



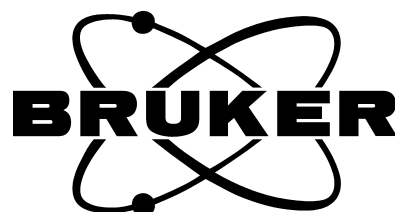
OPUS

Spectroscopy Software

Version 6

User Manual

REFERENCE



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This manual is the original documentation for the OPUS spectroscopic software.

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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*.

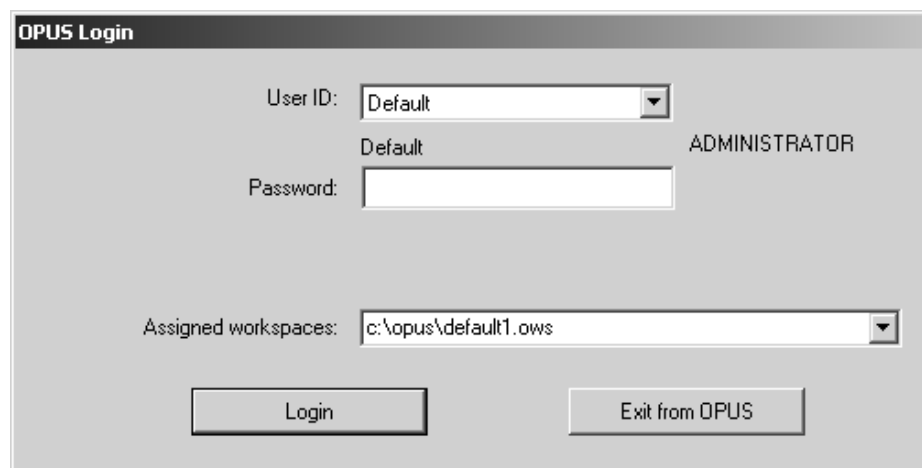


Figure 2: OPUS Login dialog

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.

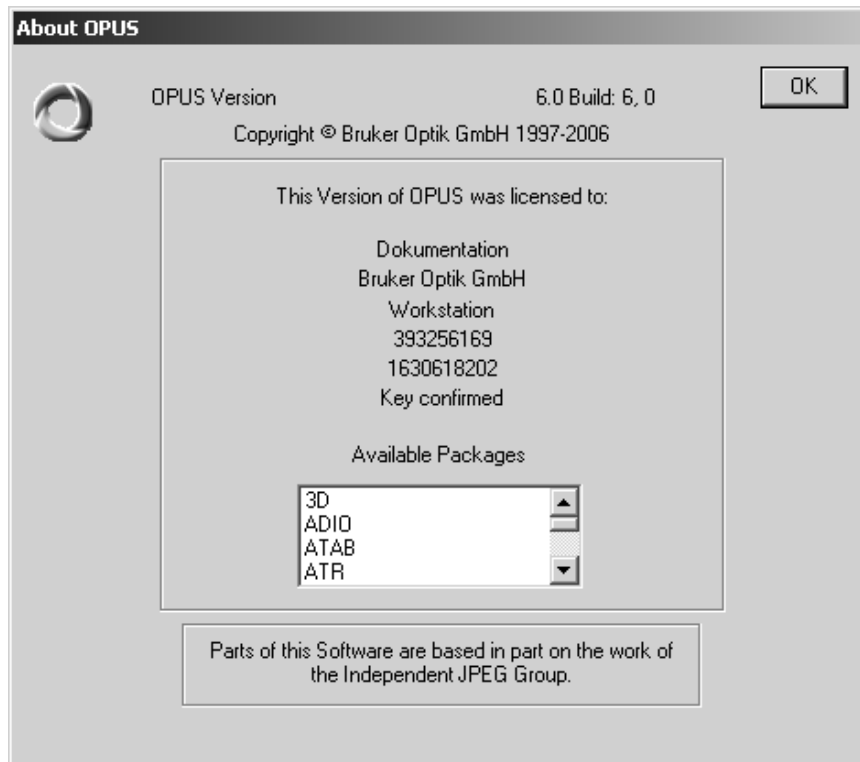


Figure 3: About OPUS dialog

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

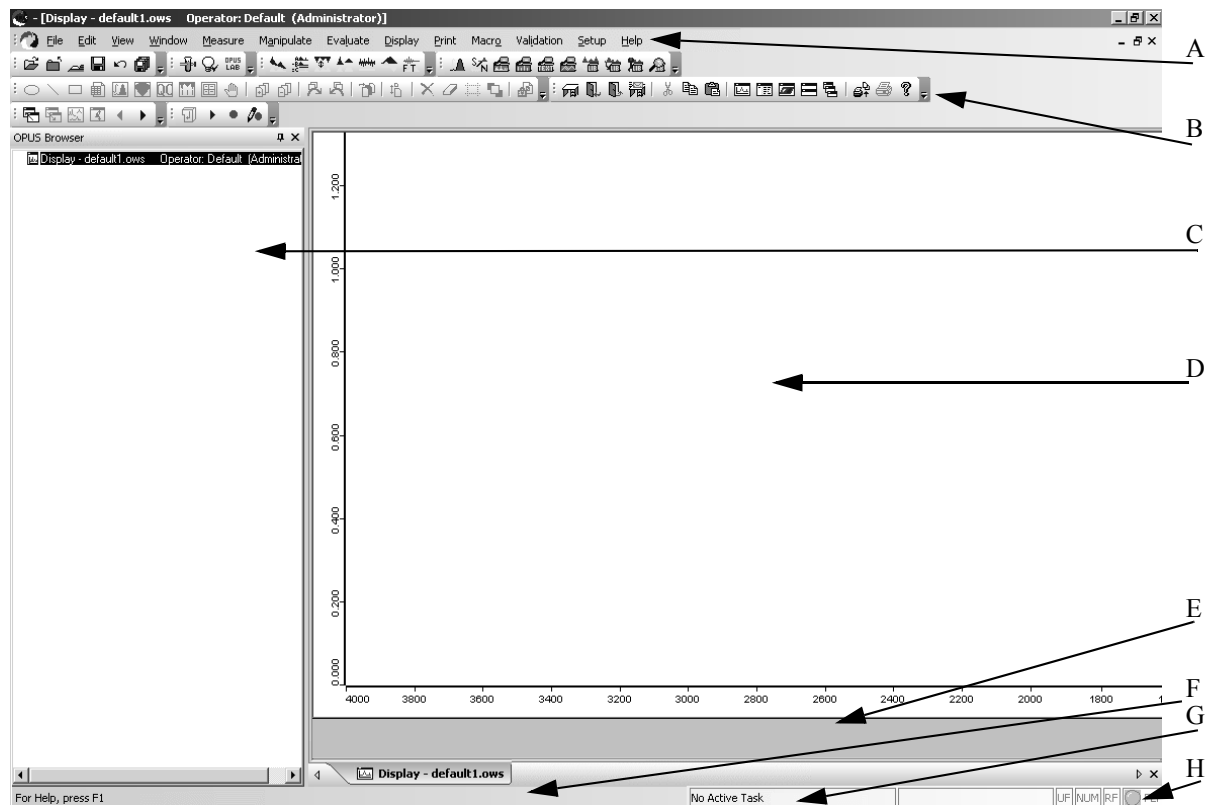


Figure 4: OPUS user interface

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.

The OPUS views which you work with are indicated by tabs. Each tab has a different color to be able to distinguish between them.

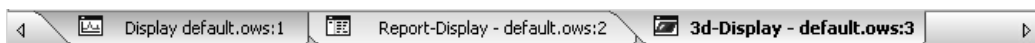


Figure 5: Tabs of different OPUS views

Click on these tabs to change from one view to the other. The frame around each view has the same color as the corresponding tab. If several views are open simultaneously, use the ◀ ▶ on the left and right to change between the different views.

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. Double clicking on the spectra file name in the OPUS browser also allows to move spectra files from there to a specific dialog.

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.

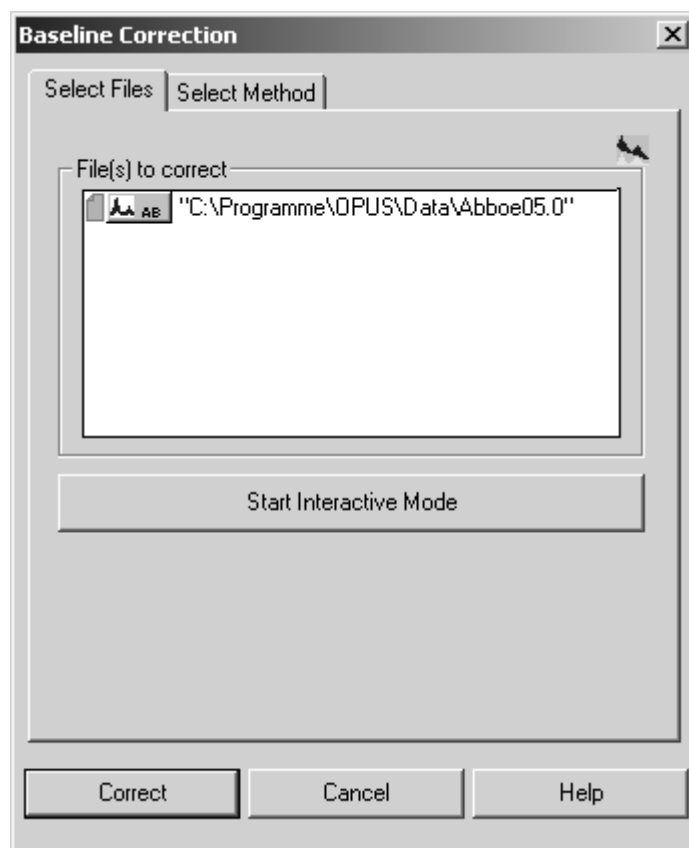



Figure 6: Example of a dialog with two tabs

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 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:

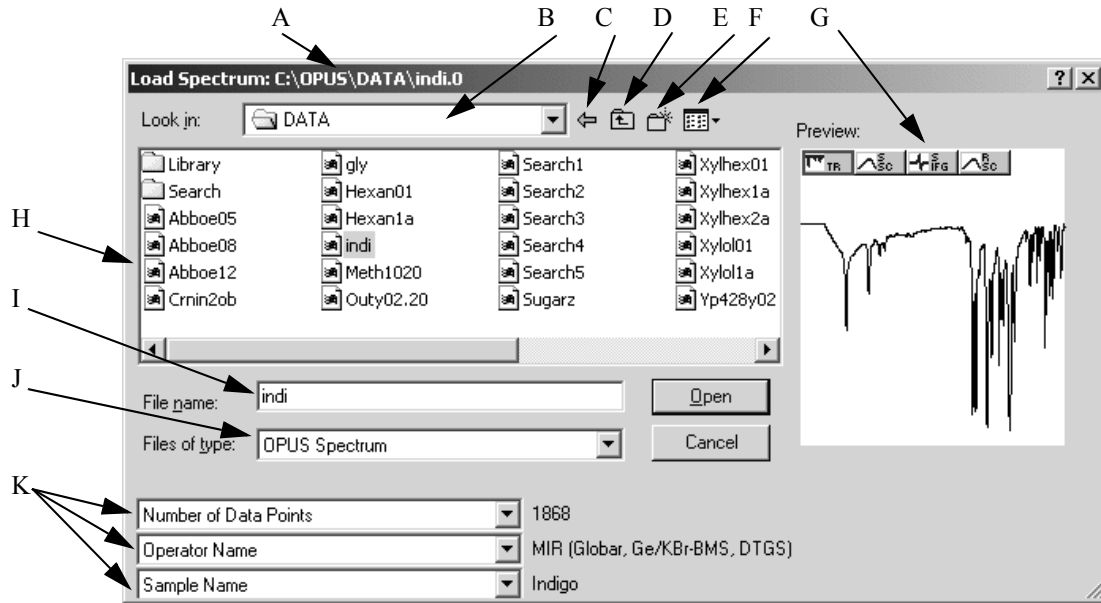


Figure 7: Load Spectrum - active preview

- 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. To open the online help click on the F1 key.
- 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. To open the online help click on the F1 key.
- I) You can also manually type the name of the file you want to load into this entry field. To open the online help click on the F1 key.
- 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. To open the online help click on the F1 key.
- 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. To open the online help click on the F1 key.

You can select several spectra in the spectra list using the *CTRL* 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 Tab

You will encounter the *Select Files* tab in various dialogs. Figure 8 shows an example of the *Select Files* tab in the *Baseline Correction* dialog.

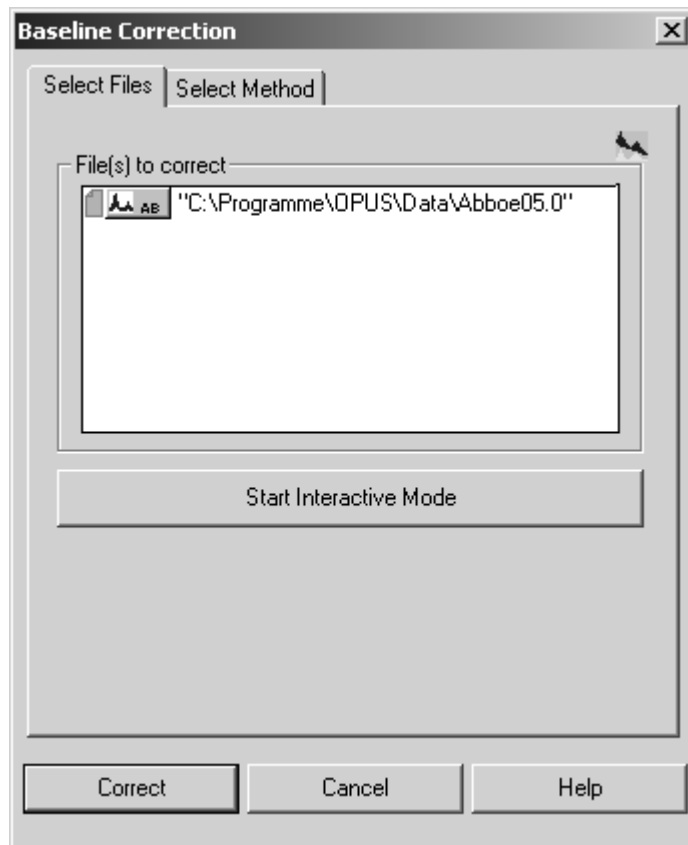


Figure 8: Example of Select Files tab

Select Files tabs include *File(s) to...* selection 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 \leftrightarrow 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 9).

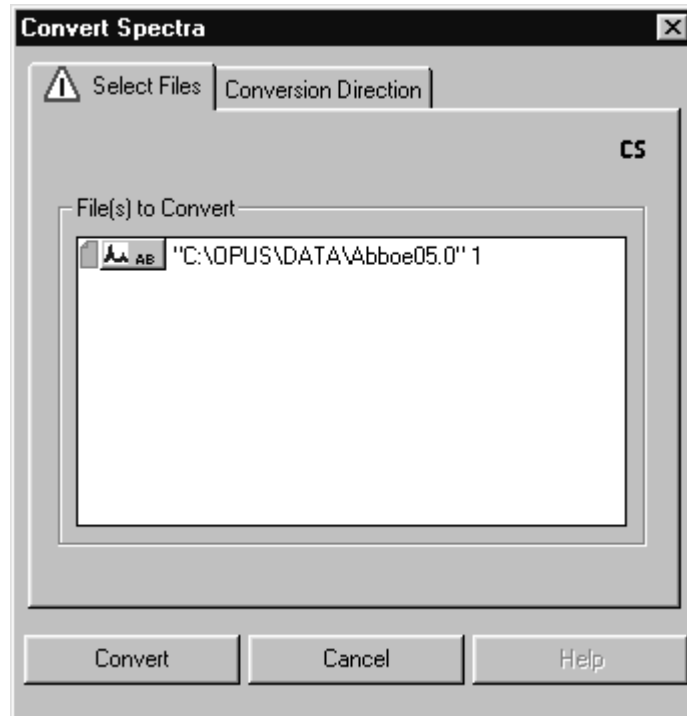


Figure 9: Convert Spectra – parameter mismatch

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...* selection field.

2.2 OPUS Browser Window

The design and functionality of the OPUS browser is similar to the Windows Explorer. To have the OPUS browser displayed click on the *Browser* command in the *View* window. A check mark is set in front of the command.

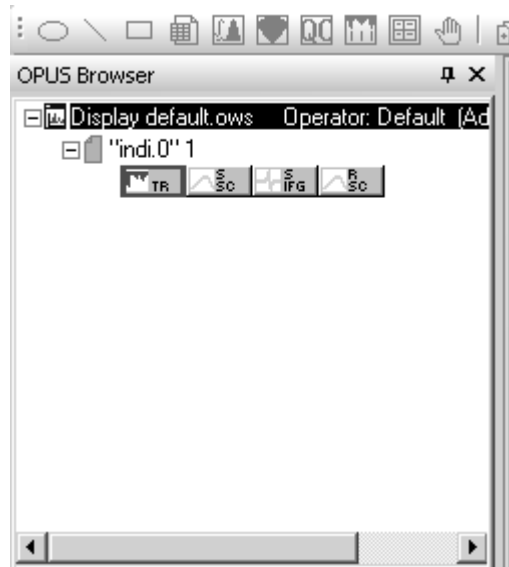


Figure 10: OPUS browser window

To enlarge or reduce the size of the browser window click between browser and spectrum window. The cursor changes into . Now, press the mouse button and drag the browser window to the size desired.

It is also possible to have the browser window displayed as drop-down list. Left click on the upper edge of the browser window and draw it underneath the toolbar. The OPUS browser window will be displayed as drop-down list, including all the files loaded (see figure 11). 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.

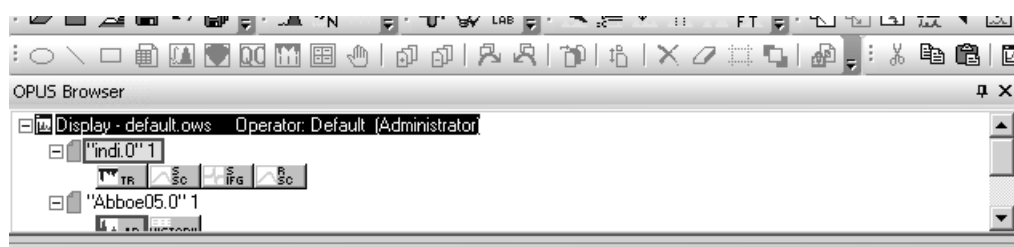




Figure 11: OPUS browser window displayed as drop-down list


The icon allows to make the browser window invisible, e.g. to enlarge the spectrum window. In this case the browser is hidden in a blue bar () on the left side. If you position the cursor on this bar, the browser will be made visible again, and the icon points to the right now. As soon as you move the cursor outside the browser on the OPUS interface, the browser will be hidden again. If

you want to have the browser displayed permanently, click on the  icon again. To permanently close the browser click on the  icon.

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 12: 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 12 indicate a transmission spectrum, single-channel spectrum, interferogram and single-channel background spectrum. For further data blocks, see the 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.

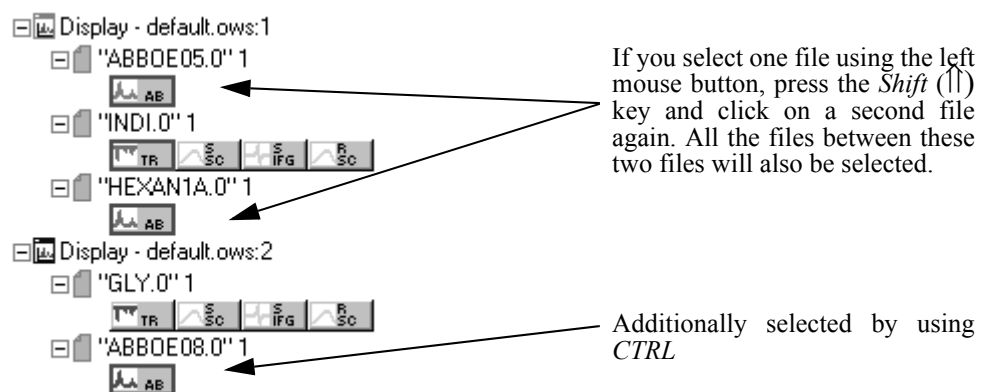


Figure 13: Selecting files

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.

