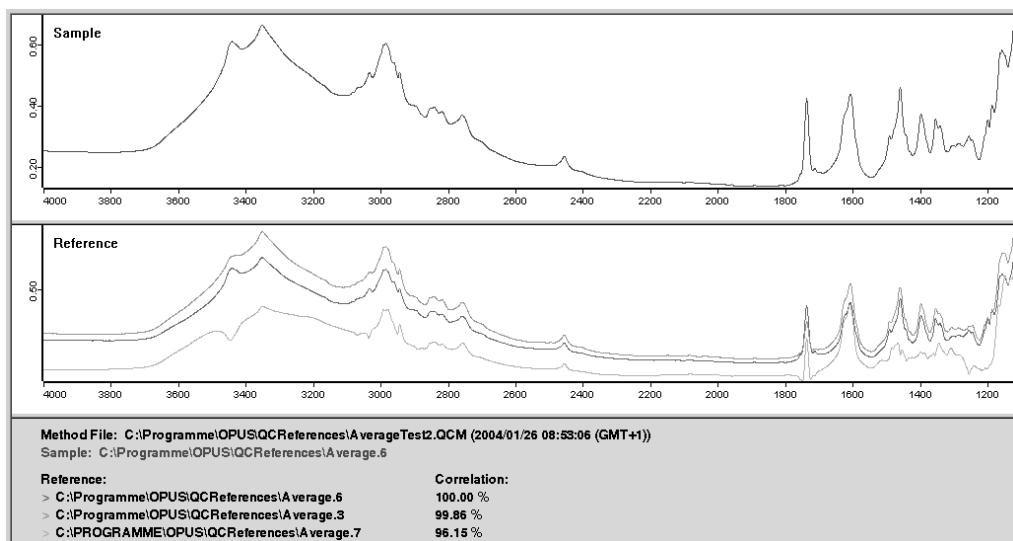
Figure 241: QC Results-Display - Several Single Spectra

If a sample spectrum is compared with the average value of several reference spectra, the *QC Results-Display* can be as follows:
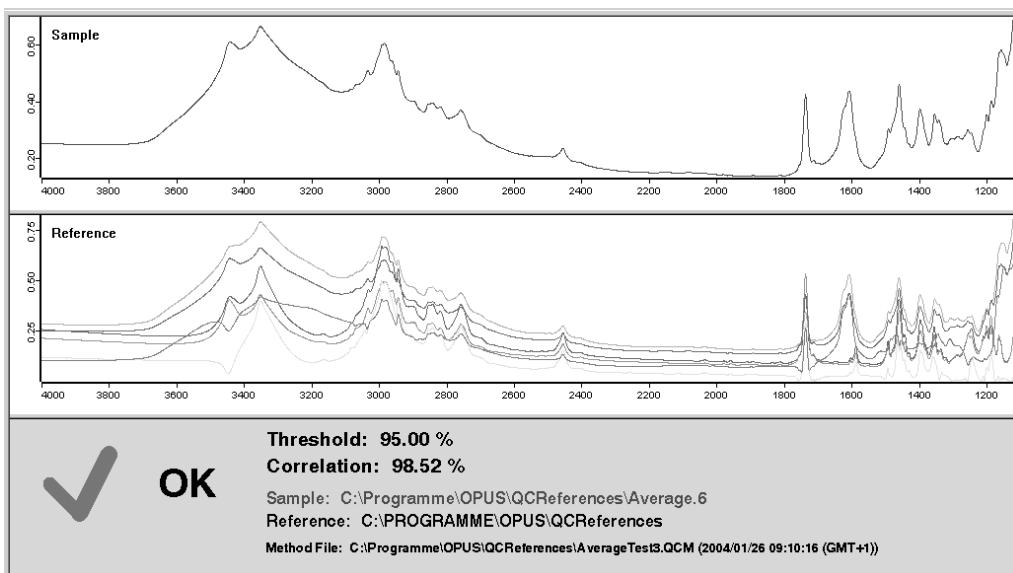

Figure 242: QC Results-Display - Average As Reference

As soon as you have activated the *Show Results Immediately* check box, the *Print Results Automatically* check box will be enabled. If you activate this check box, the comparison results will automatically be printed after the calculation has been terminated. The layout of the print is similar to the *QC Results-Display*.

To start Quick Compare click on the *Compare* button. The evaluation results are stored in a *QC* data block ( ). This data block includes the parameter values used and the result calculated which can range between 0 and 100% (0% = no correlation, 100%=full correlation), see figure 243.

Figure 243: Quick Compare Report

9.11 Spectrum Search

OPUS offers several library search commands. For details, e.g. *Library Editor* see the OPUS Search Manual which supplied with the OPUS Search package.

The aim of spectrum search is to identify unknown substances. To perform a search you need a library which is in line with your needs. BRUKER offers a variety of commercial libraries which allow to solve many analytical problems. You will find a free demo library on your OPUS CD containing 350 entries.

9.11.1 Starting a Spectrum Search

Select the *Spectrum Search* command in the *Evaluate* menu and specify the spectrum files. To do this click on the *Spectrum Search* tab. If you activate the *Show Search Report immediately* check box, a report window displaying the results opens automatically after the search run has finished. You can also limit the search to an existing search report. In this case only the substances listed in the report will be compared to the test spectrum.
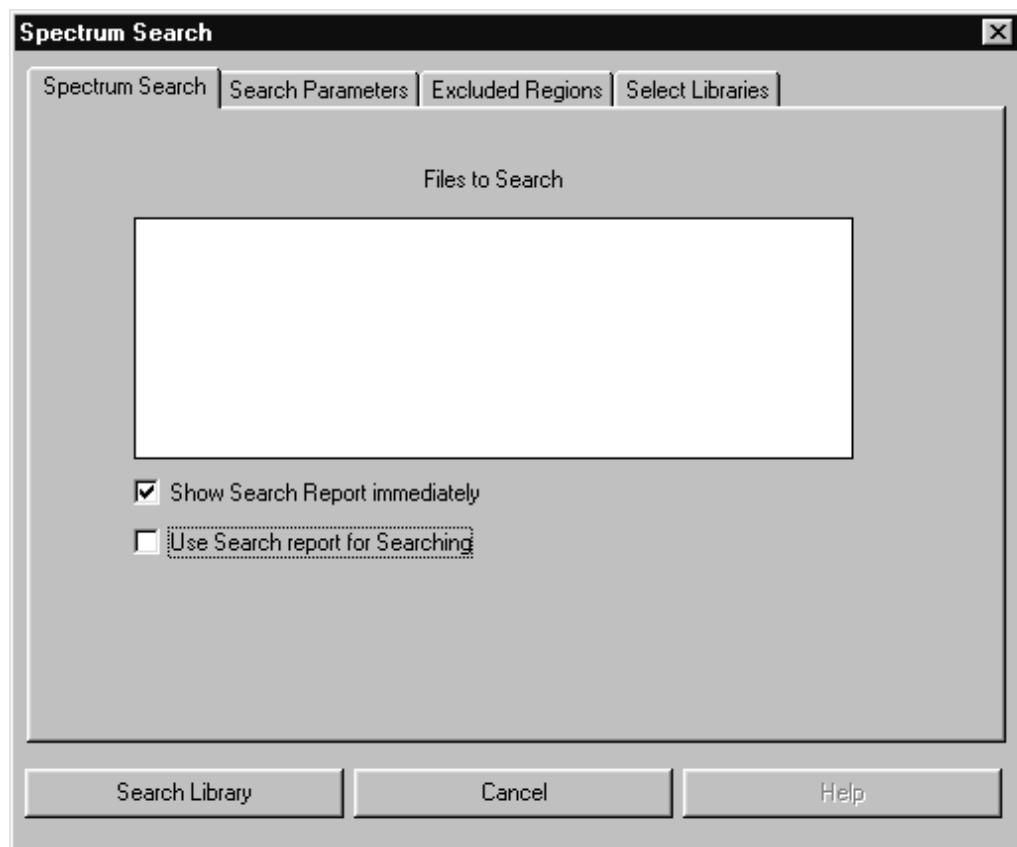
Figure 244: Spectrum Search

On the *Search Parameter* tab you define the desired search parameters.
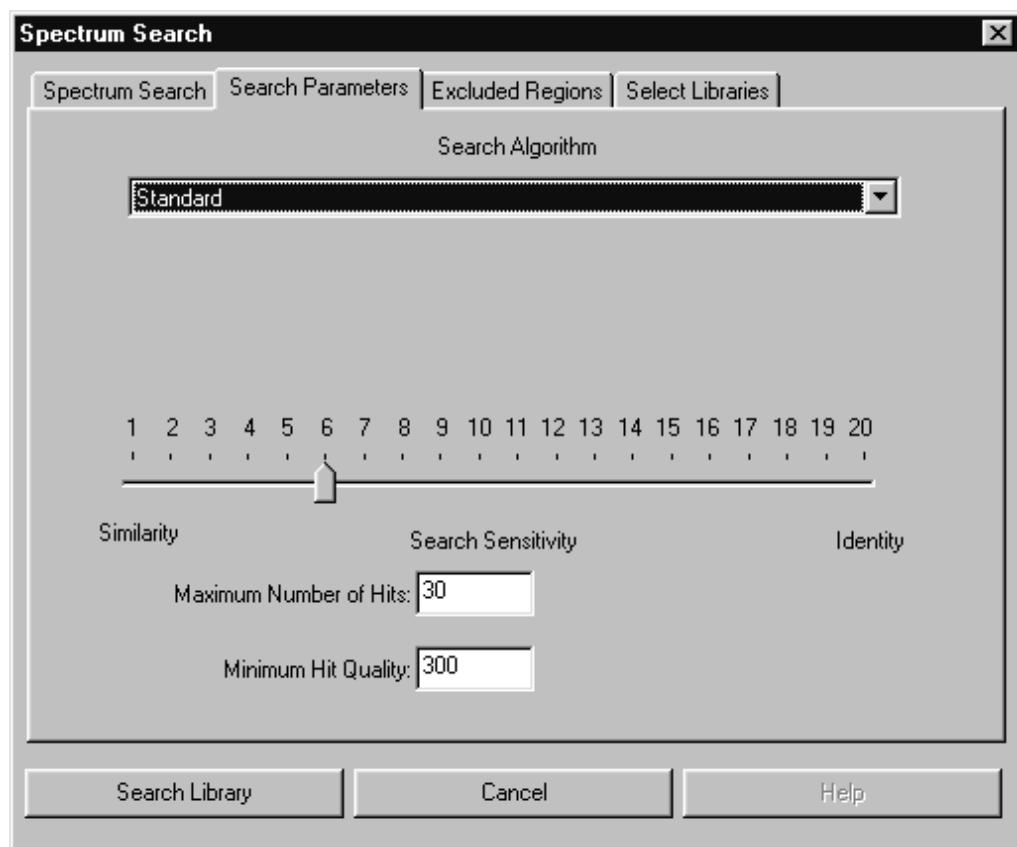
Figure 245: Spectrum Search – Search Parameters

- *Algorithm*: BRUKER search algorithm uses a peak table together with the experimental data (spectra). A temporary peak table is automatically generated during a search using the *Standard* algorithm. The second algorithm, *Use existing Peak Table* employs existing peak tables, allowing one to suppress, for example, solvent peaks.

- *Search Sensitivity:* Using *Search Sensitivity* you can control the result of your search. It is difficult to give a general recommendation for the sensitivity value, because the search result depends highly on the type of recorded spectra. For spectra taken from KBr pellets with a typical Signal-to-Noise ratio, a sensitivity setting of 6 to 10 would be reasonable. The best is, however, to learn about different sensitivity settings by doing test runs applied to known substances. As a rule of thumb, values higher than 15 rarely yield a significant result.

- *Maximum Number of Hits*: The number of hits that are to be saved in the search report can be specified. Depending on the value set in the *Minimum Hit Quality* field, the resulting number of hits can be lower than this value.

- *Minimum Hit Quality*: This field is used to enter the minimum value to qualify of a hit in the search. A value of 1000 would be a perfect match, whereas a value of 0 is obtained in the case of no correlation at all. In reality the search algorithm gives a value higher than 0 even if no (or negligible) similarities exist between spectra. Therefore, one restricts the number of hits included in the search report to a lower limit (default settings 300). This value also depends on the

sample type and should be evaluated by measuring representative samples. Only if a search yields no hits, should the *Minimum Hit Quality* be set to a lower value.

You can limit the search to certain frequency regions of the spectrum instead of comparing the whole recorded frequency range of the spectrum to the library spectra. Enter either the frequency ranges manually in the table cells or use the *Interactive Range Selection* button to directly select a frequency range in the spectrum. Once you defined a list of regions to exclude you can save them (*Save Ranges as*) for future use. *Clear ranges* clears the table and the *Restore last Ranges* button automatically calls up the last range definition you used.
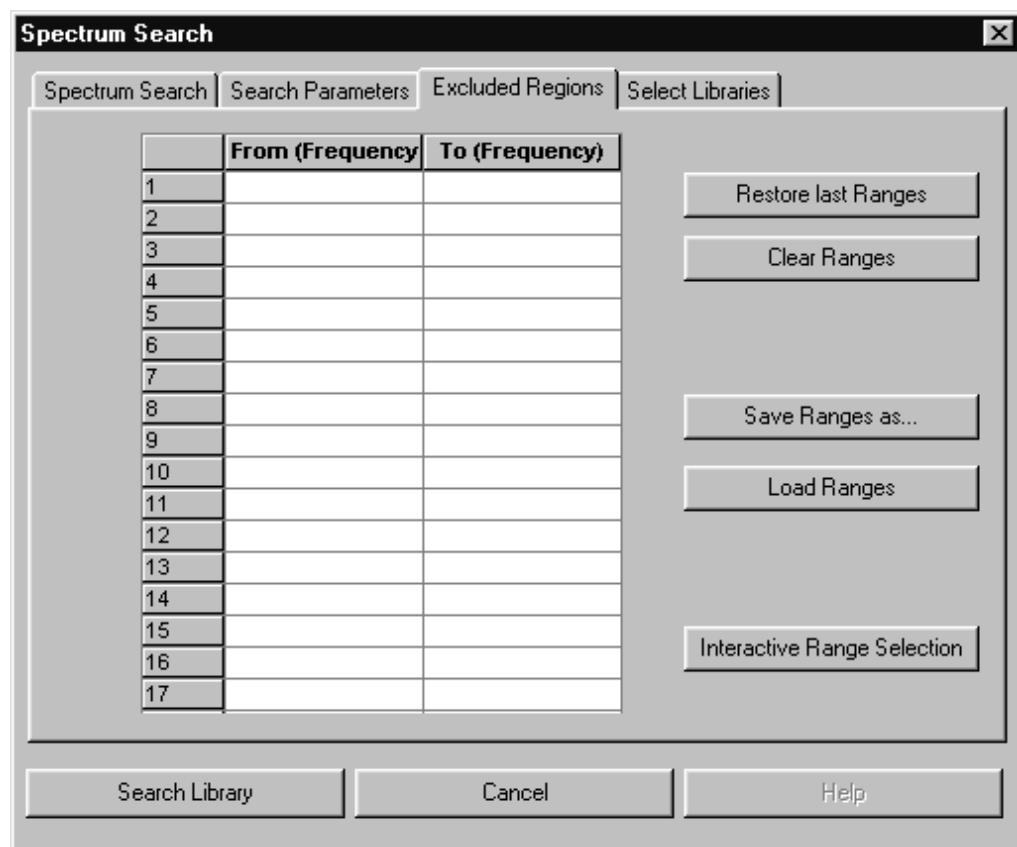
Figure 246: Spectrum Search – Exclude Frequency Regions

On the *Select Library* tab you select at least one library to apply for the search. A search can involve either one or more libraries, but creates only one search report.
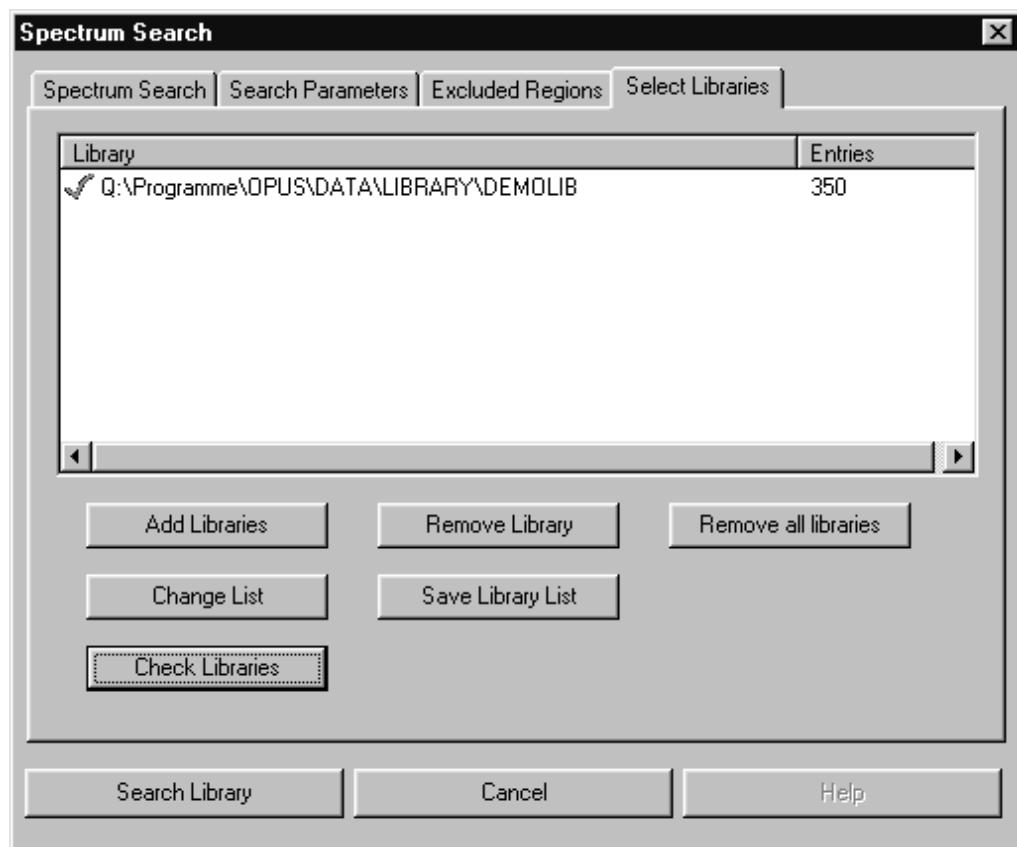
Figure 247: Spectrum Search – Select Library

Use the *Add Libraries* and *Remove Libraries* buttons to include or exclude libraries in the list. The library selection field shows only one single file for each library to ensure a clear structure. You can select several libraries from the selection field.

To remove libraries from the selection field, select them first and click on the *Remove Library* or *Remove all Libraries* button. Save a library created by means of the *Save Library List* button. To modify a library click on the *Change List* button. The library previously used will be set by default the next time when using the *Spectrum Search* function.

You can also test the integrity of a library file by the *Check Library* command. This command also updates the number of file entries. If a file passes the test, it will be checked by a green mark.

Problematic files are indicated by a red "x". This can also be caused by the fact, that OPUS cannot locate the library file (e.g. after you moved the file to a different directory).

9.11.2   Search Report

The result of a spectrum search will be saved in a report; you can read through the report by opening a report window. The report will automatically be displayed if you have checked the *Show Search Report immediately* box.

Otherwise, open the report by double-clicking on the report block.

The report window consists of four areas, which can be adjusted in size by moving the window bars. The list at the bottom of the window contains all spectra matching the search criteria. The hits are numbered consecutively (first column) and sorted by hit quality. The first spectrum is selected (red square) and automatically displayed in the display area above. The spectrum will only be displayed if the box before the spectrum name is checked. To display the substance information and the structure, the spectrum must be selected. The hit quality is marked before the name of the substance, followed by the entry number of the spectrum in the library.
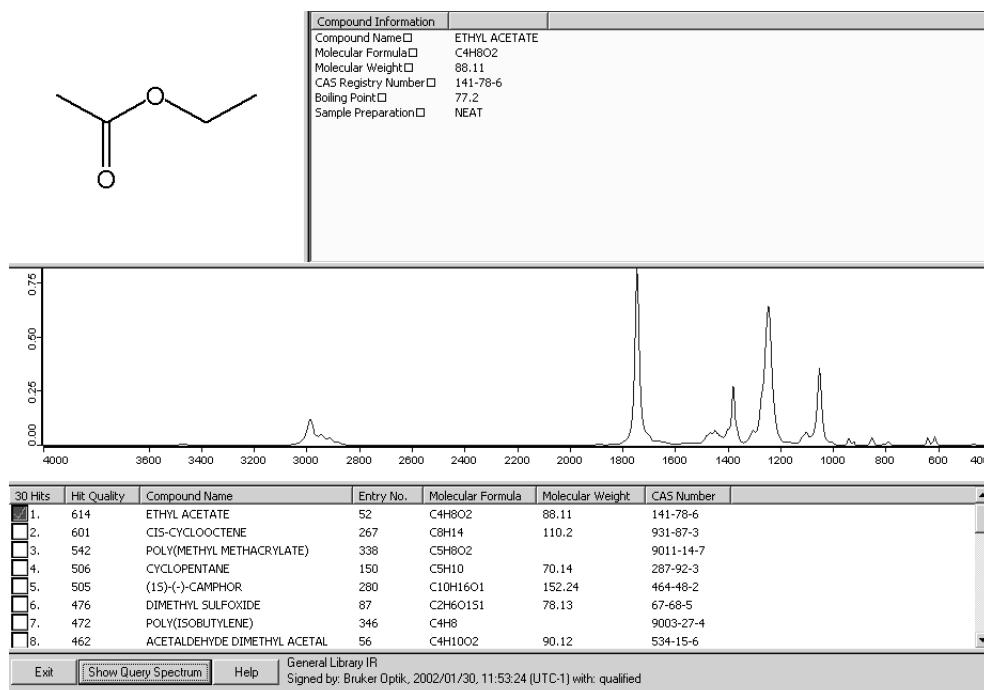
Figure 248: Search Report – Results

Display the query spectrum by clicking on the *Show Query Spectrum* button. Close the report window by clicking on *Exit*.

9.12   NeuroDeveloper Classification

For information on the NeuroDeveloper program, refer to the extensive online documentation.

10 Display

The commands within this pull-down menu are for manipulating the display of the active spectrum window. They allow you to zoom in on a detail of the display, and go back to the original display size. Some of the commands are not always available, depending on the preceding steps performed. For example, the *Forward* and *Back* commands are only active if you switched the display magnification.
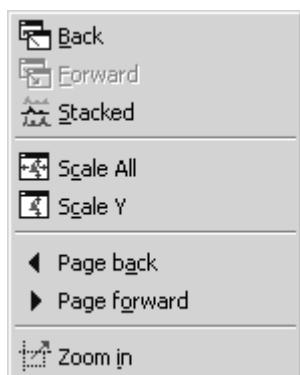
Figure 249: Display Menu

10.1 Forward, Back

Back allows you to restore the original display size on your screen after you have zoomed in on a detail of the displayed curve. *Forward* will display the zoomed in area again.

10.2 Stacked

If you loaded more than one spectrum into the same spectrum window you have the option of a stacked display i. e. the spectra will not overlap. The preview window is not affected by this command.
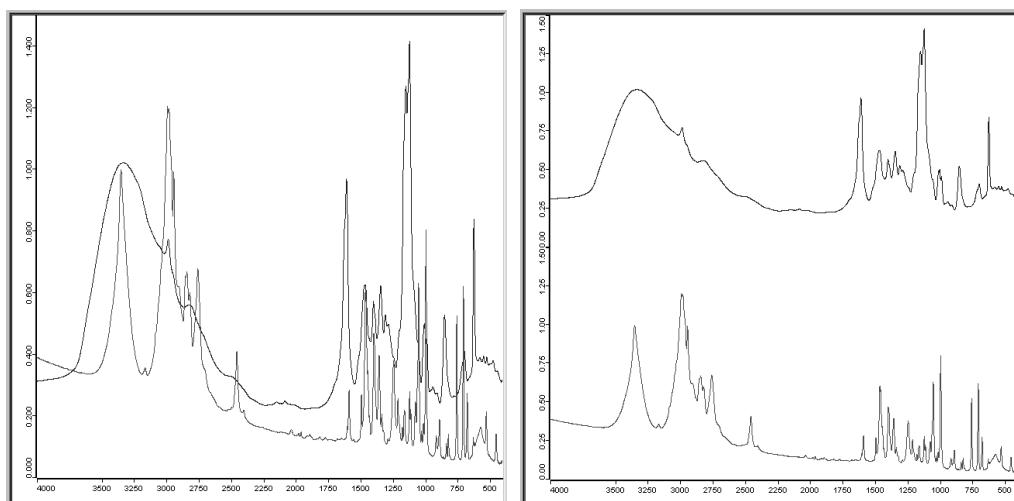
Figure 250: Spectrum Window Containing Two Spectra – Normal and Stacked View

The ordinate will be duplicated when displaying two spectra in the stacked mode. You can separate both spectra by displaying another abscissa, using the *Axis* command of the spectrum window pop-up menu (accessible by right-clicking on the spectrum window). If you expand a part of one stacked spectrum, the other spectrum will automatically be enlarged.

10.3   Scale All, Scale Y

You can fit a spectrum to the size of the spectrum window using the *Scale All* command. If you only want to scale the ordinate, you can achieve that with the *Scale Y* command.

10.4   Page Forward, Page Backward

If you have displayed only part of a spectrum you will see this part shown on a white background in the preview window, while the rest of the spectrum which is not shown appears on a gray background. You can move the displayed region along the frequency axis using the *Page Forward* and *Page Backward* commands. In this case you can browse a spectrum while keeping the displayed frequency region the same.

10.5   Zoom In

The *Zoom* option allows you to choose the magnification. Use the left mouse button to draw a frame around the region you would like to expand. After a second mouse click the crosshair cursor disappears and instead you can reposition the frame. Now left-click again and the area marked by the frame will be resized to the spectrum window.

11 Print

The *Print* menu includes printing spectra functions and allows to create new printing templates or layouts and load existing ones. It is also possible to use templates which have been created by former OPUS versions, e.g. OPUS-OS/2. They will automatically be converted.

Figure 251: Print Menu

Before being able to start printing spectra you have to set up a default printer in Windows first.

11.1   Installing Default Printer

The default printer is automatically addressed by the computer when printing. To install the printer connect it to the parallel port of your computer or make sure that a printer is available on the network. For details on the hardware connection, refer to the printer manual.

Install the printer driver as follows:

1) Click on the Windows *Start* button, select the *Settings* command and click on the *Printer* option. The *Printer* dialog opens.

2) Double click on the *New Printer* icon and follow the on-screen instructions.

3) If the installation has been successful, a new printer icon appears in the *Printer* dialog.

4) To check whether the printer has been defined as default printer double click on the new printer icon. A menu pops up in which The *Default Printer* command has to be checked.

11.2   Print Setup

Use the *Print Setup* command to define the printer and the print parameters like paper size and print quality. Clicking on the *Properties* button opens a different dialog. The settings shown will depend on the printer configuration.
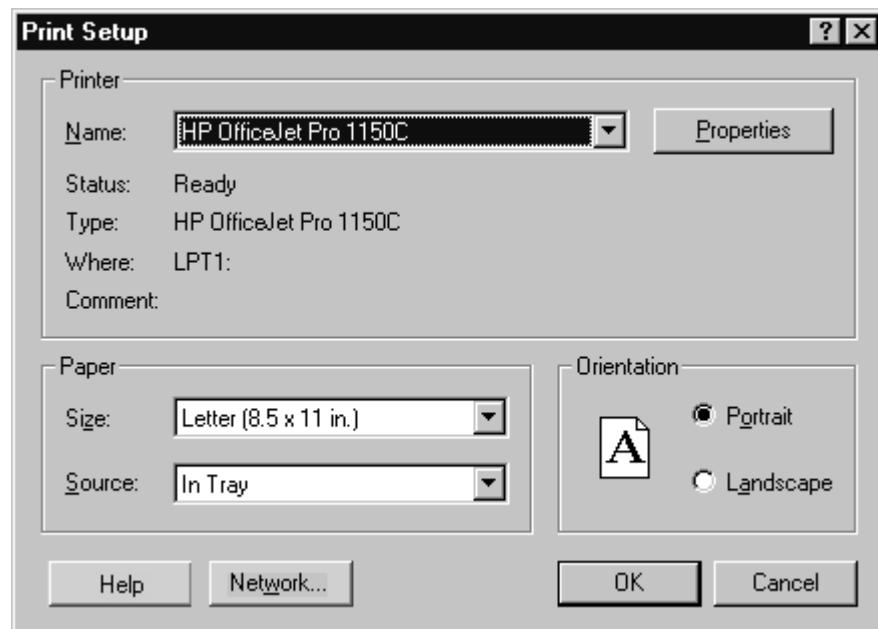
Figure 252: Print Setup

11.3   Print Spectra

Select the *Print Spectra* command to directly print spectra. The following dialog opens:
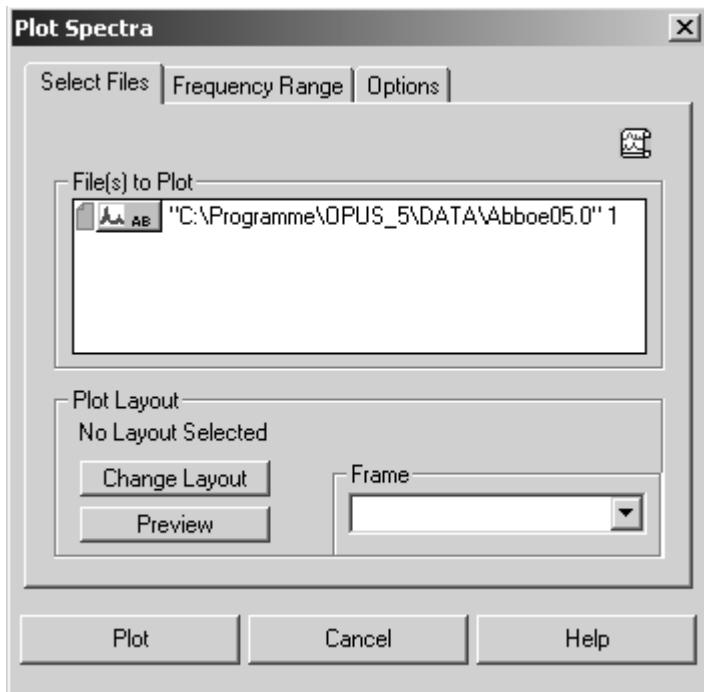
Figure 253: Print Spectra

Drag & drop the respective spectrum from the OPUS browser window into the *File(s) to Plot* selection field. Click on the *Change Layout* button to select a plot layout. If the plot layout selected consists of several frame types, use the *Frame* drop-down list to define which spectra have to be printed in each frame.

To display a preview of the plot click on the *Preview* button. If the plot consists of several pages you can select between a single and two-page display. Additionally, you can zoom in or out the spectrum previewed.
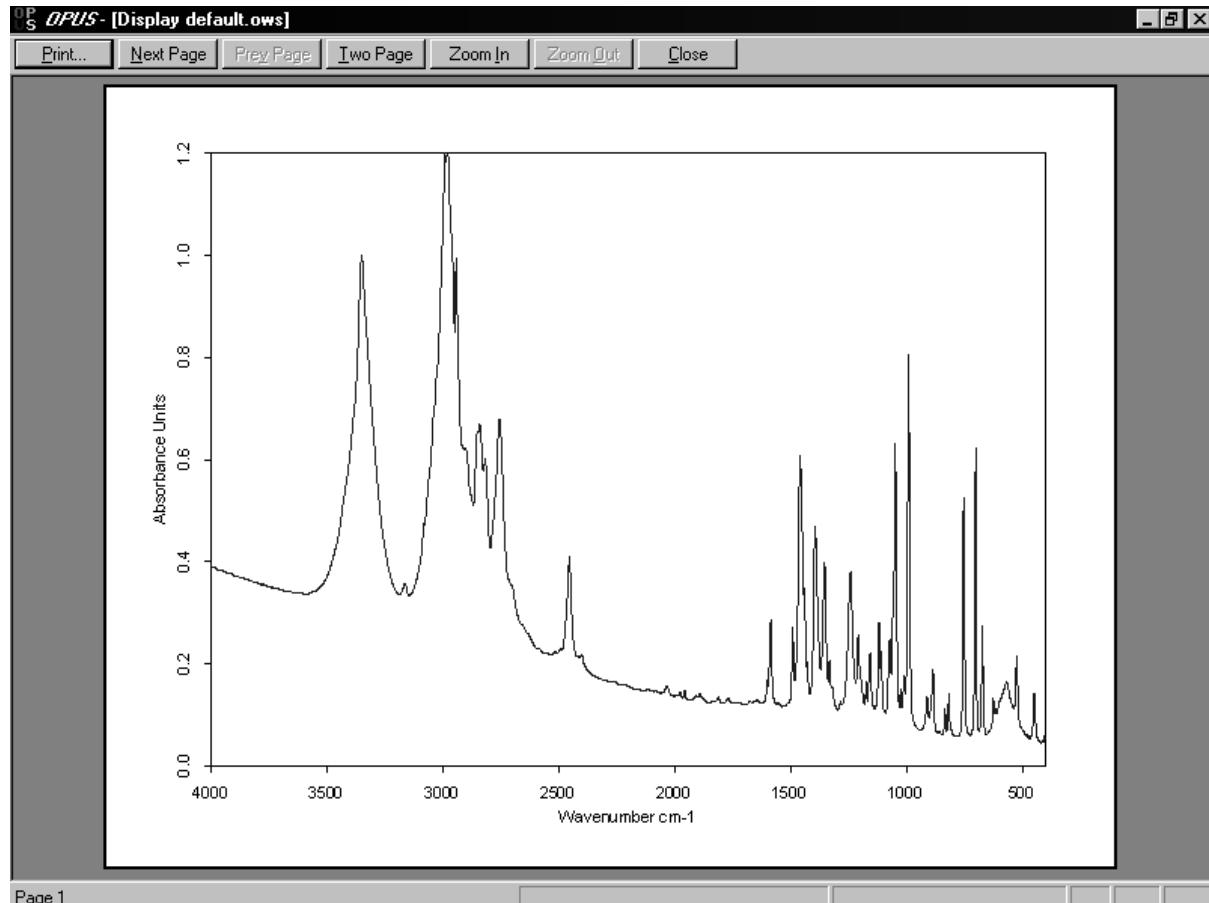
Figure 254: Print Preview

Click on the *Frequency Range* tab and either type in the limit values manually or define them interactively. If you click on the *Get Display Limits* button, the current display limits are automatically set.

Figure 255: Plot Spectra - Frequency Range

On the *Options* tab you can define the number of peak labels, scaling and printout format.
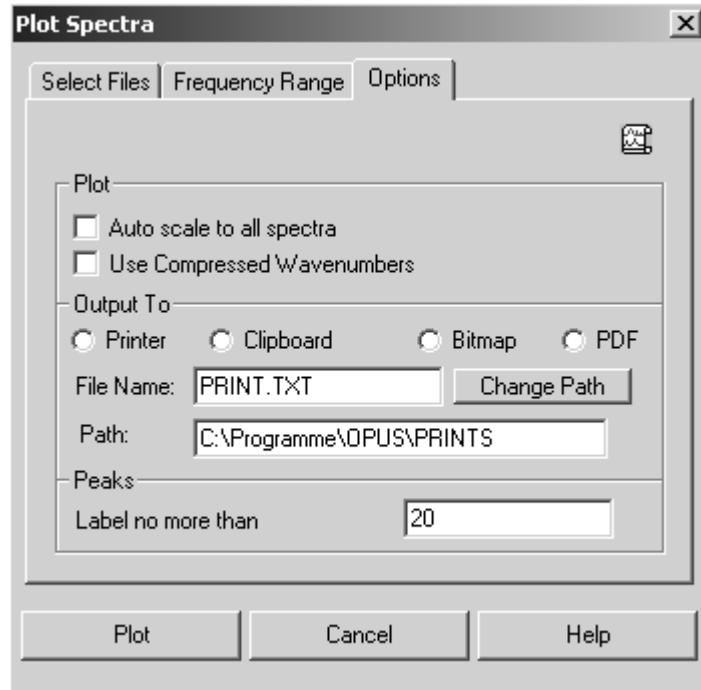
Figure 256: Print Spectra – Options

If you activate the *Auto scale to all spectra*, the x-axis of the spectrum will be linearly scaled. The *Use Compressed Wavenumbers* check box allows to plot

the with compressed wave numbers, i.e. the wave numbers above $2000\,\text{cm}^{-1}$ will be compressed by a factor of 2.

The printout can both be sent to the printer or the clipboard. It is also possible to create a bitmap or a PDF file. To save the plot define the file name and path in the respective entry field, or edit the path by means of the *Change Path* button. Click on the *Plot* button to start printing.

11.4   Quick Print

You can use the *Quick Print* command to plot the contents of an OPUS view without specifying a template. A default template suited for the currently displayed view will be used. You can change this default template by editing it or saving a different template of your choice as default. The following templates are available:

Default Template Name	Associated Window Type
3D.PLE	3D Window
3D+.PLE	3D+ Window
DEFAULT.PLE	Display (spectrum) window
LIBRARY.PLE	Library window
LIVE+OVERVIEW.PLE	Live video and overview image window
LIVEVIDEO.PLE	Live video window
MAP+SPEC.PLE	Result window of a MAP acquisition
OLDREPORT.PLE	Report window
OVERVIEW.PLE	Video overview window
ONLINE.PLE	Result window of a CHROM acquisition
REPORT.PLE	Report window
SEARCHRESULTS.PLE	Search report window
SINGLEREPORT.PLE	Report window
STRUCTURE.PLE	Structure window
VIDEOPOSTRUN.PLE	Video postrun window

The *Quick Print* command generates a printout which shows the OPUS window as it is displayed on the screen. If only part of the spectrum is displayed, only this part will be printed including all labels and annotations.

11.5 New Layout – Plot Layout Editor

Use the Plot Layout Editor (PLE) to create templates used for multiple printouts. The templates you created can be saved using the *Save as* command from the *File* menu. The PLE enables you to label peaks in a spectrum, plot details of a spectrum, print parameters and peak tables.

Start the PLE by selecting *New Layout* from the *Print* pull-down menu. Now the PLE tool bar becomes active and a new PLE window will be opened:

The PLE window consists of a black grid and a red frame. This frame represents the available print area of your printer. Located next to the PLE workspace is the PLE Browser. To the left of this window you find a column with the title *item*.

The PLE window has a *PE* tab attached. Use this tab to switch between the PLE and the spectrum window.

Since the available print area depends on your specific printer, its particular settings must now be configured. If you have already installed a printer for Windows, then you may skip the next section.

OPUS Browser   PLE Browser   PLE tool bar   PLE workspace   Active frame
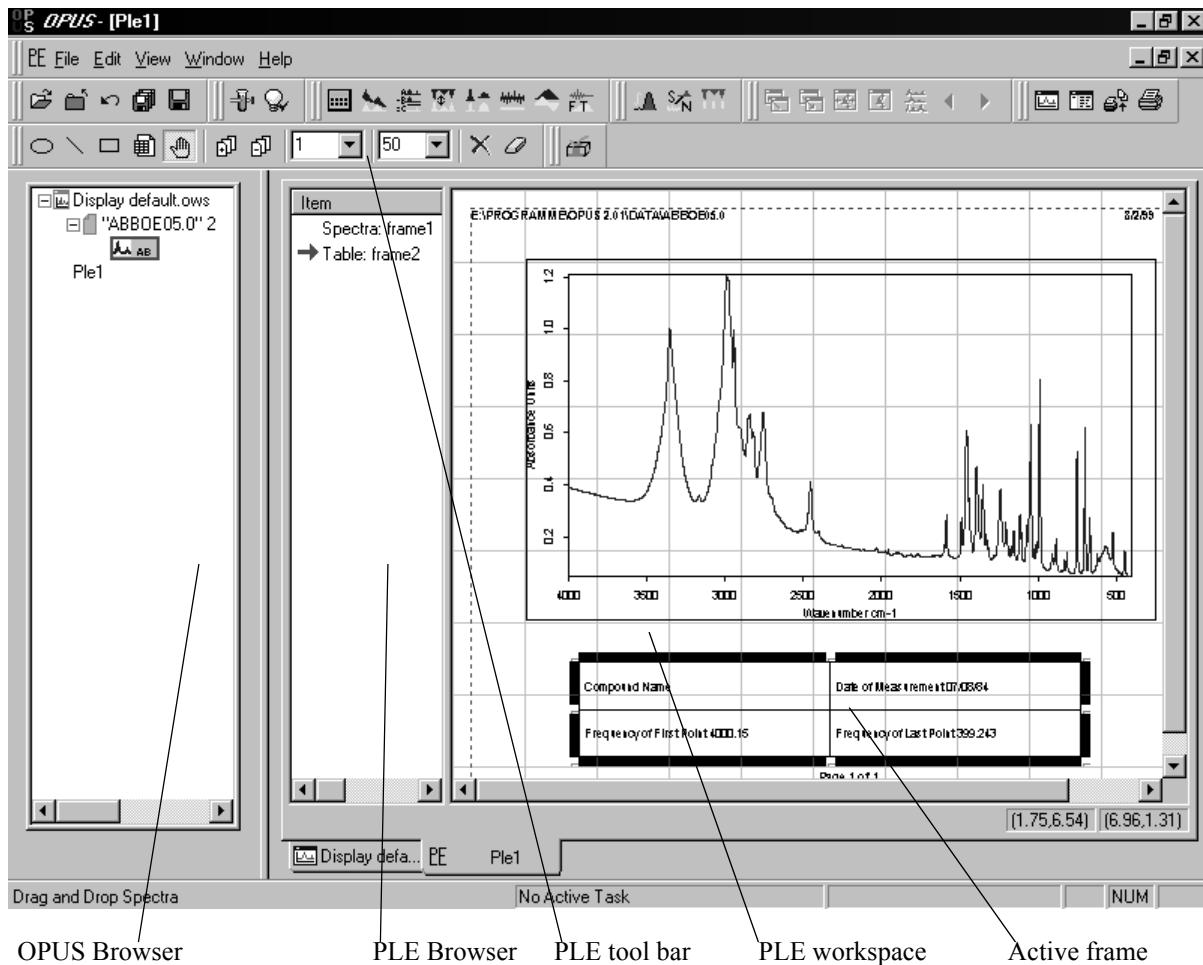
Figure 257: The PLE User Interface

- Start the PLE with *New Layout* from the *Print* pull-down menu.
- From the *File* menu choose the *Print Setup* command.
- The printer properties page will be displayed. Select the appropriate paper size and format.
- Close the dialog box by clicking on *OK*.
- Now you can start your work with the PLE.