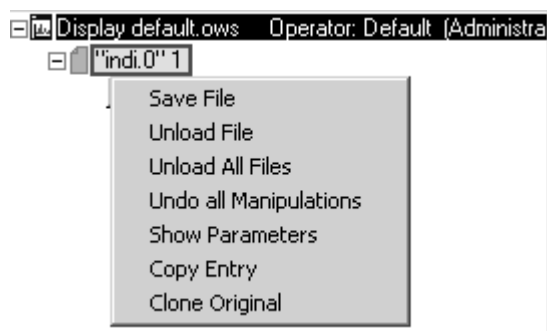


Figure 14: Pop-up menu for file manipulation

As changes made to a file are not automatically saved in the file directory, you have to store these changes using the *Save File* command. *Unload File* or *Unload All Files* 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* command 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* commands are used to duplicate spectrum files. The difference between these two commands is that *Copy Entry* copies a data file which has been manipulated, e.g. if a baseline correction has been performed. The *Clone Original* command copies the original spectrum file.

If you right click on a data block, the following menu pops up.

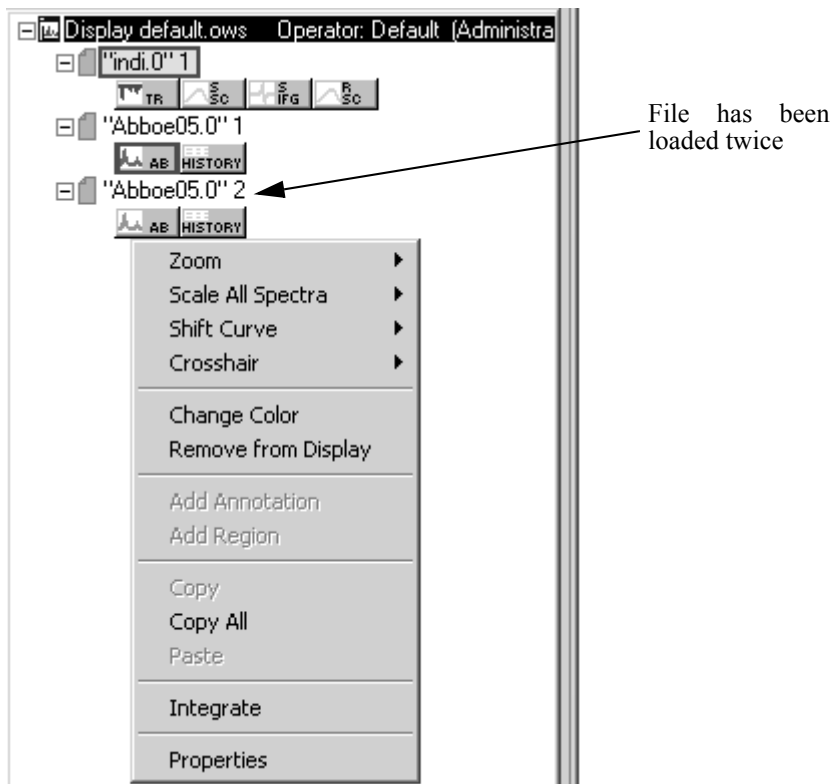



Figure 15: Pop-up menu for spectrum manipulation



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 in the middle of the OPUS user interface. When loading 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 wavenumbers 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. If a file consists of more than one data block, only the first data block is displayed in the spectrum window.

In Figure 16 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  to . Now you can move the borders of the spectral range (white) by pressing the left mouse button.

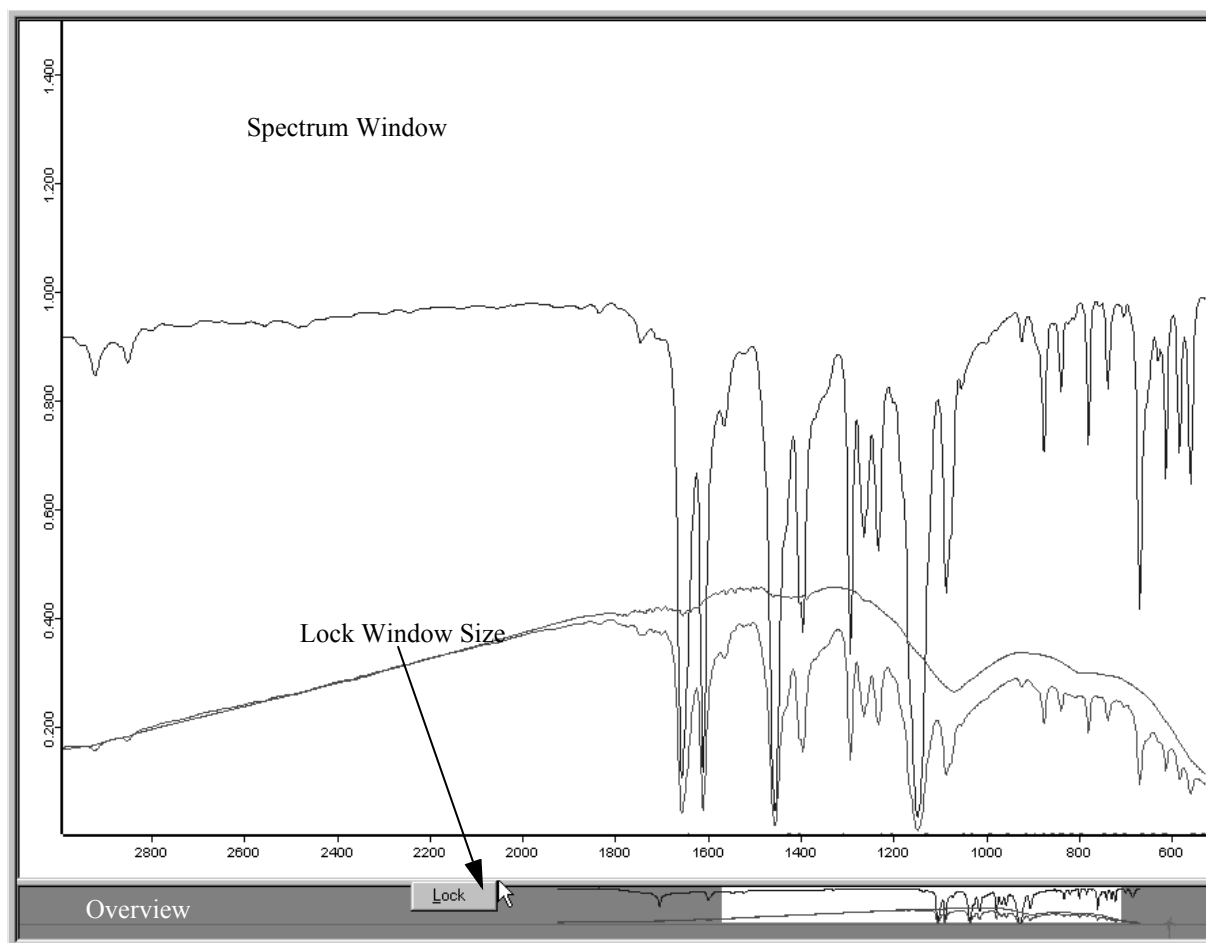


Figure 16: Spectrum and overview window showing lock button

If you position the cursor exactly 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 this boundary. If the windows are locked, 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 (figure 17). This menu allows to change the spectrum color, to zoom a specific spectral range or to shift the complete spectrum.

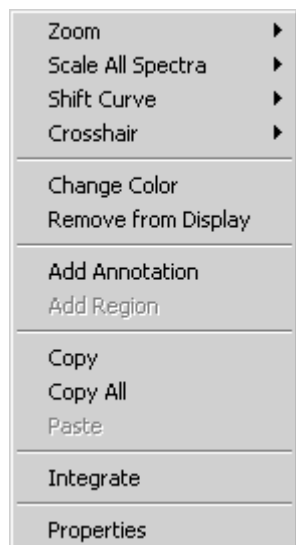


Figure 17: Pop-up menu within the spectrum window

2.3.1 Zoom

To enlarge part of the spectrum window, select the *Zoom In* command 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 enlarge. 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 enlarged part.

2.3.2 Scale

Use the *Scale all Spectra* command to return to the original view by selecting the *Show Everything (XY)* command from the pop-up menu. The *Page back* command in the *Display* menu allows to have the last 10 spectral ranges displayed again. For details on scaled spectra display, see chapter 10.

2.3.3 Shift curve

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* command. Deactivate the *Shift* mode by right clicking. To undo these changes, select *Reset* from the *Shift Curve* command.

2.3.4 Crosshair

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

2.3.5 Change color

The *Change Color* command allows to change the spectrum color by selecting an appropriate color from the color palette displayed.

2.3.6 Remove from display

To remove the spectrum from the spectrum window select the *Remove from Display* command.

2.3.7 Add annotation

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 wavenumber 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 wavenumber and select *Properties* from the menu which pops up. The *Center text lines* and *With Arrows* check boxes are activated by default.

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

2.3.8 Copy/Copy All/Paste

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

2.3.9 Integrate

This command can only be used in connection with 3D files. For further details refer to the OPUS 3D manual.

2.3.10 Properties

The *Properties* command opens the *Display Settings* dialog box.

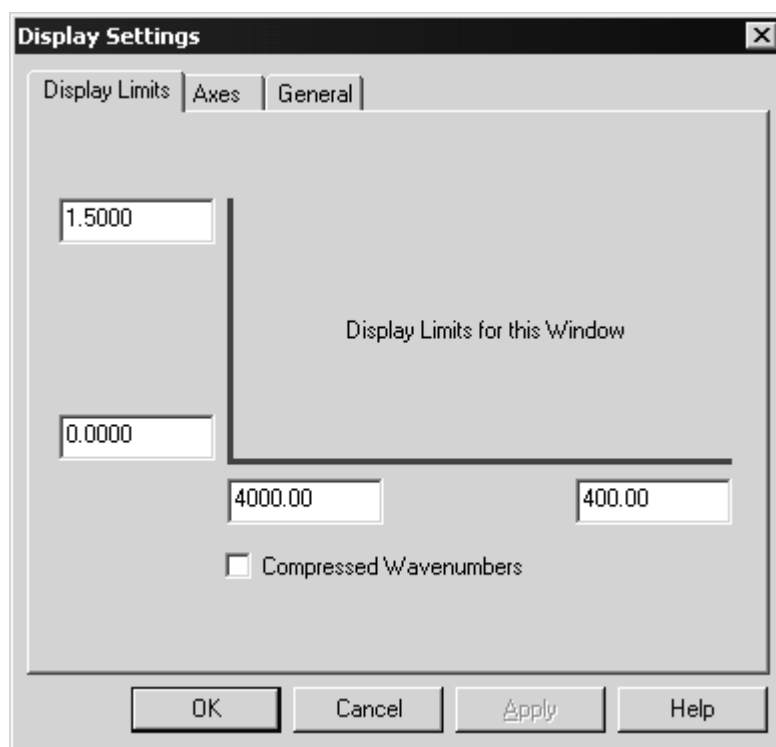


Figure 18: Display Settings – Display Limits tab

Use the *Display Limits* tab to change the size of the displayed region.

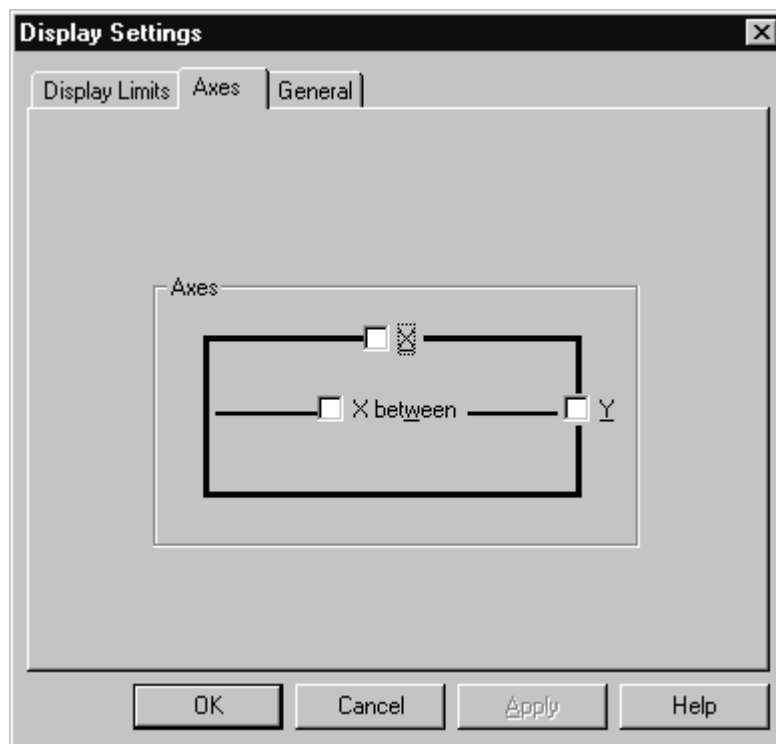


Figure 19: Display Settings – Axes tab

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*.

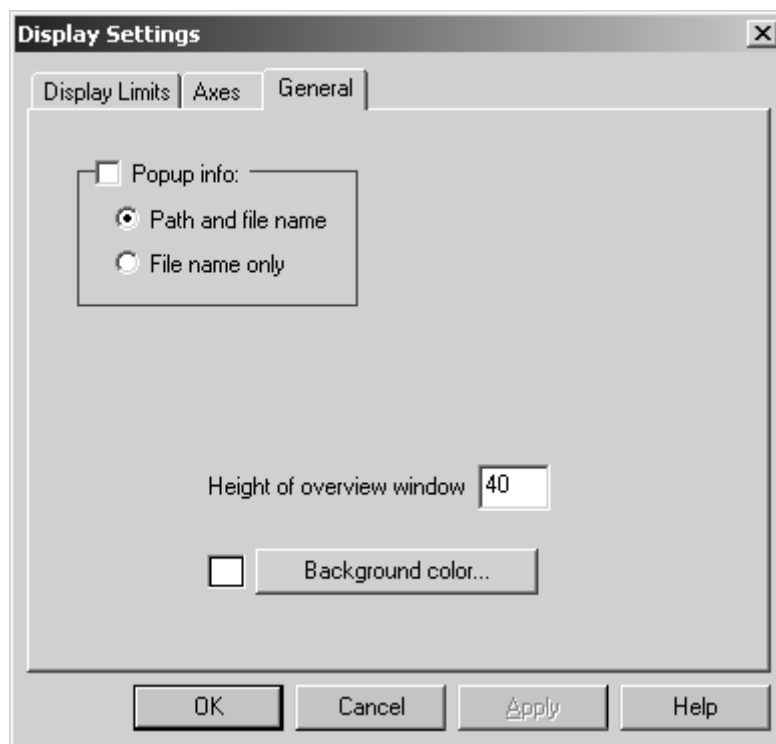


Figure 20: Display Settings – General tab

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

The report window displays numerical or text information, e.g. measurement parameters or evaluation results. This kind of information is stored in report blocks. Double clicking on such a report block (except for peak tables) opens a report window. A blank report window can be opened from the *Window* menu (see chapter 6.3).

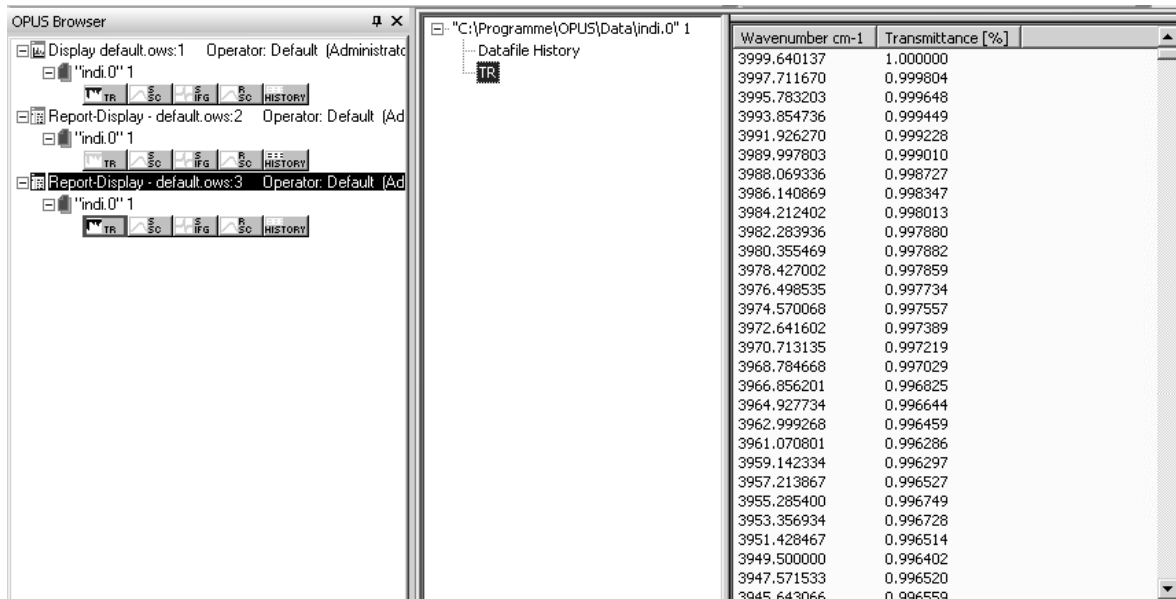


Figure 21: Report window

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.

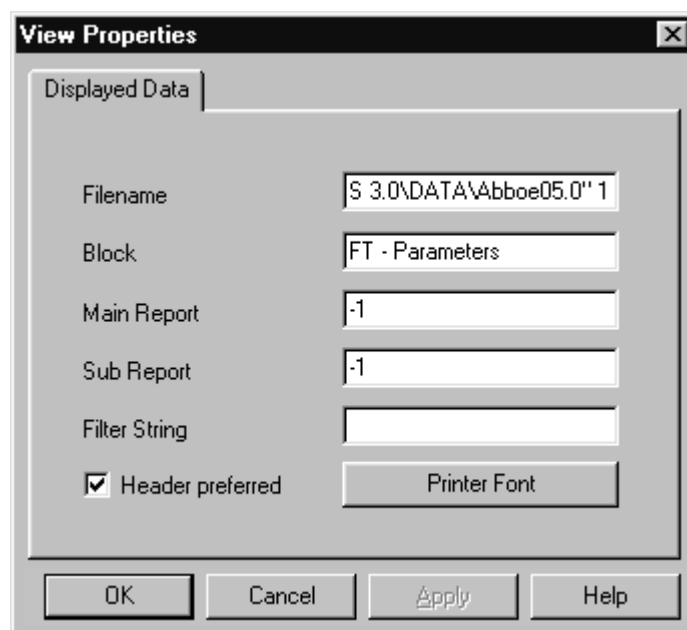



Figure 22: View Properties - Displayed Data tab

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 is recorded in a non-editable, non-deletable history datafile. Figure 23 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 () together with the edited 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.

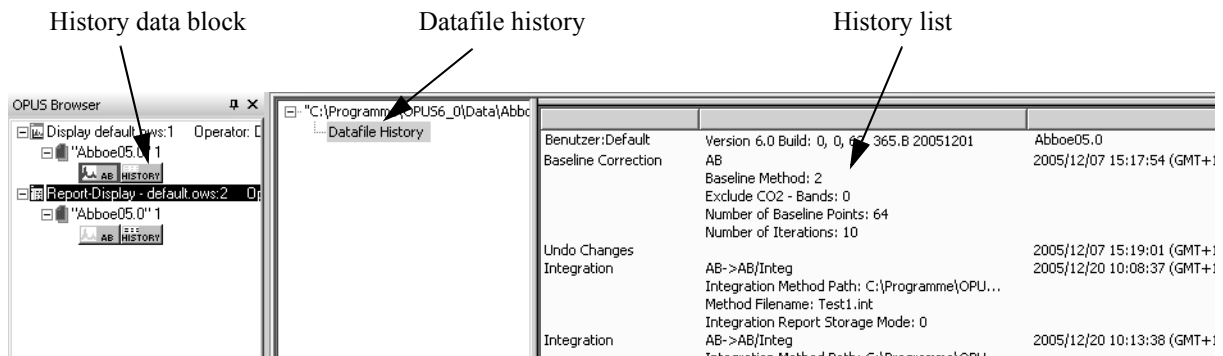


Figure 23: Report Window showing datafile history

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. There are 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 24 shows an example of the *Cut* manipulation.