OPUS Browser

The OPUS Browser lists all windows that are open, spectrum windows as well as PLE windows. The active window is highlighted. You can switch between windows by clicking on their icon in the Browser, or by clicking on the window tab.

PLE Browser

The PLE Browser lists all objects that are on the PLE workspace. A frame will be referred to by the type of object it contains (table, spectrum etc.). The active frame is indicated by a red arrow in the Browser and bordered by a thick line on

the PLE workspace. You can click on a frame to make it the active frame. This can be useful, if the item is not visible because it is covered up or is outside of the visible window area. You can right-click on an item in the Browser to bring up its properties dialog.
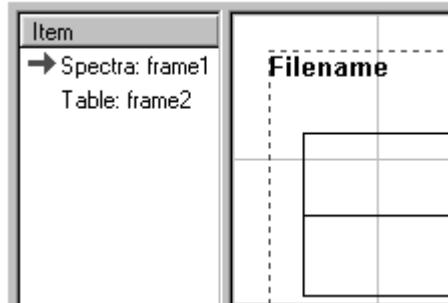
Figure 258: PLE Browser

PLE Workspace

This is a visual representation of the printed page, containing all the frames. Each frame can be scaled and positioned individually. A read-out below the workspace gives you the exact position of the activated frame (left side), while you move it around as well as size of the frame (right side).
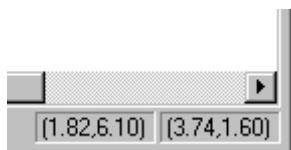
Figure 259: Read-out for Frame Size and Position

By clicking on a frame with the right mouse key, you will bring up the *Properties* dialog box of this frame. Right-clicking the mouse on the page, in a portion that does not contain a frame, will bring up the *Page Properties* dialog.

11.5.1 PLE Tool bar

The tool bar allows quick access to the most frequently used PLE commands. Select a tool by clicking on its icon before using it.

Draw a circle or ellipse on the page.

Draw a line or an arrow on the page.

	Draw a frame on the page. A frame can contain spectra, text, a bitmap or a metafile.
	Draw a frame that will contain a table.
	The selection tool allows you to use the mouse to select and move items on the page.
	Add or remove a page. This allows you to create sophisticated templates with more than one page.
	Select page number.
	Zoom factor (percentage). The zoom factor does not affect the size of the templates' printout.
	Remove objects from the workspace. These objects have to be selected before.
	Clear a selected frame.
	Open the *PLE Page Properties* dialog.
	Anchor an object to its position on the workspace.
	Open the *PLE Box Properties* dialog.
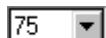
11.5.2 Pop-up Menu

If you right click on a frame, a menu will appear at the point where the mouse is clicked. This allows access to various actions, that can be performed on the frame.

Remove deletes this frame from the workspace, while *Snap to Grid* aligns this frame exactly on the closest grid lines. *Insert Legend* is only available to manipulate spectrum frames and appends a legend to a spectrum frame.

Assign lets you change the content of a frame. You can assign pictures, meta files, spectra, tables, text files or an OPUS view to a frame.

Copy duplicates the content of a frame or a page to a meta file or to a bitmap.
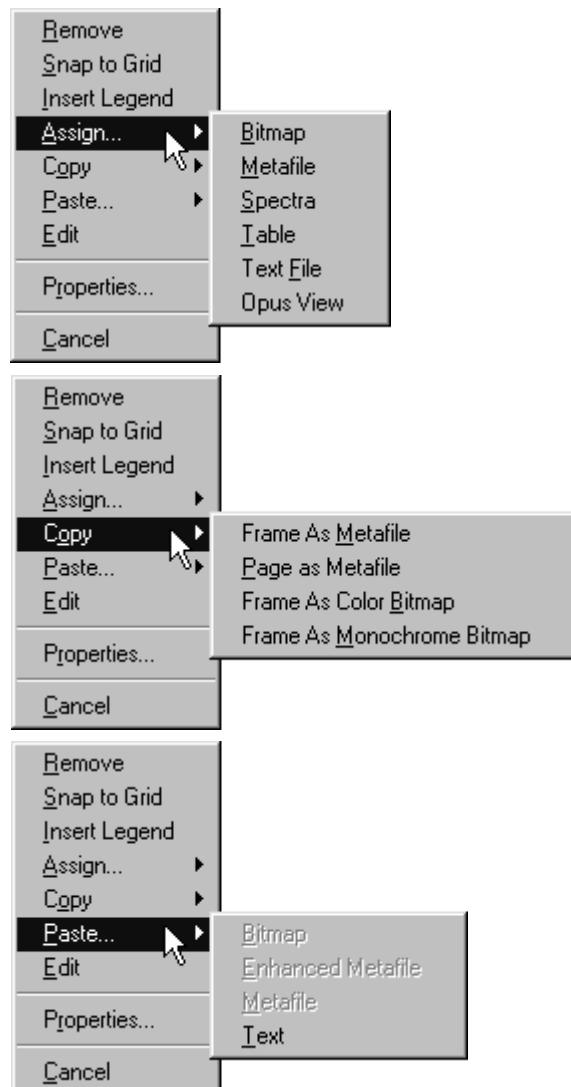
Figure 260: The PLE Pop-up Menu

Paste inserts a bitmap, a meta file or a text file from the clipboard into the selected frame.

Edit manipulates the contents of a frame. This command is only available for text and table frames.

Properties opens the dialog box associated to the selected frame.

Cancel closes the pop-up menu without performing any changes.

11.5.3   PLE Page Properties

Like all other objects the workspace itself has a property sheet associated with it. Using the *PLE Page Properties* allows you to define general settings of the PLE workspace. You call up this dialog box by right-clicking on the empty space of the PLE page.
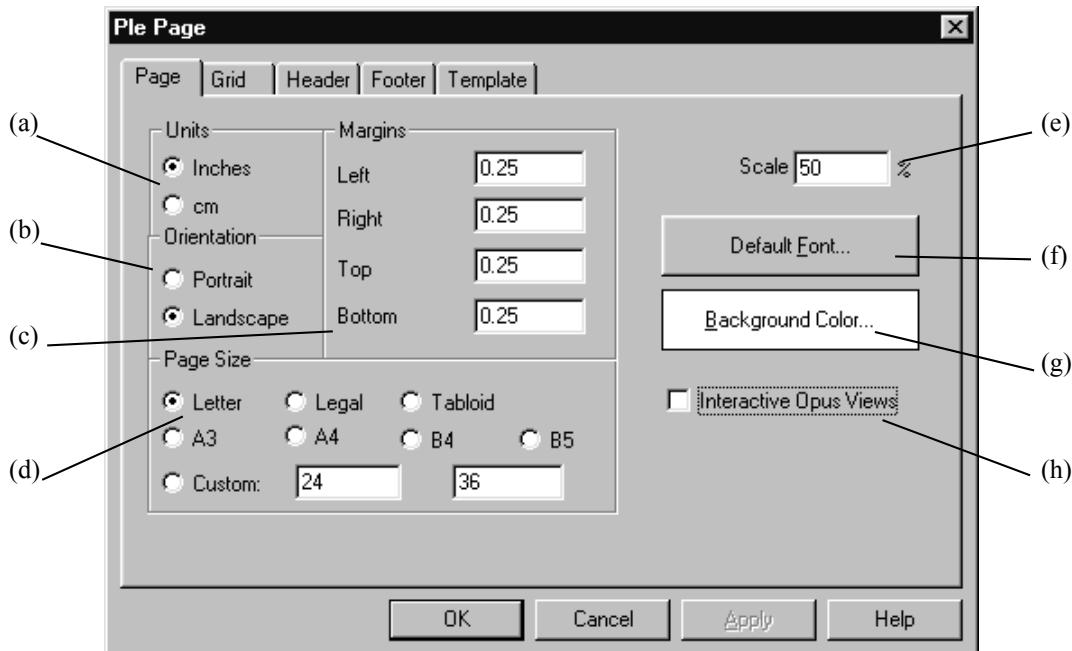

Figure 261: PLE Page Properties

General Page Properties

(a) Specify the units that you want to work with (inches or centimeters).

(b) Select the orientation of the pages in the document.

(c) The available area for printing is represented by a dotted red line on the PLE page. On account of the paper handling machinery of the printer, it cannot print to the outermost edge of the paper. To determine the corresponding unprintable area of the paper, check the manual of the printer or use empirical methods.

(d) Select the size of paper that is in the printer.

(e) This is the zoom (magnification) factor to use in viewing the PLE pages expressed as a percentage. The typical computer screen is not large enough to allow viewing the entire page at 100% scale. 75% is a good selection for documents using landscape orientation, while 50% is good for portrait orientation.

(f) This is the default font used in the document. As frames are created, they will inherit this property. Once a frame contains data, the font can be changed for that frame independently of this setting. This only determines what font will be used when a frame is first created.

(g) The background color of the page.

(h) After you assigned the desired view type to the frame, i.e. a structure view, you can drag & drop a structure data block onto the frame. To save the PLE page as a template remove the data block again; the frame will retain the view type associated to it. If the *Interactive Opus view* check box is marked, you can access an

object within a frame. You can assign any type of Opus view to a frame. Simply draw a frame on the PLE page and right-click on it to open its *Properties* pop-up menu. Selecting *Assign Opus View* will enable interactions with 3D spectra, e.g. rotating the spectrum.

Grid Properties
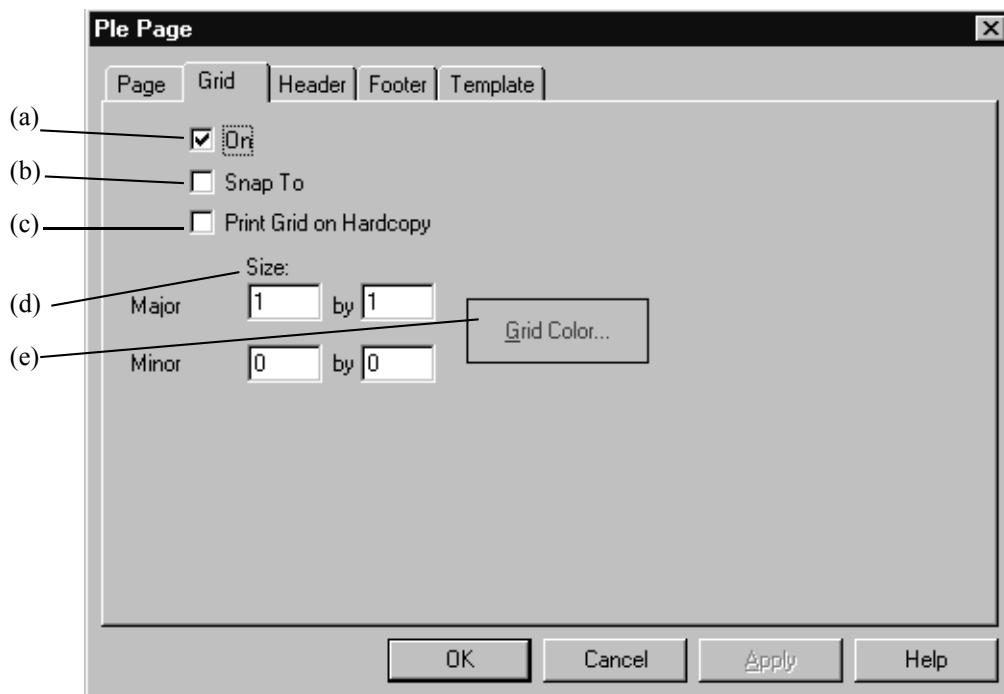
Figure 262: Grid Properties

(a) This controls whether the grid is visible on the page. A grid is useful for aligning objects. However, the grid will not be printed.

(b) As objects are created, they can be automatically positioned and sized to line up with the closest major grid lines.

(c) Usually a grid is displayed only on the screen because it is useful for alignment during document composition. If you want the grid to also be printed on the paper, select this option.

(d) This is the size of the grid, in the units that are specified in the *Page Properties* page (above). The grid can be further divided by filling in the *Minor* fields.

(e) The color used to draw the grid.

Header and Footer Properties

The Header and Footer are information that are printed on the top and bottom, respectively, of every page. The Header and Footer dialogs are identical, so only the Header dialog is discussed. Everything said about the Header applies to the Footer also.
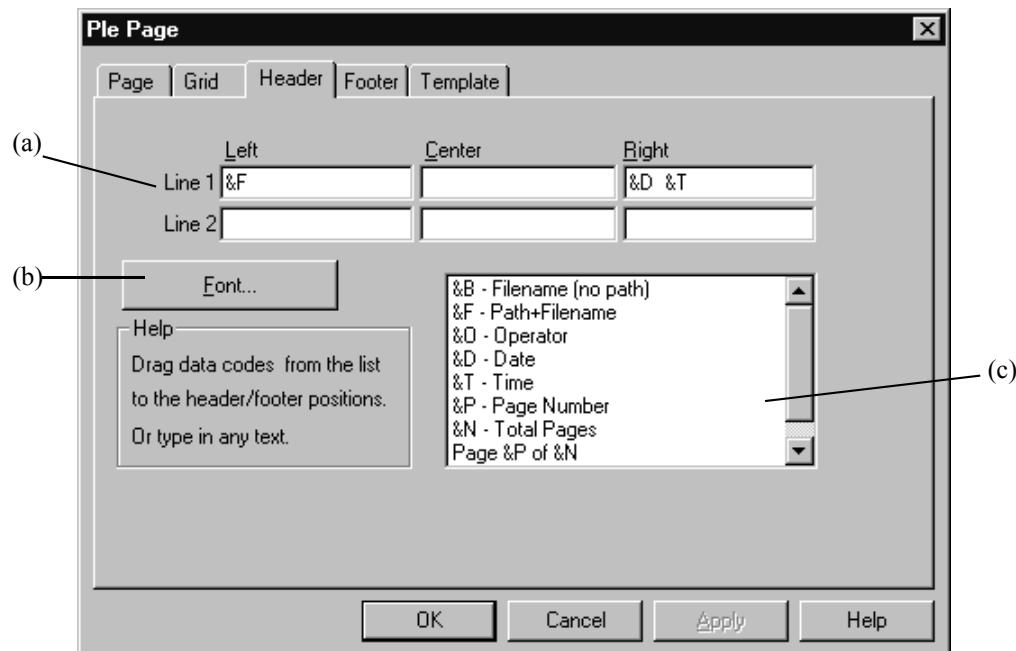
Figure 263: Header Properties

(a) The Header (or Footer) can consist of 6 fields: two rows in the left, middle, and right. The entries in the fields consist of metastrings; you can either type them in or drag them from the list (c). Of course you can also type plain text which will be displayed.

(b) The font to use to print the Header (or Footer).

(c) These are special codes that the PLE uses to identify the information that will be displayed on the page. You can use the mouse to drag the codes from the list to the field that you want information to be printed in. Or, you can type them into the fields directly.

Template Properties
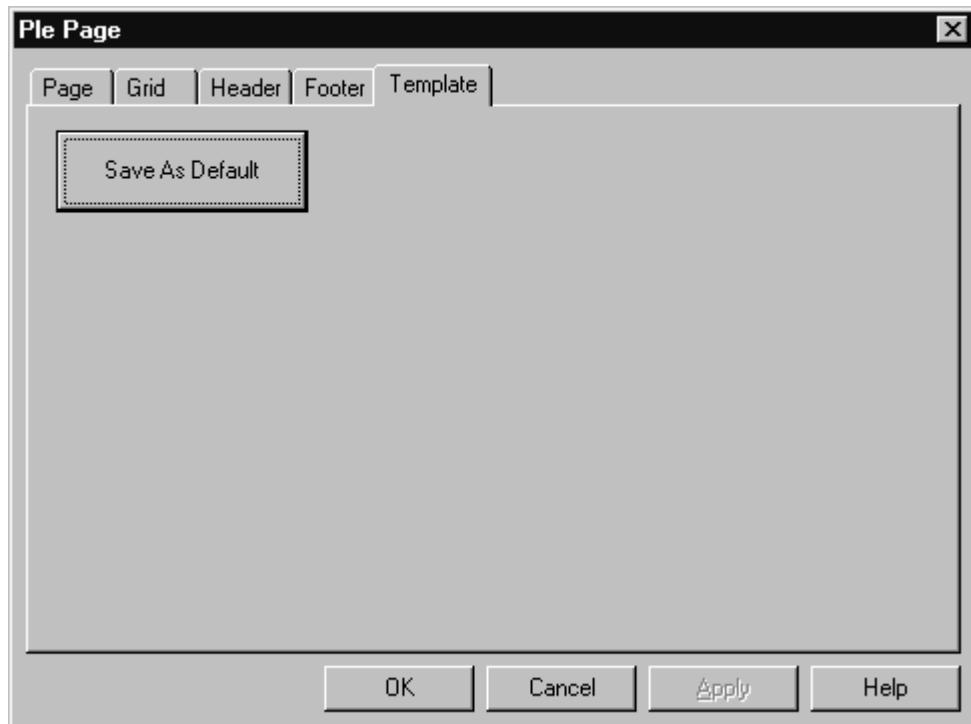
Figure 264: Template Properties

You can also save a template to be used as default. When new PLE documents are created, they will start with all of the properties of this template. The default template is automatically named "default.ple" and is located in the same directory as the OPUS executable program. Using the *Save As* choice on the *File* menu, templates can also be saved to any file name and directory. Using the *Open* choice on the *File* menu, they can be recalled for later use.

11.5.4   Loading and displaying a spectrum

A spectrum can be loaded by simply dragging it from the Browser onto the workspace. Alternatively, draw a frame by first selecting the □ icon and then using the left mouse key. Open the frames pop-up menu by clicking on the frame with the right mouse button, then select *Assign* and *Spectrum*. A file selection box will appear, in which you may choose the spectrum you want to insert. It will then show up in the frame, along with the axes and notation.
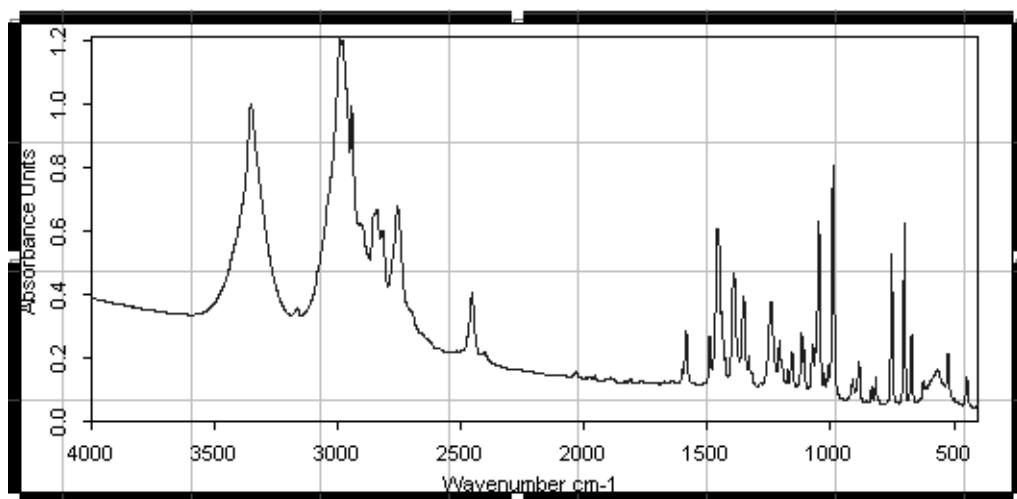
Figure 265: Spectrum Frame

In order to print the parameters of the spectrum, select the [icon] icon from the icon bar and draw a frame as done for the previous frame. This frame will contain a table which has by default two rows and two columns. Again, change the properties by calling up the *Properties* dialog (see chapter 11.5.6) with the right button. The thickness of the dividing lines between the cells and the colors, as well as the font, can be changed using the properties box. Also, you can assign titles to the rows and columns.

Using the left mouse button select a parameter from the list on the second page of the pop-up menu and move it to the cell in the table where you want it to appear. The parameter will be displayed along with its value.

Operator Name BRUKER	Frequency of First Point 4000.15
Filename ABBOE05.0	Frequency of Last Point 399.243
Sample Name COMPOUND B	Y Units Absorbance Units

Figure 266: Table with Parameters Included

Text can be included using text frames, either typed in or by assigning a text file to a frame. For manual text input draw a frame and open its pop-up menu. Use the *Change* command to transform the frame into a text frame. A text field will appear in which you now can enter the text. You close this field by left-clicking anywhere outside the field. You can re-size the text frame as usual. By selecting *Change* again you can edit the text.

To import a text file start again by drawing a frame. From the *Assign* command

of the pop-up menu choose *Text File.* A file selection box opens from which you can choose the text file to import. Currently, only files with the extension ".TXT" can be imported. Text formatting is discussed in chapter 11.5.7

11.5.5   PLE Spectral Frame Properties
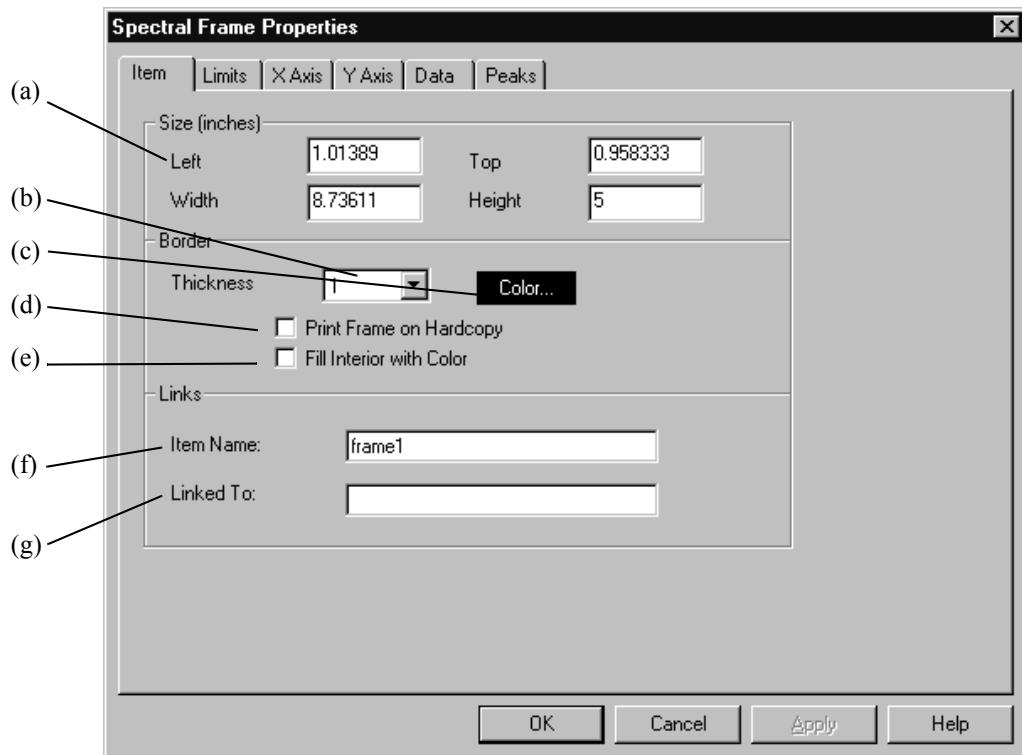
Figure 267: Spectral Frame Properties – Item

(a) Change the size and position of the frame by entering the respective values in the *Size* fields. The units used here are specified with the *PLE Page* dialog.

(b) You can select the line thickness used for the frame in pixels.

(c) The *Color* button lets you specify the color used to draw the frame, both, the background color as well as the color of the frame. A color chart is displayed from which you can either pick a color or define your own color.

(d) Normally, the border of the frame is not printed. Check this box if you would like to have the border of the frame printed.

(e) Check this box to set the frames' background color to the value chosen with (c).

(f) A name can be assigned to every object. Naming all the objects in your template simplifies their identification in complex layouts. You can use these names to link frames to each other.

(g) This field contains the target of a link operation. You can link table and text frames to spectrum frames to keep your layout organized. To establish a link, enter the *Item Name* of the target frame in the *Linked To* field.
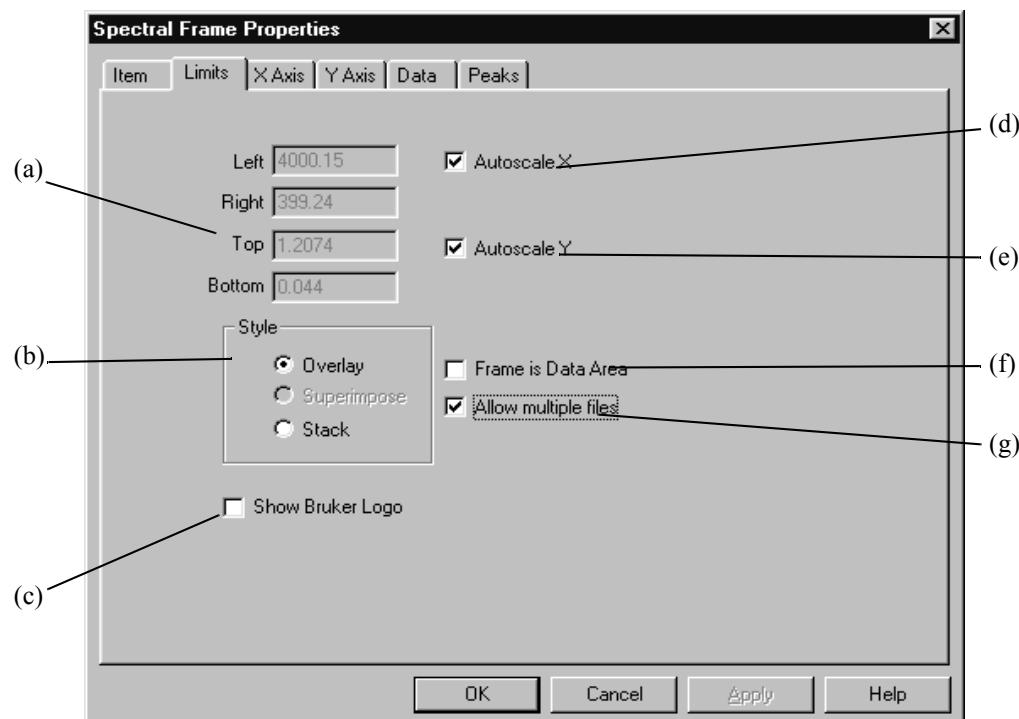
Figure 268: Spectral Frame Properties – Limits

(a) These are the limits for displaying the spectral data. The units are specified with the *PLE Page* dialog.

(b) The style selected determines the presentation of the data in frame. You can stack one spectra on top of another, or overlay them on top of each other.

(c) To add a Bruker Logo to your printout select this check box.

(d) Set the x limits (a) to the current outer limits of all the data that is in the frame.

(e) Set the y limits (a) to the current outer limits of all the data that is in the frame.

(f) When this option is selected the data is expanded to fill the area of the frame, such that the axes coincide with the border of the frame.

(g) If this is not selected, only one spectrum at a time can be displayed in the frame.

The tabs for x and y axis are identical except for the *Rotate Numbers* check box; this only exist on the y axis page. This function allows you to turn the labels of the y axis by 90°. The *Show axis for stacked spectra* and the *Compressed Wave numbers* check boxes are only available for the x axis.
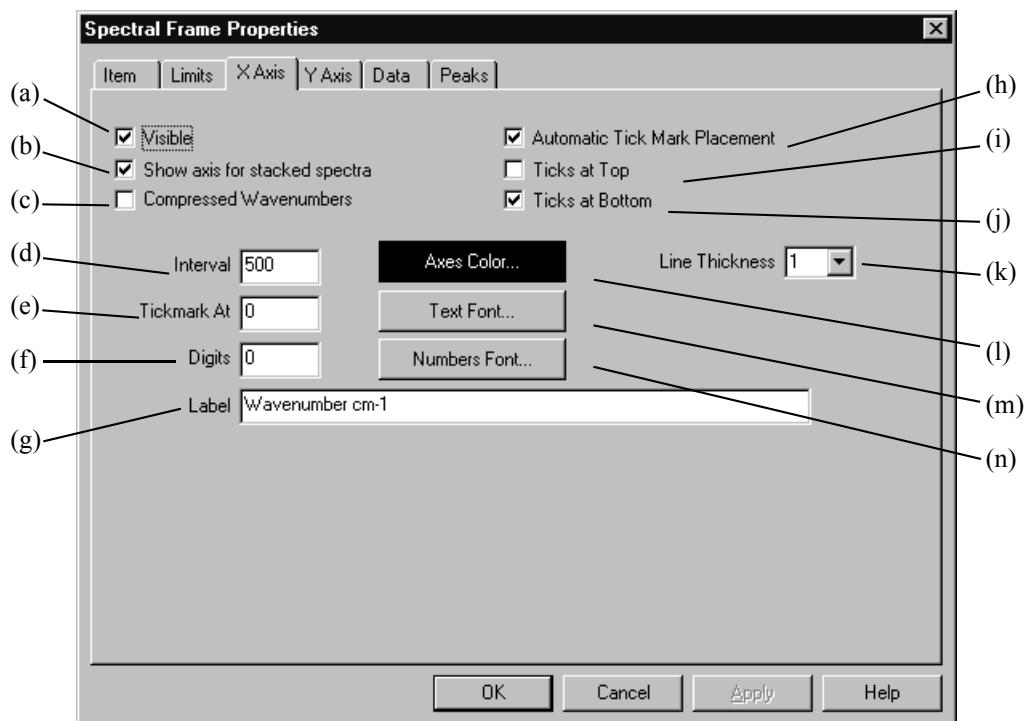
Figure 269: Spectral Frame Properties – x Axis

(a) Controls whether the axes, tick marks, and labels are displayed.

(b) You can have separate x axes drawn for every spectrum of the stack. Otherwise, one common axis will be used for all spectra.

(c) The *Compressed Wave numbers* command displays wave numbers above $2000\,cm^{-1}$ with a smaller linear scale.

(d) If automatic tick mark placement is not selected, this is the interval between the tick marks.

(e) If automatic tick mark placement is not selected, this is the position of a tick mark.

(f) If automatic tick mark placement is not selected, this is the number of decimal places used for the numeric tick mark labels.

(g) The label to display on the axis. This is automatically taken from the data file as data is loaded, but can then be changed by editing this field.

(h) Selecting this allows the PLE to alternatively determine where the tick marks are placed.

(i) If you want tick marks on top of the data area, select this.

(j) If you want the tick marks displayed at the bottom of the data frame, check this.

(k) The thickness of the axis line.

(l) The color to use for drawing the axis.

(m) The font to use for the axis label.

(n) The font to use for the tick mark (numeric) labels.
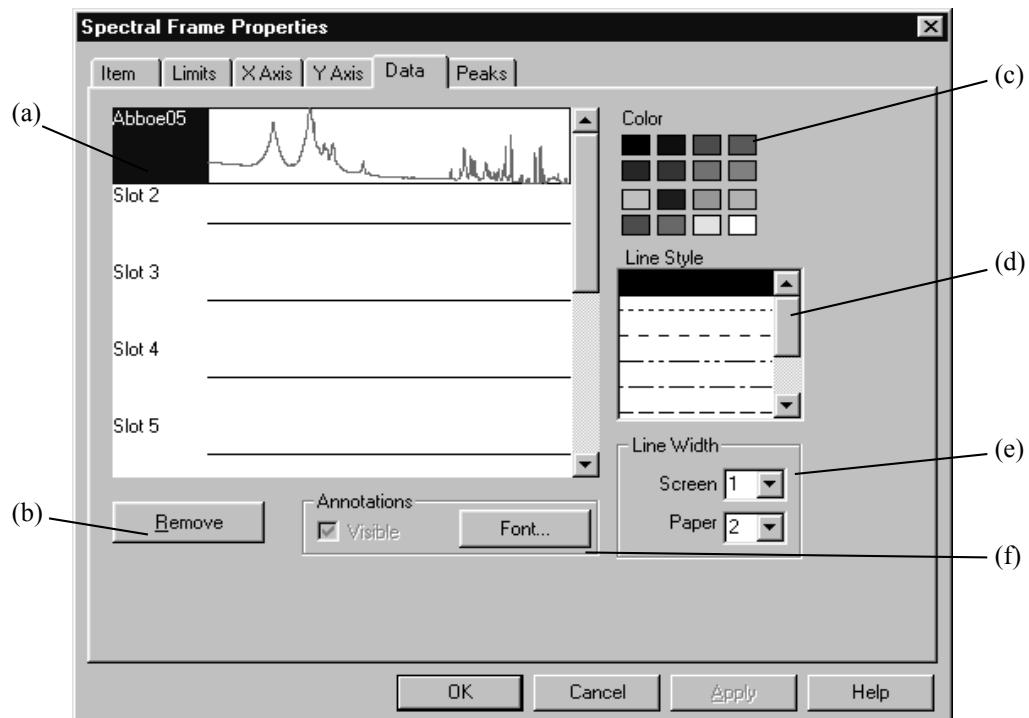
Figure 270: Spectral Frame Properties – Data

(a) As data is added to a spectral frame, it is put into a "slot", which is just a positional number. To change the look of the data in the slots, select the slot in this list box. Then define the properties for that slot, using the rest of the controls on this dialog: *Color*, *Line Type*, and *Line Width*.

(b) Remove the data that is selected in the list (a) from the frame.

(c) The color to use for displaying the data selected in list (a).

(d) The line style to use for displaying the data selected in list (a).

(e) The line width (in pixels) to use for displaying the data selected in list (a). Separate widths can be specified for the screen and the paper.

(f) In case you included annotations in your spectrum you can have them printed with the font selected via the font dialog box (*Font..* button) if you place a mark in the *Annotations* checkbooks.
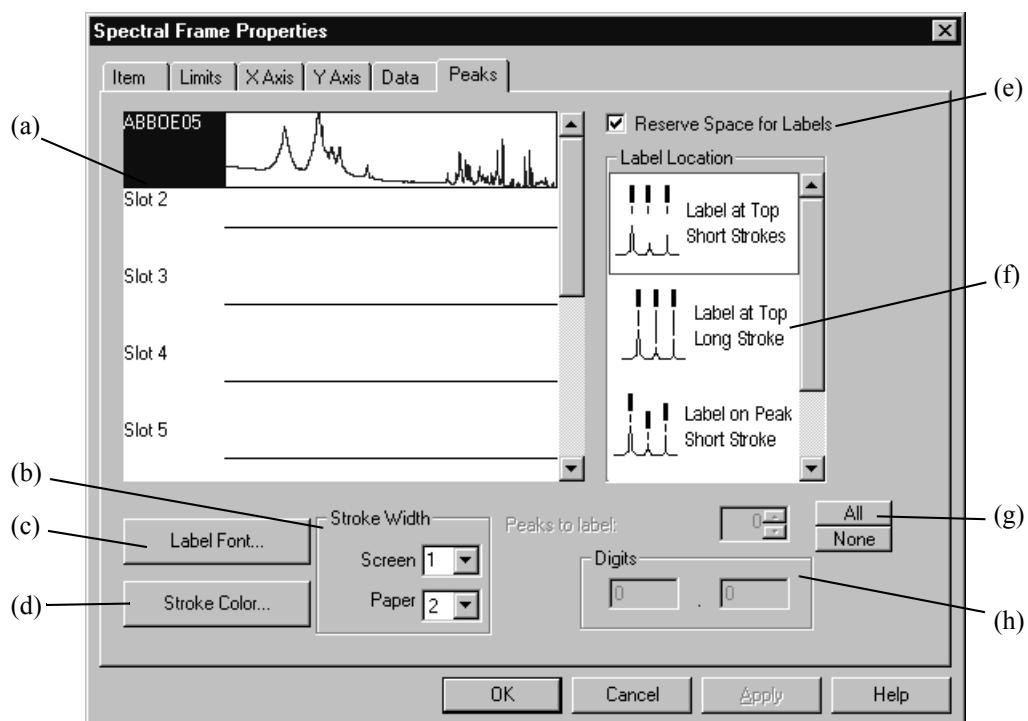
Figure 271: Spectral Frame Properties – Peaks

(a) Similar to the *Data* page the slot holding the relevant data has to be selected first.

(b) Select the stroke line thickness in pixels for the display and the printout.

(c) *Label Font* lets you control the font type used for the stroke labels.

(d) Change the color of the strokes using *Stroke Color*.

(e) Checking this box ensures extra space between the highest peak and the spectrum frame for the peak labels resulting from a peak search. The label type can be chosen from the list (f).

(f) Select the type and position of the labels you want to assign to the peaks.

(g) Specify the number of peaks to be labelled, starting with the highest peak.

(h) Set the number of digits and decimals of the peak labels.

11.5.6   PLE Table Properties

A table is created by choosing the "Table" drawing tool on the PLE tool bar, and then drawing it on the page using the mouse. Tables are linked to spectrum frames via the *Item Name* and *Link To* fields on the *Item* tab (discussed above). By default, a table of two columns and two rows is created. The number of columns and rows can be changed by right-clicking on the table and opening the corresponding *Properties* dialog box.

Cells in a table can also be edited manually, by right-clicking the mouse over the cell and selecting *Edit* from the menu that appears. When you are editing cells, you can navigate between them using the arrow keys. The return (Enter) key also switches the editing to the next cell in the column.

The first tab of the *Table Properties* dialog has been already discussed in chapter 11.5.5.
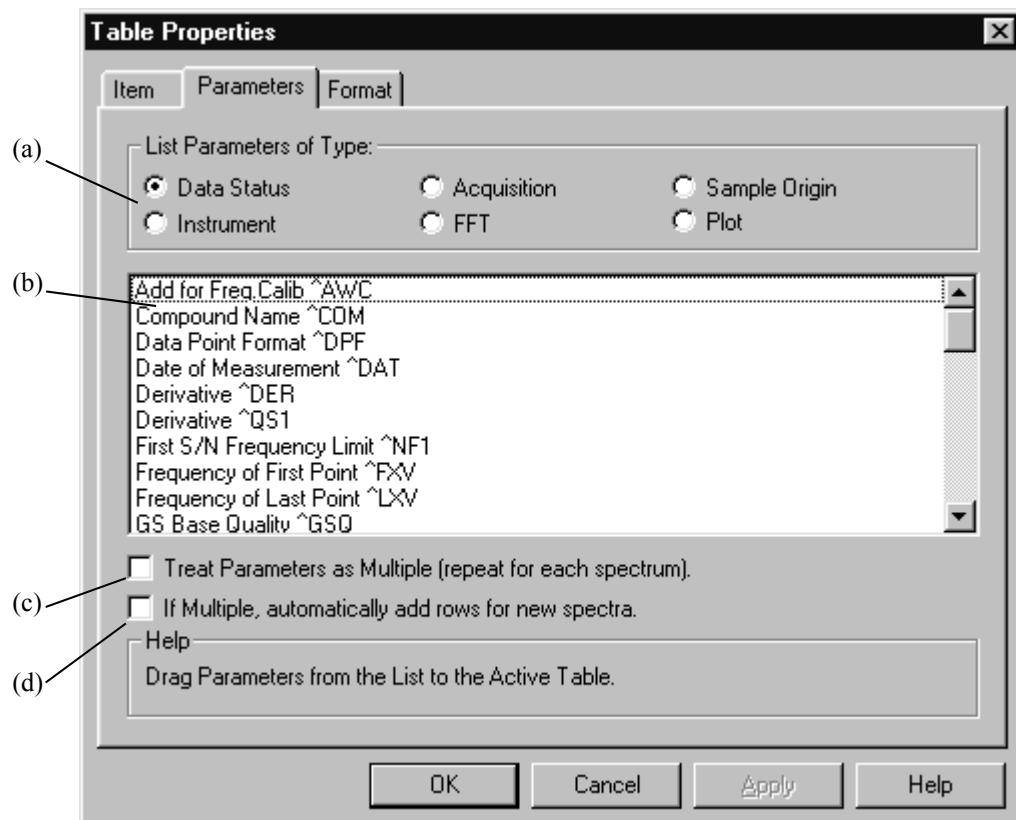
Figure 272: Table Properties – Parameters

(a) The available parameters are categorized. Depending on the category selected, the information displayed in the list box (b) will change.

(b) Available parameters of the type specified in (a) are listed here. To add information to a table, select an item from this list and then drag it to a cell on the table, and drop it there. The strings here are metastrings: a three letter code preceded by a "^" character. When PLE encounters such a code, it interprets it as an instruction to extract the information from data slot one of the linked spectral frame and substitutes that information for the code, when the table is displayed. If you edit the cell (via the *Edit* choice on the context menu, below), you will see the actual codes. When the table is displayed, you see the information that the code symbolizes. If you do not like the default format of the information, just edit the cell and change it.

(c) Normally, the information extracted by PLE to expand the metastrings is taken from the spectrum in slot one of the linked spectral frame. By choosing this option, the parameters can be repeated for each spectra in a frame, up to the number of rows you have defined on the *Format* dialog (below).