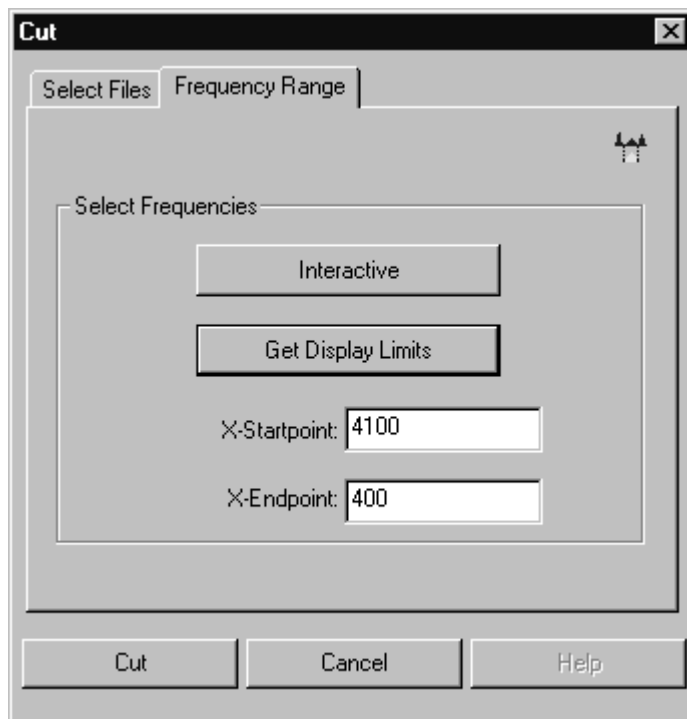


Figure 24: Frequency Range

The *Select Frequency Range(s)* window opens and displays the loaded spectra. Depending on the x-startpoint and x-endpoint defined (see figure 24), 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 complete frequency range displayed 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.

Note: The frequency range of 3D files can also be selected interactively. In this case, the first and last spectrum as well as three additional spectra which are between the first and last spectrum will be evaluated.

Figure 25 shows pre-defined display limits which do not correspond to the frequency range displayed. The frequency range between the current display limits is white.

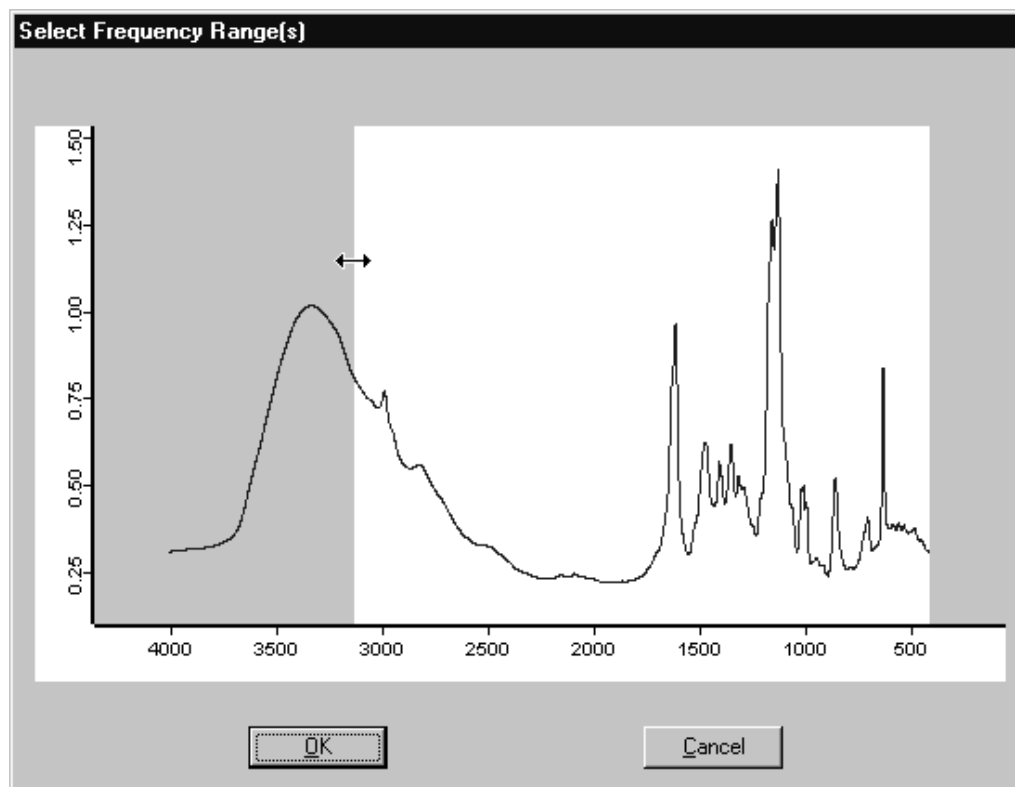


Figure 25: Interactive frequency range selection

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 (\leftrightarrow). If you press the left mouse button, you can move the entire frequency range selected.

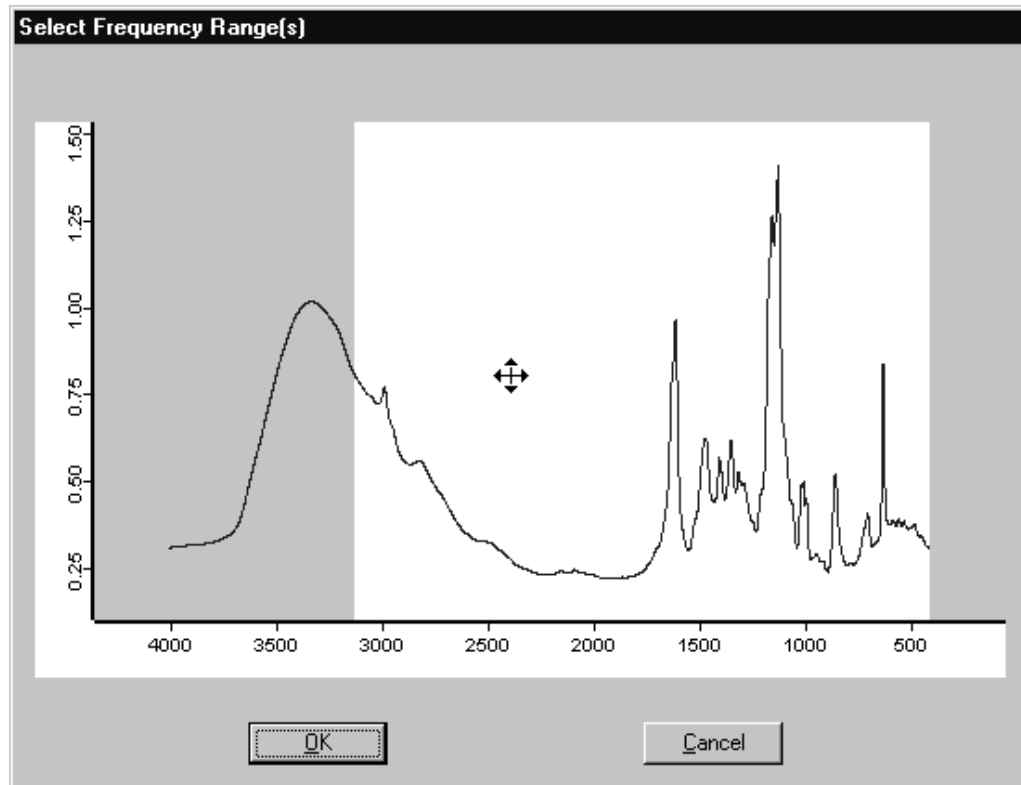


Figure 26: Interactive frequency range selection

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 on that icon.




Figure 27: OPUS toolbar showing a tooltip

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

You can customize the various tool bars to best suit your requirements. The toolbar configurations are stored together with the workspace settings in one file. This file 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 14.7. For an icons list, see the appendix A.

2.9 Instrument Status Indicator

The instrument status is shown at the right end of the status bar (). If no spectrometer is connected, a gray status light will be displayed. A green status light indicates that the instrument is OK and connected.

If the instrument status light becomes 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 texts. Options for the diagnosis can be set up using the *User Settings* command in the *Setup* menu (see chapter 14.9).

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.

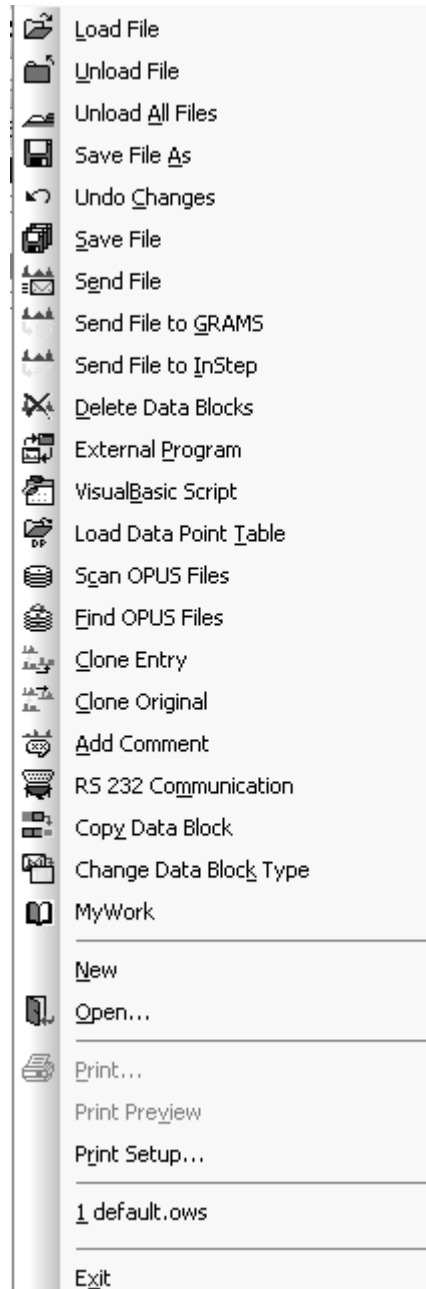


Figure 28: File menu

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 automatically deleted from hard disk. Drag and drop the respective file into the *File(s) to Unload* selection field and click on the *Unload* button.

3.3 Unload All Files

The *Unload All Files* command removes all files from the OPUS browser and spectrum window. If you have loaded several spectrum files into the OPUS browser and you want to remove them all at once, select the *Unload All Files* function. A dialog opens which automatically contains all the spectrum files in the *File(s) to unload* selection field. Click on the *Unload* button to continue.

3.4 Save File/Save File As

The *Save File* and *Save File As* commands provide different options to store files. Enter all files to be saved into the *File(s) to Save* selection field by drag and drop.

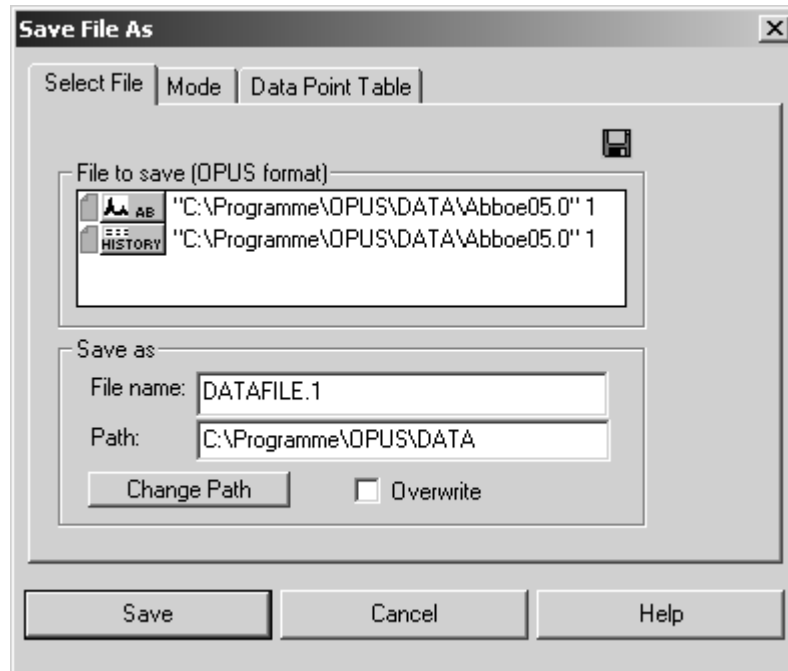


Figure 29: Save Spectrum - Select File tab

The *Select Files* tab allows to define spectral data to be stored, and the file path. Use the *Change Path* button to browse the directory on the 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 14.9.

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. GRAMS¹ or InStep². *JCAMP.DX* as an additional ASCII format can also be used.

If you activate the respective check boxes in the *Options* group field (figure 30), 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*.

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.

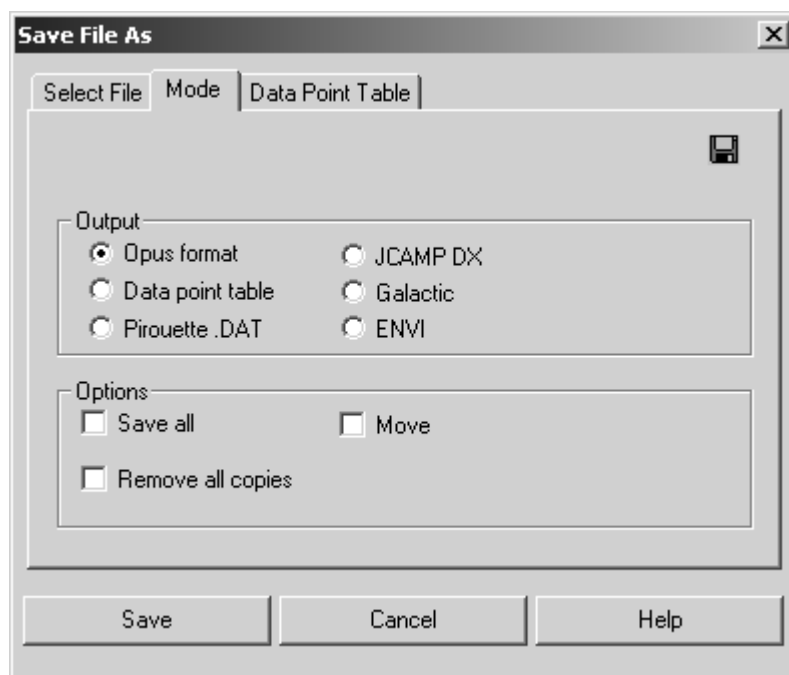


Figure 30: Save Spectrum – Mode tab

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.

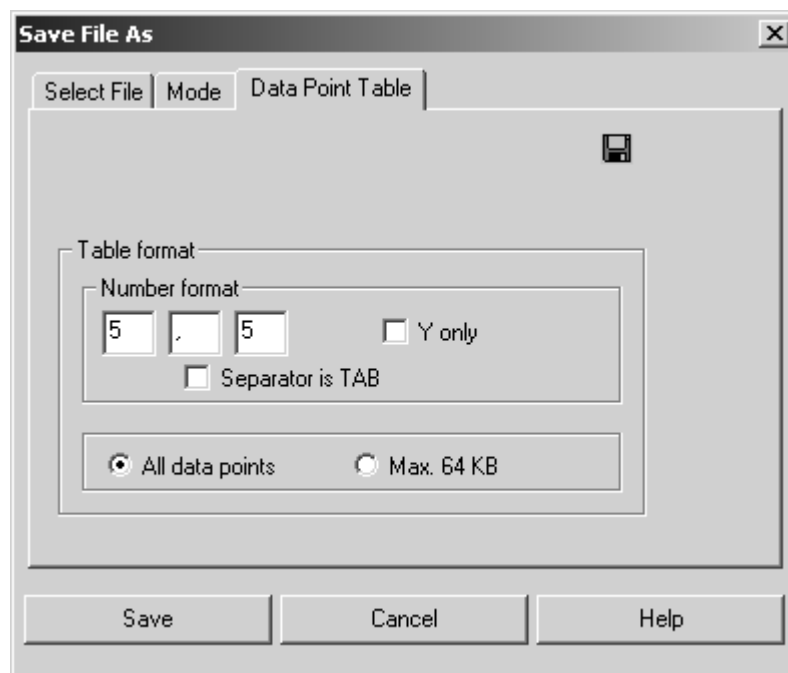


Figure 31: Save Spectrum - Data Point Table tab

3.5 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.

3.6 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.

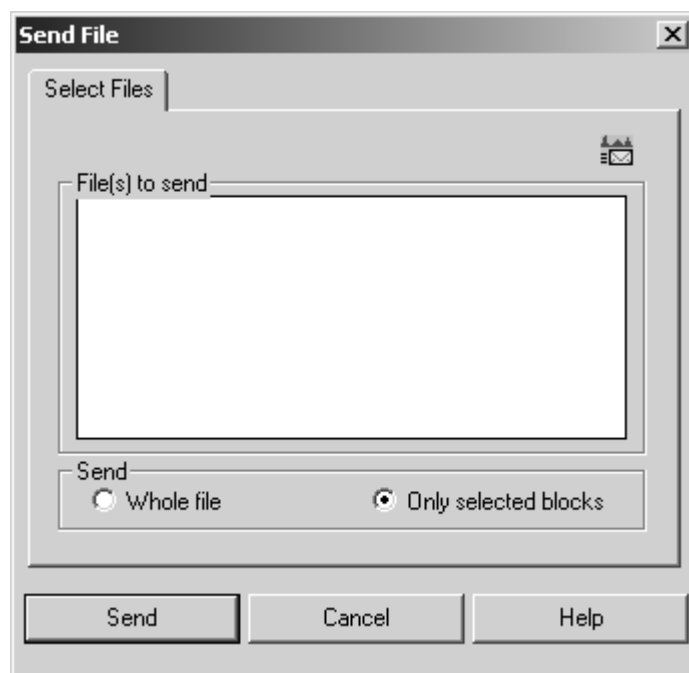


Figure 32: Send File - Select Files tab

If you check the *Whole File* option button, 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.

3.7 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.

3.8 Send File to InStep

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

3.9 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.

3.10 External Program

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

3.11 VisualBasic Scripts

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

3.12 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.

3.13 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*.

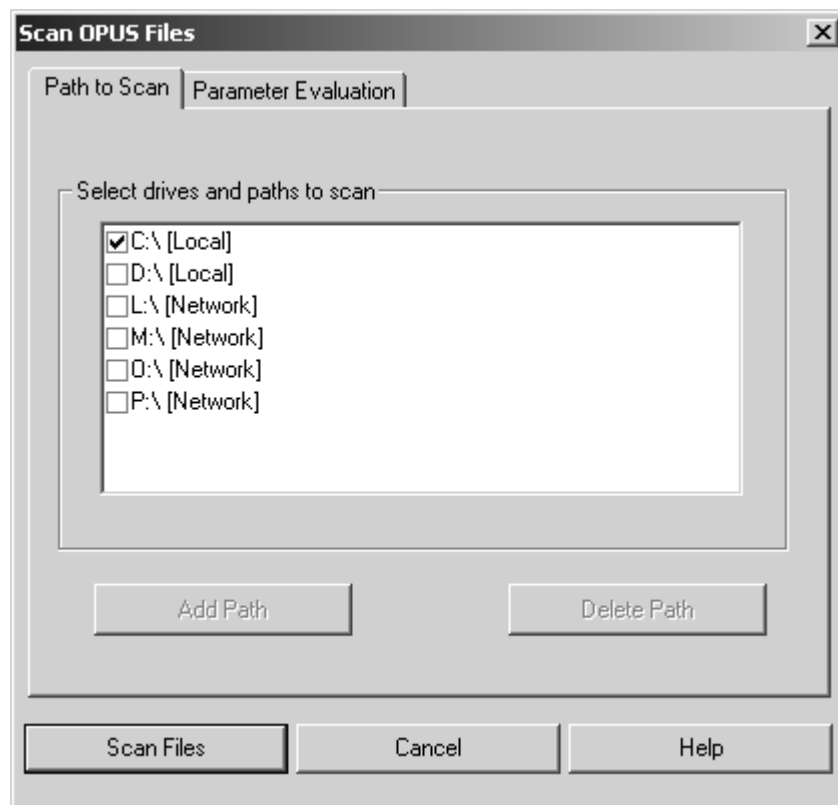


Figure 33: Scan OPUS Files – Path to Scan tab

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.

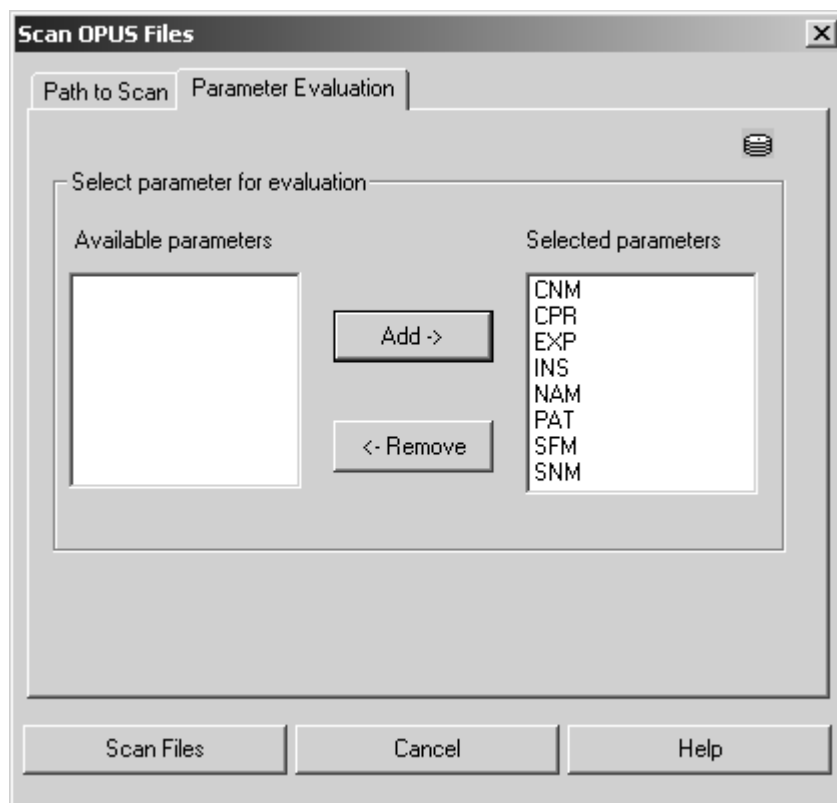


Figure 34: Scan OPUS Files – Parameter Evaluation tab

3.14 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.

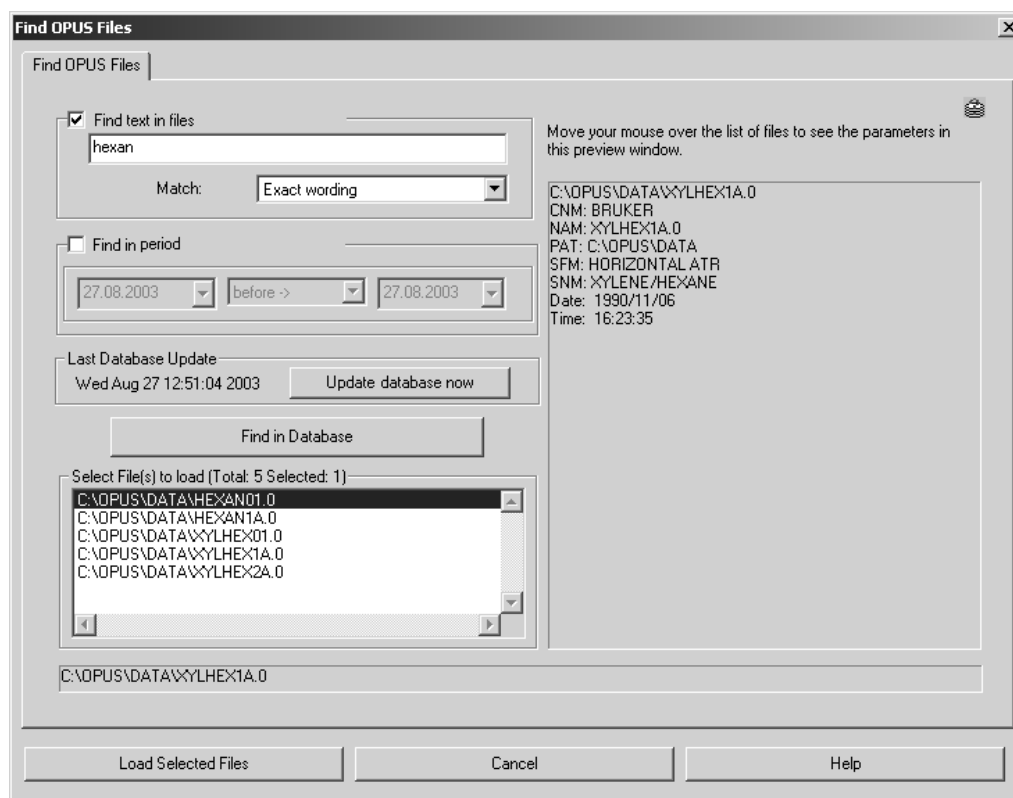


Figure 35: Find OPUS Files tab

3.15 Clone Entry and Clone Original

The *Clone Entry* and *Clone Original* commands are used to duplicate spectrum files. Use the *Clone Entry* command 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.

When storing the changes made in a cloned file you have to observe the following: use the *Save File As* command if you do not want the original file to be overwritten by these changes, and use a different file name for the cloned file.

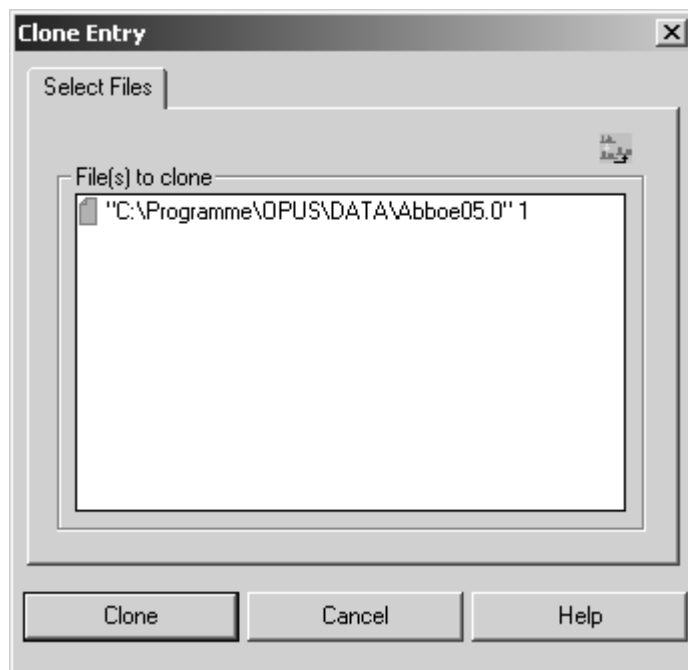


Figure 36: Clone Entry - Select Files tab

3.16 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 *File(s) to Comment* selection field. Enter the comment into the *Comment Text* entry field. The comment will be displayed in the *Report Display* under *Datafile History*.

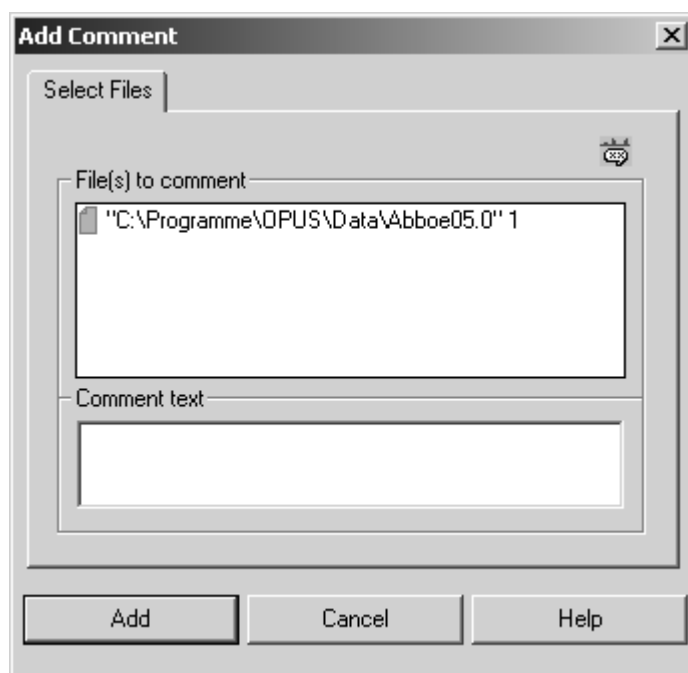


Figure 37: Add Comment - Select Files tab

3.17 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.

3.17.1 RS 232 Write/Read

If you start the command interactively, the following dialog window will be displayed:

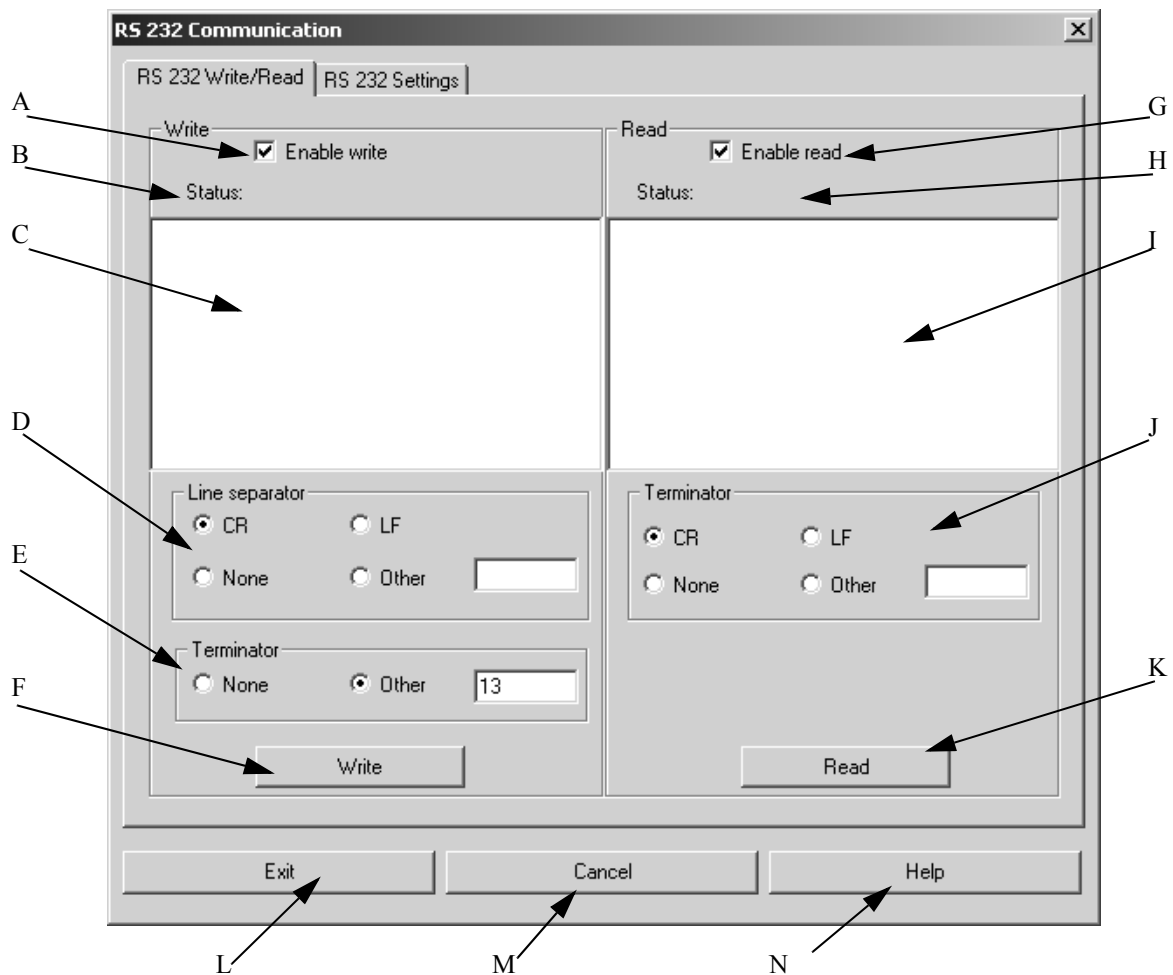


Figure 38: RS 232 Communication - RS 232 Write/Read tab

- 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.
- D) Example: **ABC@(#)039DEF** will be sent as **ABC'DEF**
- E) 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.
- F) 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.
- G) If you click on the *Write* button, the text entered in (c) will be sent to the RS 232 interface.
- H) This check box enables or disables the *Read* command.
- I) The status of the *Read* command is indicated here (e.g. Reading..., Time-out etc.)
- J) The answer sent by the external device is displayed in this entry field
- K) 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.
- L) If you click on the *Read* button you activate the read command only.
- M) Exits the *RS 232 Communication* command and stores the current settings. No write or read activity is started.
- N) Exits the *RS 232 Communication* command without saving the current settings.
- O) Shows the online help.

3.17.2 RS 232 Settings

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

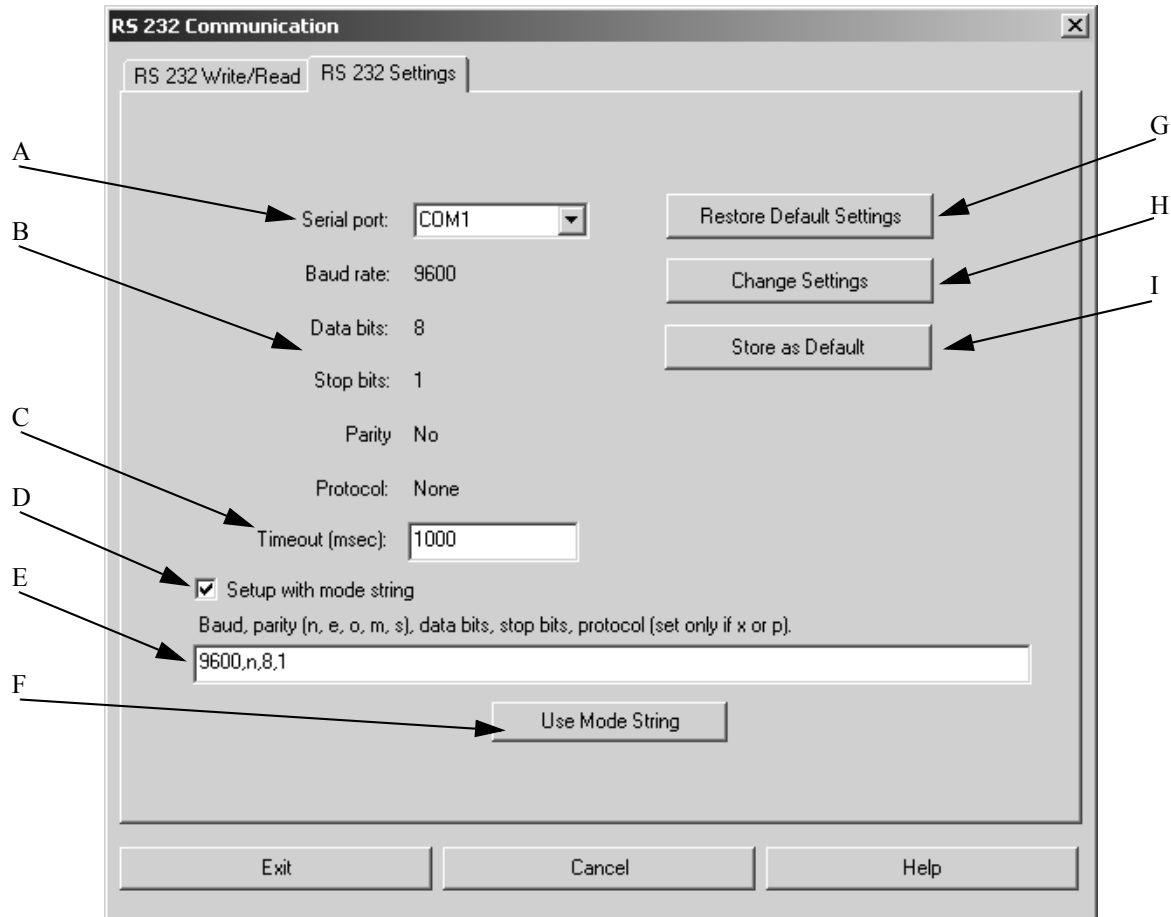


Figure 39: RS 232 Communication - RS 232 Settings tab

- 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 3.17.3.
- I) The *Store as Default* button overwrites the operating system settings by using the current settings.

3.17.3 COM1 Properties

The *COM1 Properties* dialog will be displayed if you click on the *Change Settings* button (see chapter 3.17.2):

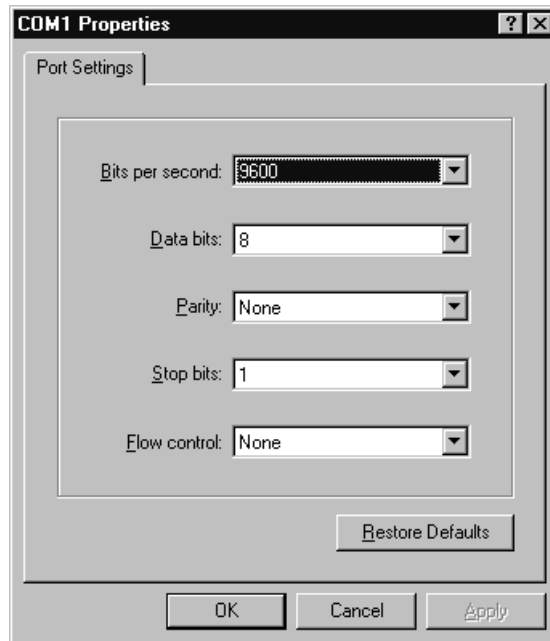


Figure 40: RS 232 Communication - Port Settings tab

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.

3.18 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.

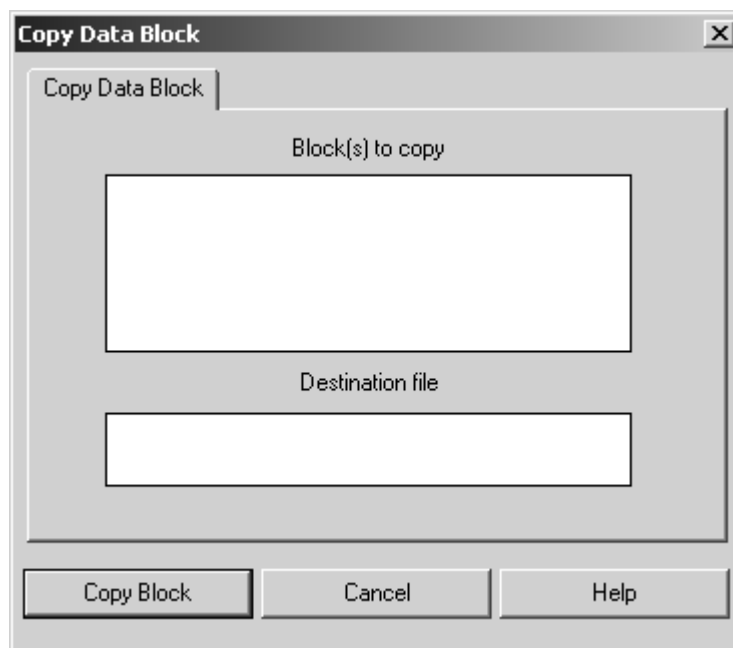


Figure 41: Copy Data Block

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.