(d) As new spectra are added to a frame, new rows can be added to the table to display the parameters for each spectrum. This setting will override the number of rows that you have set on the *Format* dialog (below).
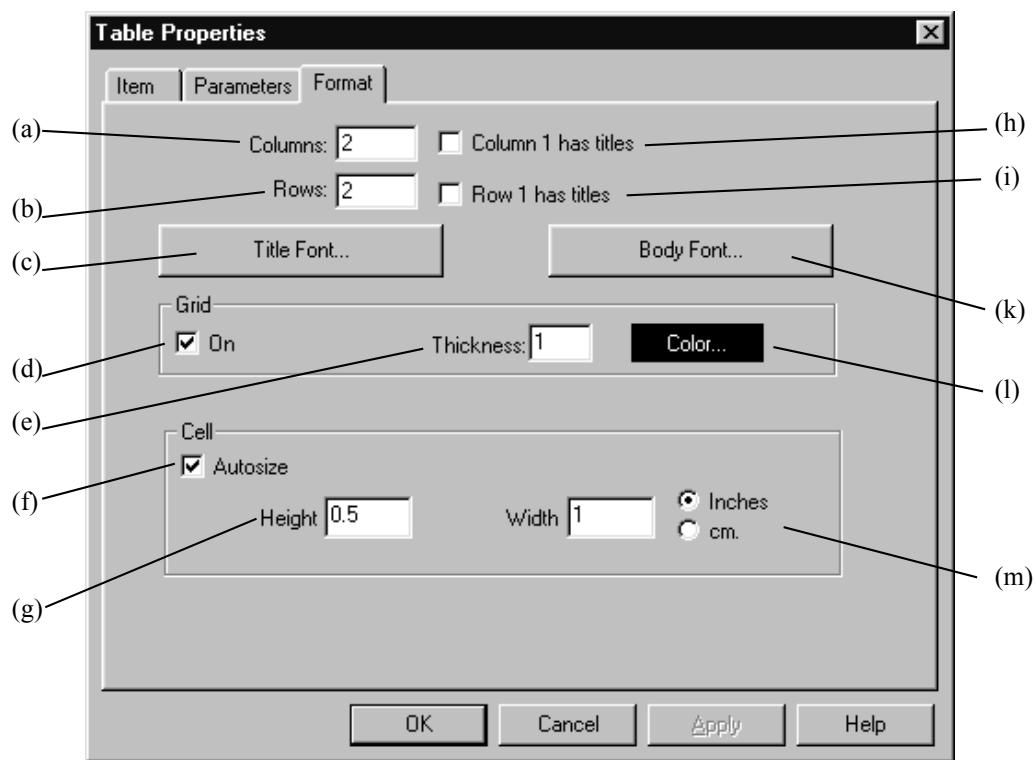
Figure 273: Table Properties – Format

(a) The number of columns in the table; the default value is two.

(b) The number of rows in the table; the default value is two.

(c) The font to use for row 1 (if the *Row 1 has titles* option is checked).

(d) A grid can be displayed, which contains each cell in the table.

(e) The thickness of the grid, in pixels.

(f) Cells can be sized automatically to fill the frame that encloses the table.

(g) If *Autosize* is not selected, this is the height of a cell (in the units specified to the right (l)).

(h) If this is checked, the text in column 1 is used as a column header, and is displayed in the font specified using the *Title Font* button (c).

(i) If this is checked, the text in row 1 is used as a row header, and is displayed in the font specified using the *Title Font* button (c).

(j) Assigns different colors to better distinguish the rows.

(k) The font to use for the body of the table. If *Column 1 has titles* and *Row 1 has titles* are both unchecked, this font will be used for every cell in the table.

(l) The color of the grid, if it is to be displayed. After a selection has been made this button will be displayed in the color of choice.

(m) If *Autosize* is not selected, this is the width and height of a cell (in the units specified to the right).

11.5.7   PLE Text Properties

If a frame contains text, its properties can be set here. The text can consist of metastrings or manually typed characters. The metastrings used for table parameters (see chapter 11.5.6) can also be typed into a text frame, and they

will be interpreted by PLE using the data from the spectrum frame linked to the text frame.

The *Item* and *Parameters* tabs have already been discussed in the previous chapter.
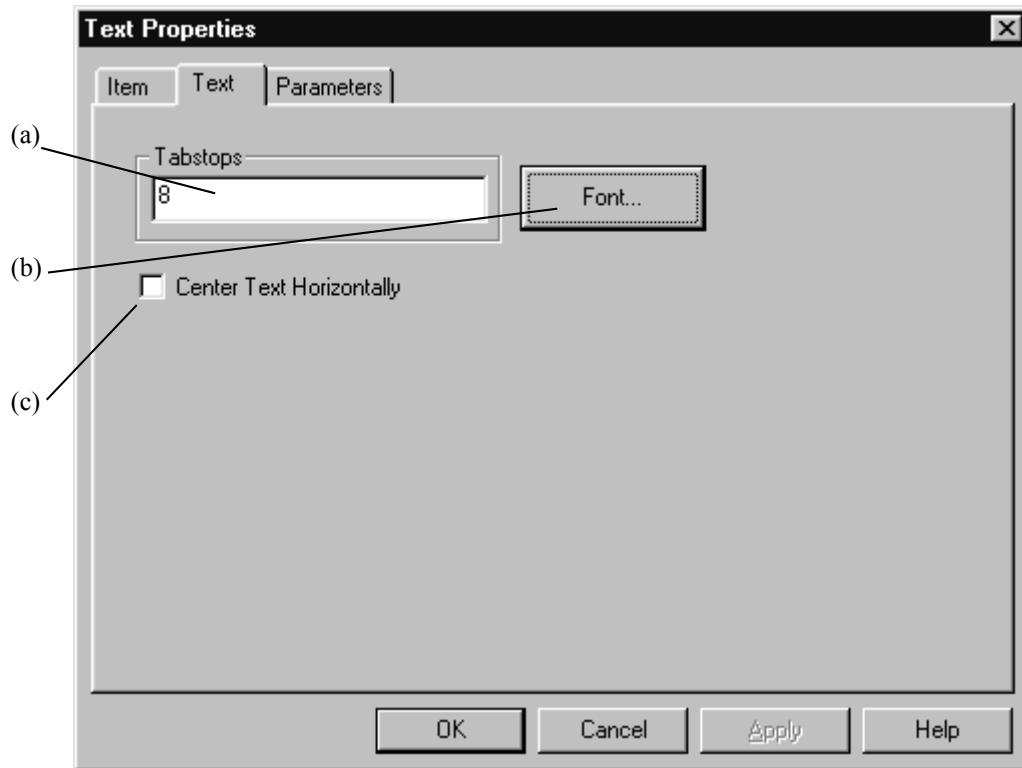
Figure 274: Text Properties – Text

(a) Defines the tab stops for the text in the frame. Multiple positions can be used, separated by spaces, such as "8 12 20 40". The last tab spacing is used for subsequent tabstops, should more be contained in the line.

(b) The font and font size to use for the text.

(c) Centers the text within the frame.

11.6   Open Layout

New Layout calls up the Plot Layout Editor, while *Open Layout* shows a list of existing templates. When using this command for the first time after the installation of OPUS you will have to navigate to the desired directory.

11.7   Print / Print Preview

You can view the result of a printout using the *Print Preview* command. *Print* will start the printing process immediately.

11.8   Print Setup

Paper orientation and the printer (in case you have more than one printer attached to your computer) are selected using the *Print Setup* menu.

12 Macro

OPUS functions you use routinely, can be automated as a macro. An OPUS macro is a sequence of OPUS commands that can be executed as one unit. Besides the regular OPUS commands a set of macro functions exists to control the macro execution, the interaction with the user and the evaluation of results.

An OPUS macro basically is a text file with the extension *.MTX,* which can be edited using any kind of text editor. A detailed description of all macro functions and the command language is given in the OPUS Programming manual.

This chapter briefly describes the commands of the *Macro* pull-down menu. It also tells you how to include macros in the OPUS tool bar.
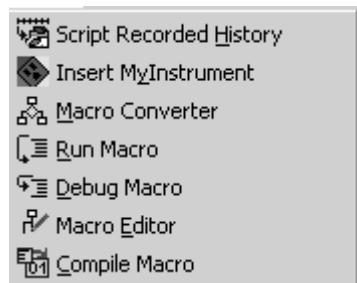

Figure 275: Macro Menu

12.1   Script Recorded History

The information stored in the history block of a file can be extracted into a script. Select the file you want to extract the performed manipulations from and load it into the upper window. Select a file name for the script and define the path, where it should be saved to. *Include Measurement* includes the measurement parameters as well.

Once the script has been saved, it can then be carried out on other files using the *Visual Basic Scipt* command from the *File* menu.
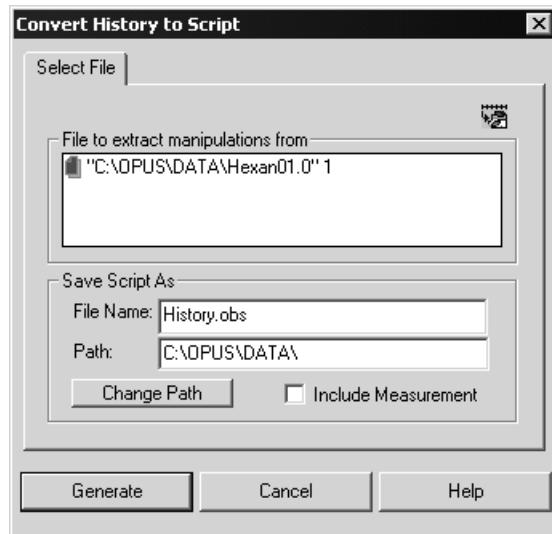
Figure 276: Macro Menu

12.2   Insert MyInstrument

My Instrument is a standardized programming interface for spectrometers running in 32-bit Windows environments. The design of this interface makes the spectrometer and the software module, which controls the spectrometer, synonymous. However, the interface clearly distinguishes between data acquisition and data processing.

The software allows to set all hardware parameters and measurement conditions which are typically useful. Special features like the detector temperature or alignment can be controlled.

Select the *Insert MyInstrument* command to create a Visual Basic Script.
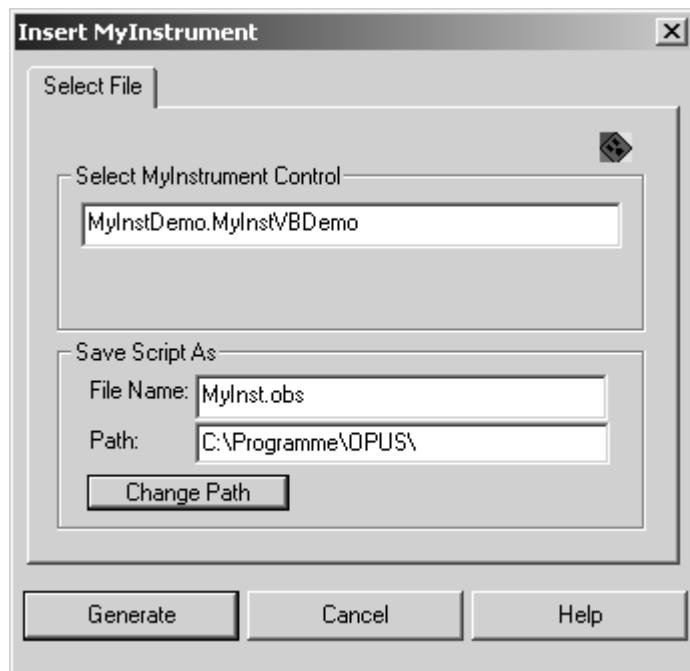
Figure 277: Insert MyInstrument - Select File tab

Enter the name of the registered *MyInstrument* control into the *Select MyInstrument Control* entry field, and define the file name and path for the resulting Visual Basic Script.

12.3   Macro Converter

Use the Macro Converter to translate macros written under OPUS-OS/2 into the OPUS format. The conversion may require some changes as a result of the different macro syntax. See the OPUS Programming manual for details.

12.4   Run Macro

To run a macro use the *Run Macro* command of the *Macro* pull-down menu. The file load box appears through which you can immediately start the macro you have selected. All further action depends on the macro you have chosen.

12.5   Debug Macro

The term *Debugging* means a step-by-step execution of a macro program with the aim of locating program errors. The program execution will continue until a stop mark is reached. This option greatly facilitates locating and analyzing errors.

12.6   Macro Editor

OPUS includes an editor to conveniently generate and edit your own macros. Start the editor with the *Macro Editor* command from the *Macro* pull-down menu. Either generate a new macro or load an existing one by clicking on the *Open Macro* button.

12.7   Compile Macro

Macros are written and stored as text files, which will be converted to executable binary code during runtime of the macro. The *Compile* command performs this step separately and generated executable binary code from a macro text file. Compiled macros are started faster than macros in text format.

12.8   Add Macro to the Toolbar

Macros which you use regularly can be added to the toolbar. To do this you have to add an entry to the USERMAC.LST file, to be found in the OPUS directory. If this file does not exist on your machine it has to be created using a text editor.

For every macro you want to include in the pull-down menu of the tool bar you have to add the following information to the USERMAC.LST file:

1) Name and path of the macro file.
2) Number of the menu (see table).
3) Text to be included in the menu.
4) Text for the tool description of the tool bar.
5) Text for the status bar.

Separate the entries by an "@" sign, e. g.:
E:\OPUS\MACRO\IT.MTX@8@Instrument test@IT-Test@Start IT

If you want to include an icon for the macro added to the tool bar you have to provide a 16*15 pixel bitmap. This bitmap must reside in the same directory as the macro.

To specify the menu you want to add a macro to, use the number indicated in the following table.

Menu	Number of Menu
Measure	1
Manipulate	2
Evaluate	3
Display	4
Print	5
Macro	6
Edit	7
Validation	8
Settings	9
File	10

13 Validation

The *OPUS Validation Program* (OVP) is a supplemental application software integrated in the OPUS software program. Its primary purpose is to provide an automated method to validate *Performance Qualification* (PQ) and *Operational Qualification* (OQ) of the spectrometer.

13.1   OPUS Validation Program (OVP)

The *OPUS Validation Program* (OVP) is part of the OPUS software and supports the 21 CFR Part 11 regulation in connection with the OPUS VALIDATION software package.

This chapter is mainly written for the system administrator who is responsible for the administration and maintenance of the spectrometer system. Details on the OVP installation, OPV setup for initial and general use by the operator are described in the following.

OVP is written in a modular, i.e. plug-in format. After installing OVP you have to configure OPUS to ensure OVP compatibility, and setup OVP to define the validation process.

OVP works in connection with OPUS as follows:

- As many as twelve test channels can be defined and assigned to OVP by specifying a unique measurement configuration for each channel. These configurations are used during the validated measurement process. Each test channel, e.g. sample compartment, integrating sphere has individual parameter settings.
- For each test channel a time period is defined which determines when a *Performance Qualification* (PQ) or *Operational Qualification* (OQ) test will be required. These tests can consist of one or more test protocols assigned by the system administrator.
- If the time period has expired for a particular channel, a warning will be displayed in OPUS. In this case the user can run OVP.
- OVP provides a simple Wizard interface which assists the user and automatically performs the test(s) assigned by the system administrator. If the test has been completed, a simple pass/fail interface will be shown with the option to view and/or print a detailed report.
- If the test has passed, the OPUS warning becomes validated. The operator can continue using the instrument as this has been properly validated.

- An unattended mode is also available which allows to run the test(s) completely automatically and without any user interaction, e.g. over night or in the early morning.

13.1.1   OVP Installation

To install OVP insert the installation CD-ROM into the computer primary CD-ROM drive. After a few moments, the installation program starts automatically.

If the installation program does not start automatically,

- click on the *Start* button on the Windows toolbar.
- select the *Run* option.
- type *D:\OVP_Install.exe* into the text field of the dialog that pops up. Substitute the proper drive letter for your CD-ROM drive.
- click on the *OK* button to start the installation.
- alternately use the *Browse* button to select the installation program on the CD-ROM.

Once the OVP installation program runs it will determine the current location of the OPUS program. By default, OVP is installed in the *Validation* sub-directory located in the OPUS directory. This path is highly recommended but not obligatory.

   Note: You must have installed OPUS before being able to install OVP.

Select the installation language and click on the *Next* button to continue. If the OPUS directory has been located, the installation start dialog appears (see figure 278). Click on the *Next* button to continue the installation, or *Cancel* button to abort the installation.
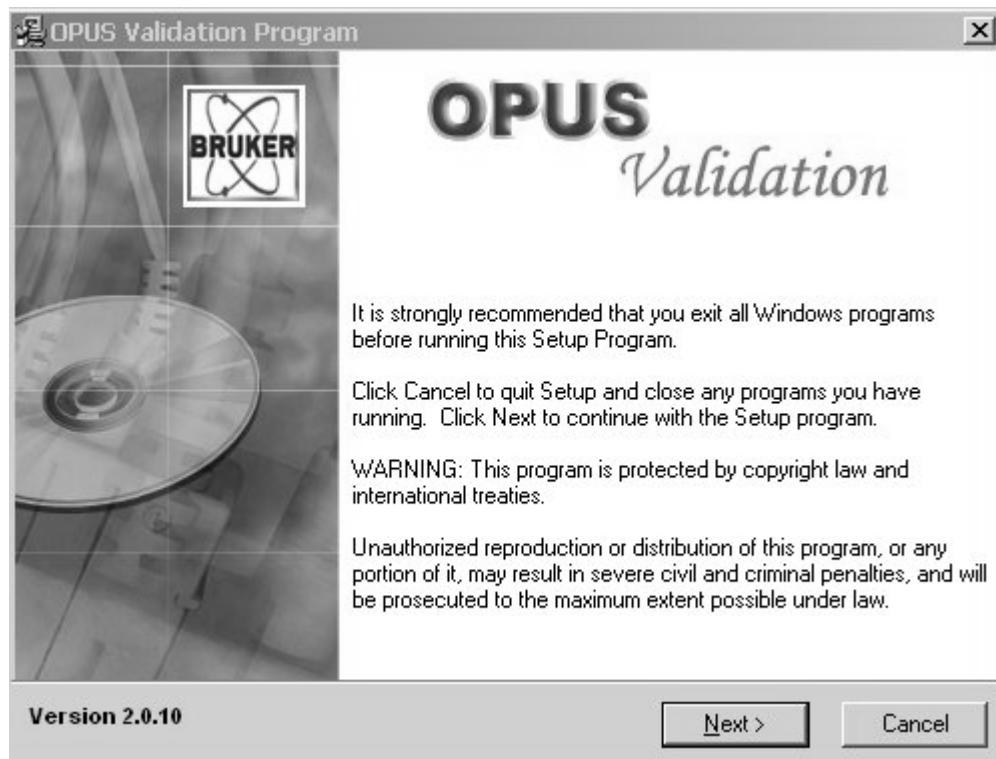
Figure 278: OVP Installation Start dialog

The next dialog displays the destination path of the OVP installation. If the *Destination* entry field does not indicate the appropriate OPUS sub-directory, use the *Browse* button to select the sub-directory. (This may be the case if you have more than one OPUS version installed).

> **Note:** OVP will only work with OPUS 4.2, build 4.2.37 or greater. If you use an earlier OPUS version, contact Bruker to get an upgrade. OVP is not compatible with OPUS versions prior to 4.2.

In case of some operating systems it may be necessary to install the latest MDAC version. If this component has been installed, the computer will reboot. Keep the OVP installation CD-ROM in the drive. After the computer has rebooted, the OVP installation process will start again. Follow the installation steps described.

13.1.2   Database Installation

Measurement and test parameters are stored in a set of databases. These databases are delivered on separate instrument-type-specific CDs and have to be installed separately after the OVP installation. Continue similarly to the OVP installation steps described.

The database installation program locates the installation path of the previously installed OVP. Make sure that you use the same path (.\OPUS\VALIDATION) for the database installation.

If the databases have been installed completely, OVP is ready to be used.

13.2   OPUS Setup (prior to OVP)

Before running OVP for the first time you have to configure the OPUS *Instrument Test* feature to be able to use OVP. Start OPUS and select the *User Settings* command from the *Setup* menu. Click on the *Instrument Test 1* tab. For further details on this subject, refer to chapter 14.10.

13.2.1   Preparing Default Measurement Experiment

This OVP version does not require individual measurement experiments for each test channel as previous versions did. Instead, a single measurement experiment is sufficient and essential when working in validated environment. In that case the measurement experiment must have a valid release signature.

The default measurement experiments for your instrument are in the *XPM* sub-directory of the OVP installation directory (.\OPUS\VALIDATION\XPM by default). The name is derived from the instrument type and must not be changed, e.g. MPA:XPM for the MPA series, TENSOR_27.XPM for the TENSOR 27 series etc.

In order to test the experiment validity select the *Advanced Measurement*, or *Setup Measurement Parameters* command if you are working in validated mode, from the *Measure* menu and load the measurement experiment(s) for your instrument.

If no error is indicated on any of the different parameter tabs, you do not have to change the experiment. If an error is shown, change the parameters which are marked red and store the modified measurement experiment. Then, sign the experiment again by a *Release* signature. For further details on signature setup, refer to the OPUS VALIDATION manual.

13.2.2   OVP Setup

Before you can setup OVP make sure that you have *Administrator* rights within OPUS. You can verify this by the OPUS title bar which has to be as follows:

Figure 279: OPUS title bar

If the title bar looks different, you only have *Operator* rights and will not have access to OVP setup functions.

Assuming you have properly configured OPUS to be used in connection with OVP (see chapter 14.10) you can now continue in order to access the

Administrative Start dialog of OVP. Left click on the status light ( ) located in the bottom-right corner of the OPUS user interface. The *Instrument Status* dialog opens which contains three rows of status icons for different instrument components to be tested by OPUS.
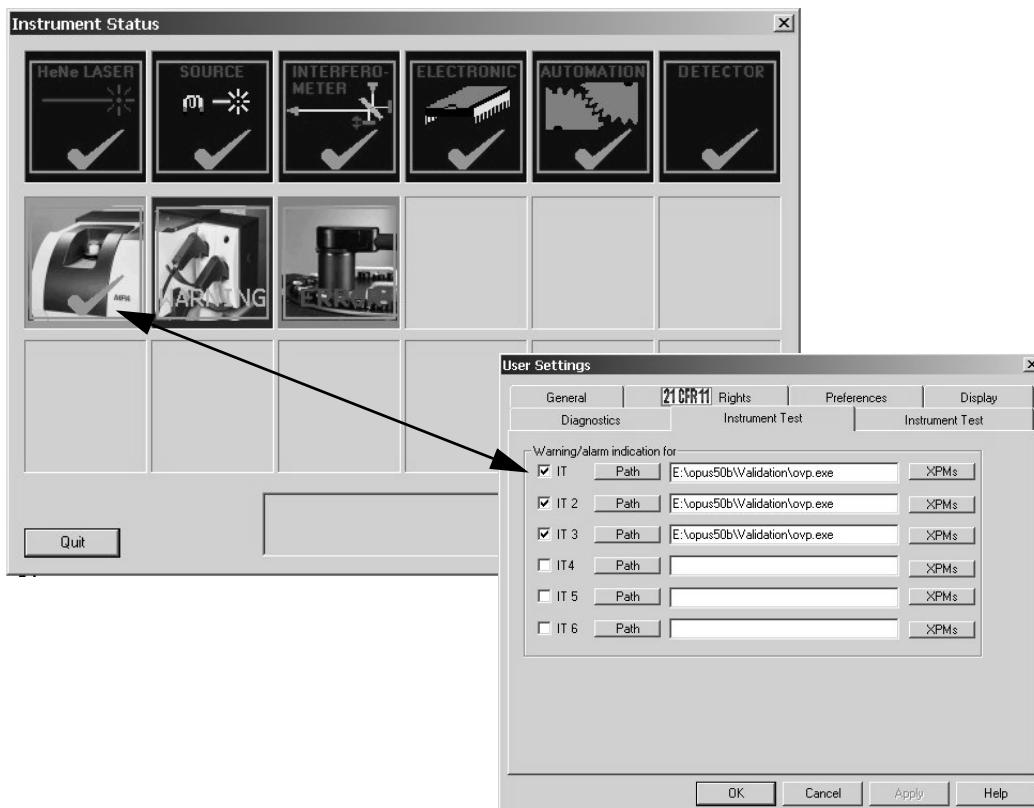
Figure 280: Correlation between User Settings and Instrument Status

The second and third row of status icons on the *Instrument Status* dialog are designed for the twelve test channels defined on the *Instrument Test 1* and *Instrument Test 2* tabs of the *User Settings* dialog box. Click on the first icon of the *Instrument Status* dialog, provided you assigned OVP to the *IT* test channel in the *User Settings* dialog. The following dialog opens, provided you have assigned OVP to the *IT* test channel in the *User Settings* dialog:
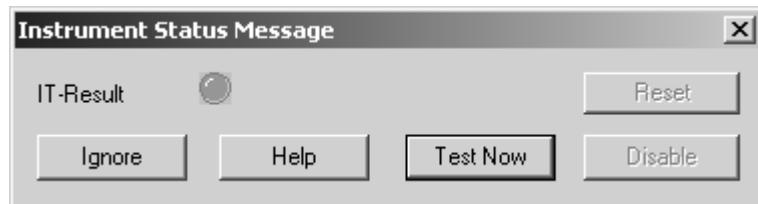
Figure 281: OVP - Instrument Status Message

Click on the *Test Now* button to open the OVP start dialog.

Figure 282: OVP - Start dialog

If you do not have OPUS *Administrator* rights, the OVP start dialog will not include the *Setup* and *Trends* buttons, and the validation wizard can directly be started by clicking on the *Measure* button.

The *About* menu option displays a list of version numbers of all main components used by OVP. Click on the *Setup* button to access the setup dialog.
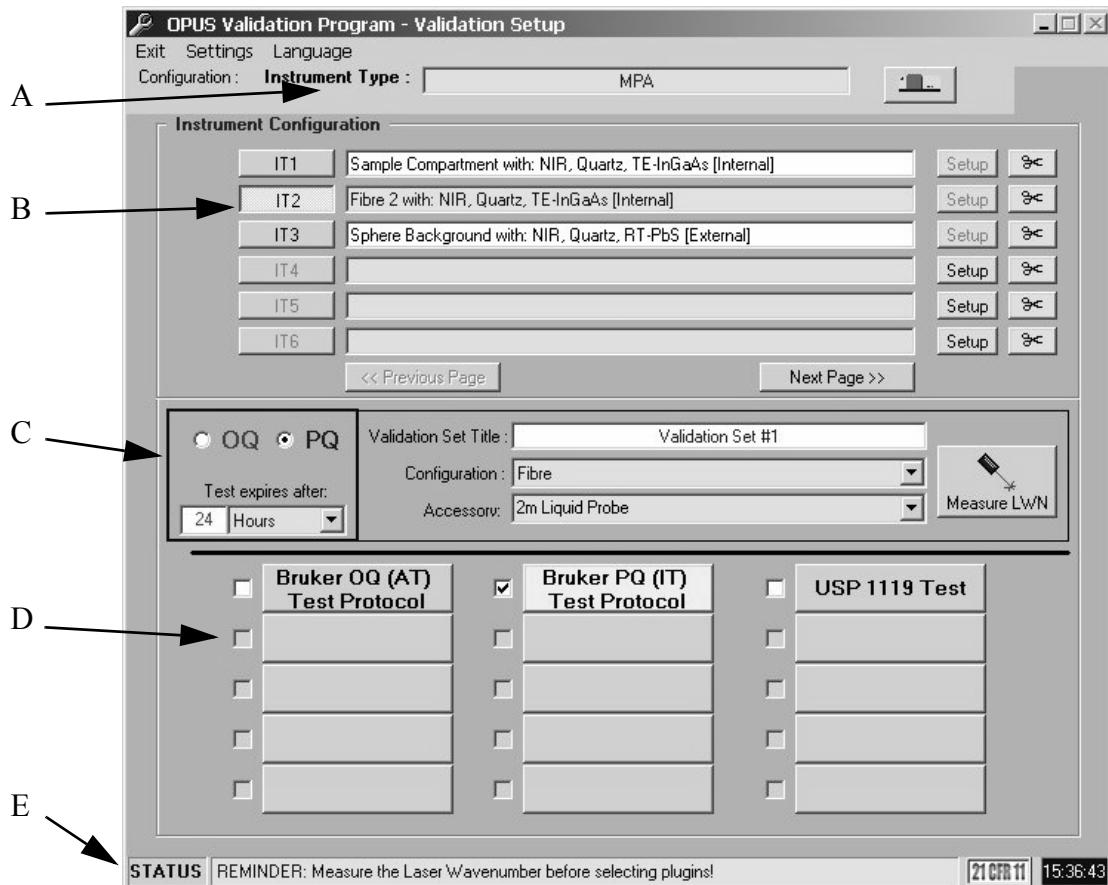
Figure 283: OVP - Setup

In the OVP setup dialog the administrator defines which tests will be performed at what intervals. The setup is the primary step within OVP before the program can be used.

Figure 283 shows the default setup dialog which is described in the following:

(A) This section displays the name of the spectrometer used. The instrument type is automatically detected by OVP. Click on the instrument button ( ) to update the setting if a different spectrometer had been previously connected.

(B) The *IT* buttons represent the assigned measurement configurations used by OVP and are similar to the buttons on the *Instrument Test* tab of the *User Settings* dialog (see chapter 14.10). Click on one of the *IT* buttons on the left to select the test assignment position.

(C) This group field defines the test category (PQ or OQ), test interval, instrument configuration and accessories, if available.

(D) This section includes a dynamic list of available tests that can be performed. Tests are included as plug-in modules which automatically are displayed in this section when installed. Activate the corresponding check boxes to select the appropriate test. The setup dialog of the selected test will open.

(E) The status bar displays the current status of the particular setup dialog. Warnings and reminders are displayed in yellow. During measurement the status bar is green. If you work in a validated environment in OPUS, the *21 CFR Part 11* logo on the right will be marked red.

The following outlines a summary of events performed within the OVP setup module.

13.2.2.1 Confirming Correct Instrument Type

This first step is to specify the instrument type used. The instrument type is selected automatically if you start OVP for the first time. The next time you start OVP the instrument type previously used will be displayed by default. To update the settings click on the instrument button, see figure 284.
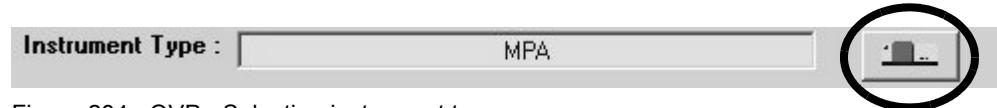
Figure 284: OVP - Selecting instrument type

An update of the settings only needs to be done the first time you use OVP with a new instrument type. If you delete the user databases, you will not need to perform an update.

> **Note:** If the instrument type is not displayed, the instrument is not supported by OVP and you will not be able to use OVP.

13.2.2.2 Adding Measurement Configuration
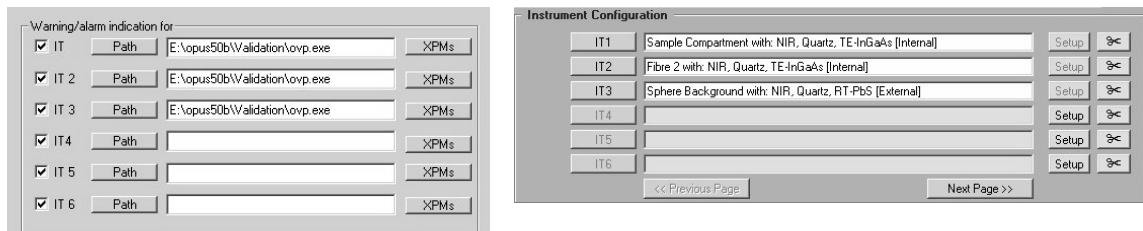
Figure 285: OPUS User Setting dialog and OVP Setup

As figure 285 shows, the six positions specified on the *User Settings* dialog directly correspond to the six positions specified for the OVP experiment method assignments. The check boxes on the left image have the same designation as the *IT* buttons on the right image. This also applies to channels 6 to 12.
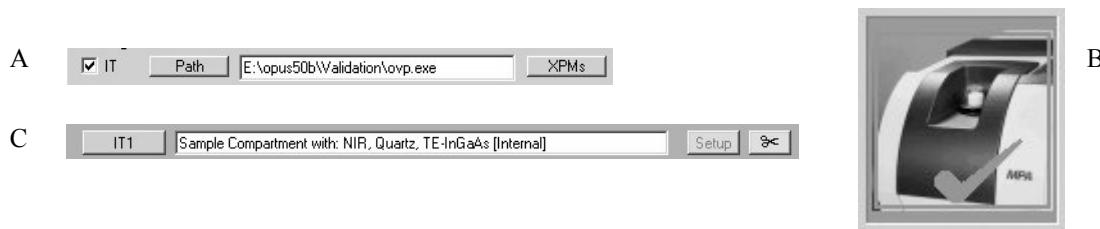
Figure 286: Test channel settings

Figure 286 compares the first IT position of each dialog. The first position in the *User Settings* dialog (A) correlates to the first icon on the *Instrument Status* dialog (B), which correlates to the first position in the OVP setup dialog (C).

For each spectrometer test channel you have to assign a measurement configuration to be used during actual validation measurement. In general, this is a valid combination of source, beam splitter, measurement channel and detector as shown in figure 287.
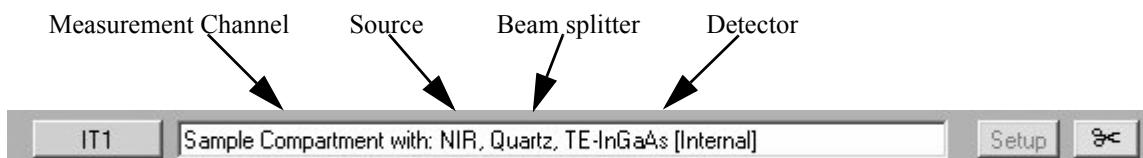
Figure 287: Test channel configuration

> **Note:** The test channel must have the same hardware configuration as the experiments defined in the *User Settings* dialog to be able to validate the hardware and optical components used during measurement.

To add an optics configuration for validation, click on the *Setup* button next to the position you would like to assign. The *Setup the Optics Configuration for a Test Channel* dialog opens as shown in figure 288.
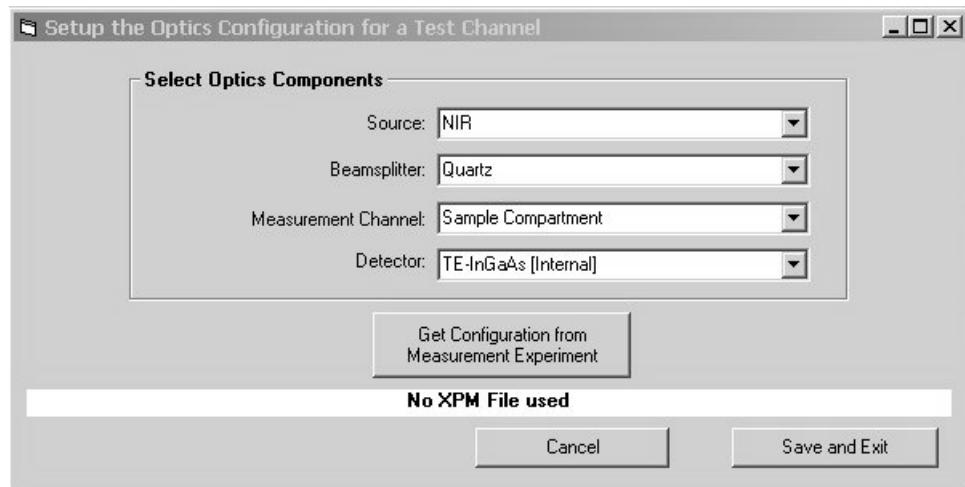
Figure 288: OVP - Optics Configuration dialog

In general, there are two possibilities to define the proper optics configuration. You can directly select the particular component from the corresponding drop-down list which include the optics components available for your instrument.
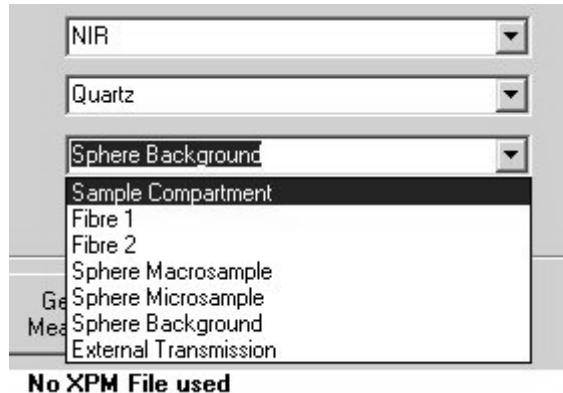
Figure 289: OVP - Optics configuration by drop-down list

Alternatively, you can use an existing measurement experiment by clicking on the *Get configuration from Measurement Experiment* button (see figure 288). Browse to the location of the measurement experiment file and select it. The optics configuration is extracted from the experiment and the name and path of the file will also be displayed, see figure 290.

Figure 290: OVP - Optics configuration by XPM file

If you have selected a wrong experiment which does not fit the instrument configuration, this will be indicated in the drop-down list (figure 291).
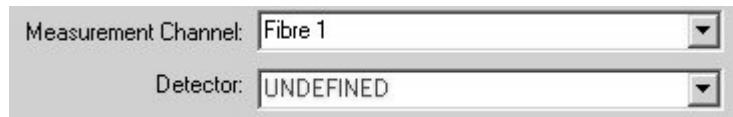
Figure 291: OVP - Wrong XPM file

To assign the configuration click on the *Save and Exit* button (figure 288). As soon as an assignment is done the *Setup* button for this test channel is disabled (figure 292). If you have to change a configuration, first permanently delete the assignment by clicking on the scissors icon ([✂]). Thus, the *Setup* button is enabled again and all settings for this assignment are deleted from the databases.
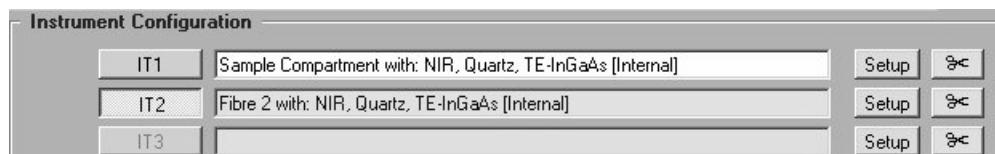
Figure 292: OVP - Disabled IT test channel

If you click on the particular *IT* button, the test channel is selected for editing turns to yellow as a visual reminder of which position is currently selected. The *IT* buttons are mutually exclusive, i.e. you can always select only one test channel. IT buttons which no optics configuration file have been assigned for are disabled and cannot be clicked on.

After assigning a new optics configuration, a warning will be displayed in the status bar to remind you to measure the laser wave number for this particular configuration before assigning any tests.

13.2.2.3 Measuring Laser Wave Number

Click on the Measure LWN button to perform a test using the optics configuration for the currently selected IT channel. In OPUS 5 (and higher) it is possible to store and use individual laser wave number values for each test channel defined. OPUS 4 uses the measurement channel assigned in the experiment file by the *Setup Measurement Parameters* command from the OPUS *Measure* menu.

Proper handling of test-channel-specific laser wave numbers may require an update of the instrument firmware as well. In case of doubt contact your local service department.

The laser wave number is affected by changes in the optical path length. This can be extremely serious when using optical fibers of different lengths. Measuring and assigning the laser wave number for each test channel ensures the accuracy of spectral data.

The test first measures a spectrum of water vapor and uses a specific water band to determine the optimum laser wave number. To verify the validity of the water band adjacent water bands are checked as well. In a second step the appropriate wave number is verified against the bands of the filter material on the internal validation unit (e.g. polystyrene or BRM 2065). After performing this test a result dialog pops up.
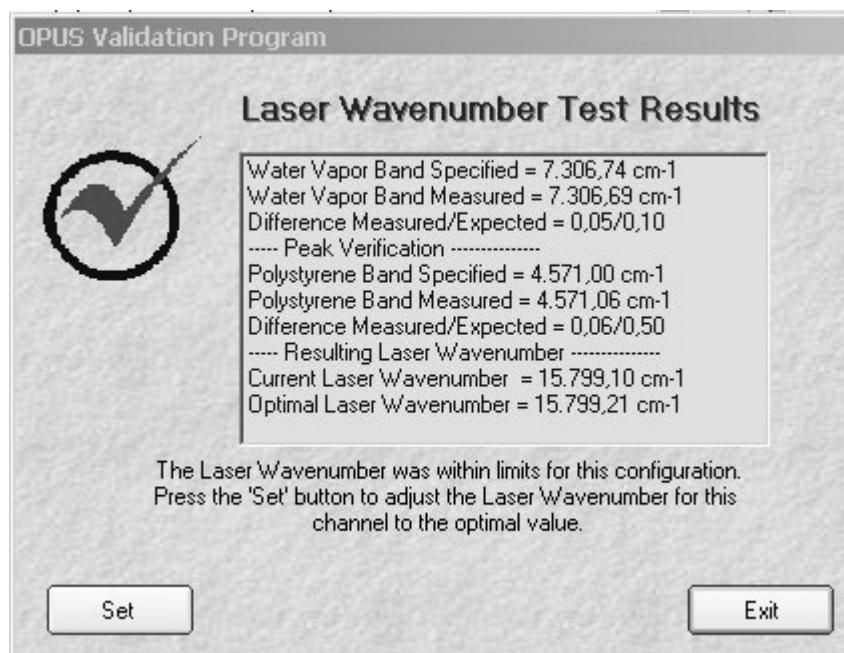
Figure 293: OVP - Test Result dialog

If the current laser wave number for this channel is within a certain tolerance, the test has passed and no changes are needed.

Click on the *Set* button to set the current measurement channel laser wave number value to the currently computed optimal value. If you do not want to update the laser wave number, click on the *Exit* button.

If the water band could not be detected properly as the water vapor concentration of your instrument is too low, first a warning pops up which will automatically disappear after one minute.

Figure 294: OVP - Water vapor warning

The result of the laser wave number determination may also indicate a problem.
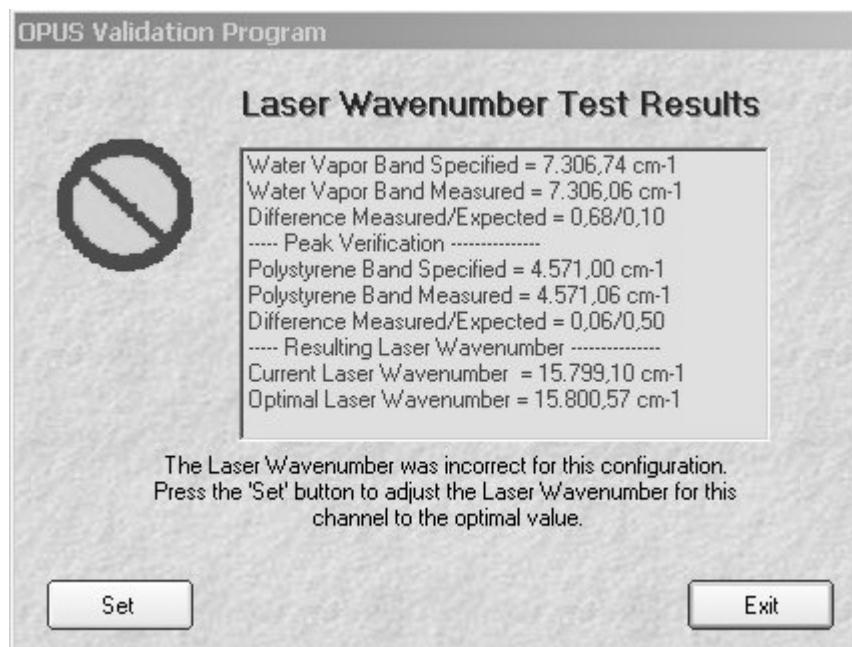
Figure 295: OVP - Laser Wave Number Test Results

In this case examine the water vapor spectrum *FR_LWN.x* (*x* being a number) which is located in the *OPUS\VALIDATION\TEMP* path. If the water vapor contents are too low, remove the desiccant cartridge for a short period of time to allow the water vapor concentration in the instrument to increase. Repeat the measurement until the result is OK.

> **Note: Changing the laser wave number after assigning tests will invalidate those tests that require reference measurements (i.e. PQ test).**

Important: As of OPUS 5 the laser wave number is stored and used based on the *IT* test channel specified in the *User Settings* dialog. It is not an OVP component. If you use one experiment to measure the empty sample compartment, a different experiment is required to measure an accessory placed in the sample compartment. These two configurations should be setup as different test channels in OPUS. The laser wave number can be different for both test channels, even if both configurations use the sample compartment as measurement channel. In that case it is important to register the measurement experiments used for measurements with the empty sample compartment, and for measurements with the accessory, in different test channels.

13.2.2.4 Configuring Test Channel

Once you have assigned an optics configuration to an IT channel, you have to configure it. Figure 296 shows the section of the OVP setup pertaining to the channel configuration.
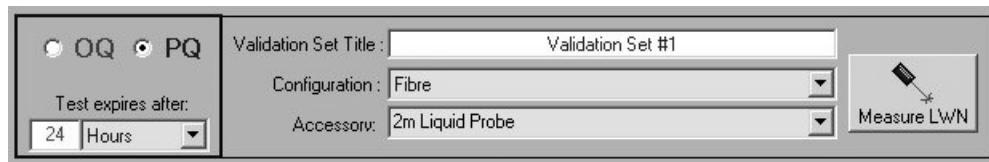
Figure 296: OVP - Channel configuration

You have two basic categories for testing:

- Operational Qualification (OQ)
- Performance Qualification (PQ)

All assignments made by the *OQ* option refer to the *OQ* test. Subsequently, all assignments made by the *PQ* option refer to the *PQ* test. Switching between these two option buttons displays the assignments for the particular test.

You have to define the test interval for both categories. Note that we recommend running *PQ* tests as a short-term test on a daily basis (24 hours). *OQ* tests should normally run after installation, maintenance or major repair, e.g. every 6 or 12 months. Type the interval period into the entry field and select the units from the drop-down list. Available units are hours, days, or months.

The *Validation Set Title* text field can be used to specify the current setup by a descriptive name. A default name is always added when a new channel is configured. The validation set title is used in the reports generated by the various test protocols.

The *Configuration* drop-down list includes currently supported hardware configurations for the particular instrument type. Depending on the instrument type the configuration is automatically selected based on the optics configuration set up. Especially, in case of older instruments (e.g. VECTOR 22/ N series), or if a configuration is available with different options (e.g. one with the standard and another with the high resolution option), the initial *Configuration* drop down list may display the *Select proper Configuration* note.

In such a case select the configuration that best matches the configuration used for this channel for both OQ and PQ. If your configuration does not match any included in the drop-down list, contact the Bruker Optics service department.

Depending on the type of instrument and the optics configuration selected an additional drop-down list for optional accessories can be displayed.
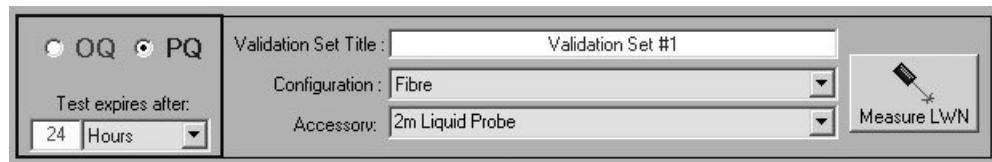
Figure 297: OVP - Channel configuration

This drop-down list includes a set of accessories which can be used in combination with the selected optics configuration. Typical accessories for different configurations can be:

Figure 298: OVP - Accessories for fiber port and sample compartment

If you select *None*, the basic configuration for that particular channel, e.g. empty sample compartment is used. In case of combinations during routine work, e.g. sample compartment with standard sample holder, sample compartment with an ATR accessory, sample compartment with a diamond cell you should set up a different test channel for each of these configurations. This allows you to validate each configuration separately.

The *Accessory* drop-down list includes Bruker standard accessories. A specific program allows you to define your own set of accessories. The program will be described in chapter 13.8.2.

13.2.2.5 Selecting Tests

The test protocols to be performed during validation measurements have to be defined.
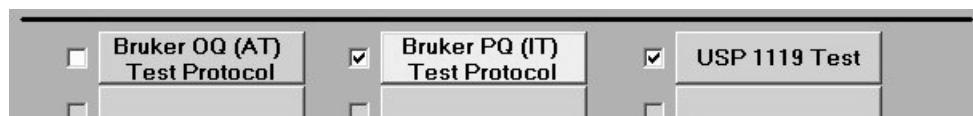
Figure 299: OVP - Test Protocol

All test protocols are plug-ins located in the *Plug-ins* sub-directory of OVP. The names of all the tests installed are automatically displayed on the respective buttons.

If you activate the check box to the left of the button, the test will be activated and the button color will change to light blue. This indicates that you want to perform this test for the current test category (OQ or PQ). The initial *Setup* dialog automatically shows these test protocols. Some tests require reference measurements to be created before the test can be used. The setup of the standard *PQ* and *OQ* test protocol will be described in the following.

If you now click on the test button, you will have access to the protocols setup dialog. Figure 299 shows that the *PQ Test Protocol* and the (optional) *USP 1119 Test* have been selected, but not the *OQ Test Protocol*.

When selecting tests you should take into account the purpose of the selected protocol, i.e. select the *PQ* test for the *PQ* category and the *OQ* test for the *OQ* category. Selecting the same tests for both PQ and OQ is needlessly redundant.

13.2.2.6 Deleting Optics Configuration from OVP

If you click on the [✄] button, the particular test channel will be deleted. You will be asked to confirm this deletion. Once deleted the settings cannot be retrieved. If you have accidentally deleted a channel, you have to complete the entire assignment process again.

13.2.2.7 Menu Options

The *Settings* menu includes two functions:

Figure 300: OVP Settings menu

The *Program Paths* function defines the path which is used to store the test spectra and PDF reports generated during validation measurement. Test spectra are stored in a structure of sub-directories. The first level uses date (YYMMDD), the second time information (HHMMSS). Reports are stored in a separate *REPORTS* directory. If you click on the *Program Paths* function, the following dialog opens:
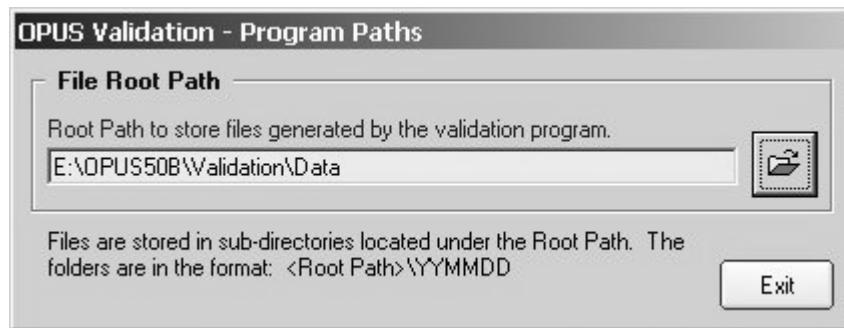
Figure 301: OVP Settings menu - Program Paths dialog

The *Change Database Password* function (figure 300) allows the administrator to modify the password to be able to access the two user-generated databases: *UserSettings.mdb*, and *UserData.mdb*. If you click on the *Change Database Password* function, the following dialog opens:

Figure 302: OVP Settings Menu - User Database Password dialog

To change the password, first enter the old password and then the new one. **The default password for the user databases is *Bruker Optics*.** This allows the administrator to access the databases from within an external program (MS Access 2000 format). The default passwords for other databases are secret as these databases can only be changed by Bruker.

13.2.2.8 Exiting OVP Setup

To exit the OPV *Setup* dialog click on the *Exit* menu item. Incomplete configurations will not be used during a validation measurement.

13.3 Validation Measurement

This chapter outlines the sequence of events encountered while validating the spectrometer. This sequence pertains to the OPUS user with *Operator* rights and is similar the one for users with *Administrator* rights.

13.3.1 Starting Validation Measurement

The OVP validation process is very simple. Once an IT channel has been assigned for validation, OPUS will store the expiration time/date.

Each time one of the measurement experiment files defined in the *User Settings* dialog is loaded, OPUS checks the stored expiration time of all tests specified for the particular test channel. The status light in the bottom right corner of the OPUS interface always indicates the following test status according to the color:

- Green: all tests are up-to-date and valid
- Yellow: at least one of the tests has expired
- Red: the last validation test has failed or has never run

Click on the status light to display the *Instrument Status* dialog.

Figure 303: Instrument Status dialog

The first row of icons represent the instrument hardware test status. The second and third row of icons are reserved for the software tests. In figure 303 OVP has

been assigned to the first three test channels, therefore three icons are displayed in the second row.

The icon results show a warning as the test for this channel has expired, a green check mark as the test for this particular channel has passed and is still valid, and an error as either the test has failed or no test has been measured for that channel.

Click one of the icons and a dialog opens indicating the current status of this particular channel:
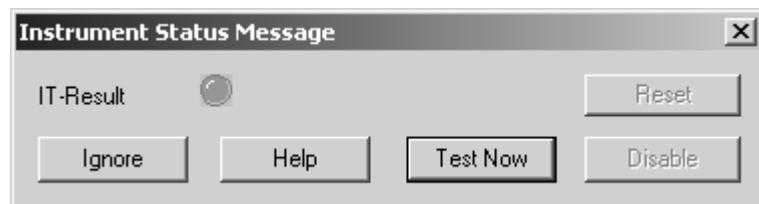
Figure 304: Instrument Status message

You can either close the *Instrument Status Message* dialog without measuring or click on the *Test Now* button to starts the OVP measurement wizard.
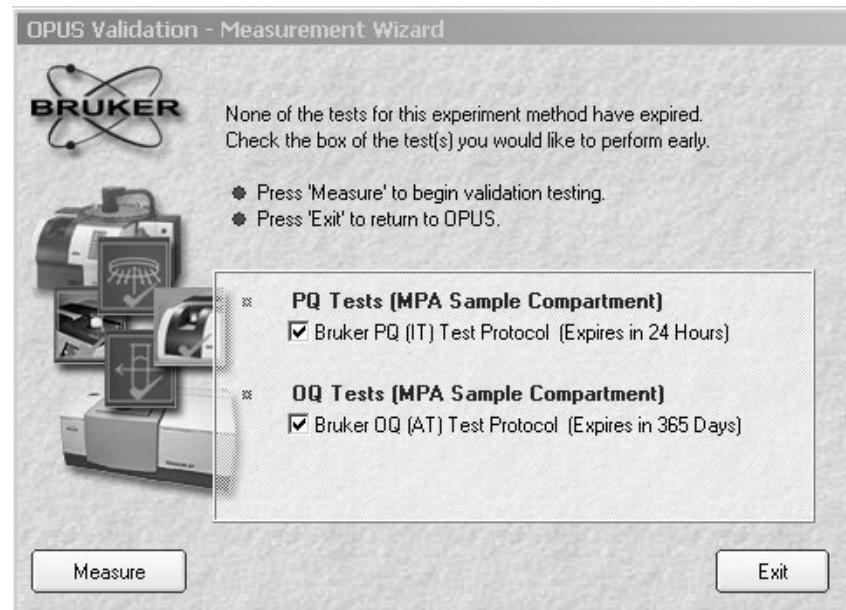
Figure 305: OVP - Measurement Wizard

Figure 305 shows a typical OVP measurement wizard dialog. To continue follow the on-screen instructions.

The group field in the middle includes all tests which have been assigned for this particular IT channel. Tests whose interval has expired are automatically

checked for measurement. Tests whose interval has not expired are not checked, and their remaining time is listed as a reminder.

For example:

If a test has not expired, but the interval has only two hours left you may wish to select that test and run it earlier.

If a test has expired, but you are not prepared to perform that test (external standards are needed), you can deactivate the check box for the corresponding test.

> **Note:** If you decide <u>not</u> to perform an expired test, the instrument status will still report a warning (yellow light) after validation testing has completed, if more than one test is assigned to the particular IT channel.

Click on the *Measure* button to start the selected validation protocols. If you do not want to perform the validation measurements, click on the *Exit* button.

13.3.2   Test Protocol Wizards

Each of the selected tests on the measurement wizard will display an individual wizard dialog customized for the prevailing test protocol. Figure 306 shows the wizard dialog for the *OQ Test Protocol*.
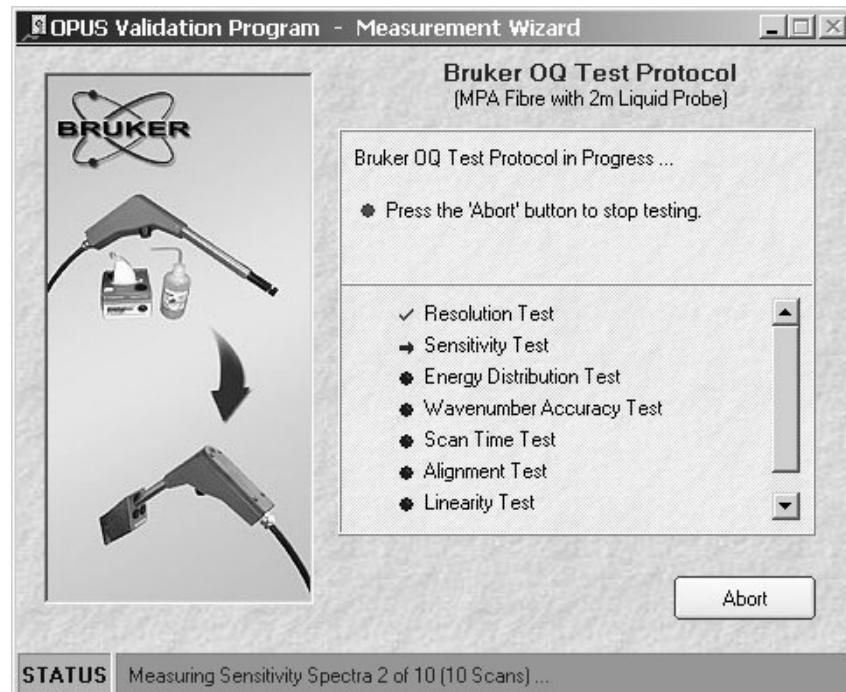
Figure 306: OVP - Measurement Wizard with OQ Test Protocol

As the test(s) are in progress, the status bar provides feedback about the current state of the measurement process.

Next to the name of each test is an icon indicating:

- ✦ Test will be performed
- ➡ Test in progress
- ✓ Test complete and passed
- ✗ Test complete and failed

At any time during measurement you can skip the current test protocol. If, however, a spectral measurement is in progress within OPUS, you will have to wait for the test protocol to be completed before being able to continue. To skip the test, click on the *Abort* button.

If the measurement wizard has been completed for each test, the *Report* button is displayed.
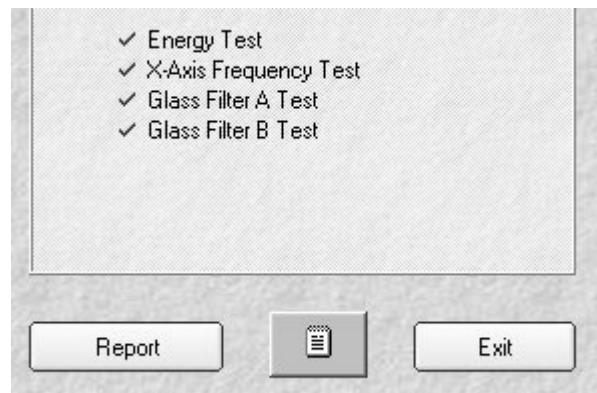
Figure 307: OVP - Measurement Wizard with Report button

Clicking on the *Report* button opens a preview window with the generated report for this test protocol (figure 308). From within this preview you can print and review the results of the test. After completing the review, close the preview window.
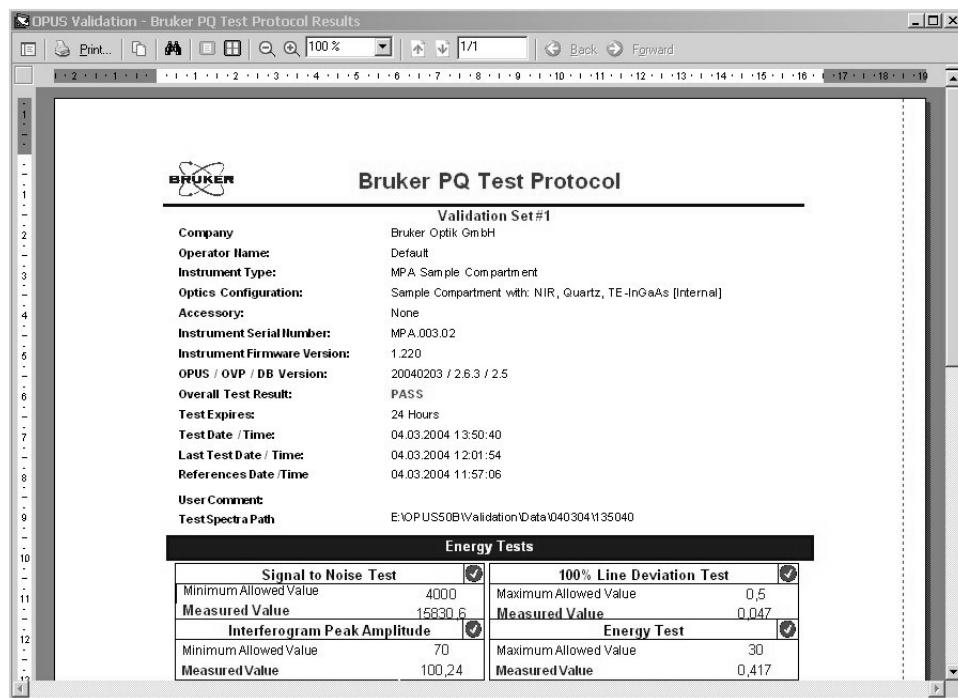
Figure 308: OVP - Test Protocol report preview

All measurement results are stored within a log table stored in the *UserData* database. To append a comment to the current log entry click on the log

comment button ( ). A dialog opens and you can type a comment for this measurement, e.g. *Measurement failed due to someone striking the instrument*.

Click on the *Exit* button to exit this protocol wizard dialog.

The next protocol wizard will start immediately, if any has been specified. For all test protocols the procedure will be the same.

If all the selected test protocols have been completed, the OVP wizard dialog will be displayed summarizing the results of all tests performed (see figure 309).
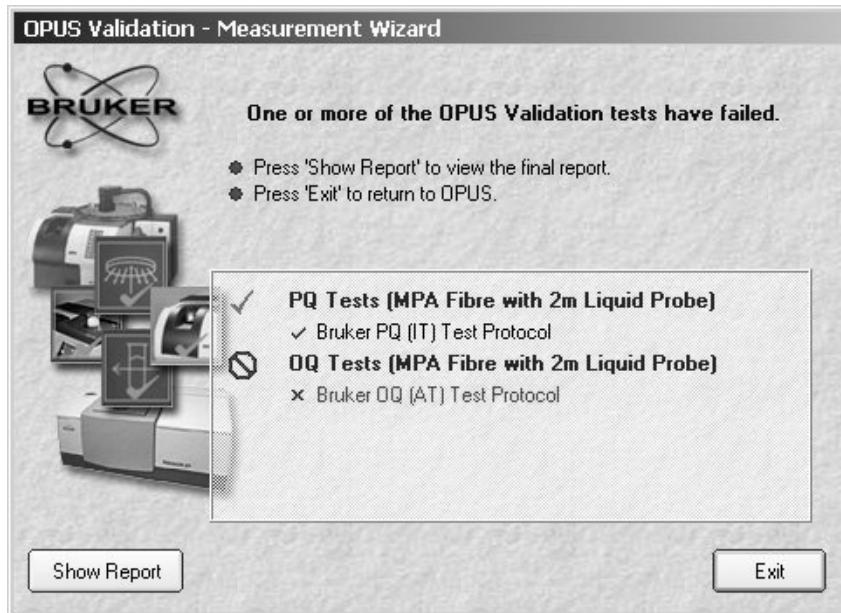
Figure 309: OVP - Measurement Wizard with summary of test results

Click on the *Show Report* button to view the final report for all tests performed. This requires the Adobe Acrobat Reader being installed on your computer. The Adobe Acrobat Reader is available on the OVP installation CD or on the OPUS installation CD.

To exit the measurement wizard click on the *Exit* button and return to OPUS. The status light will change and indicate the status of the tests.

13.4   PQ Test Protocol Plug-in

The PQ test protocol is a short-term test which verifies that the instrument performance is suited for daily operation. Most of these tests compare the measured data to a set of reference data which have been recorded after installation, major repair or exchange of optical components. The PQ test protocol is intended to be run on a day-by-day basis to ensure that the instrument is working properly.

The following single tests can be run during PQ:

- **Signal to Noise Test**
  Verifies that the signal-to-noise ratio is better than a specified limit.
- **100% Line Deviation Test**
  Verifies that the 100% line does not shift on long term.
- **Interferogram Peak Amplitude**
  Verifies that the interferogram peak amplitude is not below a certain limit.

- **Energy Test**

  Verifies that the deviation of the energy distribution of a single-channel spectrum does exceed a specified limit.

- **X-Axis Frequency Calibration Test**

  Verifies that the frequency calibration of the instrument is correct.

- **Y-Axis Reproducibility Tests**

  Verifies that the photometric accuracy is within specified limits.

13.4.1   PQ Test Protocol Setup

To set up tests for the PQ test protocol, start OVP and open the OVP setup dialog (see figure 283). Select the test channel for which you want to activate the test and make sure that the laser wave number for this channel has already been measured and set. Check the *PQ* option button and activate the *PQ Test Protocol* check box.
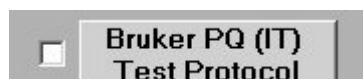
Figure 310: OVP - PQ Test Protocol check box

The *PQ Test Protocol Setup* dialog opens.
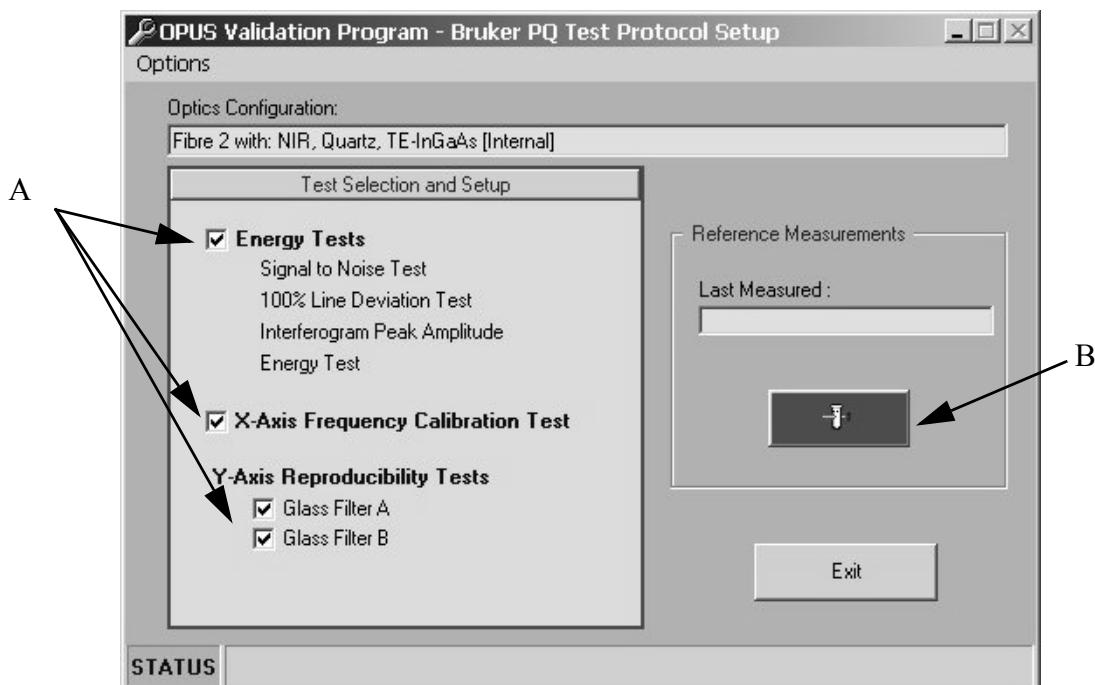
Figure 311: OVP - PQ Test Protocol Setup

The *Test Selection and Setup* group field includes the different tests which are part of the PQ test protocol (A in figure 311). Tests which are not available for the selected instrument are disabled. Tests which should not run can be cancelled by deactivating the corresponding check box. The first four tests are grouped as *Energy Tests* as these tests are all based on one spectrum.

If you start the PQ test protocol setup for the first time, the flashing *Measure* button (B in figure 311) indicates that no reference spectra have been measured. These reference data are essential to be able to run the PQ test. Click on this button to start the reference measurements. While the measurements are running the *Measure* button turns blue and shows a small animation. When the reference measurements have been finished a message dialog pops up.

Figure 312: OVP - PQ Test Protocol message

If you confirm this message, the *Measure* button becomes green. The date and time of the last reference measurement is indicated above the *Measure* button.
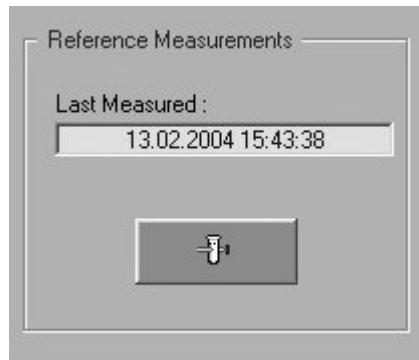
Figure 313: OVP - PQ Test Protocol reference measurements

Click on the *Exit* button. The active state of the test is indicated in the *OVP Setup* dialog by a blue *PQ Test Protocol* button and a check mark. If the reference data have not been measured in the PQ protocol setup, the test will not be activated.
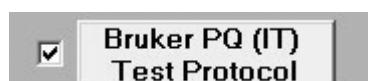
Figure 314: OVP - PQ test activated

13.4.2   Menu Options

The reference data are not stored on disk to avoid accidental deleting or overwriting. They are stored in the user database. Whenever used the reference data are temporarily extracted and afterwards removed again.

In some cases it may be necessary to have a look at the reference data, e.g. if the PQ tests fails immediately. For that purpose you can use the *Extract References* command from the *Options* menu from the *PQ Test Protocol Setup* dialog. Select the path where the reference data should be stored.
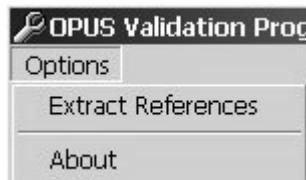
Figure 315: OVP - Options menu

The file names are *ENERGY_REF.0* for the energy spectrum and *GFA_REF.0* or *GFB_REF.0* for glass filter spectra.

13.4.3   PQ Tests Description

Signal to Noise (S/N Ratio) Ratio Test:

The signal-to-noise ratio test determines the sensitivity of the spectrometer by calculating the average signal-to-noise ratio of a 100% line.

The S/N ratio is determined by collecting and analyzing a 100% line. A 100% line is the ratio of two consecutive single-channel spectra with no sample in the beam. The ratio of these two single-channel spectra is used to generate a transmission spectrum.

The S/N ratio is determined by measuring the maximum deviation from 100% transmittance, and calculated by the OPUS *Signal-to-Noise Ratio* command in the *Evaluate* menu using peak-to-peak by means of the quadratic parabola fit option. In order to get a reliable result 10 spectra are measured (reference and sample). The S/N ratio is calculated separately for each of the spectra, using the mean value of all 10 results. The region to measure the S/N ratio will vary for systems used in the MIR and NIR region.

Figure 316 shows a peak-to-peak noise of 0.1% from 100% transmittance in MIR region. To calculate the S/N ratio take the reciprocal value multiplied by 100 (1 / 0.1 * 100). Figure 317 shows a 100% line in NIR region.
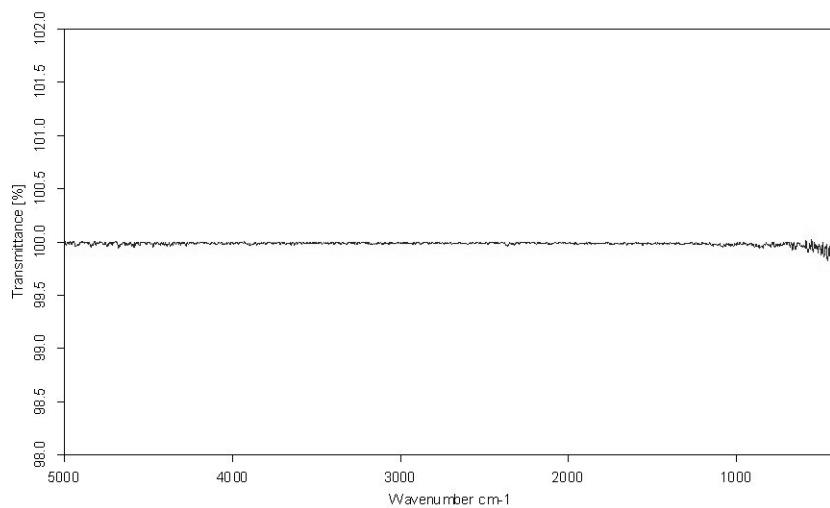
Figure 316: MIR 100% line
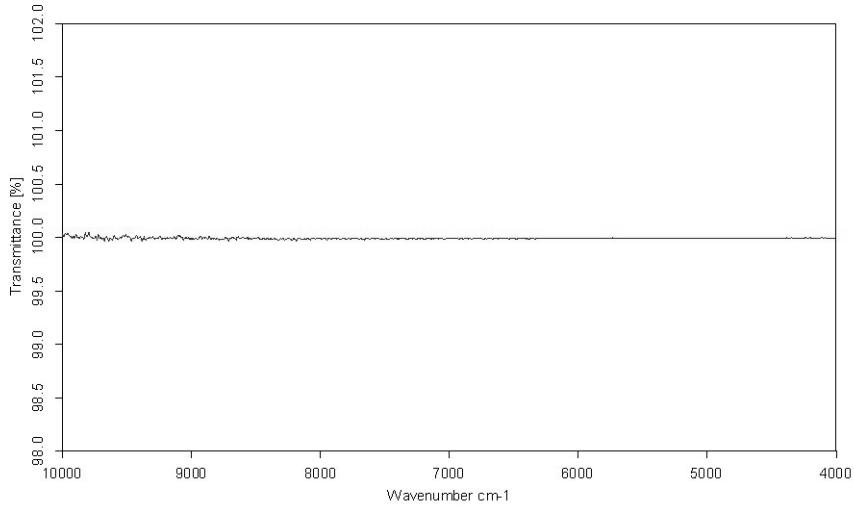
Figure 317: NIR 100% line

100% Line Deviation Test:

The 100% line deviation test is a long-term stability test which compares the minimum of the absorbance value of a 100% line to that of the stored reference spectrum.

The test is based on the spectrum generated from the S/N ratio test.

Interferogram Peak Amplitude:

The interferogram peak amplitude test is a long-term stability test which compares the amplitude of a measured interferogram to that of a stored reference interferogram.

An interferogram and a single-channel spectrum are measured and stored as reference data. For the purpose of this test only the interferogram data block needs to be considered.

The amplitude of the reference interferogram is set to 100%. In the instrument test the same measurement is repeated and the interferogram amplitude (minimum-maximum value) of this test spectrum is compared to the interferogram amplitude of the reference interferogram. The amplitude of the test interferogram is indicated in the instrument test report relative to this value. Figure 318 shows an interferogram, which has been generated by the *Double Sided, Forward-Backward* mode.
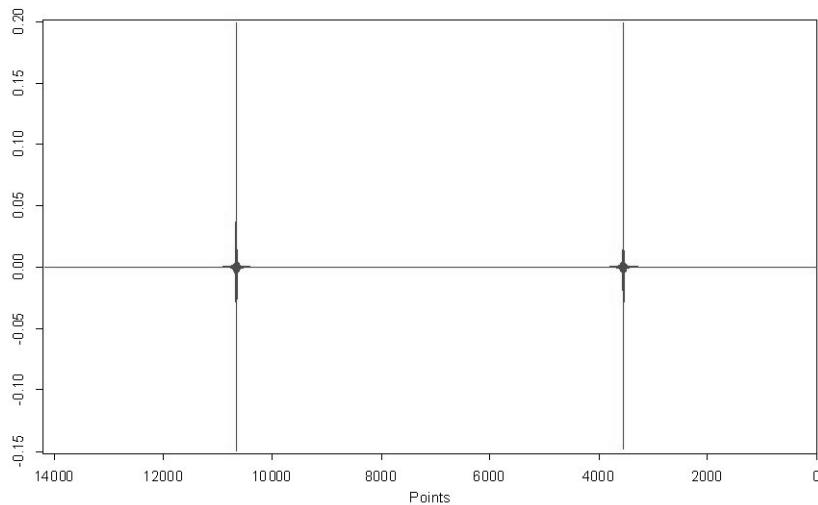
Figure 318: Double-sided interferogram

Energy Test (Single-Channel Spectrum):

The energy test is a long-term stability test which compares the amplitude of a measured single-channel spectra to that of a stored reference single channel.

Figure 319 and 320 show the single-channel spectra of the reference file and the test measurement in MIR and NIR region. The integral over the total reference single-channel spectrum is set to 100%. In the PQ test report the area between the two single-channel spectra is given relative to this value.

If the power of the spectrometer source decreases, e.g., the distance between the two single-channel spectra will increase. Therefore, this test can be used to detect changes in the source power. Like the previous test, this is a long-term

stability test. Test spectra are compared to a reference spectrum, which may have been measured several months before.

A new reference file has to be measured if the instrument has been realigned, or the source changed.
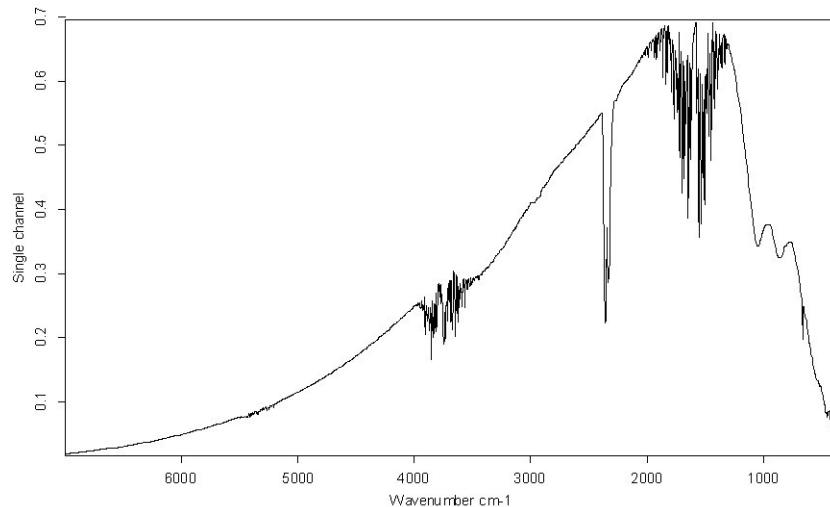

Figure 319: MIR reference and test single-channel spectra
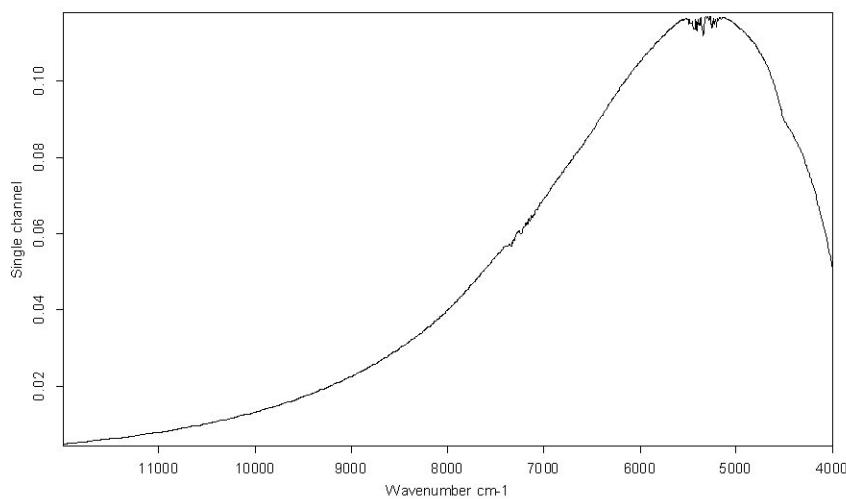
Figure 320: NIR reference and test single-channel spectra

X-Axis Frequency Calibration Test (Wave number accuracy):

The x-axis frequency calibration test ensures that the frequency calibration of the instrument is within the specified limits, if e.g. water vapor has been used to calibrate the wave number. Water vapor has the advantage of having an extremely narrow band(s) and the wavelength position can be measured to a very high degree of accuracy. To ensure that the water vapor band is completely

resolved the instrument uses a high-resolution setting. The NIR region uses the band at 7306.74cm^{-1} for calibration, and the MIR region at 1554.353cm^{-1}.

Figure 321 and 322 show a typical water vapor spectrum in the MIR and NIR region.
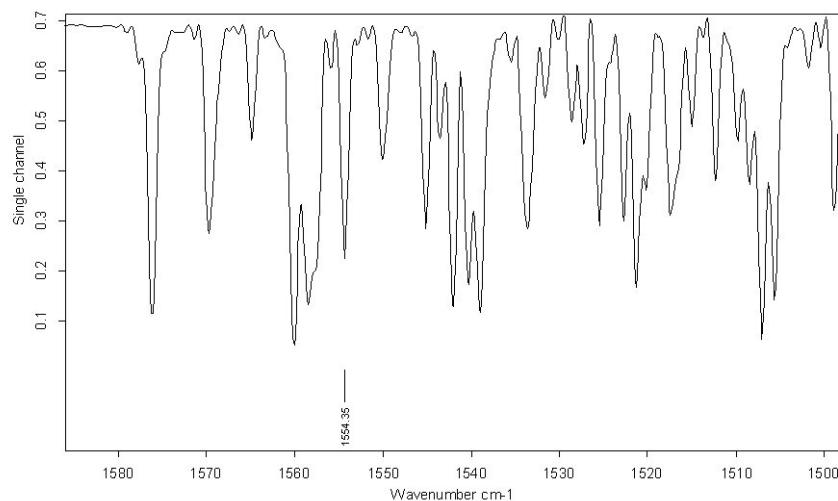
Figure 321: MIR water vapor spectrum
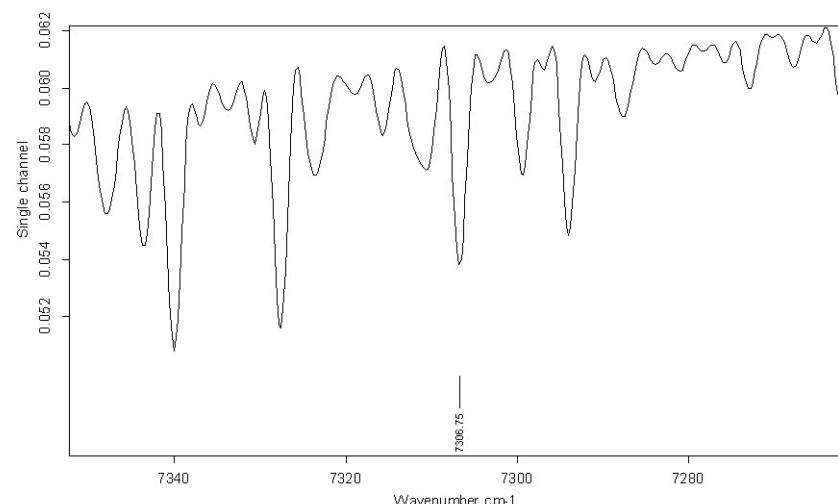
Figure 322: NIR water vapor spectrum

In addition to the water vapor test the frequency calibration is verified by measuring either a polystyrene standard sample or a glass filter with a mixture of rare earth oxides (BRM 2065) whose composition is identical to the NIST standard *SRM 2065*. The standard (either PS or BRM 2065) is mounted on the internal validation unit. Thus, no manual interaction is required for this test.