3.19 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 drop-down list.

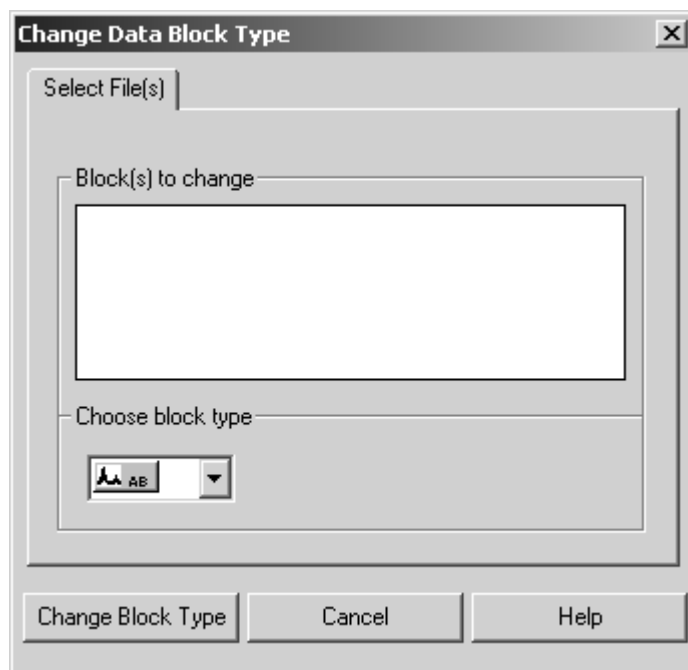


Figure 42: Change Data Block Type

3.20 My Work

OPUS provides the possibility to run a lab journal (LabJournal). This automatically-generated lab journal records what kind of evaluations or measurements have been performed in OPUS, how and when. The evaluation and measurement data stored are displayed in a special view.

The lab journal data are sorted by the name of the spectra file, type of evaluation or measurement, or date. Lab journals are files with the **.lbj* extension, which are stored in the *OPUS* directory. The lab journal file name contains the name of the user who created the lab journal and who is assigned to the journal.

3.20.1 Creating Lab Journal

To be able to create a lab journal you first have to activate the *Run a lab journal* check box (A in figure 43). Select the *User Settings* command from the *Setup* menu and click on the *Basic Settings* tab. If the check box remains deactivated, a lab journal will not be created.

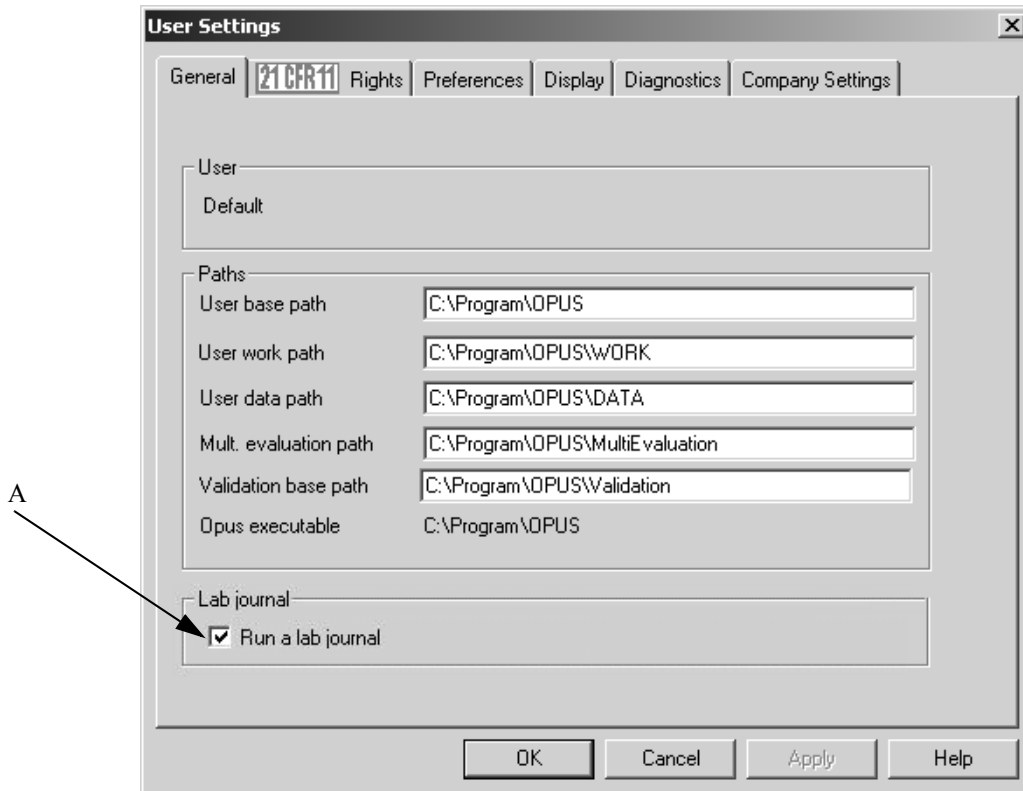


Figure 43: User Settings - Run a lab journal

Click on the *My Work* command in the *File* menu. If no lab journal can be assigned to you, you will be asked whether a new journal has to be created. Confirm the dialog that pops up by *Yes*. OPUS automatically creates a lab journal with your user name.

Note: If you have *Administrator* or *Labmanager* user rights, the *Open* dialog will first be displayed. Use this dialog to select the appropriate lab journal.

Depending on the user rights (see chapter 14.3) you can open the lab journal by means of the *My Work* command. If you have *Operator* user rights, you can only open the lab journal assigned to your account. To be able to open the lab journals of other users you require *Administrator* or *Labmanager* user rights.

3.20.2 Lab Journal View

The OPUS lab journal includes two windows. The left one shows a list with the names of the spectra files as well as the date of the different evaluations or measurements performed. These evaluations or measurements performed are in the *Block* column as follows:

- INTEG: Integration
- PEAK: Peak Picking
- QCMP: Quick Compare

- QUANT1/2: Quantitative evaluation (QUANT 1 or QUANT 2)
- MEAS: Measurement

Note: The lab journal does not contain all evaluation commands available in OPUS but only the ones mentioned above.

You can have the evaluation or measurement results displayed on the right side by clicking on the spectra file name.

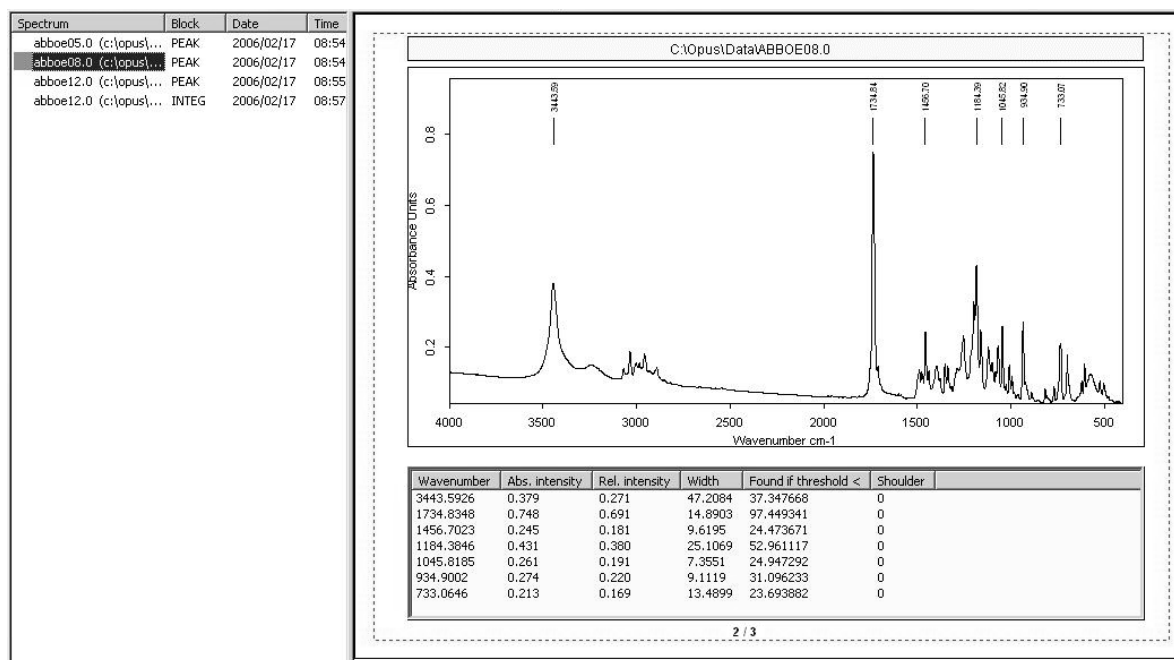


Figure 44: Lab Journal View

If you double click on a spectra file name, the spectrum window opens. This window displays the spectrum selected, together with the evaluation or measurement results.

You can sort the lab journal list entries on the left according to

- spectra file name
- block
- date

in ascending and descending order by clicking on the particular column title. Clicking again on this column title restores the original sorting order. When sorting the single actions according to date, you have the possibility to limit the search to a certain period of time. Double click on the *Date* column to open the following dialog:

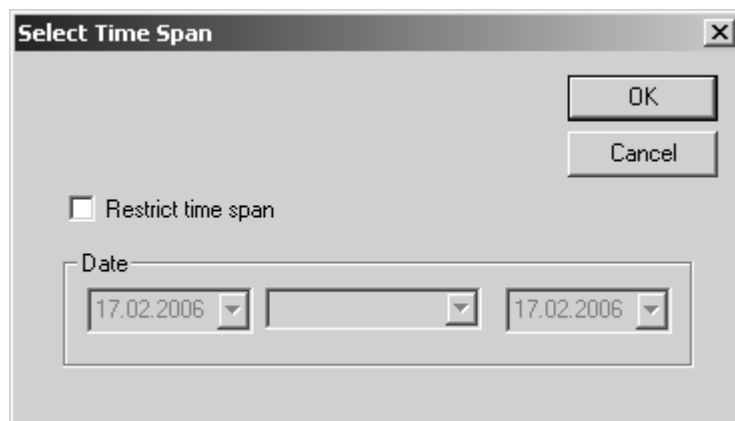
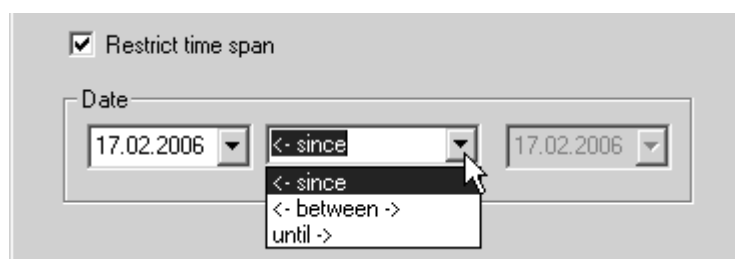


Figure 45: Lab Journal - Select Time Span

First, activate the *Restrict time span* check box. Then, determine the period of time using the drop-down lists.



Confirm the settings by clicking on the *OK* button. The list will be sorted again, considering only those evaluations or measurements selected within the defined period of time. To undo this setting double click again on the *Date* column. Deactivate the *Restrict time span* check box and click on the *OK* button.

One single lab journal contains up to 1000 entries. If the number of entries exceeds the limit of 1000, the lab journal will automatically be renamed and copied into a sub-folder for archiving purposes. When renaming, the date of the first and last entry are added to the previous file name. Thus, the new file name indicates the time period of the different entries. The following format applies to the new file name:

YYYYMMDD: *YYYY* = year, *MM* = month, *DD* = day

Example: *LabJournal_Default_2006-03-15_2006-04-10*

If the previous journal has been archived, OPUS creates a new journal using the *LabJournal_Default.lbj* name.

The lab journal can also be printed with each lab journal entry being on a separate page. Select the *Print* command from the *File* menu.

3.21 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 section 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.

3.22 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.

3.23 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.

3.24 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.

3.25 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 *Copy* and *Paste*.

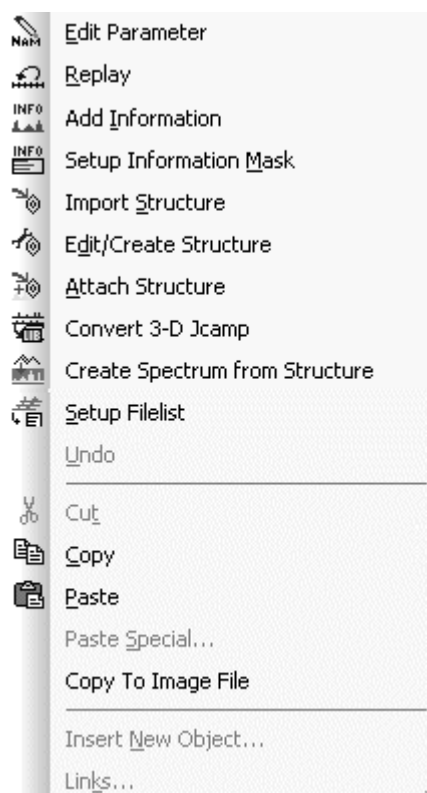
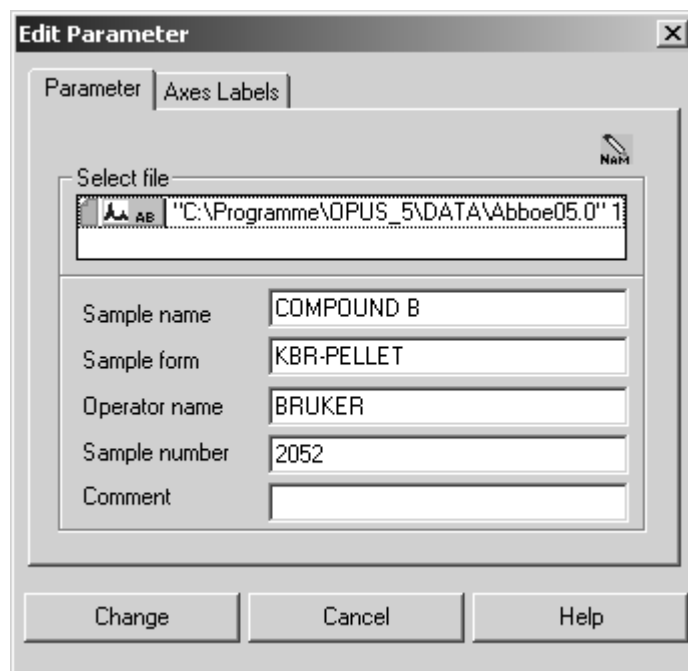


Figure 46: Edit menu

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:

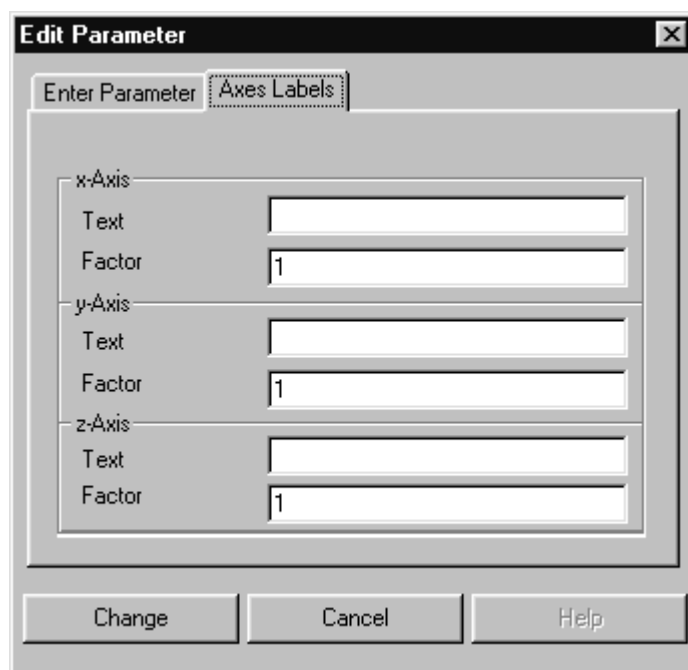


The screenshot shows the 'Edit Parameter' dialog box with the 'Enter Parameter' tab selected. The 'Parameter' tab is also visible. The 'Select file' field contains the path 'C:\Programme\OPUS_5\DATA\Abboe05.0'. Below this, there are five input fields: 'Sample name' (COMPOUND B), 'Sample form' (KBR-PELLET), 'Operator name' (BRUKER), 'Sample number' (2052), and 'Comment' (empty). At the bottom are 'Change', 'Cancel', and 'Help' buttons.

Figure 47: Edit Parameter – Enter Parameter tab

Now, change the parameters accordingly. Note that you will not be able to change these parameters when 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. The scaling factors will only be considered in case of 3D spectra.



The screenshot shows the 'Edit Parameter' dialog box with the 'Axes Labels' tab selected. The 'Enter Parameter' tab is also visible. The dialog is divided into three sections for the x-axis, y-axis, and z-axis. Each section has a 'Text' field and a 'Factor' field. The 'Factor' fields are all set to '1'. At the bottom are 'Change', 'Cancel', and 'Help' buttons.

Figure 48: 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 of this 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 repeat some manipulations.

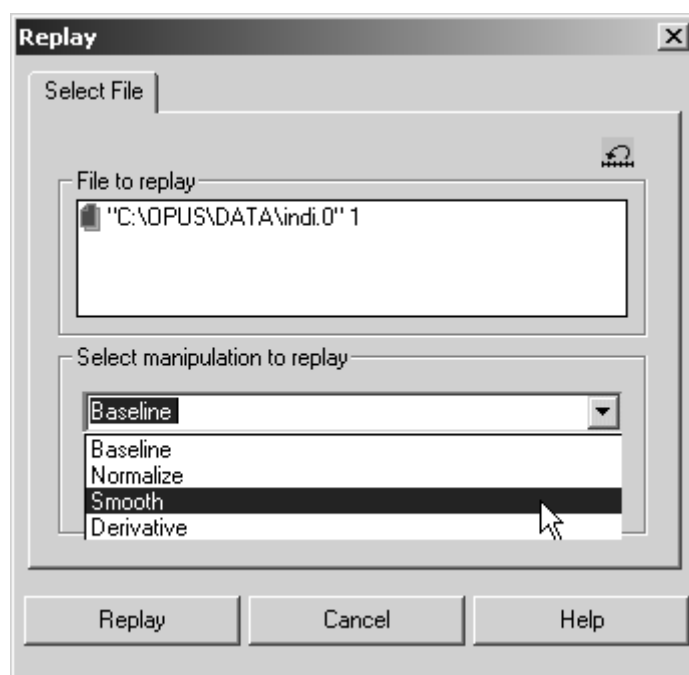



Figure 49: History Replay - Select File tab

Select the manipulation command up to which you want to restore the file. If you select *Smooth*, as exemplified in figure 49, *Baseline*, *Normalize* and *Smooth* manipulation command will be performed on the original spectrum, except the *Derivative* command.

4.3 Add Information

Apart from OPUS parameters you can also save additional information, using the *Add Information* command. This kind of information will be saved in a separate INFO (information) data block , 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 *Add Information* command. The following dialog opens:

The screenshot shows the 'Add Information' dialog box. At the top, there are two tabs: '1 - 11' and '12 - 26'. Below the tabs is a file selection field containing the path 'Q:\OPUS\DATA\SEARCH1.0' 1. To the right of this field are two buttons: 'Load Text Mask' and 'Restore Original'. Below the file field is a checkbox labeled 'New file' which is currently unchecked. Underneath the checkbox is a 'Text definition' field containing the path 'C:\OPUS\METHODS\DEFAULT.TXD'. The main body of the dialog consists of a list of input fields, each with a label and a text box. The labels and their corresponding values are: 'Compound Name' (Methylformat), 'Molecular Formula' (C2H4O2), 'Molecular Weight' (60,05), 'CAS Registry Number' (107-31-3), 'Melting Point' (empty), 'Boiling Point' (32,0), 'Sample Preparation' (empty), 'Sample Quantity' (empty), 'Manufacturer' (empty), 'Reference' (empty), and 'Charge Number' (empty). At the bottom of the dialog are three buttons: 'Add', 'Cancel', and 'Help'.