If the water vapor concentration is too low or the water band is beyond the frequency range of the instrument, the result of the polystyrene or BRM 2065 measurement is used instead.

> **Note:** If your instrument is equipped with a Germanium diode, you have to use water for the *X-Axis Frequency Calibration* test as there is no suitable polystyrene peak in the frequency range of this detector type.

Y-Axis Reproducibility Tests (Photometric Accuracy):

The y-axis reproducibility test is a long-term stability test which compares the overall intensity values of glass filter spectra to the reference spectra.

A glass filter transmission spectrum is used to test the precision of the y-axis. In the setup of the PQ qualification protocol a reference spectrum is measured. The daily filter test spectra are compared to the reference spectrum. In figure 323 and 324 the glass filter reference spectra are plotted. During the instrument test the mean difference over a large spectral range is calculated.
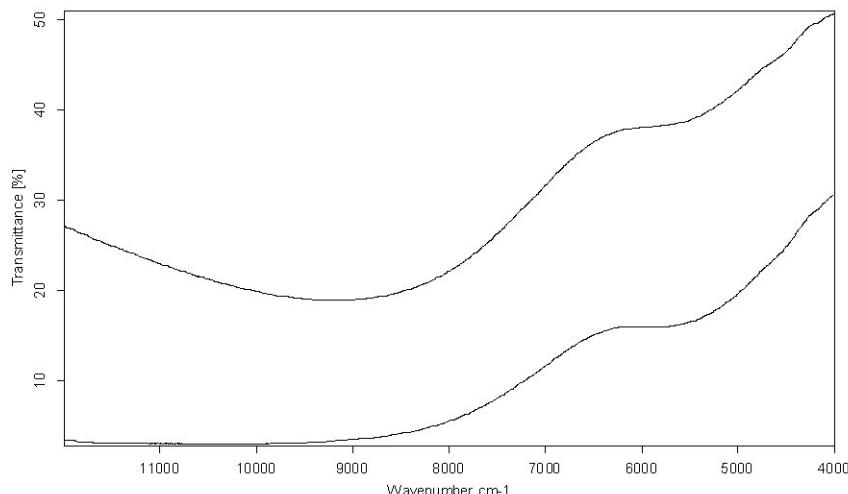
Figure 323: Glass filter NIR reference spectra
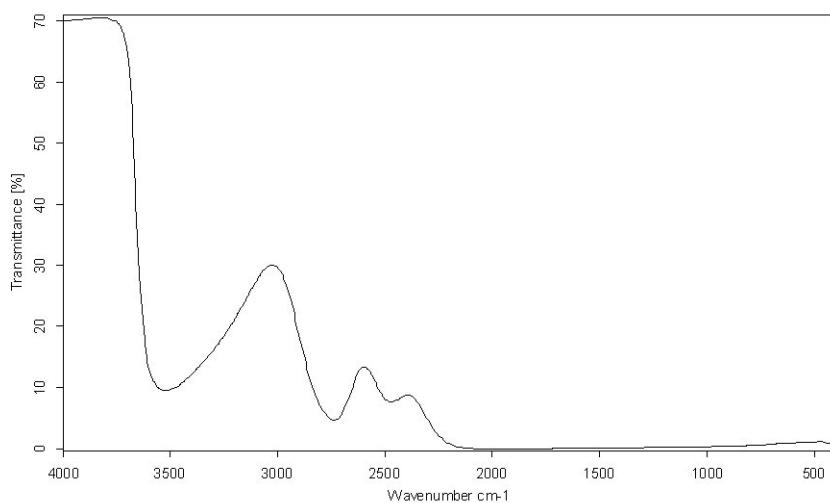
Figure 324: Glass filter MIR reference spectra

13.5 OQ Test Protocol Plug-in

The OQ test protocol is a test which checks the instrument performance and compares it to the instrument specifications. The OQ test protocol is generally run during final testing before an instrument is shipped to the customer, and after the instrument has been installed at the customer's site to demonstrate that the instrument performs as properly as before shipment. The OQ test should also be performed after each major repair, exchange of optical components which may influence the instrument performance, and on a regular yearly or semi-yearly basis after maintenance.

The following individual tests can be run during OQ:

- **Resolution Test**

  Verifies the spectral resolution achieved by the instrument.

- **Sensitivity Test**

  Verifies whether the instrument reaches the specified signal-to-noise ratio.

- **Energy Distribution Test**

  Verifies the spectrum of an empty channel, and shows the specified energy distribution over the completely achievable spectral range.

- **Wavenumber Accuracy Test**

  Verifies the absolute x-axis accuracy of the instrument.

- **Absorbance Accuracy Test**

  Verifies the detector linearity (for MIR only).

- **Scan Time Test**

  Verifies the mechanical properties of the interferometer and the controlling electronics.

- **Water Vapor Test**

  Verifies that the water vapor concentration does not exceed a specified value.

- **Alignment Test**

- Verifies that the interferogram centerburst position is within the specified range.

- **Linearity Test**

  Verifies that the detector linearity is below detector cutoff.

- **Reproducibility Test**

  Verifies the proper function of all mechanical parts which change the instrument beam path.

The individual tests depend on the type of instrument. In general, not all tests will be run for a specific instrument series. For example, the linearity test is only relevant for MCT detectors, while the absorbance accuracy test is only necessary for MID IR instruments, like TENSOR.

13.5.1   OQ Test Protocol Setup

To setup the tests for the OQ test protocol, start OVP and open the OVP setup dialog (see figure 283). Select the test channel for which you want to activate the test and make sure that the laser wave number for this channel has already been measured and set. Check the *OQ* option button and activate the *OQ Test Protocol* check box.
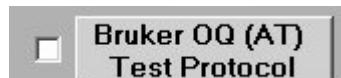
Figure 325: OVP - OQ Test Protocol check box

The *OQ Test Protocol Setup* dialog opens.
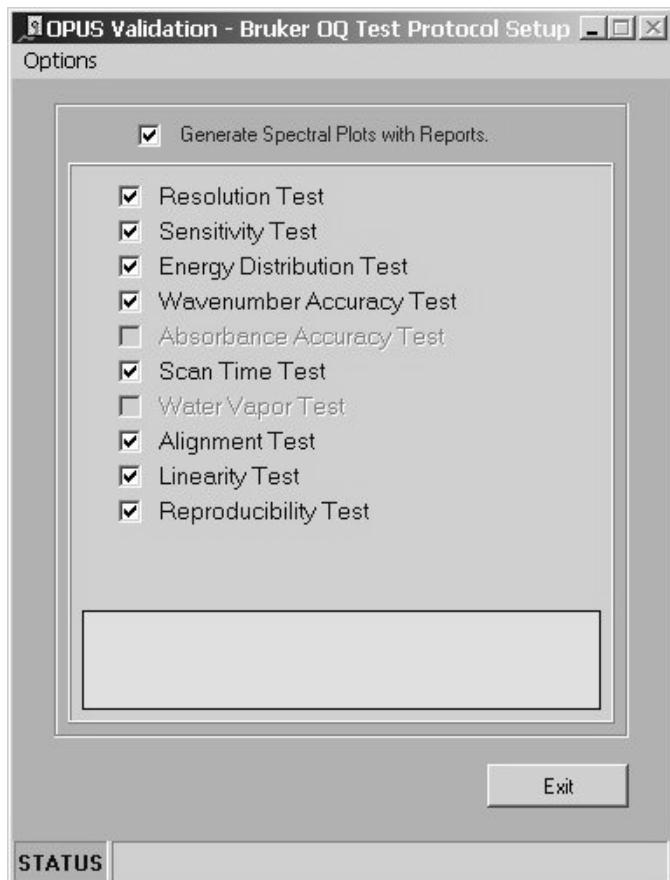
Figure 326: OVP - OQ Test Protocol Setup

Tests which are not available for the selected instrument type are disabled, all the other tests are activated. If you want to skip a test, deactivate the respective check box.

The *Generate Spectral Plots with Reports* check box will generate a multi-page report with a comprehensive test result page and subsequent pages for each test where all the test spectra are displayed. If you deactivate this check box, the report will just show the comprehensive test result page.

The *Options* menu includes the *Service Mode* command which you can use to have a measure button displayed for each test. If you click on one of these measure buttons, the particular test will run and the result will be displayed either as simple message or as full report. The output report format can be selected from the *Service Mode Options* menu.
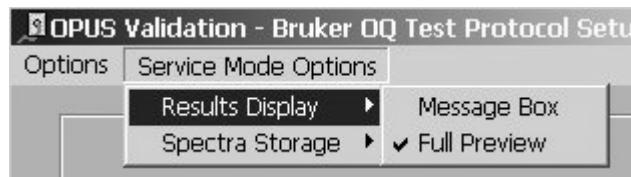
Figure 327: OVP - OQ Service Mode Options menu

If you click on the *Measure All Selected Tests* button, all tests which have been activated will run. Test spectra generated in service mode are not stored in the *DATA* sub-directory but in a temporary sub-directory which can be changed by means of the *Service Mode Options* menu. The results of the tests are temporary and will not be recorded in the user database.
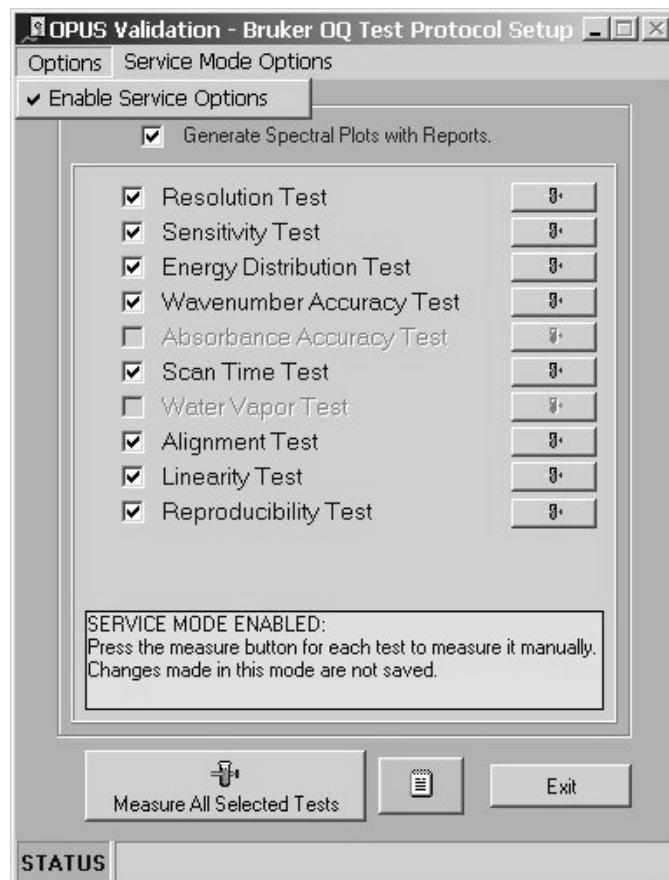
Figure 328: OVP - OQ Test Protocol Setup with service mode enabled

If all options and tests have been set, click on the *Exit* button. The *OQ Test Protocol* button in the OVP *Setup* dialog is now checked and light blue which indicates that the test has been successfully activated.

Figure 329: OVP - OQ test activated

To open the setup dialog for this test click on the *Bruker OQ (AT) Test Protocol* button. If you deactivate the check box, the OQ test will not run.

13.5.2   OQ Test Description

Resolution Test:

The resolution test verifies the achievable spectrometer resolution and records a single-channel (single-beam) spectrum of water vapor with an instrument-specific resolution. This means for most instrument types: $1cm^{-1}$ for MIR and $2cm^{-1}$ for NIR, see figure 330. The full width at half maximum (FWHM) is determined and the results are compared to the acceptance criteria of the instrument.
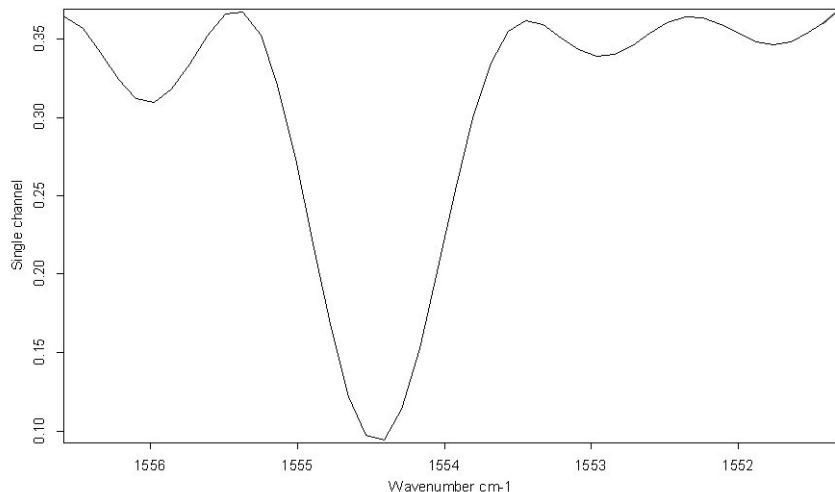
Figure 330: Water vapor band at $1553.353cm^{-1}$

Sensitivity Test:

The sensitivity test determines the sensitivity of the spectrometer by calculating the average S/N ratio of a 100% line. A 100% line is the ratio of two consecutive single-channel spectra with no sample in the beam. The ration of these two single-channel spectra is used to generate a transmission spectrum.

The S/N ratio is determined by measuring the maximum deviation from 100% transmittance, and calculated by the OPUS *Signal-to-Noise Ratio* command in the *Evaluate* menu using peak-to-peak by means of the quadratic parabola fit

option. In order to get a reproducible result 10 spectra are measured (each with separate reference and sample measurements). The S/N ratio is calculated separately for each of the spectra, using the mean value of all 10 results. The region to measure the S/N ratio will vary for systems used in the MIR and NIR region, and in case of different detectors.

The spectrum shown in figure 331 has a peak-to-peak noise of 0.1% from 100% transmittance in the MIR region. To calculate the S/N ratio take the reciprocal value multiplied by 100 (1 / 0.1 * 100). Figure 332 shows a 100% line in the NIR region.
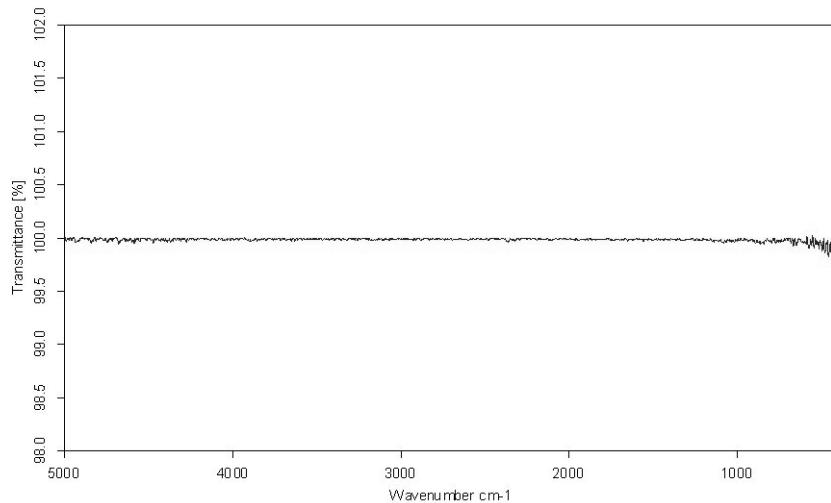
Figure 331: MIR 100% line
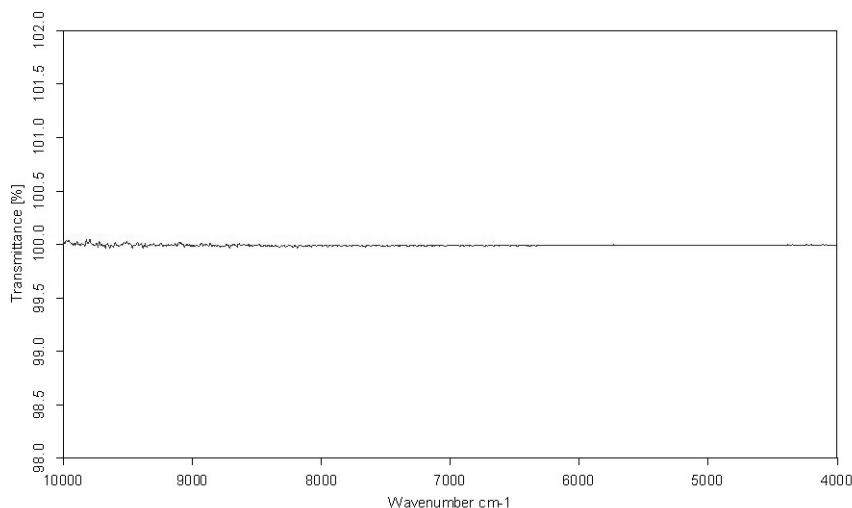
Figure 332: NIR 100% line

Energy Distribution Test:

The energy distribution test verifies the achievable spectral range high and low wave number limits, and the energy at the position of the maximum.

The test involves recording a single-channel (single beam) spectrum. The absolute values of energy measured at different wave number positions are determined, see figure 333. These values are divided by the maximum wave number value and compared to acceptance criteria expressed as a percentage.

The spectral range limits can be affected by the combination of optical components (e.g. detector, source and beam splitter) as well as the sampling accessory.

In the MIR region this test measures the energy values at $7,500 cm^{-1}$ and $370 cm^{-1}$, and compares the measured results to the acceptance criteria of 0.10% and 0.2%, respectively.
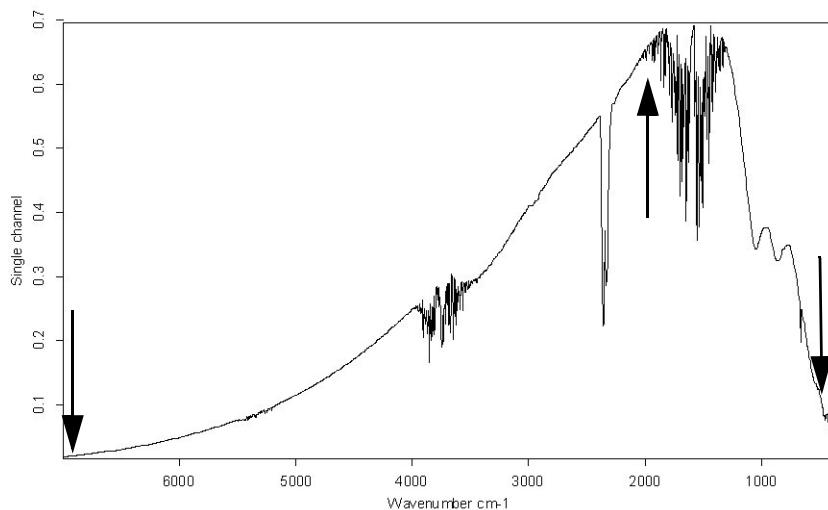
Figure 333: Single-channel spectrum

Wavenumber Accuracy Test (X-axis):

The wave number accuracy test verifies whether the frequency scale of the spectrometer is accurate. To test the wave number accuracy water vapor is used. Water vapor has the advantage of having extremely narrow bands, and the wavelength position can be measured to a very high degree of accuracy. To ensure that the water vapor band is completely resolved the test is performed by a high-resolution setting. The NIR region uses the band at $7306.74 cm^{-1}$ for calibration, and the MIR region at $1554.353 cm^{-1}$.

Figure 334 and 335 show a typical water vapor spectrum in the MIR and NIR region.
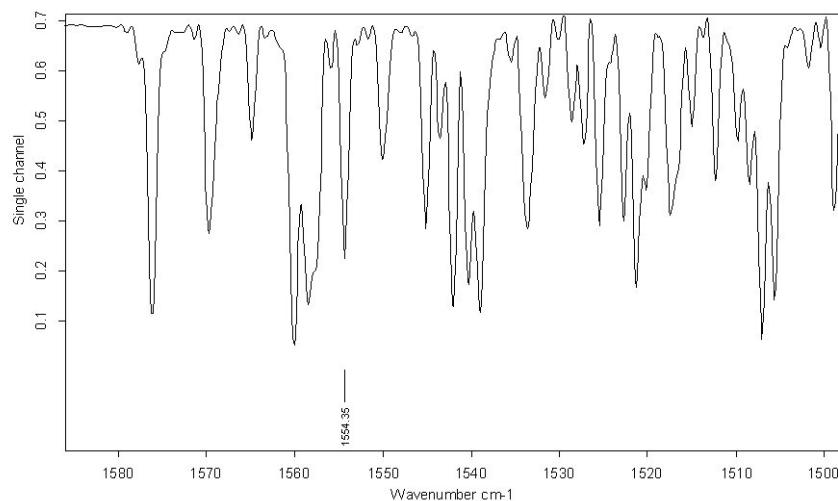
Figure 334: MIR water vapor spectrum
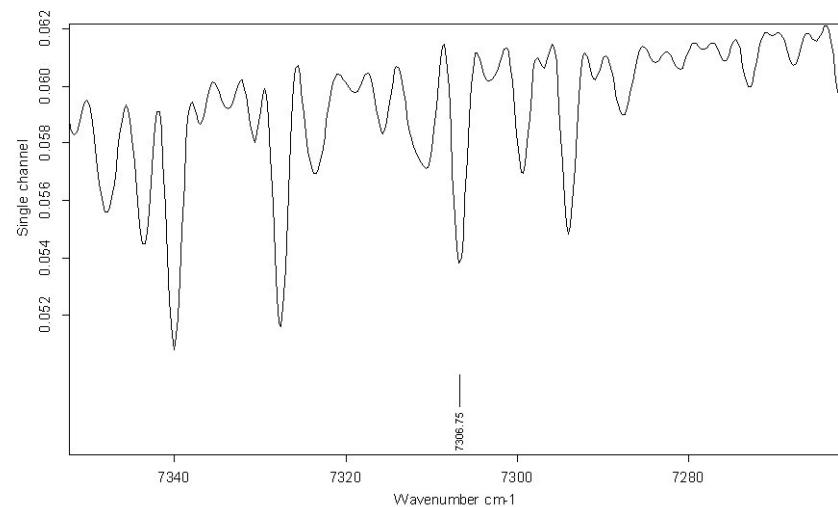
Figure 335: NIR water vapor spectrum

Absorbance Accuracy Test (Y-axis):

The absorbance accuracy test verifies whether the y-axis of a measured spectrum is accurate.

The test uses transmission spectrum of polystyrene which shows total absorption in several regions (see figure 336). At these positions the theoretical transmission of the spectrum should be 0. The absolute minimum value of the spectrum is determined and has to be smaller than the specified maximum value.
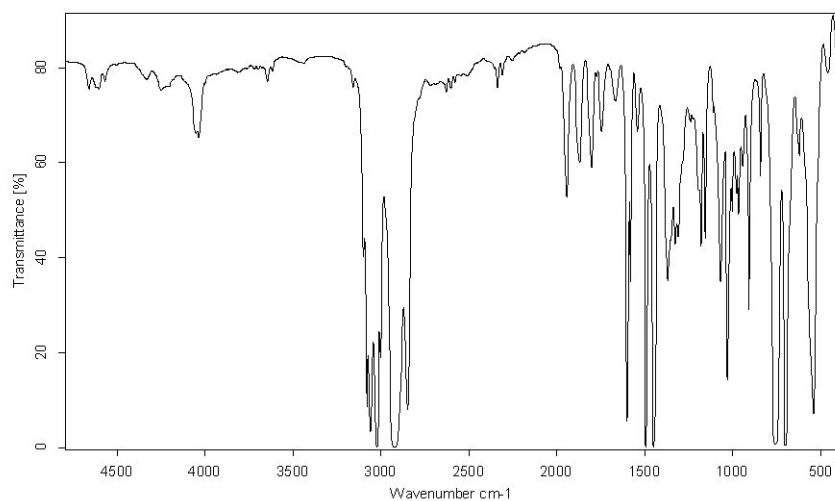
Figure 336: Polystyrene spectrum for MIR

Scan Time Test:

The scan time test is used to test the interferometer performance.

A single-channel spectrum is measured with 10 scans at the highest velocity. The time needed to measure the spectrum is determined and compared to the limit.

Water Vapor Test:

The water vapor test determines the concentration of water vapor in the instrument.

A single-channel spectrum is measured to determine the peak height of a water band within a small frequency region, i.e. 1660 - 1643cm^{-1} for MIR (figure 337) and 7315 - 7297cm^{-1} for NIR (figure 338).
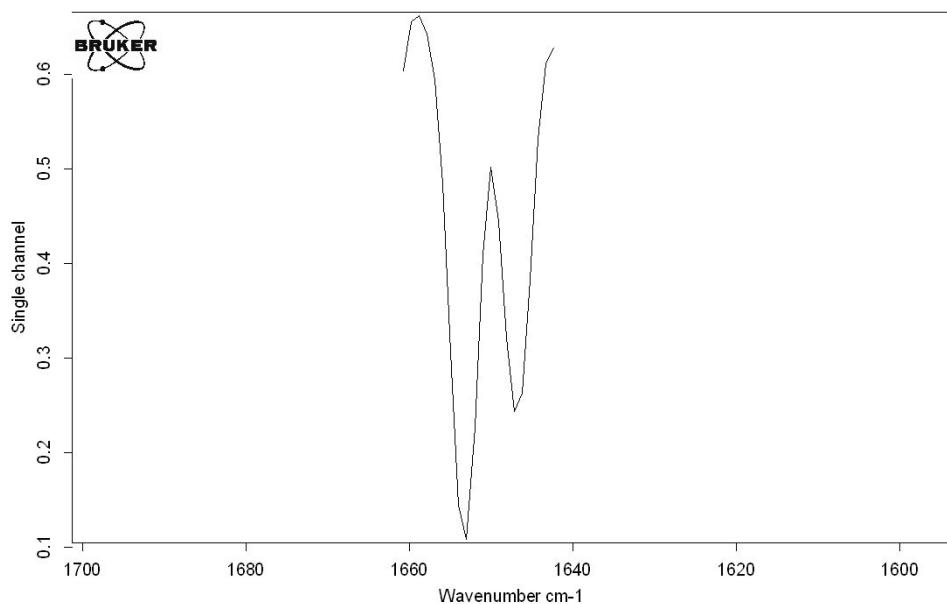
Figure 337: MIR water band, 1660 - 1643cm^{-1}
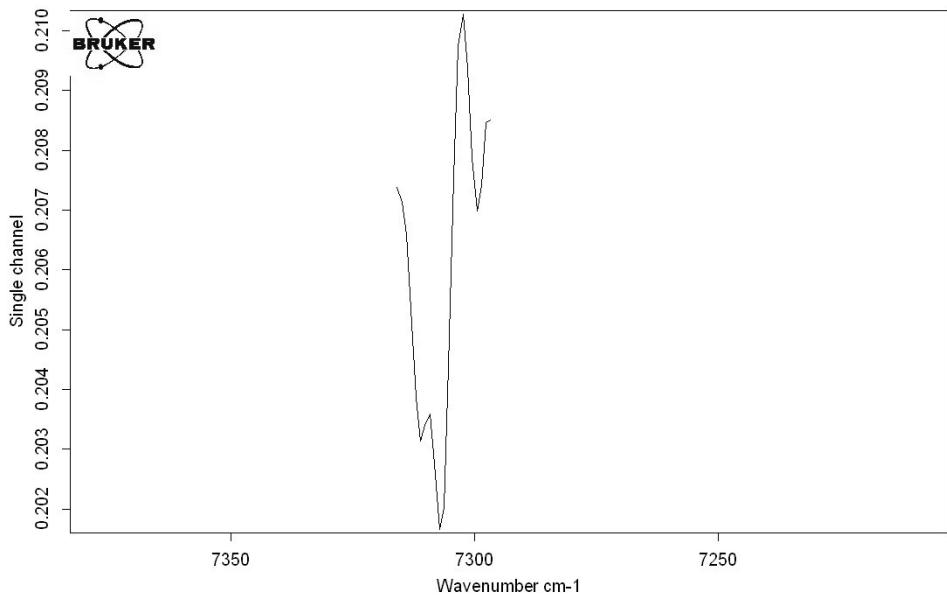
Figure 338: NIR water band, 7315 - 7297cm^{-1}

The water vapor concentration is calculated from the measured data as follows:

Water vapor concentration = 100 - ((Y_{Min} * 100)/ Y_{Max})

The limit is compared to the maximum value allowed.

Alignment Test:

The alignment test verifies whether the absolute peak position of the interferogram is within the range specified.

A single-channel spectrum is measured and the absolute peak position is read from the measurement parameters stored.

Linearity Test:

The linearity test determines the energy contribution of certain detectors below the detector cutoff frequency.

A single-channel spectrum is measured down to $0 cm^{-1}$ (figure 339). The energy contribution in the region below the detector cutoff frequency is analyzed and compared to the energy value of the single-channel spectrum at the maximum.
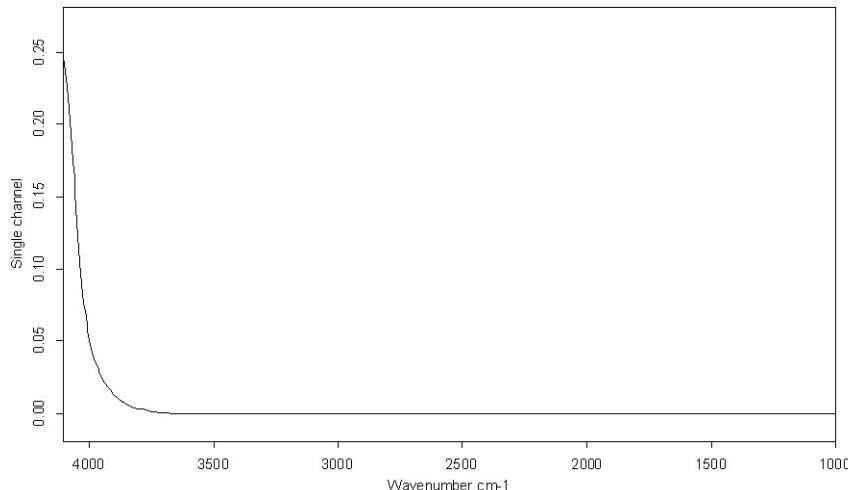
Figure 339: Single-channel spectrum around detector cutoff frequency

The following formula is used to calculate the linearity value:

$$\text{Linearity Value} = ((\text{Abs}(Y_{MaxCutoff} + Y_{MinCutoff}) / 2) / Y_{MaxSpectrum}) * 100$$

The linearity value must not exceed a maximum limit.

Reproducibility Test:

The reproducibility test confirms that all moving parts (mirrors etc.) of a multi-channel instrument are in the correct and reproducible position.

A 100% spectrum is measured for a specific channel and used as reference spectrum. After measuring the reference spectrum all moving parts relevant for the specific channel are moved and a new 100% transmittance spectrum is recorded in the channel position. This procedure is repeated 10 times. The

deviation of each of the ten 100% spectra from the reference spectrum is computed. The greatest deviation must not exceed a maximum value.

13.6   OVP Trends Module

The trends module is a long-term diagnostic tool which visualizes the test results in graphical form. Performance changes of the instrument can be detected long before the instrument does not match the required criteria. The trends module can only be accessed from the main OVP program by users with Administrator rights in OPUS.
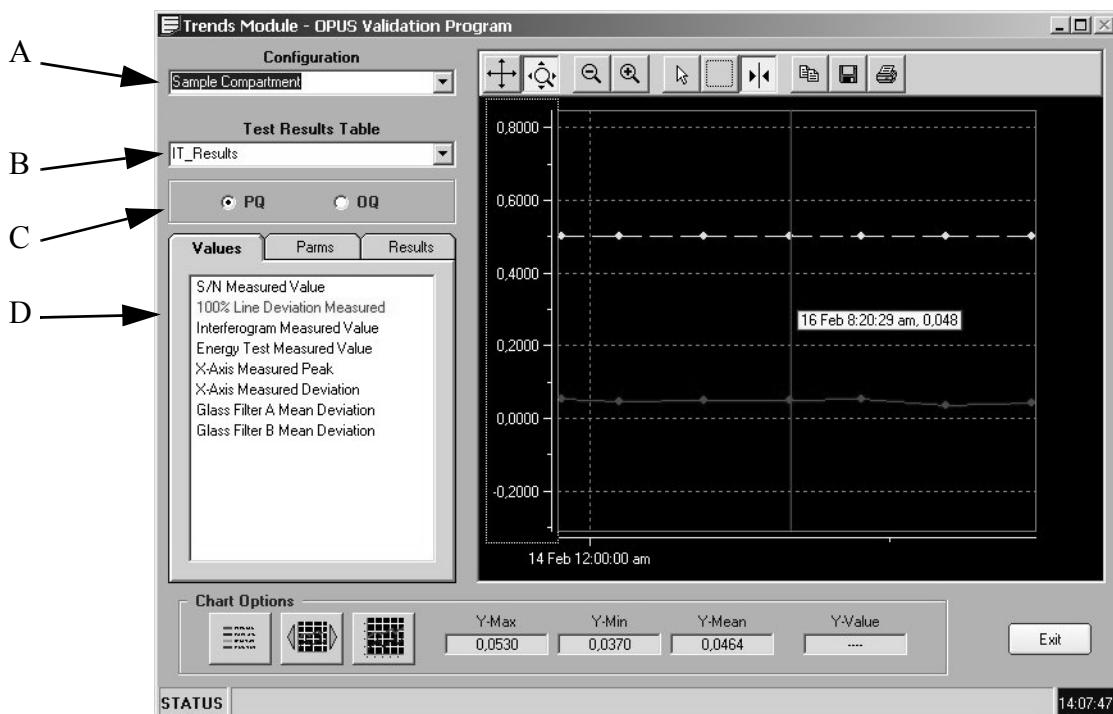

Figure 340: OVP - Trends Module

Select the instrument configuration from the *Configuration* drop-down list (A), and the test results to be shown from the *Test Results Table* drop-down list (B). Check the corresponding test category option (C). The *Values* tab (see figure 341) lists all individual tests specified for the test category. If you click on any of the tests, the test will be marked red and shown in the chart on the right side.
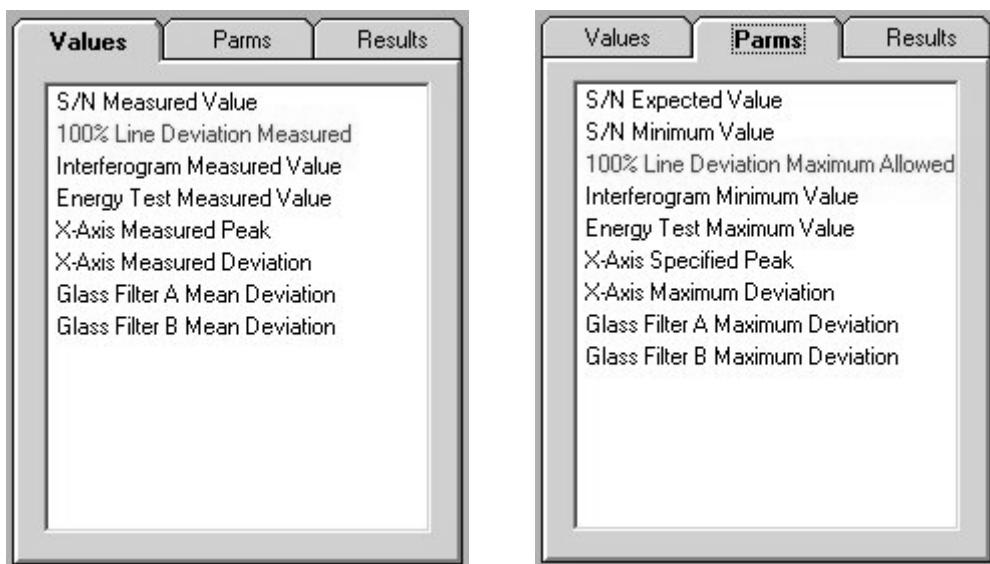
Figure 341: OVP - Values and Parms tab with tests specified

To compare the measured values with the expected values click on the *Parms* tab and select the limit for the same test which will also be shown in the chart. Multiple results and limits can be displayed in the same chart. Due to the different y-ranges, however, this might not be useful at all.

Several control options allow to customize the chart. By means of the *Chart Options* group field (figure 342) you can have the chart displayed in different views and colors.

Figure 342: OVP - Chart Options buttons

The toolbar on top allows to scale and shift the x and y-axis ( ), zoom in and out the display ( ), read out values of individual data points ( ), zoom in a particular region of the chart ( ), set time marks ( ) and copy, save or print the chart ( ).

13.7 Running OVP in an Unattended Mode

The internal validation unit (IVU) which is integrated into the spectrometers allows to run, with very few exceptions, the OQ and PQ tests without any user interaction required.

In general, there are two methods to run OVP in an unattended mode.

13.7.1 Running OVP via OPUS macro

When installing OVP the *OVP.MTX* macro is installed into the VALIDATION sub-directory. If you run this macro, the *OVP Auto Loop* dialog opens which you can use to define several options.
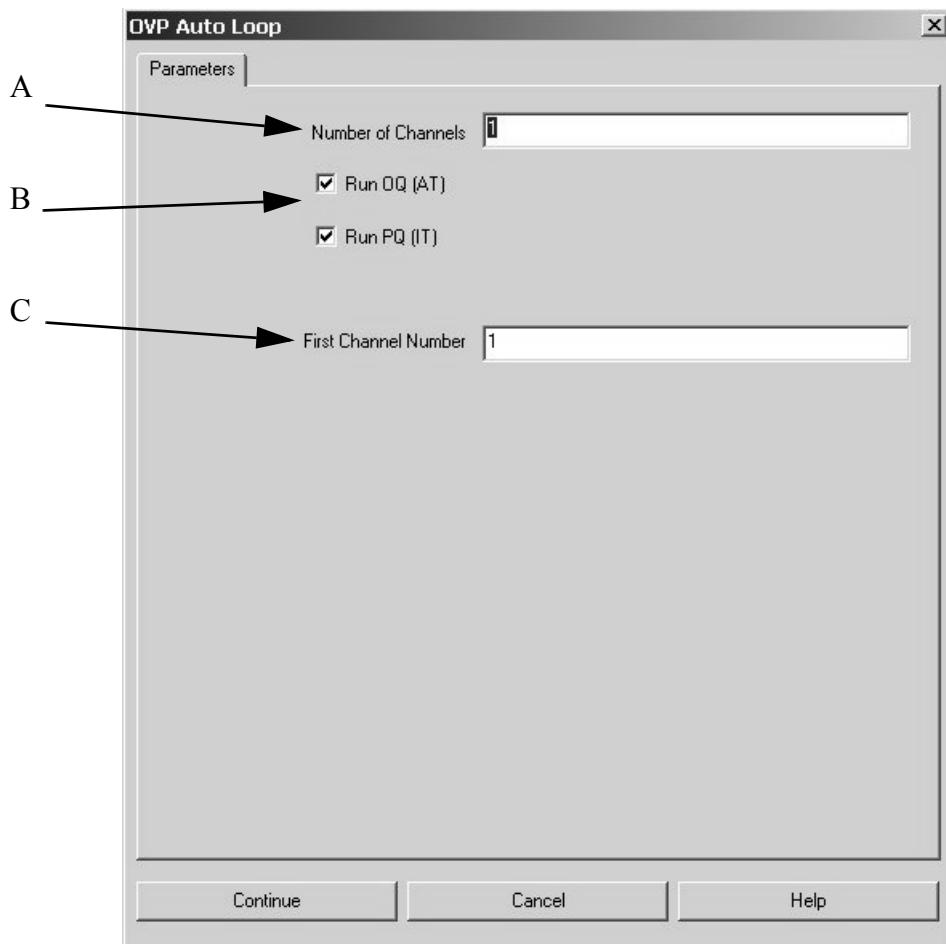
Figure 343: OVP - Auto Loop dialog

(A) Specify the number of measurement channels which you want to test. This number must not exceed the number of channels you have specified for OVP.

(B) Activate the check boxes if you want to run the OQ and/or PQ test. If a test has expired and not been activated, it will run in any case regardless of the settings made.

(C) If you have specified more than one channel but you do not want to run the test for all channels, you can specify the channel to start with. As the channel number is incremented automatically for the net channel you can only measure subsequent channels from the list.

Click on the *Continue* button to start the test. The same OVP dialogs are displayed which you can see when running the test manually. However, you do not need to click on any of the buttons.

13.7.2   Running AUTOOVP VB-Script

Instead of the macro which can be used for a one-off run of all tests you can use a VB Script which is also integrated in OVP. This script can be used to run selected tests for any of the test channels at a specified time.
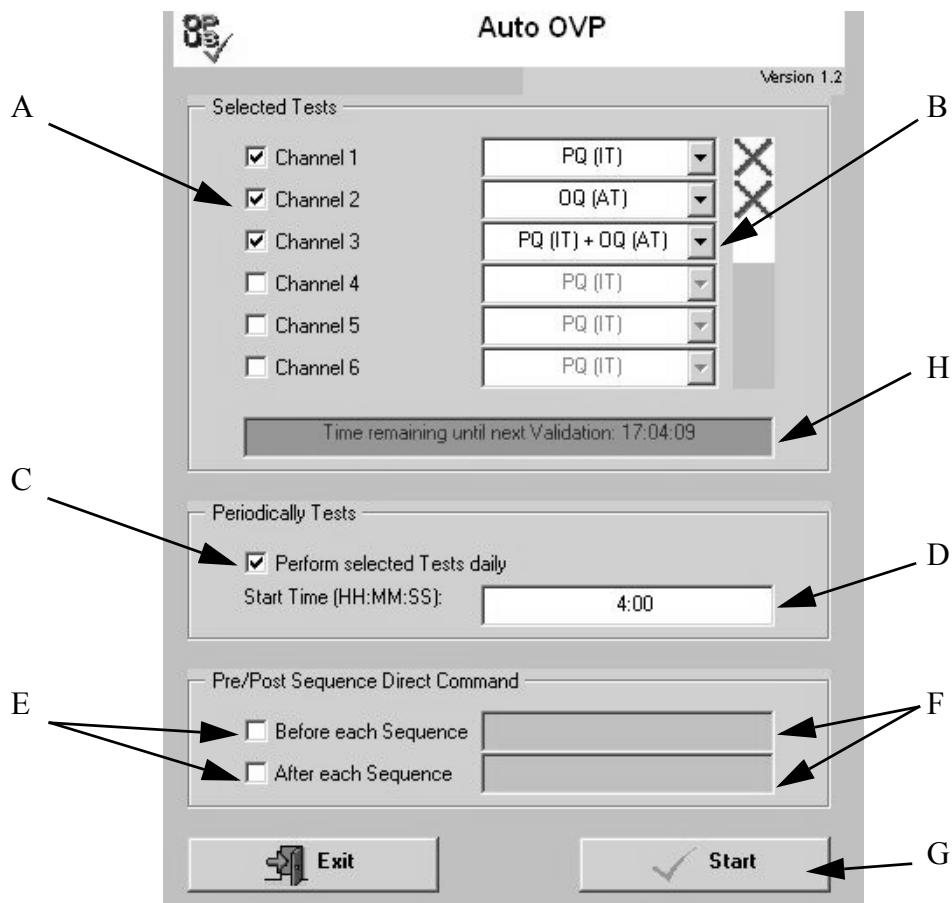
Figure 344: OVP - Auto OVP dialog

(A) Select the test channel by activating the appropriate check box.

(B) Select the tests to be run from the drop down list. You can select either PQ, OQ or both tests.

(C)If you want to run the tests on a daily basis, activate the *Perform selected Tests daily* check box.

(D)Enter the start time for the first test to be started in the entry field.

(E)If you have to define further commands, e.g. switching an external source ON and OFF, you can activate one or both check boxes in the *Pre/Post Sequence Direct Command* group field.

(F)Specify the direct command line in the entry field which shall be executed before and/or after the test measurements have been completed.

(G)Start the script by clicking on the *Start* button.

(H)If you have activated the *Perform selected Test daily* check box, the time remaining before the first test run will be indicated in the selection field below the selected test channels.

13.8   OVP Accessory Manager

Accessories are defined as additional optical components which can optionally be attached to the instruments standard configuration. Examples of accessories can be:

- A unit for special sampling technique like an ATR accessory which can be mounted in the sample compartment.
- Different types of fibre probes with different fibre lengths, e.g. a 2m liquids probe.

An accessory changes some of the basic instrument optical properties and thus the overall instrument performance. While the basic PQ and OQ tests just verify the performance and properties of the basic instrument configuration (e.g. empty sample compartment) it is obvious that these tests cannot be used to verify the performance of the same instrument if, e.g., an ATR unit is mounted in the sample compartment.

It is, however, essential to test not only the basic configuration but also instrument combinations with a built-in accessory, to be able to detect problems caused by the accessory.

Standard accessories delivered by Bruker are normally included in the separate accessory databases used by OVP. To be able to run OVP tests in case of accessories from different suppliers OVP is supported by a separate program which allows to configure test parameters for these types of accessories.

Accessory data are stored in two different sets of databases, i.e. the standard accessory databases supported by Bruker and an identical set for user-specific accessories. These databases are identified by the *User* prefix and are protected by the same password as the user databases for the test settings and results mentioned earlier. Thus, a database update will not have any impact on the contents of the user accessory data. An empty set of user accessory databases is

installed during OVP installation. The Accessory Manager will only modify the contents of these user-specific databases.

13.8.1 Accessories Influence on Tests

Accessories will change certain test results, e.g. the S/N ratio, or limit the frequency range of an instrument. In most cases these influences do not depend on the instrument type used. Therefore, the accessory properties can be specified as follows:

- Factors - influencing test limits
- Offsets for frequency limits

Depending on the type of accessory a few measurement parameters may also need to be changed compared to the basic instrument configuration. These parameters are instrument-type specific and may be:

- Number of scans, reference and sample spectrum (NSS, NSR)
- Preamplifier gain (PGN)
- Aperture setting (APT)

13.8.2 Running Accessory Manager

The *OVPACCESSORYMGR.EXE* accessory manager is located in the VALIDATION sub-directory and can be run from the Windows explorer.

Note: Do not move the accessory manager to a different sub-directory as it expects the user database to be in the VALIDATION sub-directory DATABASES.
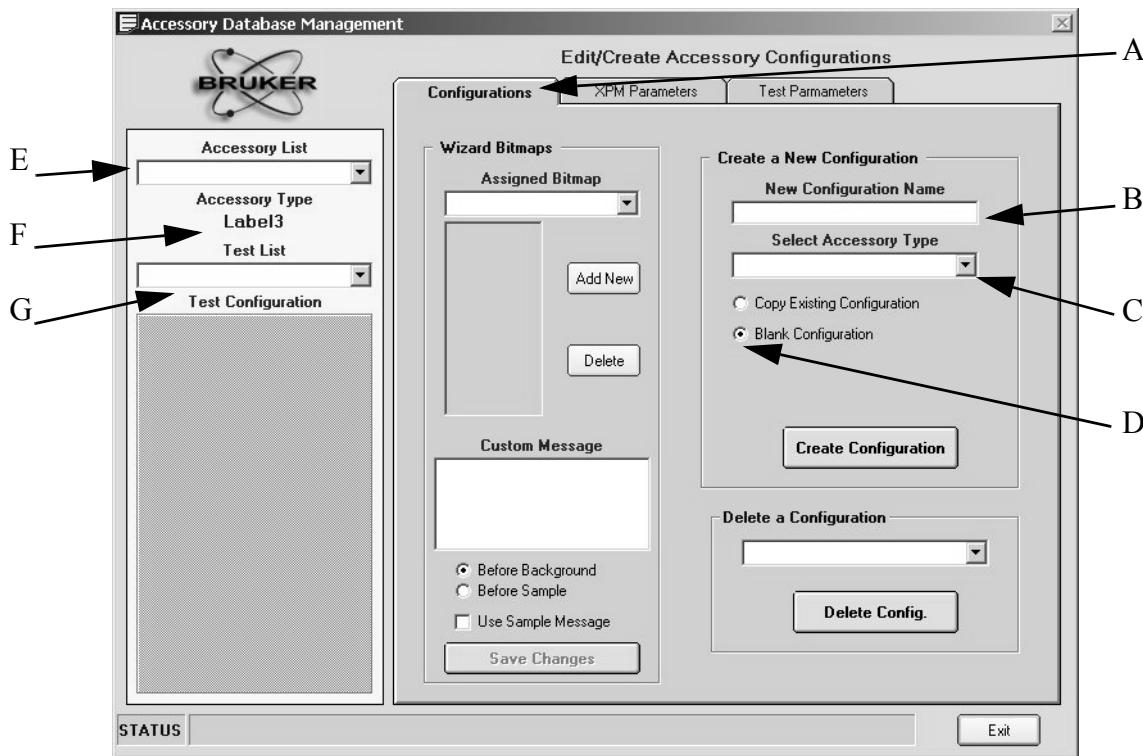
Figure 345: OVP Accessory Manager - Accessory Database Management dialog

After starting the accessory manager make sure that the *Configurations* tab (A) is selected. The following step-by-step instruction describes how to add a new accessory configuration to the database. In this example we will add the configuration for a 100m fiber liquid probe.

1) Enter the accessory name, e.g. *100m Liquid Probe,* into the *New Configuration Name* entry field (B).

2) Select the type of accessory from the *Select Accessory Type* drop-down list (C).
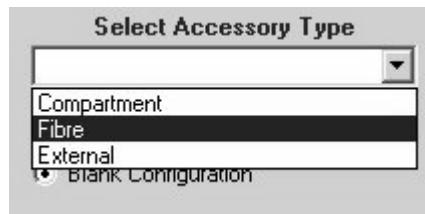
Figure 346: OVP Accessory Manager - Accessory type

The accessory type information is used to distinguish accessories which can either be mounted into the sample compartment, connected to a fiber port or mounted at an external port of the instrument. In our example select *Fibre*.

3) Make sure that the *Blank Configuration* option button (B) is selected and click on the *Create Configuration* button. The new configuration will be added to the *Accessory List* (E) and the accessory type is shown in (F).

4) Select the test protocol from the *Test List* drop-down list (G). The tests which are available will be listed in the section below. All tests are initially marked as being not available (H).
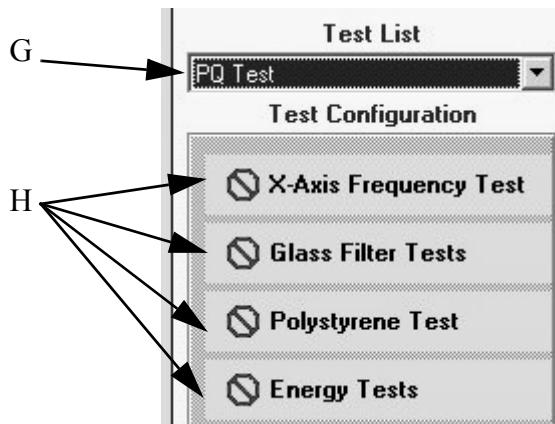
Figure 347: OVP Accessory Manager - Test configuration

5) Double click on those tests which should be made available for the accessory. The *Stop* sign will be replaced by a green check mark. Only those tests activated by a green check mark will later be accessible in the PQ test setup dialog.
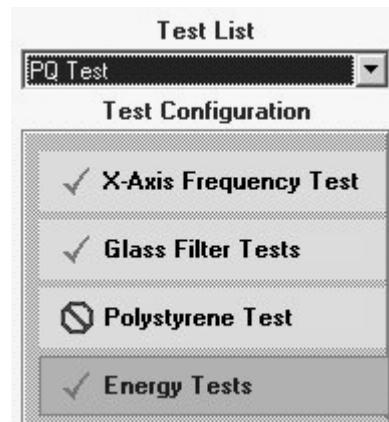
Figure 348: OVP Accessory Manager - Tests activated

6) The *Wizard Bitmaps* group field allows to select one of the existing bitmaps, or to add a new one. The bitmaps assigned will later be shown in the measurement wizard during test run. In our example we select the pre-defined *Liquid Probe* bitmap from the drop down list (I in figure 349).

Figure 349: OVP Accessory Manager - Assigned bitmap

7) If you want to add a new bitmap for the particular accessory, prepare a bitmap with the size of 150 (w) x 300 (h) pixels. Click on the *Add New* button to open a dialog which allows to add this bitmap to the database, and assign it to the particular accessory.
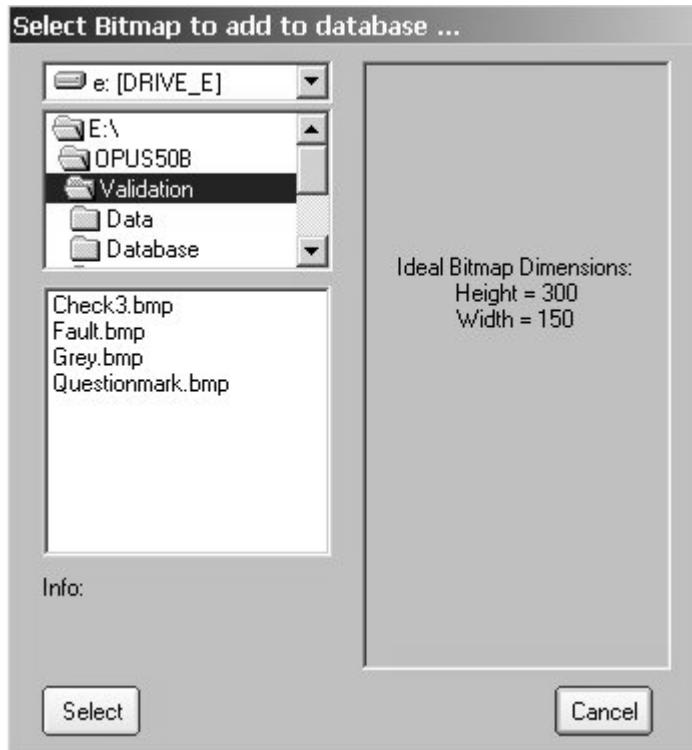
Figure 350: OVP - Add bitmap to database

8) In the *Custom Message* entry field (figure 351) you can enter a test description which will be shown in the measurement wizard before running the test measurements. The text should reflect the actions to be performed. If required, you can also add an optional test to each sample measurement. Store the current settings by clicking on the *Save Changes* button.

Figure 351: OVP Accessory Manager - Custom Message entry field

9) Select the *XPM Parameters* tab to specify required parameter changes for the particular accessory.
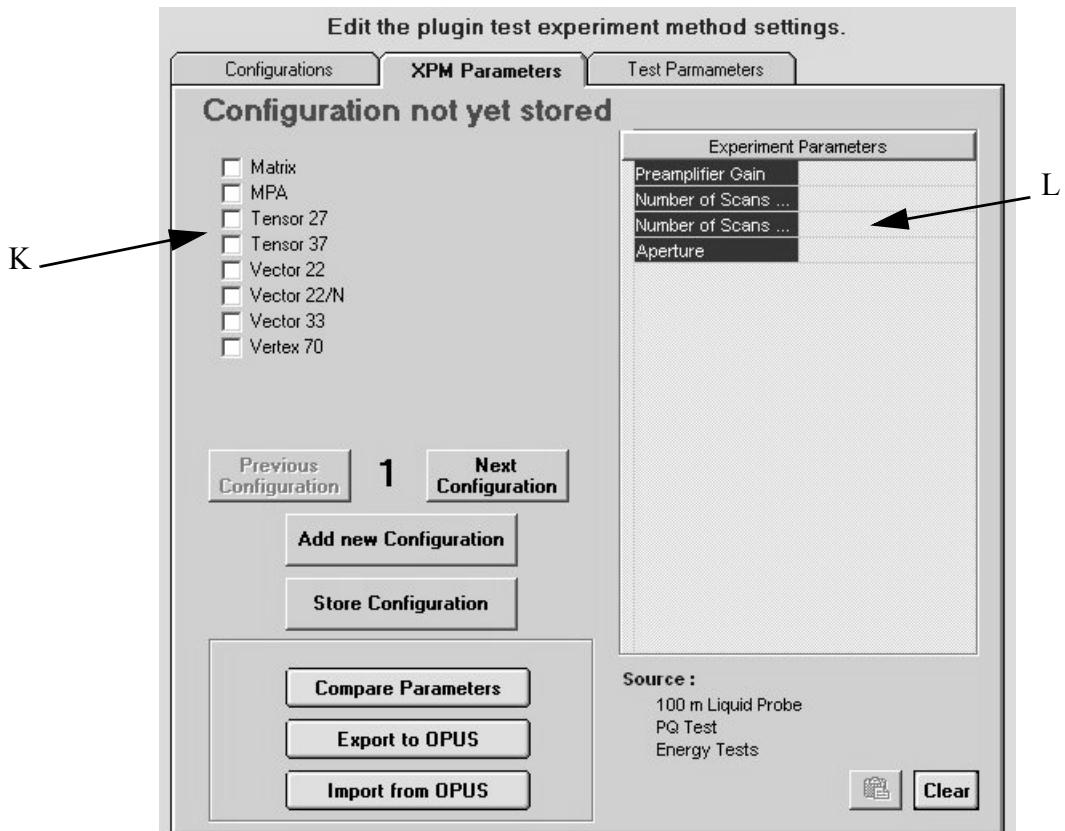
Figure 352: OVP Accessory Manager - XPM Parameters tab

10) Select the instrument (K) which you will use the accessory with. Specify only those parameters in the *Experiment Parameters* list (L), which are different from the default setting. Keep those parameter fields empty which do not have to be changed.
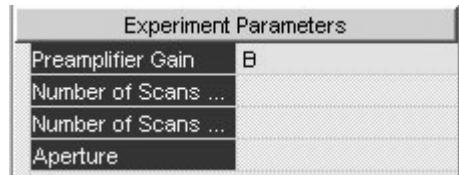
Figure 353: OVP Accessory Manager - Experiment parameters selected

11) Instead of typing parameter values you can load the parameters directly from OPUS. Load an experiment or set the parameters by the *Setup Measurement Parameters* command in the OPUS *Measure* menu. Confirm the settings. Return to the accessory manager and use the *Import from OPUS* button (O) to read the parameters from OPUS. The *Compare Parameters* button (M) can be used to compare any values entered to the current OPUS setting. The *Export to OPUS* button (N) overwrites the current OPUS settings by the parameters manually entered.

Figure 354: OVP Accessory Manager - Measurement parameters options

12) Click on the *Store Configuration* button (P).
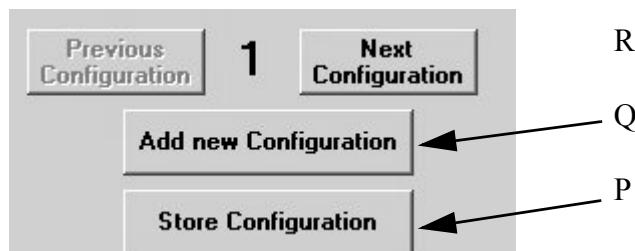
Figure 355: OVP Accessory Manager - Parameter configuration buttons

13) Steps 9 to 12 have to be repeated for each individual test. For both PQ and OQ tests.

14) If you want to use the accessory with more than one instrument type click on the *Add new Configuration* button (Q) and repeat steps 9 to 13 for each new instrument type.

15) Click on the *Test Parameters* tab which will be empty and has to be activated by clicking on the *Load Parms* button (S).
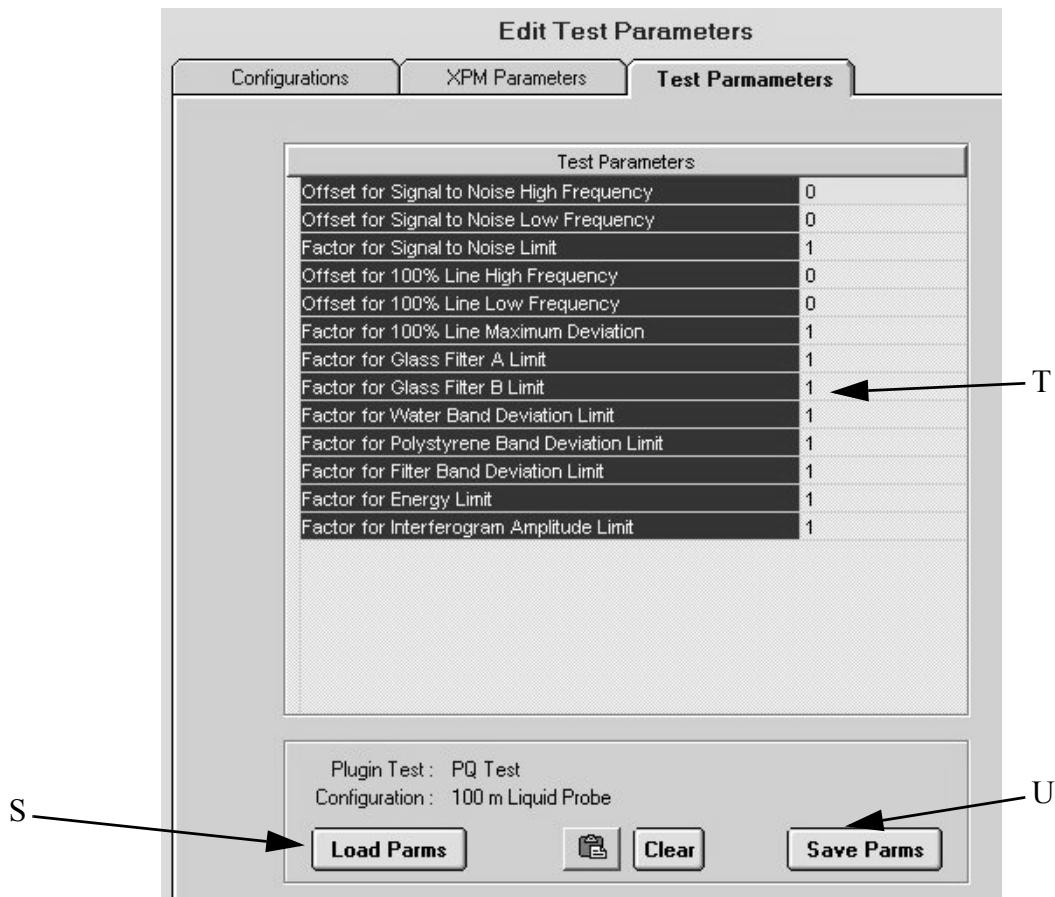
Figure 356: OVP Accessory Manager - Test Parameters tab

16) Enter appropriate offsets and factors into the parameter section (T). Offsets are entered in wave number units and will be added to the value specified for the basic instrument. If an instrument increases, e.g., the lower frequency limit for the signal-to-noise test by 100cm^{-1}, enter *100* into the appropriate field.

If a limit is decreased, enter the value with a minus sign. Factors are used to multiply test limits. In most cases the accessory will probably decrease the achievable S/N ratio of the basic instrument. If it decreases the value by 50%, enter *0.5* into the appropriate field. If the minimum S/N ratio limit of the basic instrument configuration is 10000, this limit will be decreased to 5000 as soon as you use the accessory. Offsets which are not influenced need to be set to 0, while parameter limit factors which do not change need to be set to 1.

Figure 357: OVP Accessory Manager - Test parameter settings

17) Store the settings by clicking on the *Save Parms* button (U).

18) To generate the settings for the OQ test protocol select *OQ Test* from the *Test List* drop-down list (G in figure 347). The *Test Configuration* field will now show all OQ tests. Proceed for the OQ test protocol and follow the steps as described for the PQ tests.

Once you have generated a complete accessory configuration you can set up another configuration by copying the existing one.
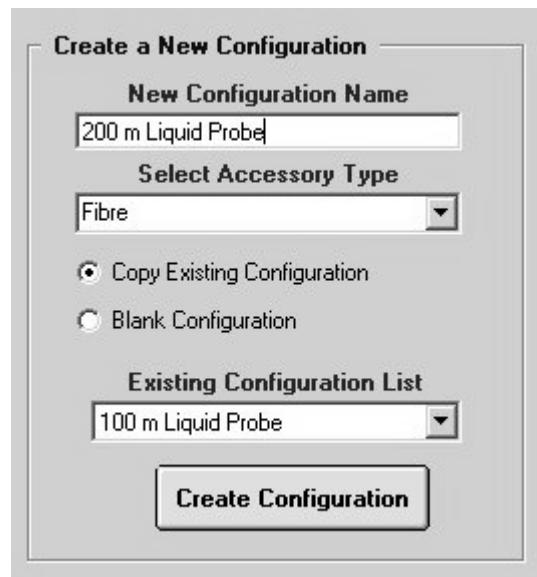
Figure 358: OVP Accessory Manager- Create new configuration

Enter the name of the new configuration into the *New Configuration Name* entry field. Select the accessory type from the drop-down list and activate the *Copy Existing Configuration* option button. Select the configuration to be copied from the *Existing Configuration List* drop-down list. Click on the *Create Configuration* button to make the copy. Instead of defining all parameters you just need to make the required modifications.

In the OVP setup you will immediately find the accessories listed in the *Accessory* drop down list
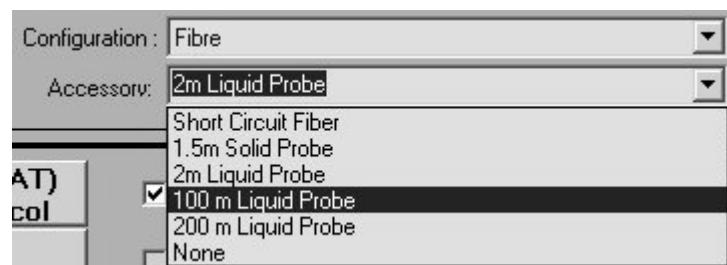
Figure 359: OVP Setup - Accessory List

13.9 Adding New Test Channel

This chapter exemplifies step by step a typical first-time use of the OVP setup. Assuming that the program has been properly installed, make sure that you meet the following conditions:

- OPUS has been installed in the *C:\PROGRAMS\OPUS* path.
- OVP has been installed in the OPUS *VALIDATION* sub-directory.
- Set up a test channel for the MPA spectrometer with a 2m liquid fiber probe.

13.9.1 OPUS Setup

1) Select the *Optic Setup and Service* command from the OPUS *Measure* menu.
2) Select the *Interferometer/AQP* tab and make sure that the *Channel Specific Laser Wavenumber* check box is activated.
3) Close the dialog.
4) Select the *User Settings* command from the *Setup* menu.
5) Select the *Instrument Test1* tab.
6) Click on the *Path* button to locate the OVP installation path.
7) Type *\OVP.EXE* at the end of the path. The *IT* entry field should now read *C:\PROGRAMS\OPUS\VALIDATION\OVP.EXE*
8) Close the dialog.
9) Select the *Advanced Measurement* from the *Measure* menu, or the *Setup Measurement Parameters* command when working in validated mode.
10) Load the default measurement experiment located in the *XPM* sub-directory of the OVP installation directory. In case of our example this means: *MPA.XPM* in *C:\PROGRAMS\OPUS\VALIDATION\XPM*.
11) Make sure that none of the tabs indicates an error or warning symbol (e.g. STOP sign).
12) If an error is indicated on any of the parameter tabs, click on this tab, correct the error and store the experiment using the same file name. Add a *Release* signature to the experiment if you are working in validated mode

13.9.2 OVP Setup

1) Click on the status light on the OPUS interface. The *Instrument Status* dialog opens.
2) Click on the first icon in the second row to open the *Instrument Status Message* dialog.
3) Click on the *Test Now* button to open the OVP start screen.
4) Click on the *Setup* button to open the OVP setup dialog.
5) Check the instrument type and make sure that the correct instrument

(MPA) is indicated. If the instrument type is not correct or if the *Instrument Type* entry field is empty, click on the [button] button to update the automatic selection. If the entry field still shows the wrong instrument type, check if the correct instrument is selected in the OPUS *Optics Setup and Service* settings in the *Measure* menu.

If the entry field is still empty, the instrument selected is not supported by OVP. In this case contact your local service department for more information. Currently, the following instrument types are supported: VECTOR, VECTOR 22/N, TENSOR, MATRIX, MPA and VERTEX.

6) Click on the *Setup* button in the first row (*IT1*) of the OVP setup dialog to open the *Setup Optics Configuration* dialog. Select *Source*, *Beam-splitter*, *Measurement Channel* and *Detector* from each of the four drop-down lists for your configuration. The following settings apply to our example:

- Source = NIR
- Beam splitter = Quartz
- Measurement Channel = Fibre 1
- Detector = TE-InGaAs [Internal]

7) Close the dialog by clicking on the *Save and Exit* button.

8) Select the new entry. Click on the *IT1* button. The entry field becomes yellow.

9) Make sure that the *Configuration* entry field shows the correct configuration, i.e. *Fibre* in case of this example. If the configuration is not automatically selected or wrong, select the correct configuration from the drop down list. If the drop-down list does not include the configuration required, contact your local service department for more information.

10) If the configuration has not been detected automatically, make sure that the configuration is still the same even after selecting the respective test category. Activate the appropriate *OQ* or *PQ* option button.

11) If the *Accessory* drop-down list is enabled, select the accessory you want to use, or the *None* option if no accessory is used. In case of this example select the *2 m Liquid Probe* accessory.

12) Press the [Measure LWN] button to measure a new laser wave number (LWN). As soon as the result is displayed click on the *Set* button to set the new LWN value. If the LWN has already been correct, click on the *Exit* button.

13) Activate the *PQ* option button.

14) Define the time interval between the tests. Generally, PQ tests are performed once every 24 hours.

15) Activate the *OQ* option button.

16) Define the time interval between the tests. Generally, OQ tests are performed once every 6 or 12 months.

17) Enter a unique title into the *Validation Set Title* entry field. This title is used in reports to help to identify the configuration used, e.g. *Liquids Probe on Chemical Vat #3*.

13.9.3   PQ Test Protocol Setup

1) Activate the test channel by clicking on the *ITx* button. The entry field will turn yellow.

2) If the *PQ* category has not yet been activated, check the *PQ* option button.

3) Activate the *PQ Test Protocol* check box. The *PQ Test Protocol Setup* dialog opens.

4) Click on the *Measure* button and start the reference measurements.

5) If the reference measurements have finished, click on the *Exit* button.

13.9.4   OQ Test Protocol Setup

1) Activate the test channel by clicking on the *ITx* button. The entry field becomes yellow.

2) If the *OQ* category has not yet been activated, check the *OQ* option button.

3) Activate the *PQ Test Protocol* check box. The *PQ Test Protocol Setup* dialog opens.

4) Make sure that all the respective tests are activated.

5) Click on the *Exit* button.

Repeat all steps for any other channels which you want to be validated.

13.10   OVP Program Modules and Databases

The main programs and databases required for OVP, and their meaning are outlined in the following:

\VALIDATION	**Main OVP Directory:**
OVP.EXE	Main OVP program
OVP.MTX	OPUS Macro for OVP Automation
AUTOOVP.OBS	OPUS VB-Script for OVP Automation
OVP_MANUAL.PDF	This Manual in PDF Format

\VALIDATION\MODULES	**Directory for OVP Modules:**
OVPSETUP.EXE	OVP Setup Program
OVPWIZARD.EXE	OVP Measurement Wizard
OVPTRENDS.EXE	OVP Trends Module

\VALIDATION\PLUGINS	**Directory for OVP Test Protocol Plug-ins:**
IT_BVP.EXE	Plug-in for PQ Test Protocol
AT_BVP.EXE	Plug-in for OQ Test Protocol

\VALIDATION\DATABASE	**Database Directory:**
SYSTEMDB.MDB	Instrument Configuration Database
IT_DATA.MDB	PQ Test Protocol Database
AT_DATA.MDB	OQ Test Protocol Database
ACCESSORY.MDB	Accessory Configuration Database
PQ_ACCESSORY.MDB	PQ Accessories Test Protocol Database
OQ_ACCESSORY.MDB	OQ Accessories Test Protocol Database
USERACCESSORY.MDB	User-specific Accessory Configuration Database
USERPQ_ACCESSORY.MDB	User-specific PQ Accessories Test Protocol Database
USEROQ_ACCESSORY.MDB	User-specific OQ Accessories Test Protocol Database
USERSETTINGS.MDB	Test Channel Configuration
USERDATA.MDB	Test Data
\VALIDATION\XPM	Directory for Default Measurement Experiment
instrument.XPM	Instrument-specific Measurement Experiment
\VALIDATION\DATA	Main Data and Report Directory:
\<YYMMDD>\<HHMMSS>	Data Sub-Directory named with test date and time
\REPORTS	Reports Sub-Directory
PQ_*configuration_Testtype*.0	PQ Test spectra named by instrument configuration and test (e.g. PQ_MPA_SAMPLE_ COMPARTMENT_ FREQTEST.0)
OQ_*configuration_Testtype*.0	OQ Test spectra named by instrument configuration and test (e.g. OQ_MPA_SPHERE_LINEARITY.0)
PQ_*configuration_date_time*.pdf	PQ Test Report (e.g. PQ_MPA_FIBRE_040217_124909.pdf)
OQ_*configuration_date_time*.pdf	OQ Test Report (e.g. OQ_MPA_FIBRE_040216_103545.pdf)
\VALIDATION\TEMP	Directory for Temporary Data

13.11   Instrument Status Indicators

OPUS has two types of status indicators. The status light located in the bottom right corner of the OPUS interface, and the icons displayed on the *Instrument Status* dialog. To access the *Instrument Status* dialog click on the status light.

The status light indicates the status of the active channel as defined by the currently loaded measurement experiment file (XPM).

While the first row of icons on the *Instrument Status* dialog indicates the state of the instrument hardware, the second and third row of icons refer to each of the 12 possible active test channels. The program assigned to the channel position determines the status indicated on the *Instrument Status* dialog.

These are two important distinctions. The status light indicates the status based on the measurement experiment loaded. The icons on the *Instrument Status* dialog indicate a status returned by a program assigned to that channel position.

13.11.1   Status Light Setup and Operation

Primarily designed for the latest Ethernet-based spectrometers, the status light indicates the status of the active test channel. This status is stored on the instrument, not on the PC.

Each time the user loads an experiment file, the corresponding channel is set as active channel. The status of this new active channel is checked and indicated by the status light.

The active test channel refers to one of 12 IT channel positions defined on the *Instrument Test* tabs of the *User Settings* command in the *Setup* menu.
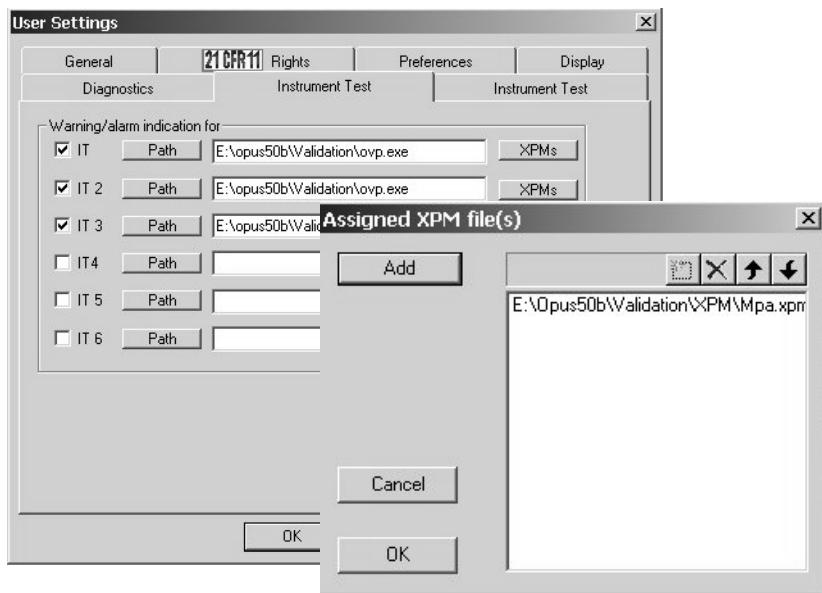
Figure 360: Instrument Test tab and XPM file assigned

To activate a channel, select a path by clicking on the *Path* button. You can also manually enter the path.

If you select a path, OPUS will be informed that you want to assign the *Instrument Test* macro (which can be installed during OPUS installation) to a particular channel. OPUS assumes that the *IT.mtx* macro is located in this path. If the macro cannot be found, a *Runtime Error in Macro* message pops up when you attempt to run the test.

Entering an executable program file name, e.g. *OVP.EXE* informs OPUS to run that program instead of the macro.

If you have entered a path (and *exe* name, if desired) into the appropriate *IT* entry field on the *Instrument Test* tab, an icon is assigned for that particular channel on the *Instrument Status* dialog.

For the status light to operate, you have to assign measurement experiment files (xpm) by using the *XPMs* button. Click the *XPMs* button to the right of the path assignment. A dialog opens. All experiment files listed in this dialog are registered for this particular channel. Therefore, you should only select experiment files that have the same basic configuration of the spectrometer (source, beam splitter, measurement channel, detector).

If you load an experiment file, OPUS checks all the experiment files registered. If a match is found, that channel (1 to 12) becomes the active test channel. OPUS polls the spectrometer to detect the status of that channel. That channel is set *Active* in the spectrometer as well. The status light changes its color as follows:

- **GREEN:** The active test channel is active, the tests have passed and not expired.
- **YELLOW:** The time interval for one or all the tests for the active test channel has expired.
- **RED:** One or all the tests for the active test channel have failed.

If you deactivate one of the *IT* check boxes, that particular channel becomes inactive. OPUS does not update the status light if that particular channel is selected as the active channel.

The following summarizes situations which may have an effect on the status light:

- User loads an experiment file.
- The XPM lists for each channel are scanned for the first position containing that experiment.
- If a match is found, this match becomes the active test channel.
- The status for the active channel is read from the spectrometer web server.
- The status light is changed to reflect that status.

13.11.2 Instrument Status Icon Operation

If you click on the status light, the *Instrument Test* dialog opens. The status light will change to reflect the state of the active channel icon.

If a path (and exe name, if desired) has been entered into an *IT* entry field on the *Instrument Test* tab, an icon is assigned for that channel position in the second or third row of icons on the *Instrument Status* dialog. The first row indicates the results of the instrument diagnostics test performed when the *Instrument Status* dialog opens.

The first row of icons can have three possible status indicators. A green check mark indicates that the hardware component has passed the diagnostic test. A yellow warning is displayed if a limit is nearly reached, e.g. source lifetime has nearly expired. A red error message indicates that the diagnostics have failed.

The second and third row of icons can have three possible status indicators. A green check mark indicates that the tests have passed and are still valid. A yellow warning indicates that the tests have passed, but expired. A red error indicates that a test has failed.

If you click on the first row of icons in the *Instrument Status* dialog, the *Instrument Status Message* dialog pops up and displays the *Service Info* button.

Figure 361: OVP - Instrument Status Message with Service Info button

Clicking on the *Service Info* button opens a window in OPUS indicating the diagnostics page from the instrument Web server. On non-Ethernet instruments the Bruker Web page is displayed, provided you are connected to the Internet.

If you click on the second and third row of icons in the *Instrument Status* dialog, the *Instrument Status Message* dialog pops up and displays the *Test Now* button. Clicking on the *Test Now* button tries to run the macro or program assigned to this particular test channel.
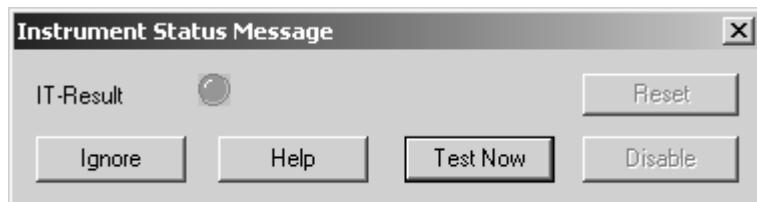
Figure 362: OVP - Instrument Status Message

If you have not assigned any program name, OPUS assumes that you are running the *IT.mtx* instrument test macro. The results of this test are stored in the *IT.log* text file. This file is located in the *IT* sub-directory. If OPUS cannot locate the *IT.log* file, the *Instrument Status Message* dialog displays the message: *Test log not found*. OPUS reads the *IT.log* file to determine the status of the particular channel.

If the file listed is an executable program, OPUS runs the program and transfers a parameter to the program requiring the status of the current channel. The program then returns the test channel status.

This program status check is performed for each channel assigned at the time the *Instrument Status* dialog is accessed. The results returned are displayed as icons.

The following summarizes situations which may have an effect on the icons displayed in the *Instrument Status* dialog.

- The user clicks on the status light.
- OPUS polls the programs listed for each of the 12 positions, if assigned.

- The program returns the test status for that channel to OPUS.
- OPUS changes the icon for that channel to reflect the result returned.
- OPUS performs an instrument hardware diagnostics check.
- The user clicks on an icon to run the tests previously assigned.
- If the tests have been completed, the program directly writes the test results of the active channel to the spectrometer.

13.11.3 Status Indicator for Non-Ethernet Based Spectrometers

The status light and icons are intended to be used in connection with Bruker Ethernet-based spectrometers. In case of previous spectrometer types and research spectrometers the functionality is different.

A command line option must be added to the OPUS icon to specify a time (in minutes) that OPUS should use to poll the program for the current status of the active channel. Once during each interval, the program is polled to request the status and the status light is updated.
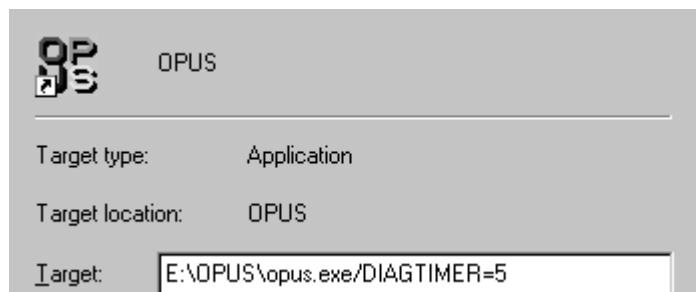
Figure 363: OPUS Property dialog

In figure 363 the */DIAGTIMER=10* command polls the status once every 5 minutes.

The status is not updated when loading an experiment file, it is updated if the time interval has expired and the assigned program polled.