Figure 50: Add Information

You can only select one spectrum file at once 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 *Add Information* dialog (see figure 50) can include up to 7 pages. Enter the requested information. You do not need to fill in all the fields.

Clicking on the *Add* 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 *Add Information* dialog (see figure 50).

Compound Information	
CAS Nummer	107-31-3
Molmasse	60,05
Siedepunkt	32,0
Substanzname	Methylformat
Summenformel	C2H4O2

Figure 51: 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 *Add Information* dialog (figure 50) 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 50).

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 50). 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 *Inn* 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 *Tnn* as parameter name (e.g. T01 = text in first line, T12 = text in twelfth line).

4.4 Setup Information 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 *Information Mask*.

If you select the *Setup Information Mask* command, the corresponding dialog will be displayed (figure 52), and the last-accessed *Information Mask* is automatically loaded. The file name and path of the *Information Mask* is displayed in the *Current Info Mask* line.

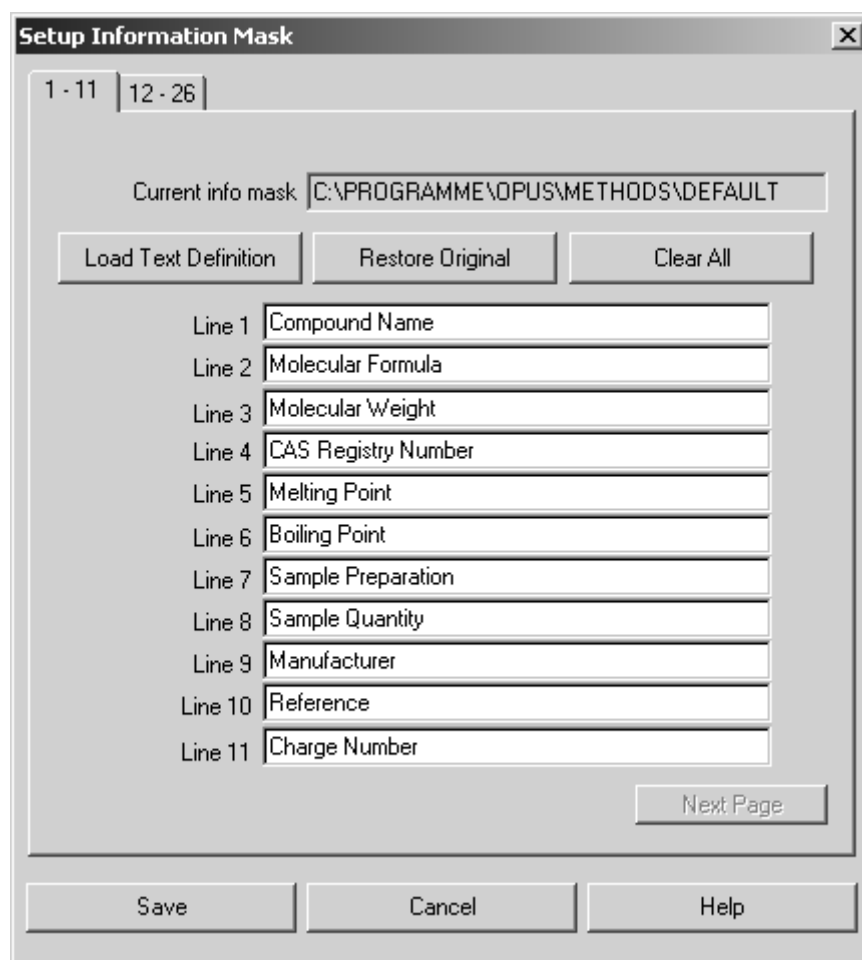


Figure 52: Setup Information Mask

Depending on the number of lines up to 7 pages can be displayed, similar to the *Add Information* 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 53).

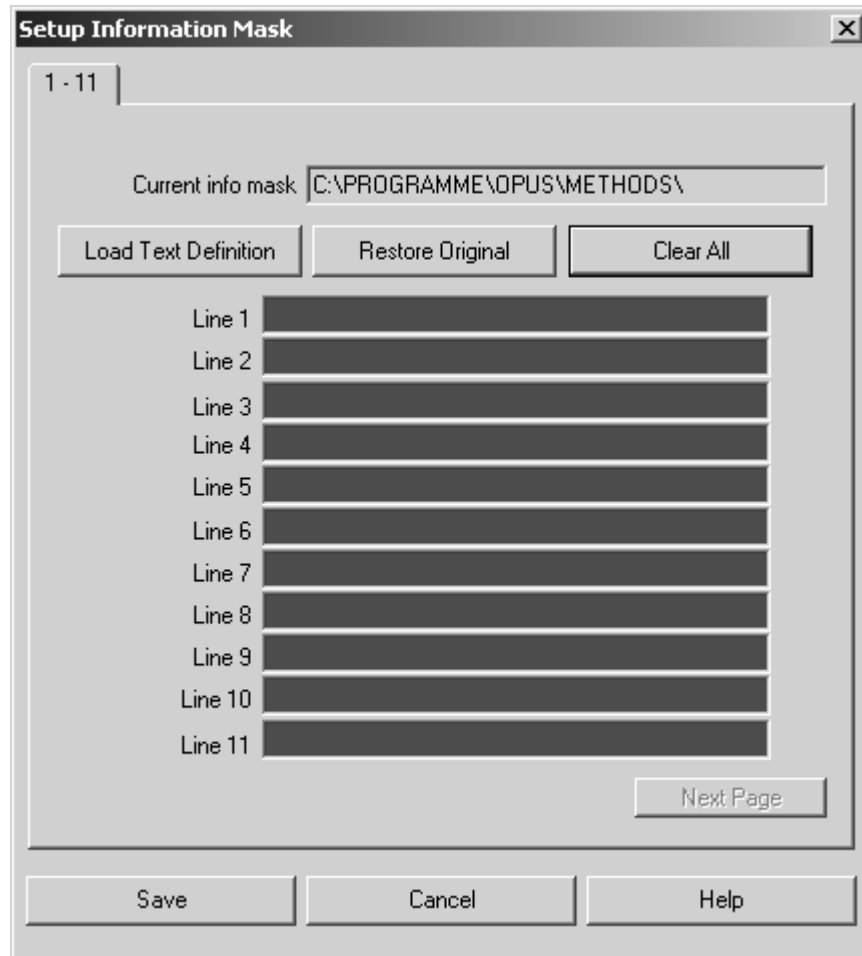


Figure 53: Setup Information Mask - defining entry fields

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.

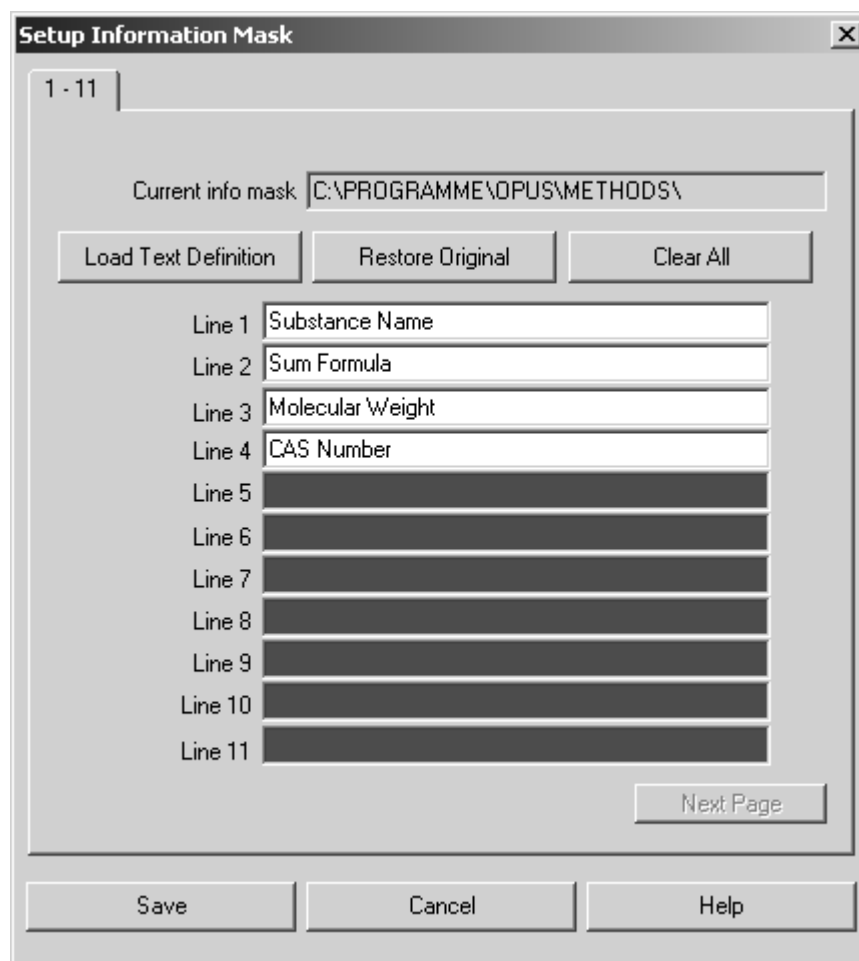


Figure 54: Setup Information Mask - defining entry fields


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 Import Structure

The *Import Structure* command can be used for chemical structural formulae created in Molfile format. These formulae can be imported to OPUS. Select the *Import Structure* command to open the respective dialog, and 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 STR 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.

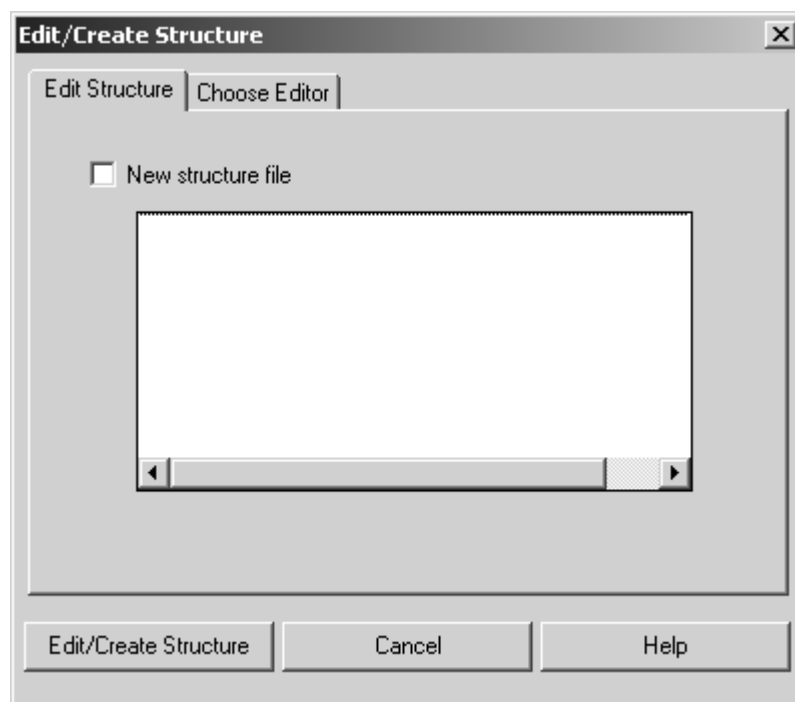


Figure 55: Edit/Create Structure – Edit Structure tab

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. The dialog changes as follows:

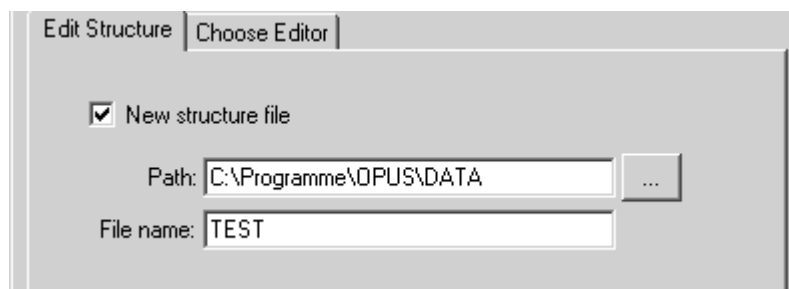


Figure 56: Edit Structure - path and file name

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 55), and click on the *Edit/Create Structure* button.

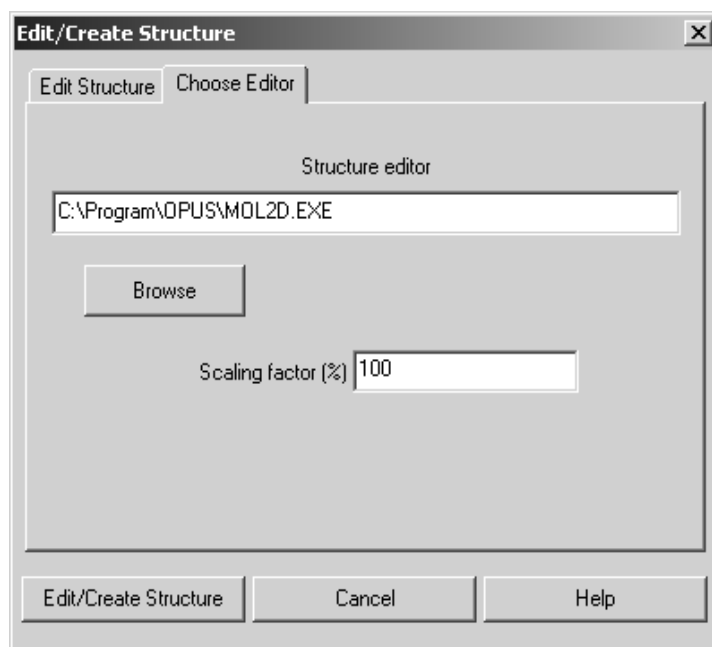


Figure 57: Edit/Create Structure – Choose Editor tab

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.

If you want to use the *Mol2d Version 1.0* structure editor provided by OPUS, you require the OPUS STRUCTURE software package. If this software package is available, you can open the structure editor by clicking on the *Browse* button and selecting the *Mol2d.exe* file from the *C:\OPUS* directory.

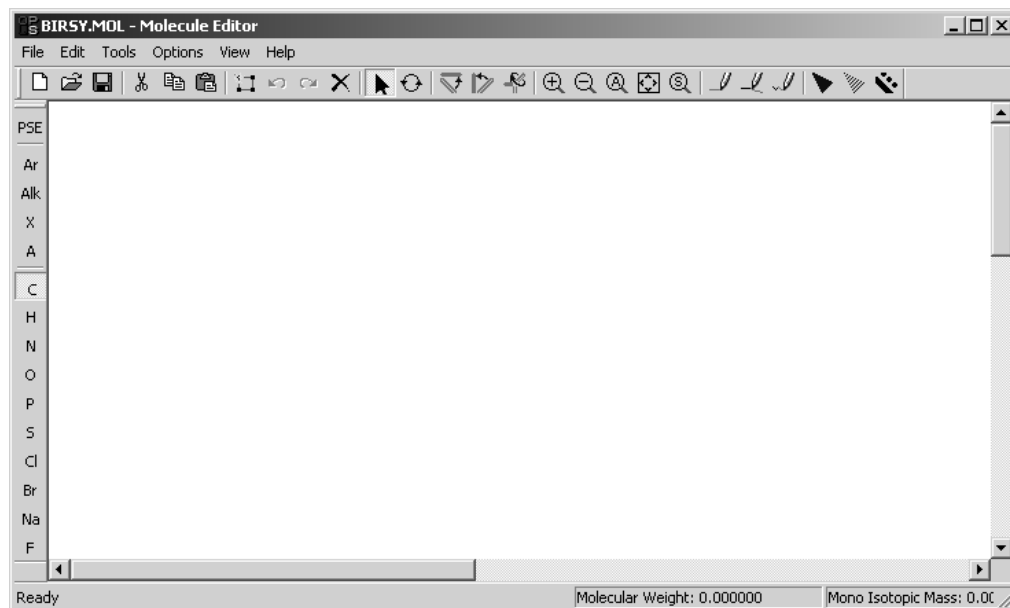


Figure 58: OPUS structure editor

The Windows-based menus include, apart from standard commands (e.g. *Copy* and *Paste*), specific editing commands used to create molecular structures. The most frequently used commands can be found in the icon bar.

- Drawing/Editing bonds:
- Scaling bonds:
- Arranging bonds:
- Refining/Rotating bonds:

On the left side you find the abbreviations of the most important atoms. If you click on *PSE*, the periodic table of elements opens.

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.

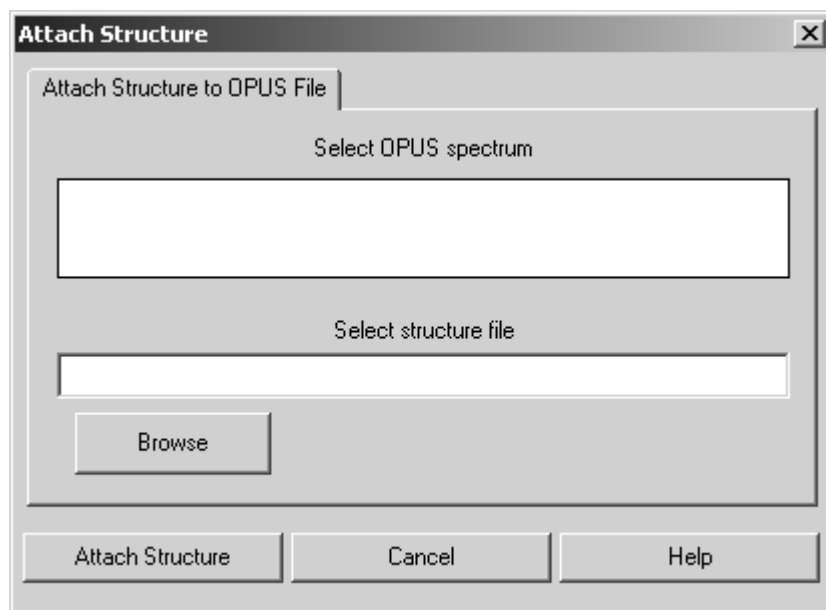



Figure 59: Attach Structure

Load the spectrum into the OPUS browser window and drag and drop it into the *Select OPUS Spectrum* selection 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 Create Spectra from Structure

The *Create Spectra from Structure* command calculates a theoretical IR spectrum resulting from a chemical structure. In this case the structural formula is searched for chemical groups which create characteristic bands within IR spectra. The information extracted from these bands is used to calculate a spectrum.

Load the file(s) which include structure data blocks and select the *Create Spectra from Structure* command. Drag & drop the data blocks () into the *Structures used to create spectra* entry field.

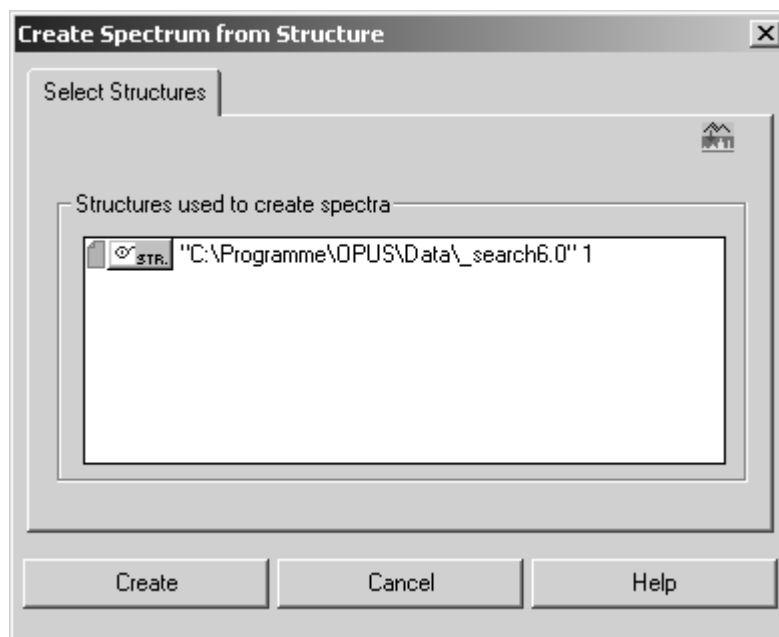


Figure 60: Create Spectra from Structure

To start the calculation click on the *Create* button. The result output will be an absorbance spectrum, and stored in the AB data block (📄 AB). If there has already been a ratio spectrum (AB, TR etc.) in the file selected, this spectrum will be overwritten.

The additional INTERPR report data block (📄 INTERPR) will be created and attached to the file. All band information included in this data block are written as text, and used to calculate the spectrum. The band information may comprise:

- Name of chemical group
- Consecutive numbers of atoms included in the group
- Band position and band height


4.9 Convert 3-D Jcamp

The *Convert 3-D Jcamp* 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 data block ().

If you click on the *Convert 3-D Jcamp* command, the following dialog opens:

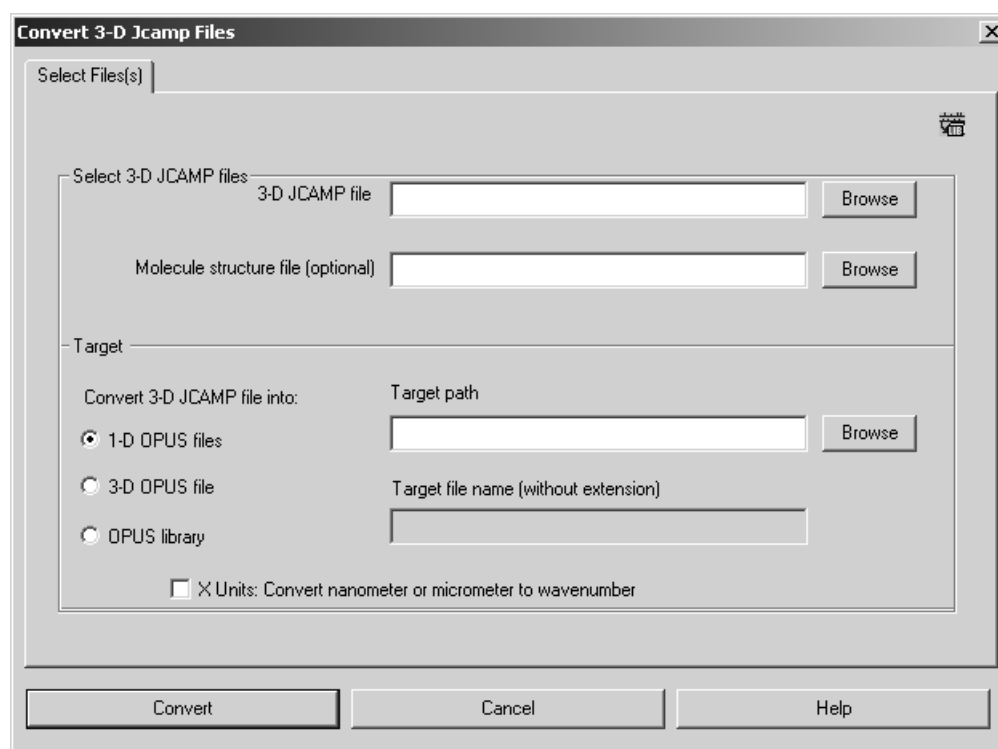


Figure 61: Convert 3-D Jcamp Files - Select File(s) tab

In the *Select 3-D JCAMP files* group field you define the file name of the 3D 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 61) 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 3D JCAMP file is converted into a 3D 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 differ-

ent 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 3D 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.

JCAMP files with x units being indicated in wavelengths (i.e. nm or μm) cannot be used in OPUS without converting the x units into wavenumbers (cm^{-1}). In this case activate the corresponding check box.

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.

4.10 Setup File List

Several spectra of a particular spectrum type can be combined into one file list, and edited as one single spectrum. The list which consists of different spectra is stored in the LIST data block () and displayed when selecting the respective data block.

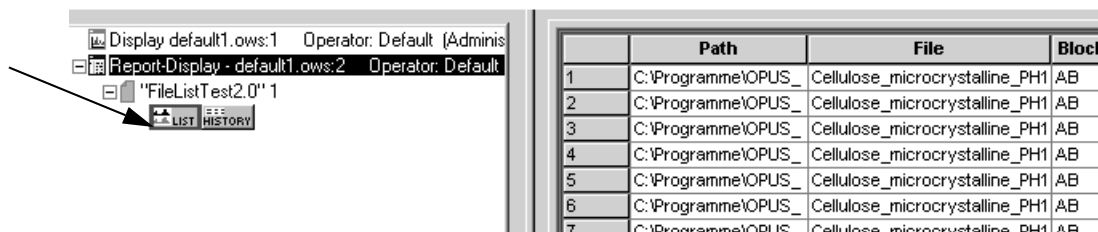


Figure 62: LIST data block

All OPUS commands available for manipulating and evaluating spectra data can be used for the complete spectra file list in the same way as being used for single spectra files.

To create a spectra file list click on the *Setup File List* command, and click on the *Add Spectra* button to load the particular spectra.

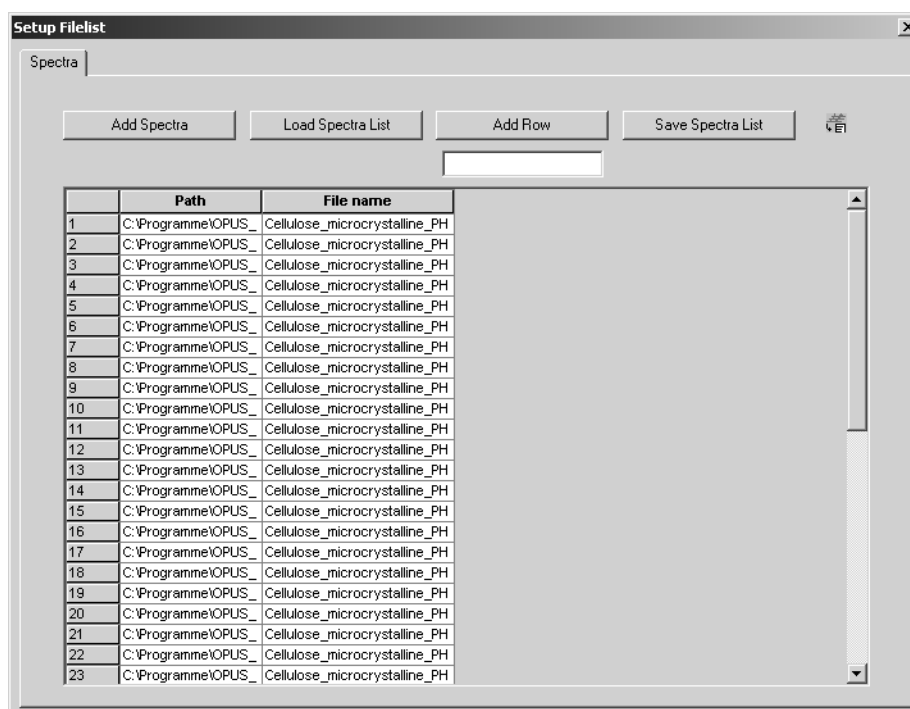


Figure 63: Setup File List - Different spectra

By default, the path and file name of each spectrum is displayed in a table. This table can be customized, i.e. enlarged by as many columns as you like, e.g. to be able to store parameters and input values required for evaluation functions. Enter the name of the column into the entry field below the *Add Row* button. If you click on this button, the new column will be added to the table.

To store the spectra file list click on the *Save Spectra List* button. Define a specific name for the list. Spectra file lists are stored as reports in the OPUS format. The file extension of the list may be incremented, i.e. automatically increased by 1. This is especially helpful if you want to use the same name for different spectra file lists.

In case of evaluating single spectra you can also add specific parameter values to the table in the form of a column. Make sure that you always enter the right parameter code for the specific value into the entry field. The parameter code can be obtained from the Macro Editor, also see the OPUS Programming manual.

If you want to add, e.g. the Mahalanobis distance in case of a QUANT evaluation, or the outlier identification for each single spectrum from the QUANT report to the spectra file list, you first have to create an INFO data block (see also chapter 4.3).

Select the *Add Information* command. Enter the following data into the *Compound name* line (figure 64): name of the OPUS function (A), result data block (B) as well as the corresponding element from the QUANT report (C), i.e. main report number, sub-report number, line, column.

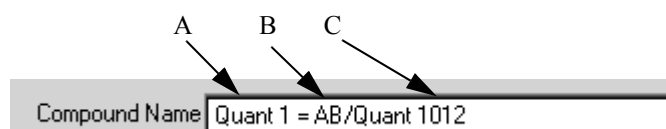



Figure 64: Example of an information input

Evaluation results for files within the spectrum file list are stored in the TRC data block () which is attached to the list. The data block gives a survey about the results of all single spectra.

When loading a spectrum file which contains a TRC (Trace) data block the results are displayed within separate columns. Figure 65 exemplifies the results of an integration recently performed.

	Path	File name	Integrate :
1	C:\data\Toluol	Toluol IA.0	44.629761
2	C:\data\Toluol	Toluol IA.1	45.441830
3	C:\data\Toluol	Toluol IA.2	41.914082
4	C:\data\Toluol	Toluol IA.3	41.442970
5	C:\data\Toluol	Toluol IA.4	42.938992
6	C:\data\Toluol	Toluol IA.5	41.415459
7	C:\data\Toluol	Toluol IA.6	43.086977

Figure 65: Setup File List with integration results

4.11 Copy To Image File

The command *Copy To Image File* allows to store the current OPUS view as image file, with the following formats being available:

- **.bmp* (Bitmap)
- **.pdf* (Portable Data Format)
- **.emf* (Enhanced Metafile)

If you select the command, a dialog opens in which you define the file name and path as well as the file format.

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.

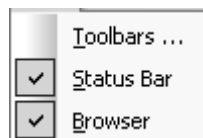


Figure 66: View menu

5.1 Toolbars

If you click on the *Toolbars* command, the *Customize* dialog opens. The options provided allow to customize toolbars, configure single icons or even complete pull-down menus. For further details refer to chapter 14.7.

5.2 Status Bar

The status bar informs about the background tasks of programs running in 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. To deactivate the browser remove the check mark. Besides, you can also reposition the OPUS browser window. For further information refer to chapter 2.2 and 6.4.

6 Window

The *Window* menu allows to open new windows and 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.

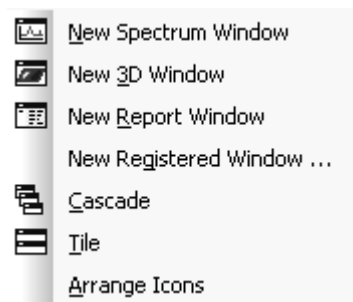




Figure 67: Window menu

6.1 New Spectrum Window

OPUS allows to display several spectra in one spectrum window, and in different spectrum windows. If you select the *New Spectrum Window* option, a new spectrum window opens, indicated by the  **Display default.ows** 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 contain 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 data block () 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
ChromPostrun	CHROM postrun window
Cluster Analysis	To display a dendrogram or histogram (part of OPUS IDENT)
CorrelChart	To display a band assignment chart
Display	To display spectra
EvalResults	To display IDENT results
Factor3d	Score plot window
FPA Measurement	To display FPA measurements
GridReport	GridReport window
Library	To display libraries and their detailed information
Live FPA	To display live FPA measurement
Live+Overview	Live video and overview window
LiveVideo	Live video window
Macro	Macro editor window
Map+Spec	To display the results of an MAP measurement
Online	To display the results of a CHROM measurement
OldReport	Shows report in the OPUS/OS2 format
Overview	Video overview window
Process Control	To display a standard trend chart (part of OPUS PROCESS)
QCompResult	To display Quick Compare results
Report	To display report blocks
SearchResults	To display the result of a search performed using <i>Spectrum Search</i> and other Search commands
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.
VideoPostrun	Video post-run window

6.3.1 Text View

To enter text select the *Text View* window from the drop-down list, which is indicated by the  **Text-Display - default.ows** 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 *I* arrow key to mark a text passage. If you want to delete text, 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 68 and 69.

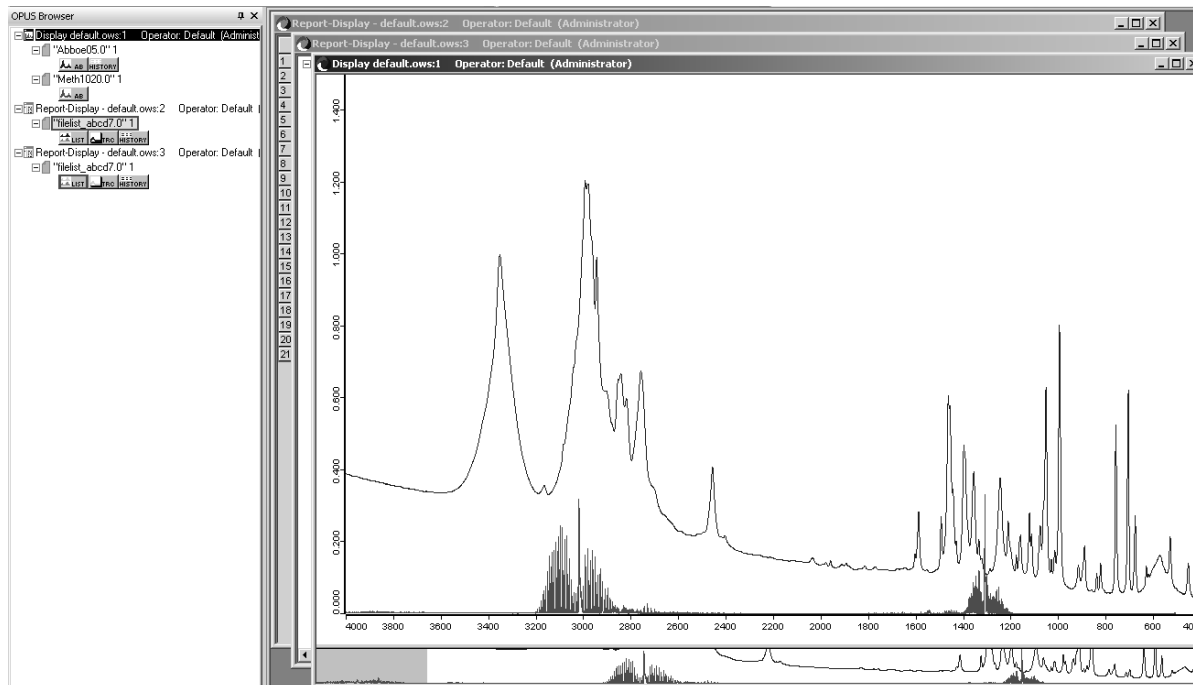


Figure 68: OPUS user interface - Cascaded windows

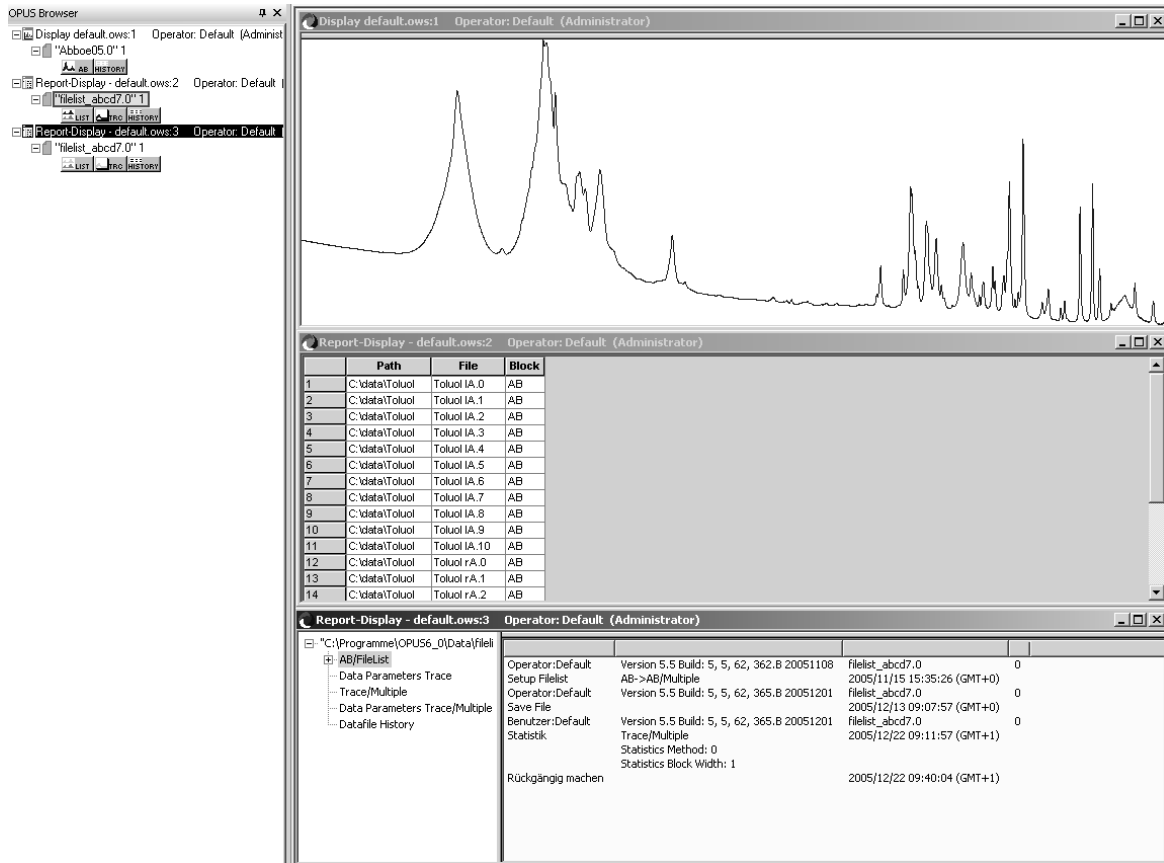


Figure 69: OPUS user interface - Tiled windows

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 70: 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.

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.

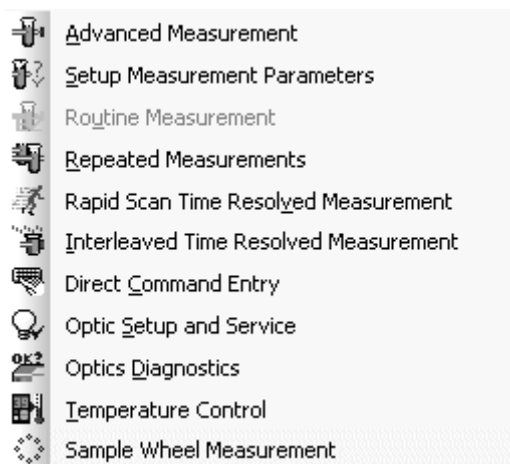


Figure 71: Measure menu

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 72 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 72), provided no Ethernet connection has been used.