14 Setup
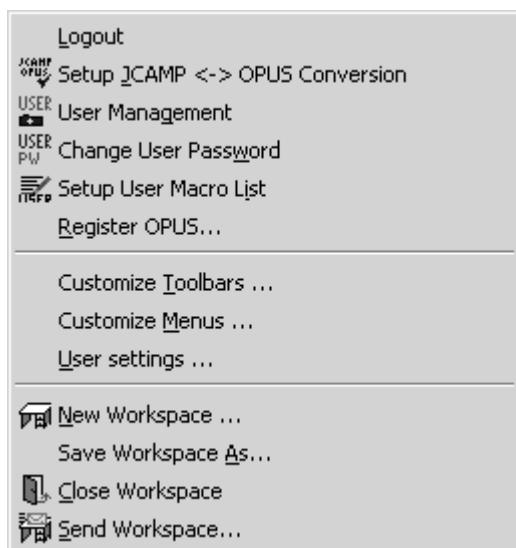
Figure 364: Setup Menu

14.1 Logout

To login a new user or to logout and terminate OPUS chose Logout from the Setup menu.
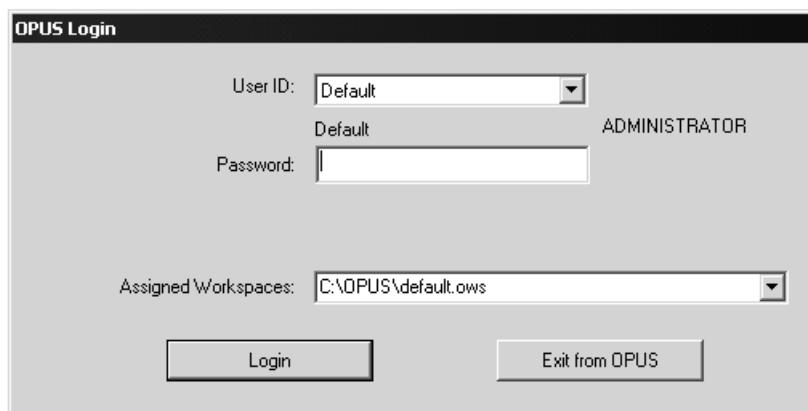
Figure 365: Logout Screen

To log in, choose the User ID from the combo box. The last user is always shown. Enter the proper user password. The password is displayed as a series of "*". The user type (Operator or Administrator) for the currently selected user is displayed.

Choose one of the workspaces from the combo box. The contents of the combo box depends on the selected user. In case of Operators only the assigned

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workspaces are shown while in case of Administrators all workspaces in the OPUS root directory are shown. Click on the *Login* button to log in the new user. Click on *Exit from OPUS* to cancel the login procedure and leave OPUS.

14.2   Setup JCAMP/OPUS Conversion

Use this command to set the conditions for the conversion of JCAMP files into OPUS files. The settings made apply to the *Convert3dJCAMP* command in the *Edit* menu as well as to the *Load File* command in the *File* menu. To avoid the loss of information conversion tables are used to correlate JCAMP labels with OPUS parameters and information lines. These tables are text files and have the extension *.PCT* which can be generated using any kind of text editor. In addition, the file containing the info text definition has to be specified. The general syntax for each line is as follows:

#Ixx:yyy:LABEL

Ixx   defines the number of the line in the info block, xx being a two-digit number starting with 01
yyy   a three character OPUS parameter
LABEL   the name of the JCAMP label

It is mandatory to determine the consecutively numbered info line. Each line need to have two colons. The parameter name and the JCAMP label definition are optional.

The following example refers to the DEFAULT.PCT file which is stored in the *OPUS Methods* directory.

#I01::SNM:TITLE
#I02::MOLFORM
#I03::MW
#I04::CAS REGISTRY NO
#I05::MP
#I06::BP
#I07:SFM:SAMPLING PROCEDURE
#I08::
#I09:CNM:ORIGIN
#I10::CROSS REFERENCE
#I11::CHARGE NO
#I112:HIS:DATA PROCESSING

Use the *Setup JCAMP/OPUS Conversion* command to define the conversion table required for the JCAMP file conversion. If you click on the *Change* button, you can load the relevant file from the dialog that pops up. Localize the files which include the conversion tables desired.
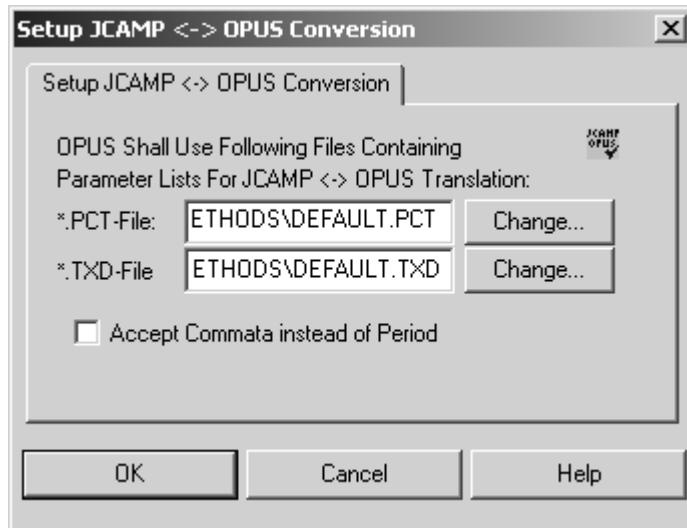
Figure 366: Setup JCAMP - OPUS Conversion

If you activate the *Accept Commata instead of Period* check box, a comma is used as decimal separator during conversion.

14.3 User Management

An essential part of quality regulations is the access control to computer systems and software packages. While the operating system ensures a high level of access control to the computer system it might be desirable to have further levels of access control to the different software packages. This allows to establish access control for one user group within the operating system, and have individual access control levels in case of application software. Thus, several users can work simultaneously with the same software and do not have to reboot the system each time a different user wants to access a certain software package.

14.3.1 Definitions

- **User Database**
  A database with different user records.
- **User Record**
  An entry in the user database, which includes user ID, user name, password, user type, workspaces.
- **User ID and Password**
  Required to be able to log into OPUS.
- **User Name**
  The user name is stored in measured spectra and indicated in all audit trails.

- **User Type**

  Specifies the access rights of a user.
- **Workspace**

  User environment in OPUS.
- **Assigned Workspaces**

  Workspaces assigned to a certain user.

14.3.2   Default User Database

To allow immediate access to OPUS after the installation a default user database is available. This default database includes three pre-defined user records, which allow full access to OPUS and all workspaces. These records include the following user data:
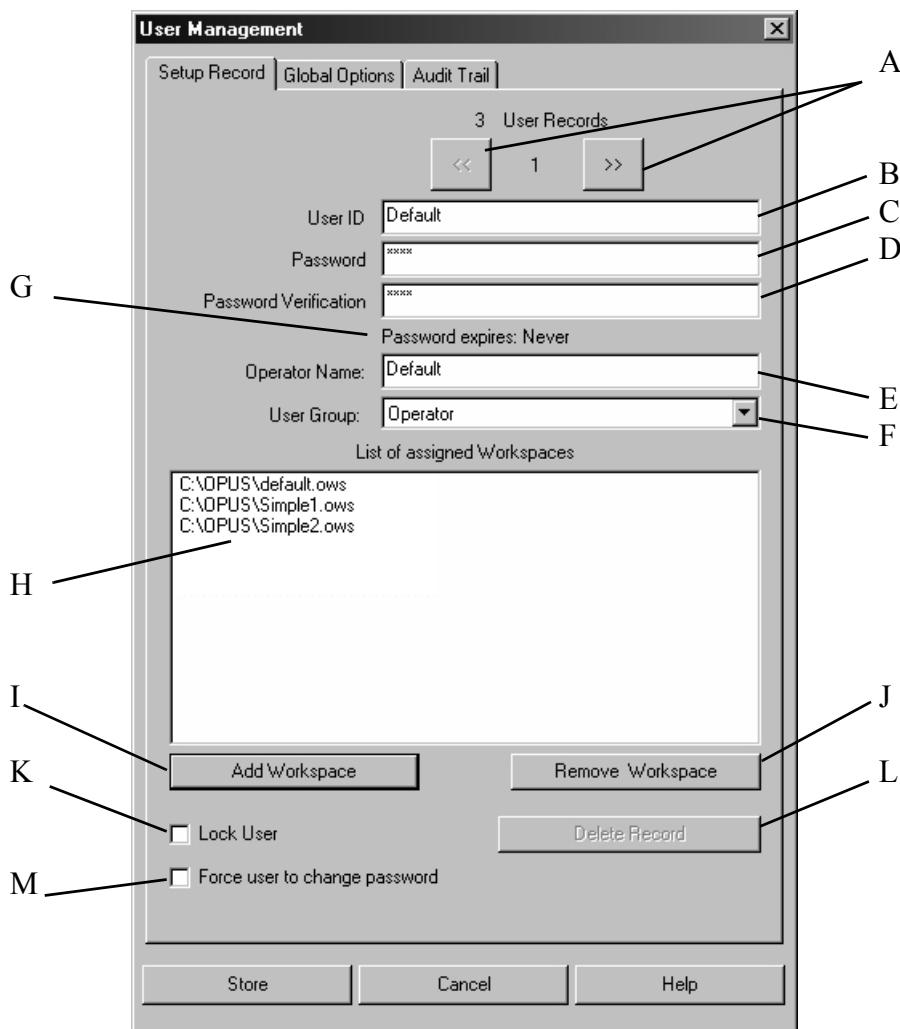
User ID	Default	Administrator	Labmanager
Password	OPUS	OPUS	OPUS
Operator name	Default	Administrator	Labmanager
User group	Administrator	Administrator	Labmanager
Assigned Work-spaces	Unlimited access to all user workspaces		

We recommend not to delete these user records or to change the password to be able to use the user management features.

14.3.3   Setting up User Records

Make sure that you are logged in to OPUS with administrator rights to be able to create, modify or delete user records. Otherwise, the *User Management* function will not be accessible in OPUS.

Select the *User Management* command from the *Setup* menu. The following dialog opens.

(A) Buttons to go to the previous and next user records.

(B) Enter the user ID for the user. The user ID must have a minimum length which can be specified on the *Global Options* tab. It is not possible to log in to OPUS without any user ID.

(C) Enter the password for the user. The password must have a minimum length which can be specified on the *Global Options* tab. The entry in the *Password* entry field is indicated as a sequence of "*".

(D) Re-enter the password for verification. The entry in the *Password Verification* entry field is indicated as a sequence of "*".

(E) The user name is stored in newly measured spectra and in the audit trail of spectra and methods.

(F) The user group can be defined either as *Operator, Labmanager* or *Administrator*. Each user group has the following rights:

	Workspaces	User and Signature Management
Administrator	All	Yes
Labmanager	All	No
Operator	Only those assigned	No

In OPUS 4 and even more previous OPUS versions the access rights had been as follows:

	Workspaces	User and Signature Management
OPUS Administrator and operating system admini-strator (NT, XP...)	All	Yes
OPUS Administrator and user/power user of opera-ting system (NT, XP...)	All	No
OPUS Operator	Only those assigned	No

If the previous OPUS access rights have to be valid, start OPUS by the */CHECKWINADMIN=ON* option. In this case the OPUS operating system rights will also be checked.

(G)Password duration (if any). The password duration can be specified on the *Global Options* tab.

(H)This selection field includes all workspaces which can be accessed by the user. The selection field is only visible for users with *Operator* rights, as users with *Administrator* or *Labmanager* rights both have unlimited access to all workspaces.

(I) Use this button to add a workspace to the selection field (H). Workspaces are always stored with the complete directory path. If you move a workspace to a different directory, you will no longer have access to this workspace.

(J) Use this button to remove a currently selected workspace from the selection field (H).

(K)If you activate this check box, the user will be locked. This check box is automatically activated if a user tries to log in by using a wrong password several times. The number of login attempts can be defined on the *Global Options* tab.

(L)Button to delete the current record.

(M)Activate this check box if you want to force the user to change his password when logging in the next time.

The total number of user records is displayed in the top line of the dialog box.

The number of the current user record is displayed between the [>>] and

[<<] buttons.

All entry fields which must be filled in are initially marked red. If you start typing into any of the red entry fields, the color of the entry fields changes to yellow. The color of the entry fields remains yellow as long as the number of characters typed in is lower than the number specified for the current field. If the minimum number of characters is reached, the entry field color changes to white indicating a valid input.

The default settings for the different fields are:

- **User ID:**   3 characters
- **Password:**   4 characters

The default settings can be changed on the *Global Options* tab. Any changes made will have an immediate effect on all user records.

The *Password Verification* entry field will only change to white if the text entered is identical to the text defined as password. The password can be empty if the appropriate check box is activated on the *Global Options* tab. In this case the *Password* entry field will be yellow and the *Password Verification* entry field white.

Double user IDs are not allowed and will be indicated by red entry fields.

User records cannot be stored, unless all obligatory fields have been filled in properly. For operators at least one workspace must be displayed in the workspace selection field.

The user records are stored in the USERDATABASE.DAT file in the USERDATABASE sub directory of the OPUS directory. The file is encrypted and cannot be modified externally. Make sure that this file is protected against accidental deletion using Windows' security options. Make a backup copy whenever you modify this file, **but you must not set this file to *read only*.**

Click on the *Global Options* tab to define further user management options.
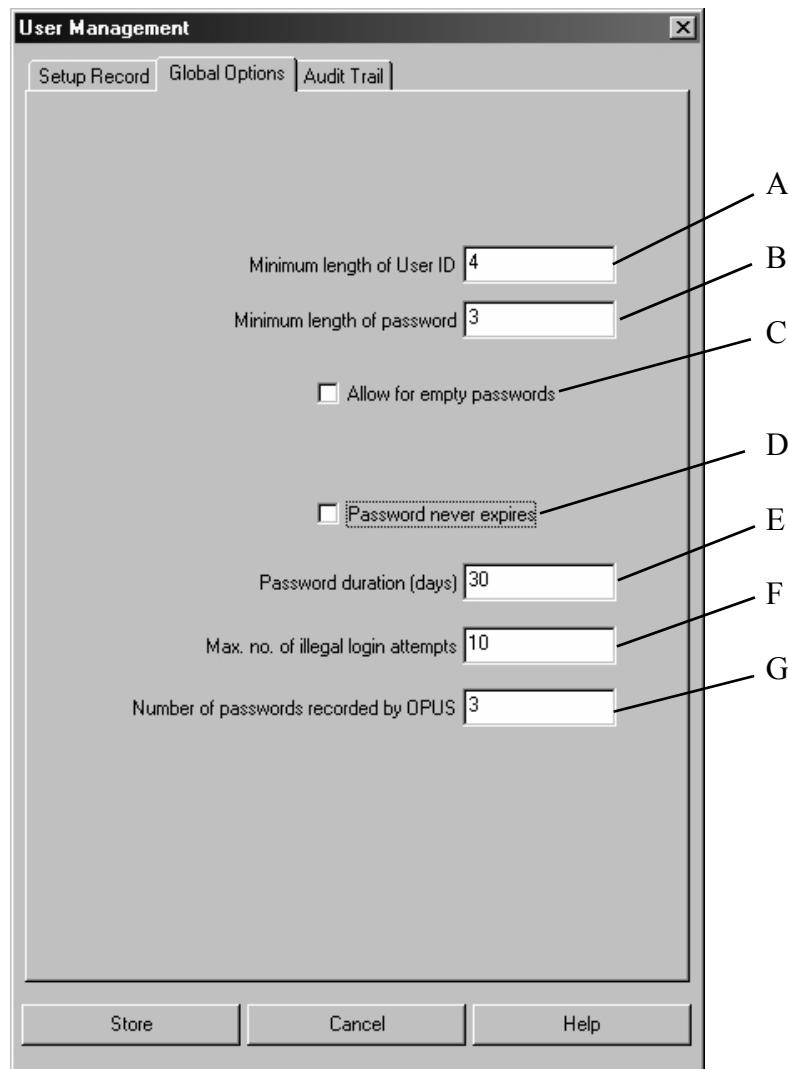
Figure 368: User Management - Global Options tab

(A) Minimum length of User ID.

(B) Minimum length of password.

(C) If you activate this check box, empty passwords are allowed. Note that empty passwords will never expire, regardless of the password duration set.

(D) This check box either activates or deactivates the password duration option, i.e. the password never expires or expires after the number of days defined.

(E) Password duration in days. This entry field is only visible if the *Password never expires* check box has been deactivated. The duration period starts with the date when the user record is created or modified.

(F) Maximum number of illegal login attempts, i.e. entering a wrong password during login. The user gets a warning indicating how many attempts are left. If the last attempt has not been successful either, the user will be locked and not be able to run OPUS anymore. The

administrator only can undo this lock by deactivating the *Lock user* check box on the *Setup Record* tab.

(G) Number of passwords previously used by the user, and not allowed to be used anymore when changing the password. Thus, the user is forced to use a completely new password if the duration of his password has expired.

Any changes made have an immediate effect on all user records in the data base. Therefore, check all user records after changing any of these settings. Illegal entries will be marked in red.

The *Audit Trail* tab indicates the audit trail of all actions for each user. The following actions are recorded:

- Successful login
- Login attempt of a locked user
- Login with password expired
- Password change

For users with *Administrator* rights the following actions are additionally recorded:

- Creating or changing a user record
- Deleting user record
- Locking user record
- De-locking user record
- Creating or changing signature record
- Deleting signature record
- Locking signature record
- De-locking signature record
- Exporting audit trail
- Exporting all audit trails
- Deleting one audit trail
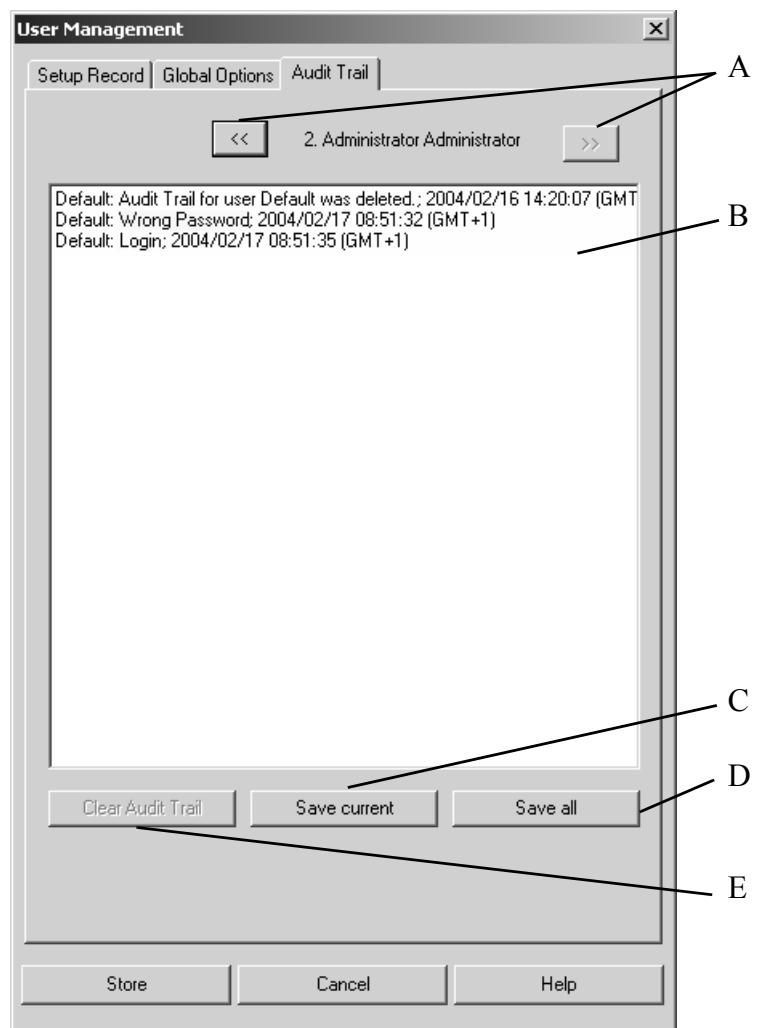
Figure 369: User Management - Audit Trail tab

(A)Buttons to go to the previous or next user record.

(B)Audit trail

(C)Use the *Save current* button to store the current user data recorded in the audit trail.

(D)Use the *Save all* button to store all user data recorded in the audit trail. If you click on the *Save all* button, a dialog opens. Define the file to be used to store the audit trail data and confirm the entry. Audit trail data are stored in ASCII format.

(E)If you click on the *Clear Audit Trail* button, the audit trail data of the current user will be deleted. This button is only enabled if the audit trail data have been stored.

The *Save* and *Clear Audit Trail* actions are recorded in the audit trail of the user currently logged in.

14.4   Change User Password

Each user can change his password. There are different reasons for changing a password:

- A new user record has been created. In this case the administrator defines the initial password which will be changed by the user.
- The *Password Expiration* option is enabled and the password has been expired after the period of time defined. In this case the user cannot log in to OPUS anymore.
- A user assumes that someone else knows his password.

Select the *Change User Password* command. The following dialog opens:

A

B

C

D
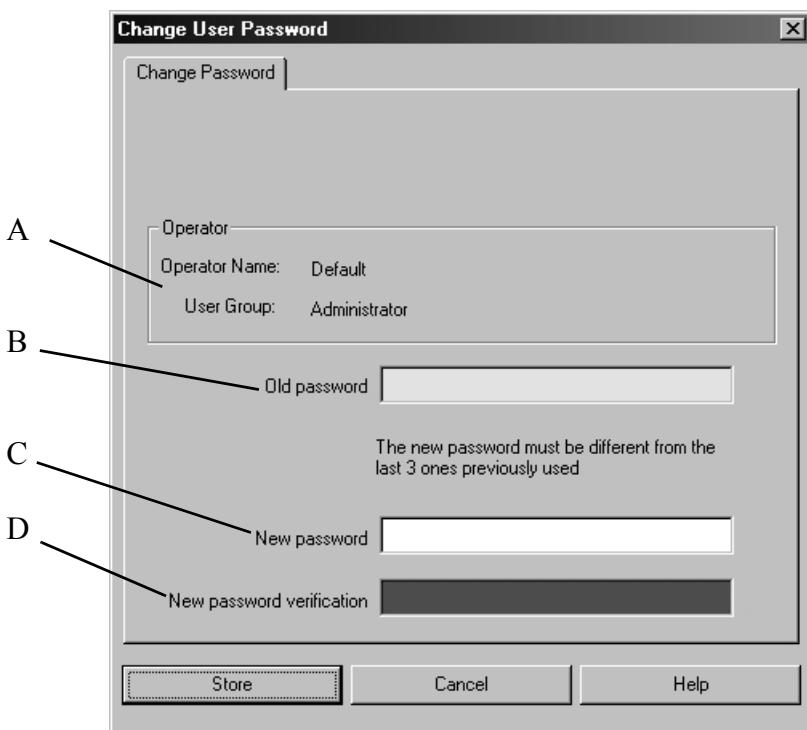
Figure 370: Change User Password

(A)User name and user group
(B)Entry field for the old password
(C)Entry field for the new password
(D)Entry field to confirm the new password

When defining a new password make sure that it is different from the last ones previously used. Furthermore, the new password has to have the minimum length defined on the *Global Options* tab of the *User Management* dialog.

If your password has already expired and you attempt to start OPUS, a warning pops up.

Figure 371: Warning - Password expired

If you click on the *OK* button, the *OPUS Login* dialog opens. Enter the new password and verify it.
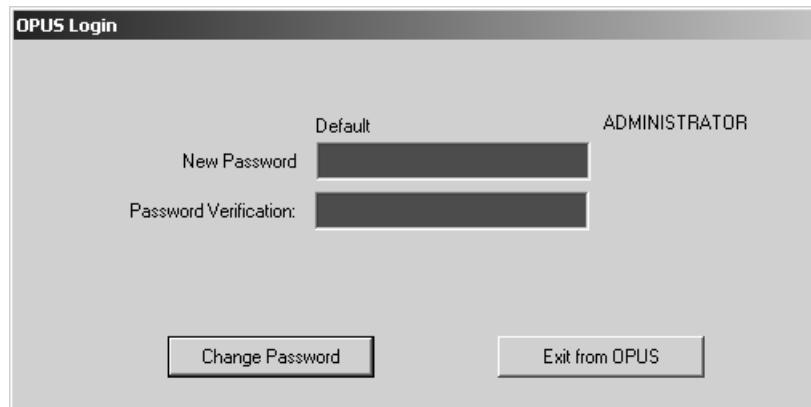
Figure 372: Change Expired Password

Click on the *Change Password* button. The *OPUS Login* dialog opens again. You can now log in to OPUS by using the new password.

14.5 Setup User Macro List

This function can be used to integrate macros or VB-Scripts into OPUS. The user own macros/scripts are integrated in the menu and can be added to the toolbars. It is possible to add macros/scripts in different languages.
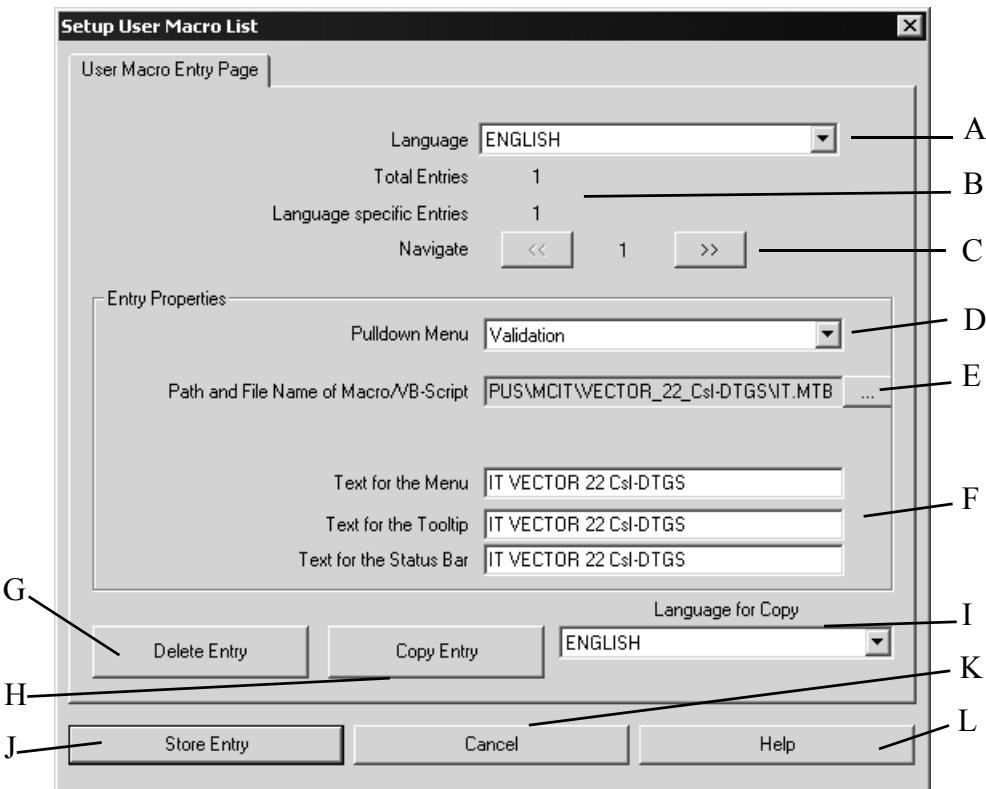
Figure 373: Setup User Macro List

(A) Select the language for the entry. The default language is the language in which OPUS was started. Only the entries for the selected language can be edited. When the language is changed the entries for the newly selected language are accessible.

(B) Shows the total number of entries and the number of entries for the current language

(C) The navigate buttons allow to scroll between the different entries for the current language

(D) The menu where the macro/script shall be added to can be selected from the combo box.

(E) Use the browse button to select the macro/script for the entry. To prevent errors the path and name of the macro/script cannot be entered manually.

(F) Three different text fields have to be specified: The text shown in the menu, the text shown as tooltip and the text displayed in the status bar

(G) This button deletes the current entry from the list

(H) An entry can be copied into the list for a different language by clicking on that button. After copying an entry the language can be changed in A and the entry can then be translated or otherwise modified.

(I) This combo box specifies the target language for copying. Copying into the same language as specified in A is not possible.

(J) This button stores all entries for all languages in the USERMAC.LST file

(K) Exit from the function without storing any modifications

(L) Shows the online help for this function

Contents of the USERMAC.LST File

The USERMAC.LST file in the OPUS directory is stored as a plain text file.

[ENGLISH]
.\macro\it.mtx@8@Instrument Test@Instrument Test@Run the Instrument Test
[GERMAN]
.\macro\it.mtx@8@Gerätetest@Gerätetest@Gerätetest durchführen
[FRENCH]
.\macro\it.mtx@8@Test d'instrument@Test d'instrument@Lancer le test d'instrument

The key words in square brackets specify the different language sections. Within the sections each line represents a macro/script. The different parts of the lines are separated by the "@" character. The different parts have the following meanings:

.\macro\it.mtx@8@Instrument Test@Instrument Test@Run the Instrument Test
   (1)   (2)   (3)   (4)   (5)

(1) Path and filename of the macro/script

(2) Menu number

(3) Text for the menu

(4) Text for the tool tip

(5) Text for the status bar

14.6 Register OPUS

After installing OPUS you can test the program for 30 days without registering. After this trial period you have to register your copy of OPUS. Furthermore, you can use libraries and additional OPUS packages only after you have registered your copy. To register you have to obtain the necessary information (key, serial number etc.) from Bruker. The registration has to be only performed once and is valid for all users of the system. You must be a Windows power user to register.
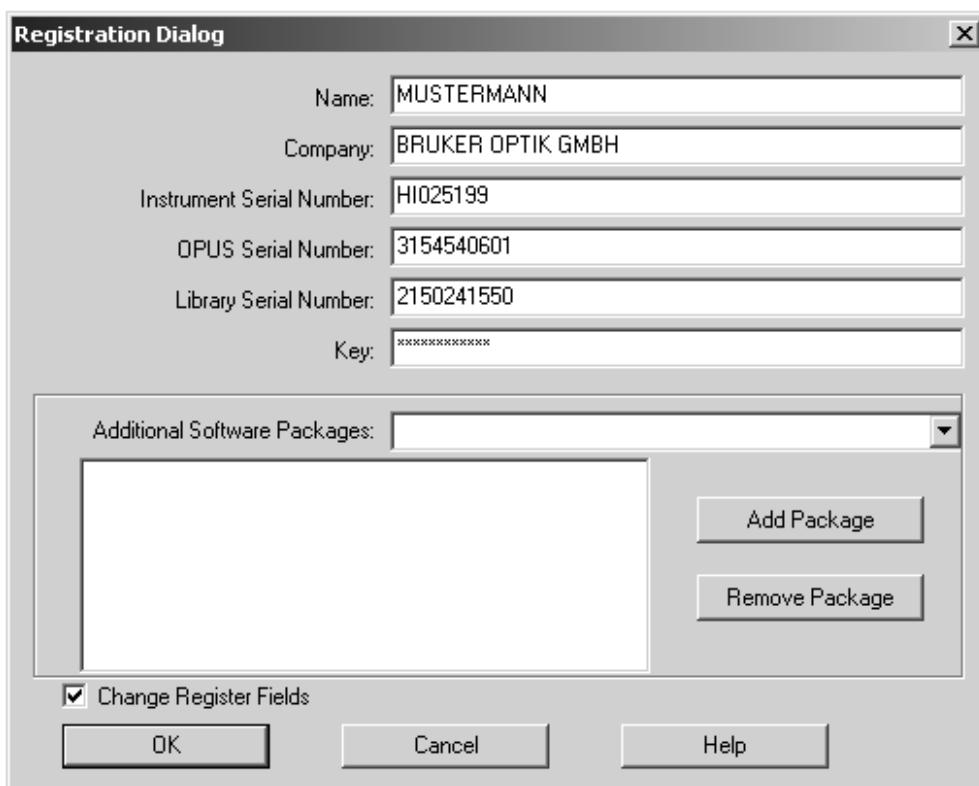
Figure 374: Registration Dialog

The key will be only visible while you type, later on it will be masked. The serial number of OPUS and the OPUS library consist of numbers only. The key also includes characters; be sure to type capital letters when required.

After registering OPUS these fields will be grayed out unless the *Change Register Fields* check box is marked. When you buy additional OPUS packages or libraries you may have to re-enter some of the information in order to use these packages.

14.7 Customize Toolbars

You can personalize your OPUS workspace by configuring the toolbars to suit your requirements. Open the *Customize Tool bars* command of the *Setup* pull-down menu. Alternatively, right-click on the empty space of a tool bar to obtain the dialog box.
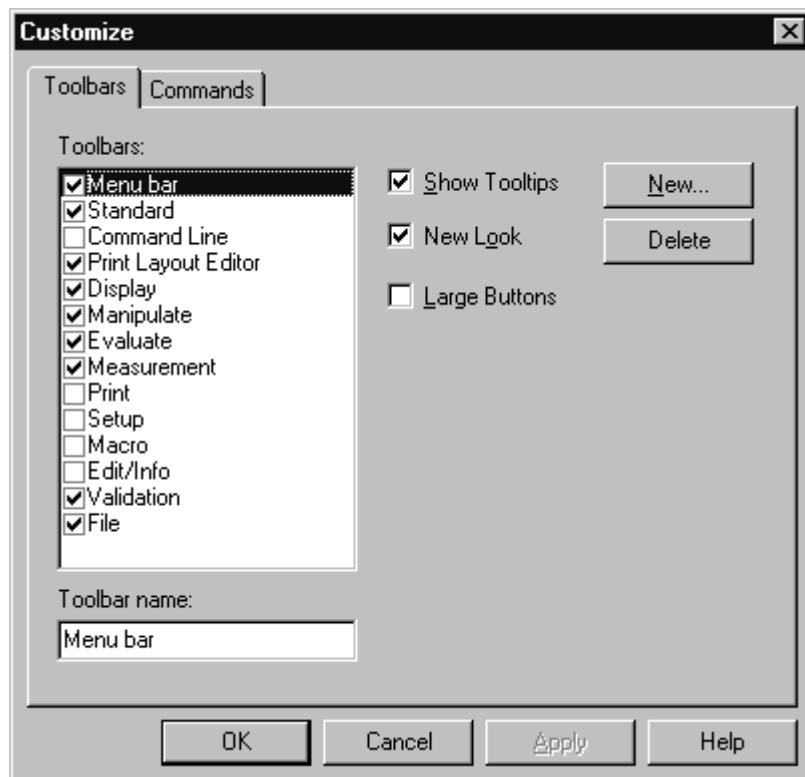
Figure 375: Customize Toolbars

You can

- move bars by the mouse.
- generate new bars or load existing bars.
- use the *Show Tooltips* check box to display help texts.
- turn separators on and off (*New Look*).
- include descriptions in the icon (*Large Buttons*).

Add or remove icons to a tool bar using *Commands* tab of the *Customize Tool bars* dialog box.
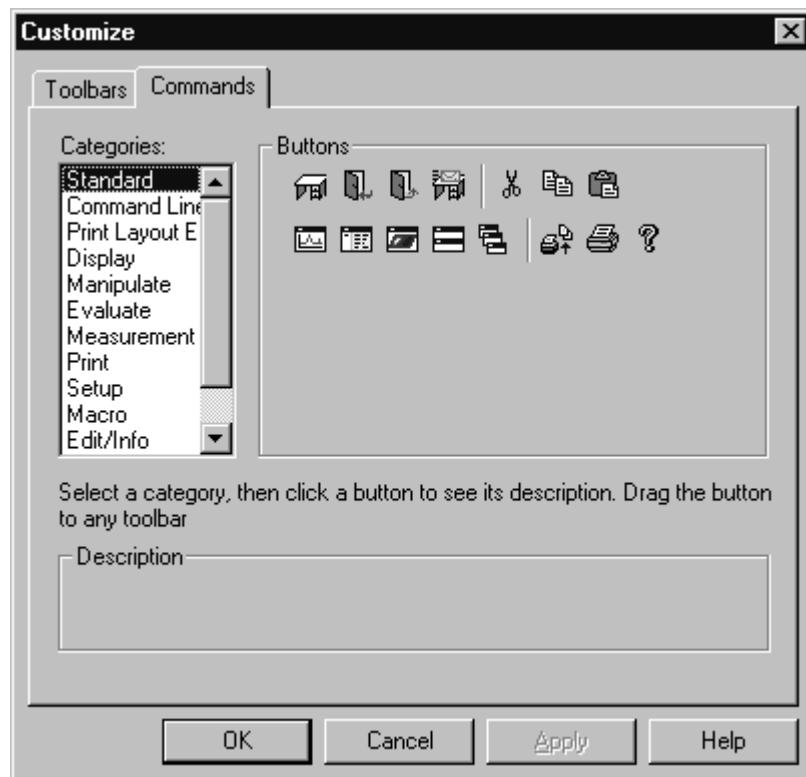
Figure 376: Customize Toolbars – Commands

14.8   Customize Menus

Like the tool bars you can also customize the pull-down menus. By default the *Show All Functions* check box is marked during the OPUS installation. As a result the menus include all available OPUS functions. However, you can create your personal profile (if your rights according to 21CFR11 allows a customizing of the workspace) by choosing the functions you wish to use.
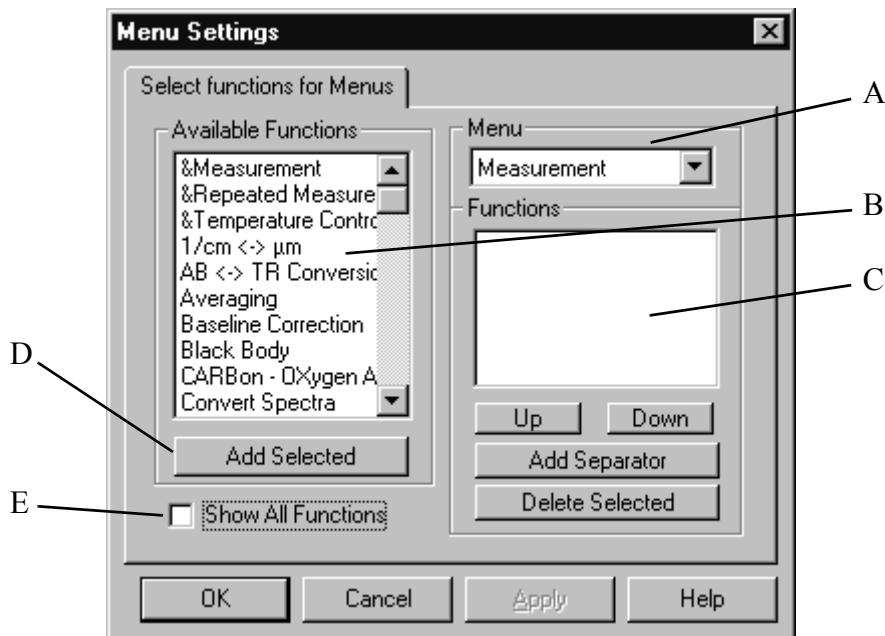
Figure 377: Menu Settings

To customize the menus first remove the tick from the *Show All Functions* check box which is selected by default. Select the menu you want to configure from the menu list (A) and then add the functions you would like to include by selecting them from the *Functions* selection field. Use the *Add Selected* button to include them in the *Functions* selection field. You can change their order of appearance in the menu with the *Up* and *Down* buttons and add separators to structure the menu.

Your individual settings will be saved in your user profile. However, you can only customize your profile when you were granted the necessary rights to do so.

You also can use the *Menu Settings* to configure the display pop-up menu. To do this, deactivate the *All Functions* check box and choose *Display Popup* from the menu drop-down list. Add the functions you would like to include in the pop-up menu and activate the *All Functions* check box again.

Shown in figure 378 is the display pop-up menu in which three functions have been added. To facilitate the identification of these functions they have a small tag on the left side.
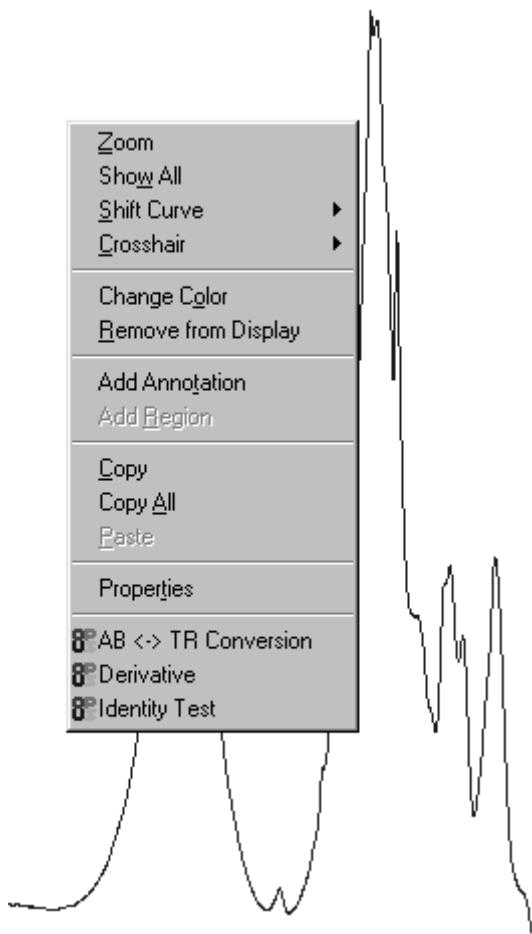
Figure 378: Display Pop-up Menu with Added

14.9   Display Settings

Change the appearance of the spectrum window by calling up its pop-up menu. This is discussed in chapter 2.3.

14.10   User Settings

Create and manage OPUS user accounts by means of the *User Settings* command. Make sure that you have the necessary user rights to do so.
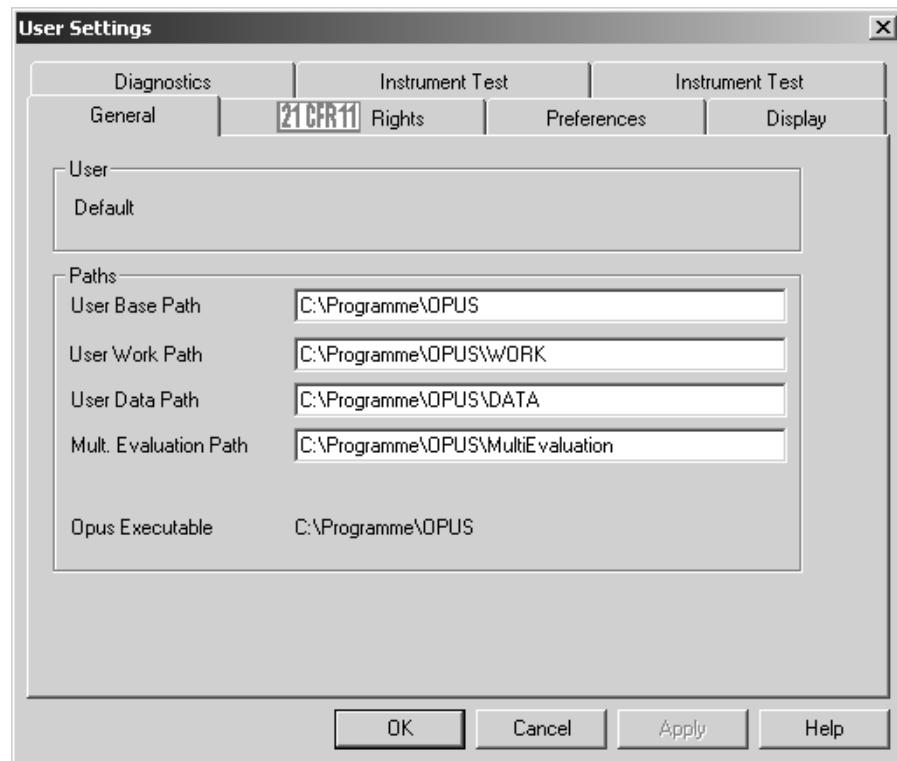
Figure 379: User Settings – General tab

The *General* tab indicates the user status as well as the paths for the most frequently used OPUS directories. If you want to edit the multi evaluation path, make sure that you have the right to change parameters.

Click on the *21CFR11 Rights* tab to assign the rights for the account.
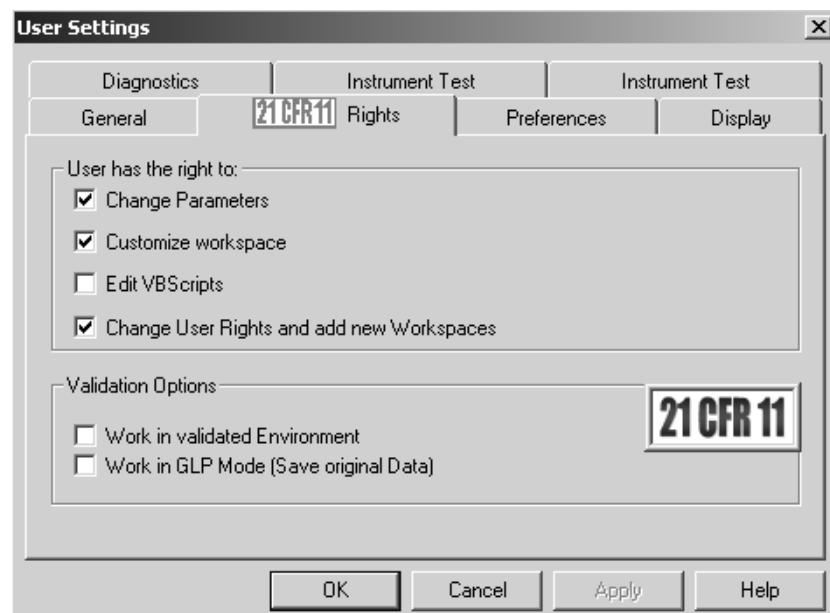
Figure 380: User Settings – 21CFR11 Rights tab

Select the user rights by means of the different check boxes and define whether you want to work in GLP mode or in validated environment. Make sure that at least one administrator account includes all the user rights which can be assigned to.

To select the file name incrementation type click on the *Preferences* tab.
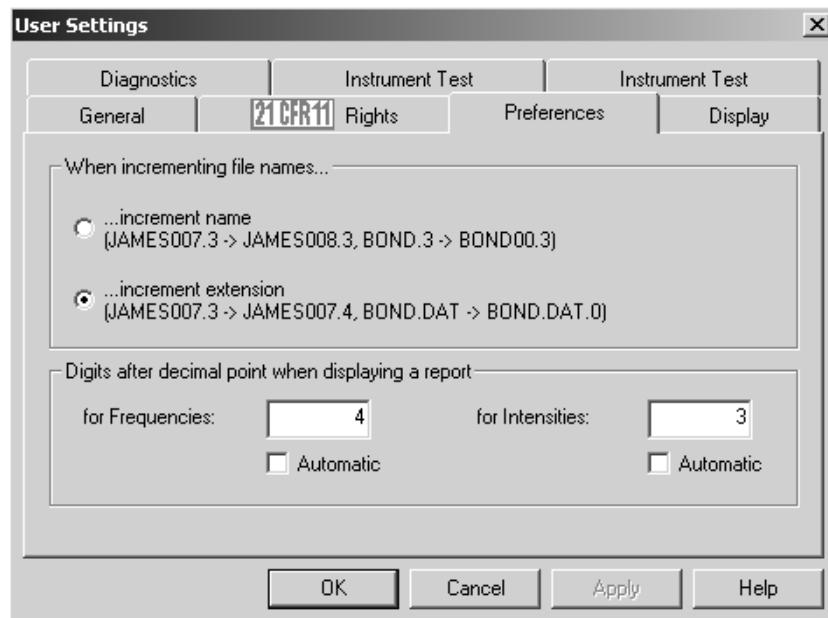
Figure 381: User Settings – Preferences tab

You can either increment the file name or file name extension. Set the number of decimals for frequencies and intensities to be displayed in the report. The default decimals for frequencies are *4* and for intensities *3*. If you want to have the number of decimals automatically set, activate the *Automatic* check box for both frequencies and intensities.

Click on the *Display* tab to set the default display limits and define whether the axes should have legends.
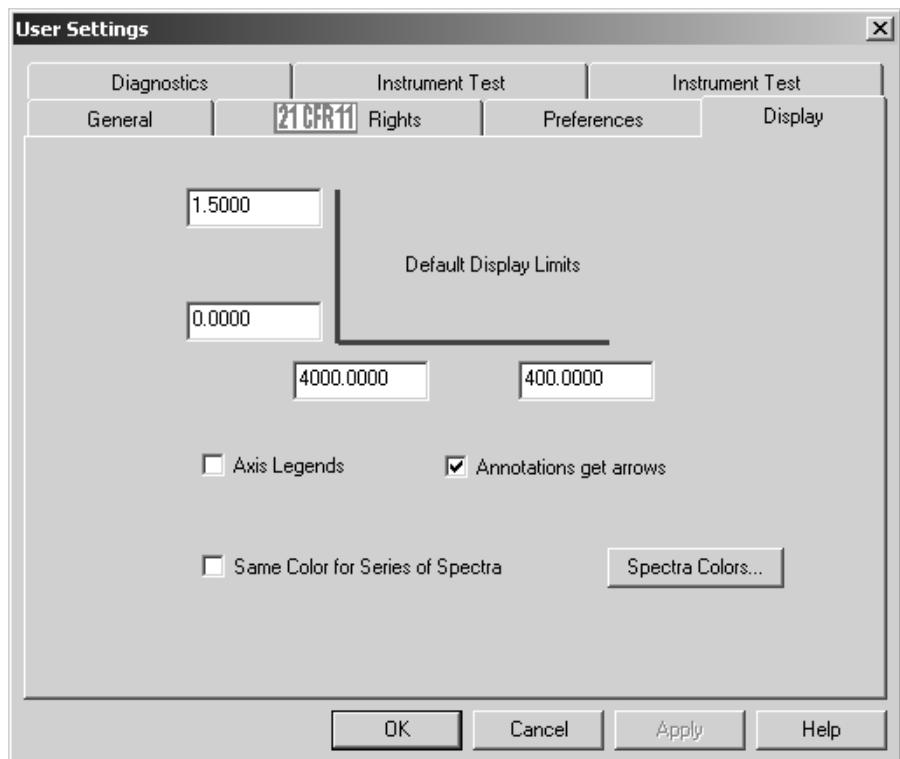
Figure 382: User Settings –Display tab

To add arrows to the annotations activate the *Annotations get arrows* check box. The *Same Color for Series of Spectra* check box allows to display spectra, which have the same basic file name, in one specific color during a particular loading procedure. Usually, the spectral curve colors are automatically assigned when loading spectra into the OPUS browser window.

If you activate the *Same Color for Series of Spectra* check box, two additional option buttons will be displayed.
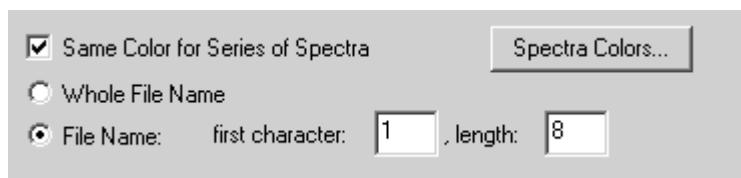
Figure 383: User Settings - Display tab with additional features

The *Whole file name* option button indicates that the file name (without extension) of the spectra series has to be identical to assign spectra colors. Activate the *File Name* check box if only a specific number of file name characters has to be identical. If, for example, a file name has 12 characters and you enter 1 into the *First character* entry field and 8 into the *Length* entry field, the first 8 characters of any file name will be checked to see whether they are conform with the file name series.

Click on the *Spectra Colors...* button to assign a color sequence to the spectra. The following dialog opens:
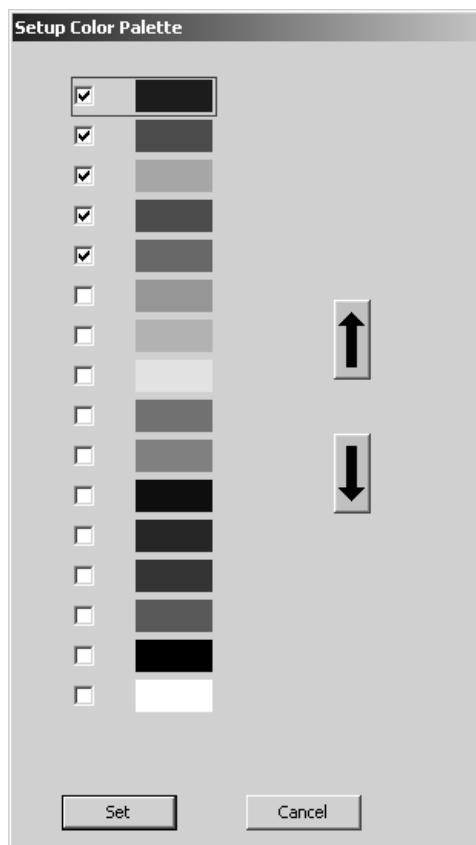
Figure 384: User Settings - Color Palette

The standard range of colors include 16 colors defined by default, whereby only those colors checked will be assigned to spectra.

If you have checked a color, use the arrow buttons to move it to the appropriate position, either upwards or downwards. The color sequence defined on the color palette correlates with the spectra color displayed in the spectrum window. Therefore, the first color on the color palette corresponds to the color of the first spectrum displayed, the second color corresponds to the color of the second spectrum and so forth. To save the settings click on the *Set* button.

Click on the *Diagnostics* tab and define which warning indications or alarms you want to set for which spectrometer component:
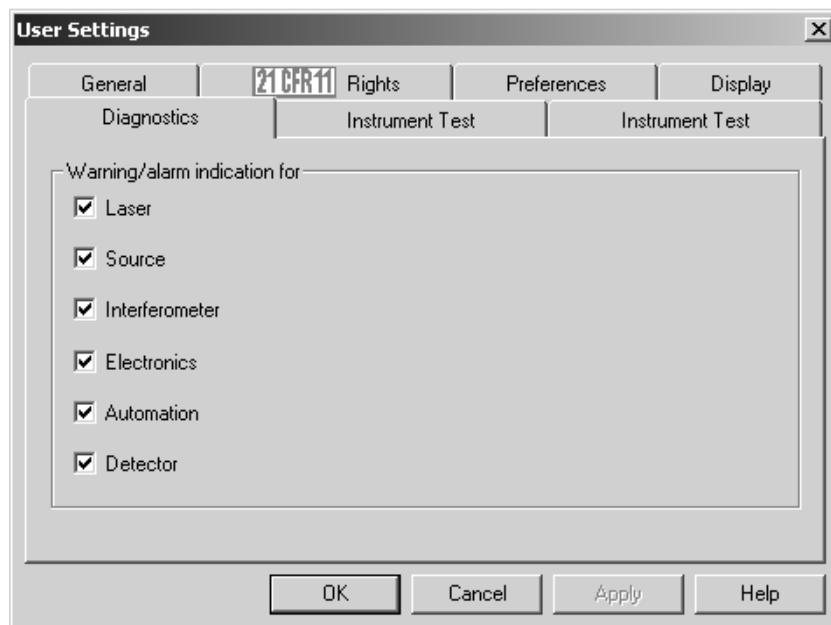
Figure 385: User Settings – Diagnostics tab

Each of the *Instrument Test 1* and *Instrument Test 2* tab includes six test channels. Each of these test channels can assign one program, e.g. OVP (see chapter 13), to be used from within OPUS for validation purposes, and correlates with an icon position on the second row of the *Instrument Status* dialog, see chapter 7.7. The *Instrument Status* dialog can be accessed by clicking on the status light in the bottom right corner of the main OPUS spectrum window.

The test channels of the *Instrument Test 2* tab correlate with the third row of the *Instrument Status* dialog. Thus, a total of 12 different test channels can be assigned, if required.

Note: OPUS 5 and higher versions only allow to configure twelve test channels. In previous OPUS versions you can only assign a maximum number of six channels. Thus, these versions only have one *Instrument Test* tab in the *User Settings* dialog.
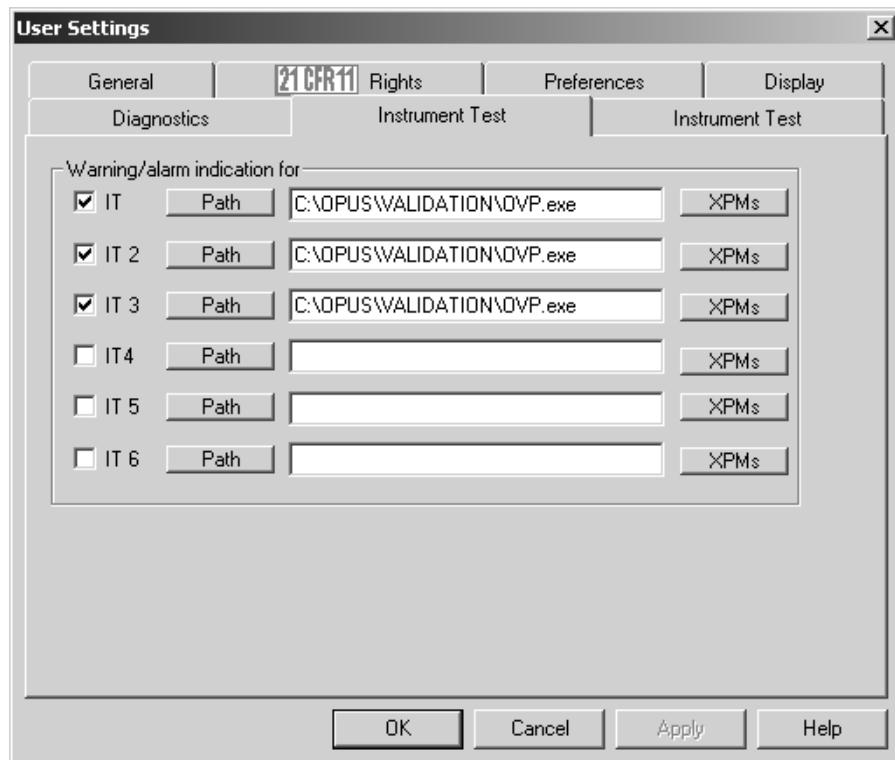
Figure 386: User Settings – Instrument Test 1 tab

First, activate the *IT* check box which represents the active test channel, and either enter the path manually or click on the *Path* button. If you work with OVP, select the OVP path which is normally located in the *Validation* sub-directory of the OPUS directory. Enter the program file name manually, including the extension.

Example:

Assuming the instrument has both a sample chamber and a fiber optic probe, to validate both configurations you would assign OVP to two IT channels on the *Instrument Test* tab.
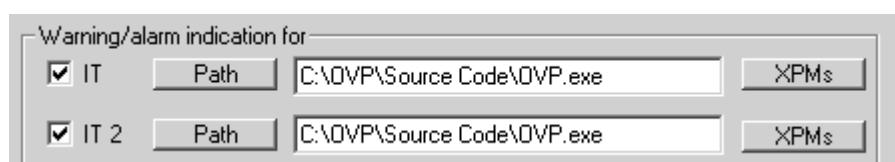
Figure 387: Two Configurations Assigned for OVP

In this example we would arbitrarily designate the first position (IT) to be used for all experiment files that use the sample compartment, assuming that these experiments use the same detector, beam splitter, etc. All experiment files that use the fiber optic probe channel will be designated for the second position (IT2). This only completes the assignments required by OPUS. Further OVP settings are required. For further details, refer to chapter 13.

Use the *XPMs* button to register one or more measurement experiment files to the validation channel. These are the experiment files you will use for normal daily measurement. Each time you load one of the registered experiment files into OPUS, this list is checked. If a match is found, the status for the particular channel (IT 1-12) is polled. If it is determined to be valid, the status light will be green.

You can add as many *XPM* files as you like. It is important that you only select experiment files which have the same basic spectrometer configuration (source, beam splitter, measurement channel etc.). Further details on preparing default measurement experiments can be obtained from chapter 13.2.1.

If you click on the *XPMs* button the following dialog opens:
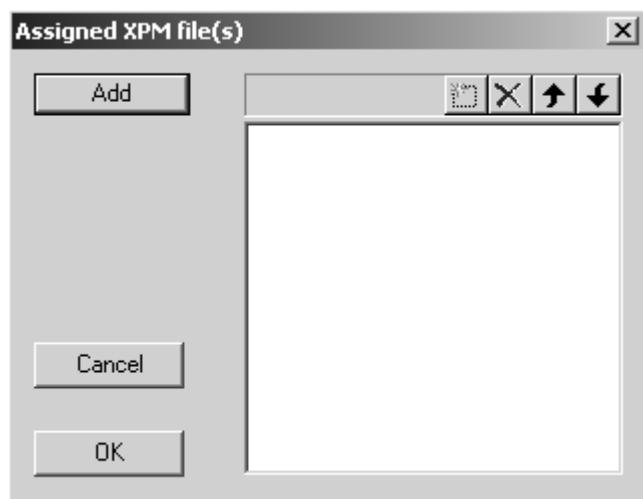
Figure 388: Assign XPM file(s)

Click on the *Add* button to add XPM files from particular directories into the selection field. By means of the icon bar on the right you can either define a new *XPM* file, or cancel existing ones. Use the arrow buttons to scroll up and down the entries in the list. Confirm the selection by clicking on the *OK* button. Undo the selection by clicking on the *Cancel* button.

14.11   New Workspace

OPUS is able to manage several user profiles which can be password protected. A profile contains information OPUS about the users rights, his customized desktop (tool bars, menus), the parameters of all commands as well as the users name and password. Create a new profile with *New Workspace*. See chapter 14.10 for details.

14.12   Save Workspace as

If you changed anything concerning the settings saved in your profile, e.g. the position of the tool bars, your profile will automatically be updated when you exit OPUS. If you created a new profile OPUS will ask you for the profiles name.

15 Help
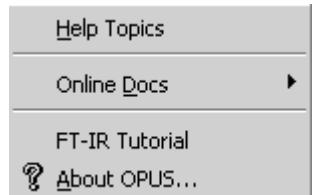
Figure 389: OPUS Help Menu

The OPUS *Help* commands are available either from the *Help* menu or by clicking on any *Help* button of a dialog box. By means of the *F1* button on the PC keyboard you can activate the online help. To be able to use the online help function you have to install Microsoft Internet Explorer 4.0 (or higher).

If you select the *Online Docs* command, you all OPUS manuals available are indicated on a different menu. They are provided as PDF files. In order to read these PDF files you have to install the Acrobat Reader from the OPUS CD.

The *FT-IR Tutorial* imparts basic knowledge about FT-IR spectroscopy. Click on the *About OPUS* command to learn something about the OPUS version used, the registered user name and the OPUS packages available. For further details on this subject, see chapter 1.

15.1   Setting the Language

When installing OPUS you define the OPUS directory and select between three languages (English, French and German) to be used for the installation dialogs.

The procedure to set the OPUS system language depends on the Windows version used. Therefore, the following steps described may be different in your case. Click on the Windows *Start* button and right click on the OPUS icon. Select the *Properties* command and the following dialog will open:
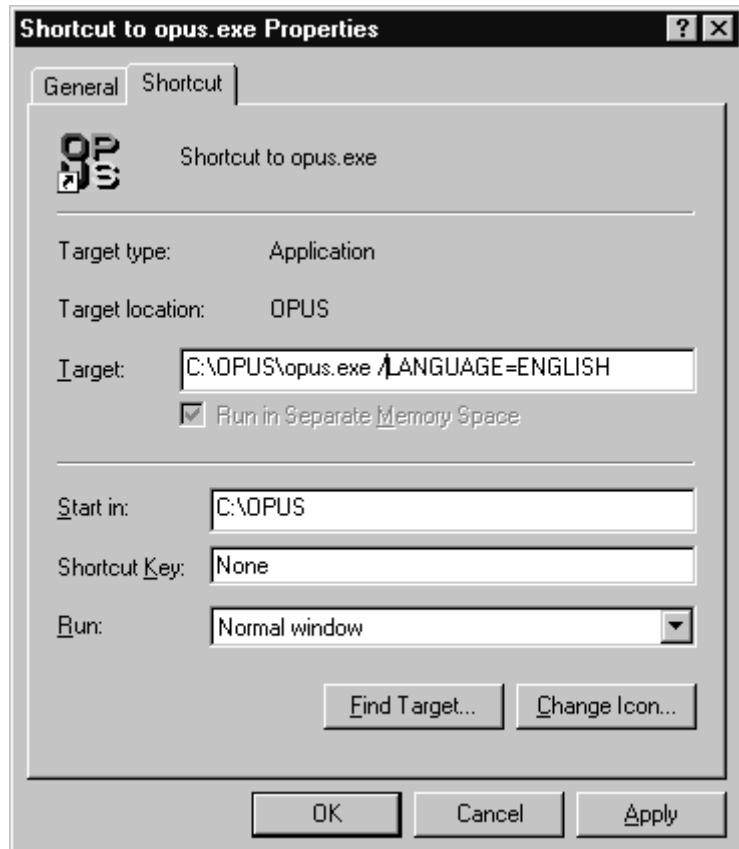
Figure 390: Properties Dialog - Shortcut tab

Depending on your Windows version this dialog may look slightly different. Add the correct language parameter into the *Target* entry field on the *Shortcut* tab. Make sure that you type the parameter in capital letters. If the parameter is not recognized, OPUS will use the default language, i.e. English. The following parameters are possible:

- OPUS/LANGUAGE=ENGLISH starts the English language module
- OPUS/LANGUAGE=FRENCH starts the French language module
- OPUS/LANGUAGE=GERMAN starts the German language module

To confirm the setting click on the *OK* button. The language setting will be transferred to OPUS as parameter when starting the program next time.

15.2   Rebooting the AQP

Sometimes it may be necessary to reboot the acquisition processor (AQP). A simple way to reboot is to change any of the configurations in the *Optics Setup and Service* command in the *Measure* menu. Any change of these parameters causes the AQP to reboot.

15.3   Abort OPUS

If OPUS hangs for quite some time and cannot be closed by the ☒ button, you can abort the program by using the Windows Task Manager. Data not stored before aborting the program will be lost. This also applies to the workspace settings made during the program run (e.g. toolbar configuration, directory name etc.)

To open the Task Manager simultaneously press the *ALT*, *CTRL* and *DEL* keys on the PC keyboard. The Windows Task Manager will be displayed.

Figure 391: Windows Task Manager

Select OPUS from the *Applications* tab and click on the *End Task* button. **OPUS will terminate without saving any data.**

Appendix

Data Block Icons

OPUS files can consist of several spectra, data blocks and reports which all will be stored in OPUS using the same file name.

The OPUS browser window and some other types of windows display the file components by small icons. The following table describes the different icons and their abbreviations which can be used in connection with macros.

1a	Single channel spectrum, reference	ScRf
1b	Report	Report
1c	Reflectance spectrum	Refl
1d	Raman spectrum	Raman
1e	Quant report	Quant
1f	Quality test	QTest
1g	Sample, power spectrum	PwSm
1h	Reference power spectrum	PwRf
1i	Sample, phase spectrum	PhSm
1j	Reference, phase spectrum	PhRf

2a	Unknown block	
2b	Peak table	Peak
2c	Photoacoustic spectrum	PAS
2d	n th derivative	n.Der
2e	Logarithm of reflectance	lgRefl.
2f	Kubelka-Munk spectrum	KM
2g	Integration report	Integ
2h	Information block	Info
2i	Sample, interferogram	IgSm
2j	Reference interferogram	IgRf

3a	Protocol	History
3b	Transmittance spectrum	TR
3c	Video image	Graphics
3d	General report	GenRep
3e	Fit report	Fit
3f	Emission spectrum	Emis
3g	3D spectrum	3D
3h	Average report	AvRep
3i	ATR spectrum	ATR
3j	Arithmetical result, transmittance	AriTR

4a	Arithmetical result, absorbance	AriAB
4b	Absorption spectrum	AB
4c	Trace	Trace
4d	First derivative	1.Der
4e	Second derivative	2.Der
4f	Subtraction report	Subtract
4g	Molecular structure	Strc
4h	Search result	Search
4i	Unknown spectra type	Spec
4j	Single channel spectrum, sample	ScSm

5a	Annotation	ANNO
5b	Cluster Analysis	Clus
5c	Signature	Sign
5d	Quick Compare	QC
5e	Quick Compare results for 3D files	TRC
5f	Multi Evaluation	ME
5g	Conformity Test	CONF

These basic data block icons can also be combined with other types of icons. Furthermore, modifications of the above icons exist. For example, the **R** character represents the real part and the **I** character the imaginary part of a complex data block. A data block icon accentuated by a shadow indicates a 3D data block.

Icons Used For OPUS Commands

The OPUS commands listed are included in the different menus and can be called up by means of the tool bar. In the following the most common OPUS commands are described.

New workspace		Draw ellipse
Open		Draw line
Close workspace		Draw rectangel
Send workspace		Insert table
Cut		Move
Copy		New page
Paste		Delete page
New spectrum window		Delete
New report window		Clear frame
New 3D window		Page properties
Tile		Object properties
Cascade		Lock
Quick print		Back (frequency range)
Print		Forward (frequency range)
About OPUS		Scale all
		Scale y
		Stacked
		Page back
		Page forward

	Baseline correction		Integration
	Spectrum subtraction		Quantitative analysis 1
	AB <–> TR conversion		Set up Quant 1 method
	Straight line generation		Signal -to-Noise ratio
	Spectrum calculator		Peak picking
	Cut		Quick identity test
	Normalization		Conformity test
CS	Make compatible		Spektum search
	Convert spectra		Peak search
	Smooth		Information search
	Derivative		Structure search
Corr	Frequency calibration		Initialize library
	Raman correction		Store spectrum in library
	Black body		Library editor
FT	Interferogram to spectrum conversion		Library browser
iFT	Inverse FT		Quantitative analysis 2
2F +0	Post zerofilling		Quant 2 analysis / file list
	Fourier self-deconvolution		Set up Quant 2 method
SFT	Symmetric FT		Identity test
KKT	Kramers-Kronig Transformation		Set up Identity test method
LiM	Extrapolation		Cluster analysis
cm⁻¹	1/cm <–> µm	CO	Carbon Oxygen Analysis
	Averaging		2D Correlation
	Merging spectra ranges		DMA
	Atmospheric compensation	QC	Quick Compare Setup
	Straylight correction	QC	Quick Compare
	Noise generation	Multi Eval	Multi Evaluation Setup
	Moving mean	Multi Eval	Multi Evaluation Test
	Make monotone		

Measurement		Edit parameters
Repeated Measurement		Information input
Rapid Scan TRS		Set up Info mask
Direct command entry		Structure import
Optic setup and Service		Edit / create structure
Optics diagnostic		Attach structure
Temperature control		Instrument test
Motorised stage control		Load file
Video assisted measurements		Unload file
Time resolved step scan		Undo changes
Chromatography		Save file
Step scan modulation		Save file as
Data extraction		Send file
Add traces		Send file to GRAMS
Assemble GC file		Send file to InStep
Assemble Map file		Delete data blocks
Print spectra		External program
Setup JCAMP/OPUS conversion		VisualBasic Script
Macro converter		Load data point table
Run macro		Scan OPUS files
Debug macro		Find OPUS files
Macro editor		Clone entry
Compile macro		Clone original

Parameters

The main parameters which may be included in the parameter data blocks are listed

Data Status Block

General

DPF = "Data Point Format"
NPT = "Number of Data Points"
FXV = "Frequency of First Point"
LXV = "Frequency of Last Point"
CSF = "Y - Scaling Factor"
MXY = "Y - Maximum"
MNY = "Y - Minimum"
DXU = "X Units"
DYU = "Y Units"
DER = "Derivative"

QS1 = "Derivative"
SMO = "Smoothing points for der."
QS0 = "Smoothing points"
DAT = "Date of Measurement"
TIM = "Time of Measurement"
XTX = "X - Axis Label"
YTX = "Y - Axis Label"
ZTX = "Z Axis Label"
XAF = "X axis factor"
YAF = "Y axis factor"
ZAF = "Z axis factor"
GSQ = "GS Base Quality"

Mapping

AOX = "Map Origin X"
AOY = "Map Origin Y"
DDX = "Map Delta X"
DDY = "Map Delta Y"
NPX = "Map Points in X"
NPY = "Map Points in Y"

S/N

NF1 = "First S/N Frequency Limit"
NF2 = "Second S/N Frequency Limit"
SN1 = "S/N (RMS)"
SN2 = "S/N (Peak-to-Peak)"
SN3 = "Max. Ordinate in S/N region"
SN4 = "Min. Ordinate in S/N region"
SNF = "S/N Flags"

Frequency calibration

MWC = "Mult. for Freq.Calib"
AWC = "Add for Freq.Calib"

Search

HQU = "Hit Quality"
COM = "Compound Name"

Display

DST = "Display text"

Instrument Block

General

DPH = "Demod. Phase (Degrees)"
MOF = "Modulation Frequency"
NLA = "NL Alpha"
NLB = "NL Beta"
HFL = "High Folding Limit"
LFL = "Low Folding Limit"

DFR = "Digital Filter Reduction"
DFC = "Number of Filter Coef."
HFF = "Digital Filter HFL"
LFF = "Digital Filter LFL"
ASG = "Actual Signal Gain"
ARG = "Actual Ref. Signal Gain"
ALF = "Actual Low Pass Filter"
AHF = "Actual High Pass Filter"
ASS = "Number of Sample Scans"
ARS = "Number of Background Scans"
GFW = "Number of Good FW Scans"
GBW = "Number of Good BW Scans"
BFW = "Number of Bad FW Scans"
BBW = "Number of Bad BW Scans"
DUR = "Scan time (sec)"
RSN = "Running Sample Number"
PKA = "Peak Amplitude"
PKL = "Peak Location"
PRA = "Backward Peak Amplitude"
PRL = "Backward Peak Location"
SSM = "Sample Spacing Multiplicator"
SSP = "Sample Spacing Divisor"
SGP = "Switch Gain Position"
SGW = "Gain Switch Window"
INS = "Instrument Type"

AQP and OPTIC special settings

ITF = "Interface Type for Optic"
SIM = "Simulation Mode"
DEB = "Debug Printer Mode"
LOG = "Logfile for Measurement"
ADR = "AQP Adress"
AD2 = "AQP2 Adress"
RMX = "Resolution Limit"
PLL = "Maximum PLL Setting"
FFT = "Maximum FT Size in K's"
MXD = "Maximum ADC Sate in Hz"
FOC = "Focal Length"
ABP = "Absolute Peak Pos in Laser*2"
ABP = "Absolute Peak Pos"
LWN = "Laser Wavenumber"
RLW = "Raman Laser Wavenumber"
RLP = "Raman Laser Power in mW"
RDY = "Ready Check"
RC0 = "Raman Background Corrected"
RC1 = "Raman Scattering Corrected"
SRT = "Start time (sec)"
ERT = "End time (sec)"
MAX = "X Measurement Position"
MAY = "Y Measurement Position"
AN1 = "Analog Signal 1"
AN2 = "Analog Signal 2"

Acquisition Block

General

CH2 = "Channel 2"
SGN = "Signal Gain, Sample"
SG2 = "Signal Gain, Sample"
RGN = "Signal Gain, Background"
RG2 = "Signal Gain, Background"
GSW = "Gain Switch Window"
GSG = "Gain Switch Gain"
NSS = "Sample Scans"
NSR = "Background Scans"
REP = "Repeat Count"
DLR = "Delay Between Repeats in Sec."
MIN = "Sample Meas. Duration in Min."
MIR = "Background Meas. Duration in Min."
SOS = "Scantime or Scans"
SOT = "Sample Scans or Time"
STR = "BG Scans or Time"
COR = "Correlation Test Mode"
DLY = "Stabilization Delay"
DEL = "Delay Before Measurement"
HFW = "Wanted High Frequency Limit"
LFW = "Wanted Low Frequency Limit"
RES = "Resolution"
RE2 = "Resolution Ch.2"
TDL = "To do list"
PLF = "Result Spectrum"
SPO = "Sample Number"
RPO = "Background Number"
SPO = "Sample Number"
RPO = "Background Number"

Transient Recorder Parameters (nur OPUS-NT)

General

WTR = "Tr.Rec. Resolution"
WAS = "Tr.Rec. Slices"
WRC = "Tr.Rec. Repeat Count"
WTD = "Tr.Rec. trigger Delay in points"
WPD = "Tr.Rec. Stab. Delay after Stepping"
WXP = "Tr.Rec. Trigger Mode"
WSS = "Tr.Rec. Sampling Source"
W2W = "Tr.Rec. Channel 2 Weighting"
WXD = "Tr.Rec. Experiment Delay"
WDV = "Transient Recorder"
WIR = "Tr.Rec. Input Range"
WTH = "Tr.Rec. Weighting Threshold"

TRS

TRR = "TRS Resolution in micro sec"
TRS = "TRS Slices"
TRC = "TRS Repeat Count"
TRD = "TRS Exp Delay in msec"
TRP = "TRS Positioning Delay"
TRM = "TRS Experiment Trigger Mode"
TRX = "TRS Sampling Source"

Interleaved TRS

ITS = "Interleaved Time Slices"
ISP = "Interleave Time Res. æsec"
IDL = "Interleave Trigger Delay æsec"
ITR = "Max. Exp. Trigger Rate Hz"

Step Scan

STD = "Step Scan Pos. Delay in msec"
STC = "Step Scan Coadd Count"
SMX = "Multiplexer positions"
SMD = "Modulation (0=OFF 1=MOD 2=MOD-DEMOD
        4=OLD PHASE 8=AMPL)"
SMA = "Scanner Modulation Amplitude"
SMF = "Scanner Modulation Frequency"
AMF = "Ampl. Modulation Frequency"
ADA = "Ampl. Demodulation Angle"
PDA = "Phase Demodulation Angle"

Chrom

CIN = "Chrom Integrate Trace"
CIM = "Chrom Integration Method"
CDT = "Chrom Display Trace"
CDS = "Chrom Display Spectrum"
CTM = "Chrom Start Trigger Mode"
CSV = "Chrom Save Mode"
CSV = "Chrom Save Mode"
CTL = "Chrom Trigger Level"
GSS = "Gram Schmidt Size"
GSO = "Gram Schmidt Offset"
GSP = "Gram Schmidt Points"
CLD = "Limit Run Duration"
CMD = "Max Run Duration"

Map

MLS = "Map XY List"
MPO = "Map Port (com 1...n)"
MSH = "Map Shape (1..6)"

OS/2 Specific

MDV = "Map Device"
MOX = "Map Origin X"
MOY = "Map Origin Y"
MDX = "Map Sample Dim. X"
MDY = "Map Sample Dim. Y"
MSX = "Map Spacing X"
MSY = "Map Spacing Y"
MGX = "Map Gram Schmidt X Base"
MGY = "Map Gram Schmidt Y Base"

NT Specific

NDV = "Map Device"
NOX = "Map Origin X"
NOY = "Map Origin Y"
NSX = "Map Spacing X"
NSY = "Map Spacing Y"
NGX = "Map Gram Schmidt X Base"
NGY = "Map Gram Schmidt Y Base"
MEX = "Map Measurement Experiment"

OS2 and NT

MUN = "Map units"
MPX = "Map # Pos X"
MPY = "Map # Pos Y"
MSS = "Map Save Spectra"
MCI = "Map Compute Integrals"
MIM = "Map Integration Method"
MCM = "Map Macro"
MEM = "Map Evaluation Macro"
MSV = "Map Save Video"
MVM = "Map Video Method"
MRL = "Map Relative Origin"
MGT = "Map Gram Schmidt"
MGS = "Map Gram Schmidt Size"
MGO = "Map Gram Schmidt Offset"
MGP = "Map Gram Schmidt Points"

Display

MXS = "Meas x-Startpoint Display"
MXE = "Meas x-Endpoint Display"
MYS = "Meas y-Minimum Display"
MYE = "Meas y-Maximum Display"
MDM = "Meas Display Mode"
MDP = "Meas Display Product"

Display Channel2

XS2 = "Meas2 x-Startpoint Display"
XE2 = "Meas2 x-Endpoint Display"
YS2 = "Meas2 y-Minimum Display"
YE2 = "Meas2 y-Maximum Display"

FT Parameter

AF2 = "Apodization Function"
HQ2 = "End Frequency Limit for File"
LQ2 = "Start Frequency Limit for File"
PH2 = "Phase Correction Mode"
SP2 = "Stored Phase Mode"
ZF2 = "Zero Filling Factor"
APF = "Apodization Function"
HFQ = "End Frequency Limit for File"
LFQ = "Start Frequency Limit for File"
PHZ = "Phase Correction Mode"
PHR = "Phase Resolution"
NLI = "Non Linearity Correction"
NL2 = "Non Linearity Correction"
DIG = "Digital Filter"
DI2 = "Digital Filter"
SPZ = "Stored Phase Mode"
ZFF = "Zero Filling Factor"

Optic Parameter

IRS = "Iris Aperture (micron)"
UNI = "Command string for UNI"
APT = "Aperture Setting"
AP2 = "Aperture Setting"
AP2 = "Aperture Setting"
BMS = "Beamsplitter Setting"
DTC = "Detector Setting"
DT2 = "Detector Setting"
OPF = "Optical Filter Setting"
OPF = "Optical Filter Setting"
PGN = "Preamplifier Gain"
PGN = "Preamplifier Gain"
CHN = "Measurement Channel"
DMX = "Multiplexed Data"
ADC = "Ext. Analog Signals"
SON = "External Synchronisation"
SRC = "Source Setting"
VEL = "Scanner Velocity"
HPF = "High Pass Filter"
LPF = "Low Pass Filter"
SRL = "Raman Laser Power(mW)"
RFL = "Raman Flags"
POL = "Polarizer"

Sample Origin

SNM = "Sample Name"
SFM = "Sample Form"
CNM = "Operator Name"
HIS = "History of Last Operation"

Additional Information

OPUS Macro Language

For further details on the OPUS macro language, refer to the OPUS Programming manual.

Additional Commands in the Evaluate Menu

Depending on your requirements you can add additional evalution modules to OPUS. As these evaluation modules may be very complex they are documented in separate manuals.

List of File Name Extensions

The following list includes the OPUS file name extensions. This list is by no means complete and will be permanently extended. File name extensions used in OPUS-OS/2 are only listed if they are also used in OPUS-NT.

Extension	Used By[a]	Description
.CLA	X	Cluster analysis
.CLG	N	Scan/find OPUS file
.CON	X	Conformity test
.DAT	N	Pirouette file, used by InStep software
.DX	X	JCAMP file, also DX1, DX2...
.INT	X	Integration method
.MAC	O	Macro file
.MTB	N	Macro file
.MTD	X	Library method
.MTX	N	Macro file

Extension	Used By[a]	Description
.NTI	N	Optical bench configuration file
.OWS	N	OPUS workspace
.PCT	X	Parameter correlation table used for JCAMP-DX
.PLE	N	Printing template
.PLT	O	Printing template
.Q1	X	QUANT 1 method
.Q2	X	QUANT 2 method
.QCM	N	Quick compare method
.RED	N	OPUS help file
.S01	X	Spectrum library, also S02, S03...
.SPC	N	GALACTIC spectrum library
.TXD	X	Information mask
.XPM	X	Experiment file
.TRS	N	TRS Experiment
.QT	N	Quality Test
.0	X	OPUS file (any numerical extension)

a. O: used by OPUS-OS/2   N: used by OPUS   X: used by both programs

Index

User Settings 371
USERMAC.LST File 366

V

Vector Normalization 218
View
    Menu 55
VisualBasic Scripts 28

W

Window
    3D 18
    Allow Docking 62
    Cascading 61, 253
    Crosshair 13
    Floating In Main Window 62
    Hiding 62
    Lock 13
    Menu 59
    Resize 13
    Scaling 254
    Tile 61
    Zooming 13, 253
Workspace 38

X

XPM Files 378

Z

Zerofilling 135, 140
Zooming 254