7.1.1 Optical Bench

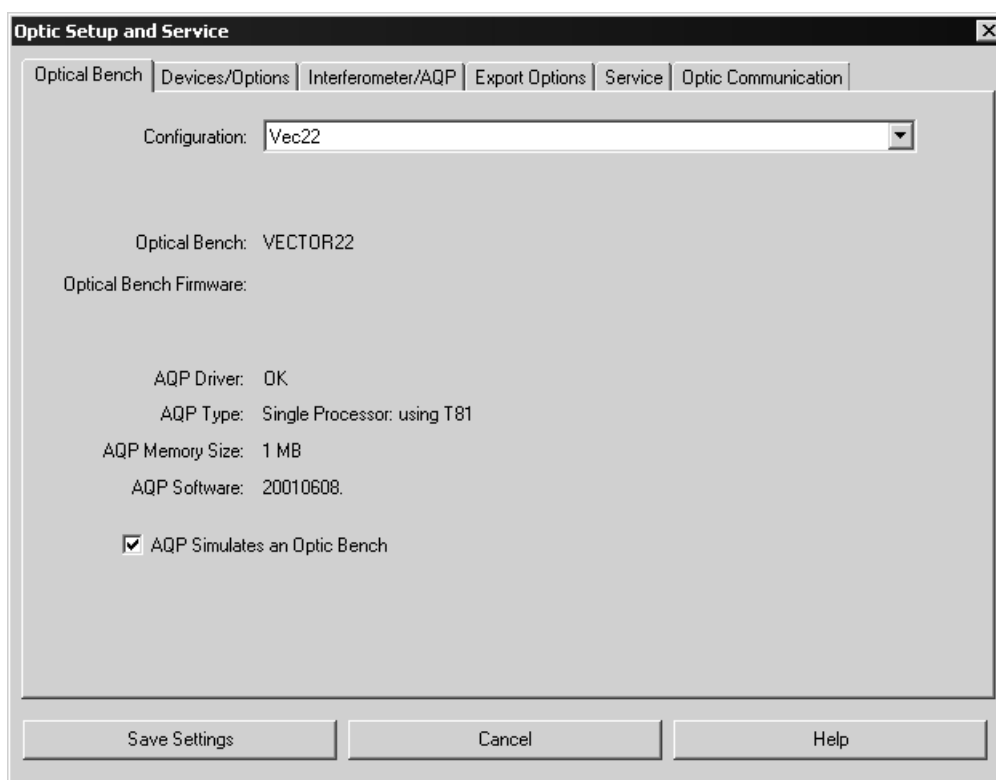


Figure 72: Optic Setup and Service – Optical Bench tab with VECTOR configuration

If the *AQP simulates an Optic Bench* check box is activated, the communication between OPUS and the 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 73).

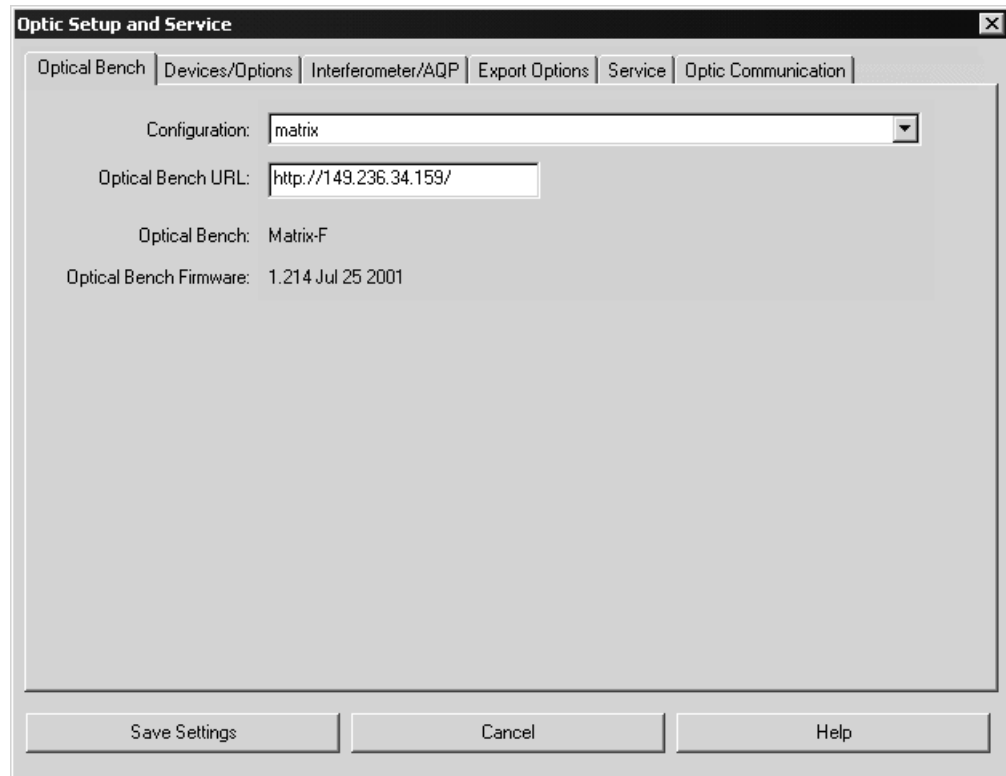


Figure 73: Optic Setup and Service – Optical Bench tab with MATRIX configuration

7.1.2 Devices/Options

On the *Devices/Options* tab you specify the components installed on the spectrometer. Make sure that the settings correspond to the spectrometer configuration. To activate a component, select the respective check box (see figure 74).

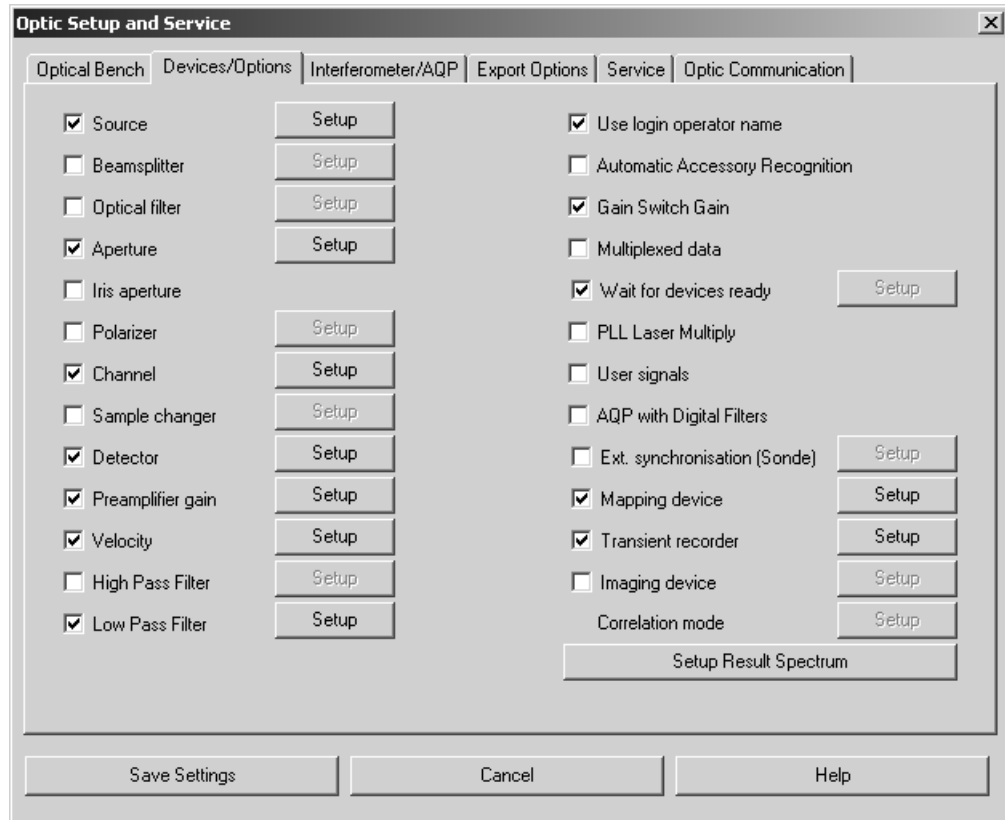


Figure 74: Optic Setup and Service – Devices/Options tab

All available options can be configured using the *Setup* button. Figure 75 exemplifies a detector configuration.

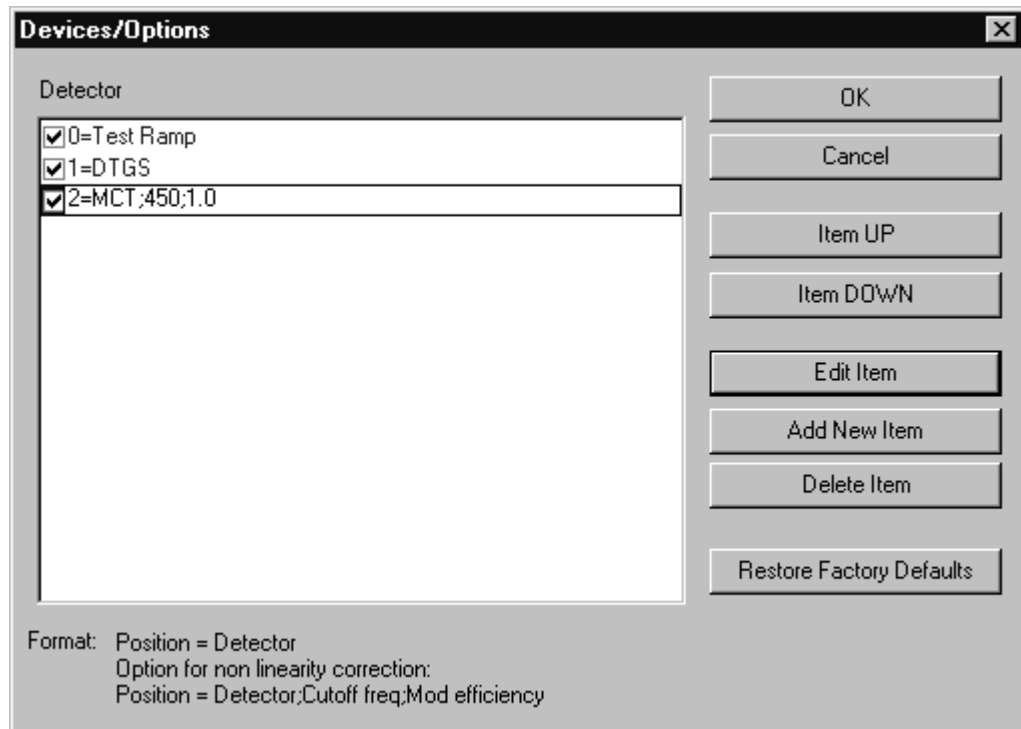


Figure 75: Detector configuration

Figure 75 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 76).

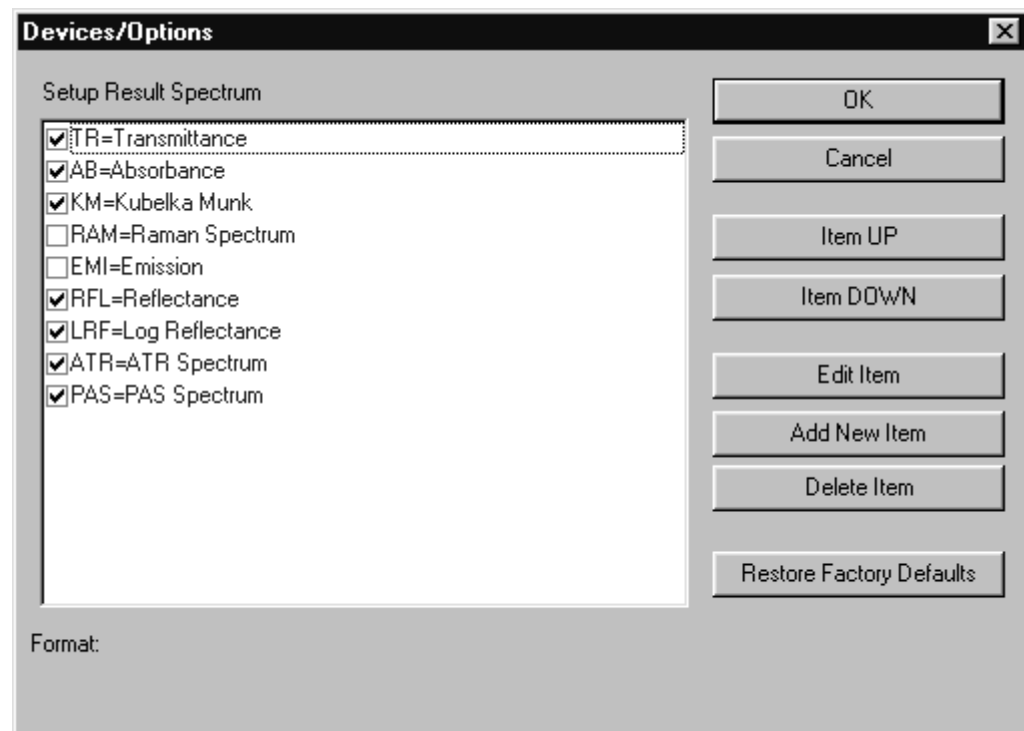


Figure 76: Setup Result Spectrum

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 a 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 77).

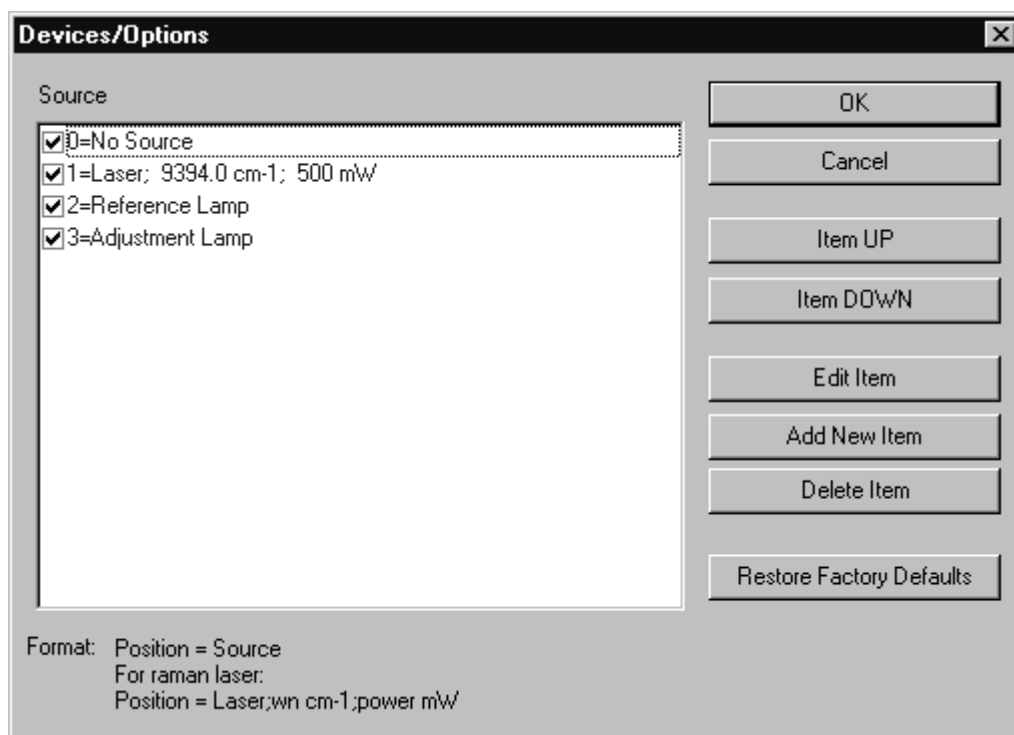


Figure 77: Source settings in case of Raman instruments

7.1.3 Interferometer/AQP

On the *Interferometer/AQP* tab of the *Optic Setup and Service* dialog (see figure 78) you can set the values for the absolute peak position, laser wavenumber, resolution, data rate and the maximum FT size.

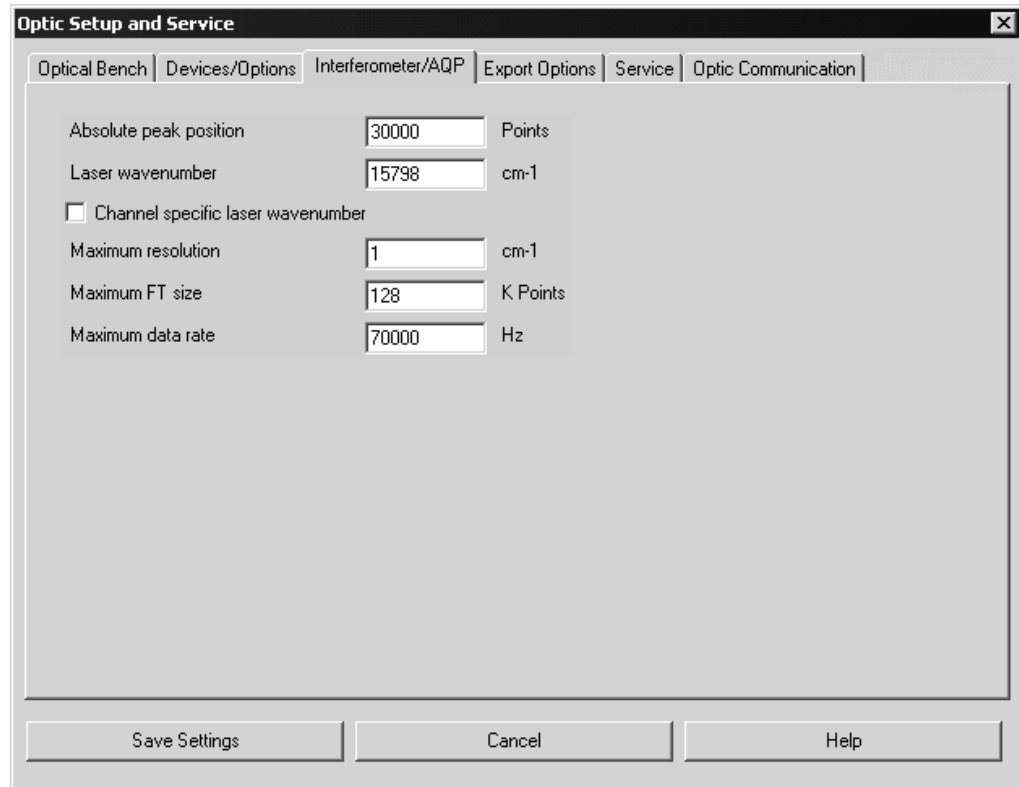


Figure 78: Optic Setup and Service - Interferometer/AQP tab

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 measurements, the laser wavenumber 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 79). 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.

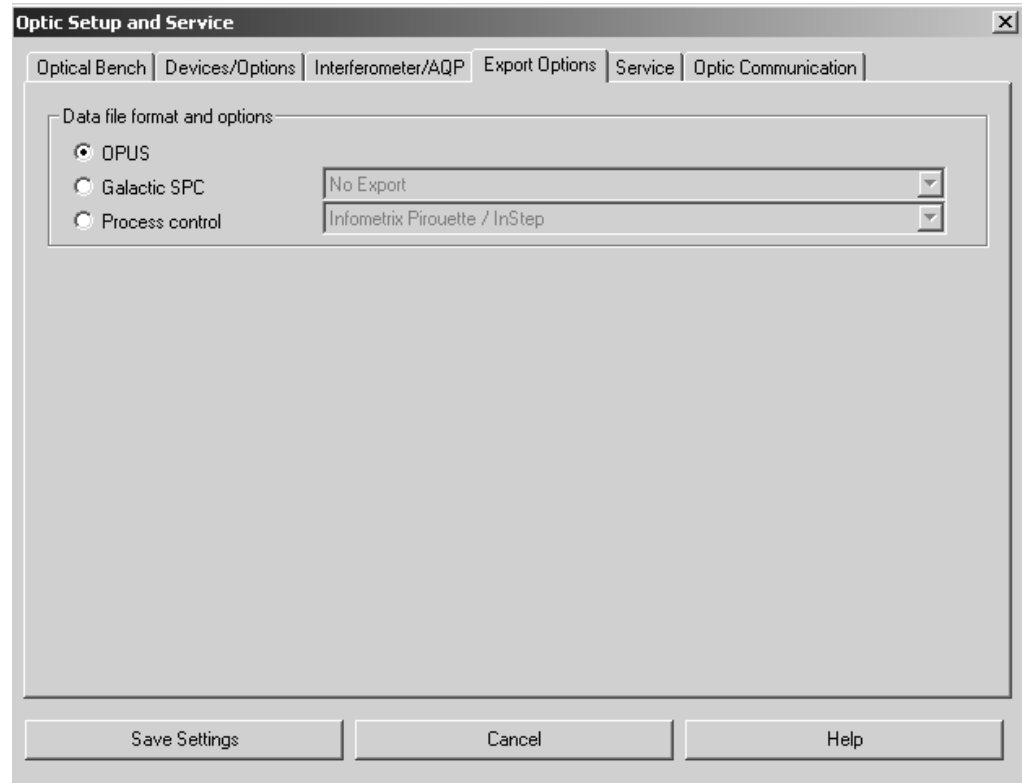


Figure 79: Optic Setup and Service - Export Options tab

7.1.5 Service

The *Service* tab (see figure 80) 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.

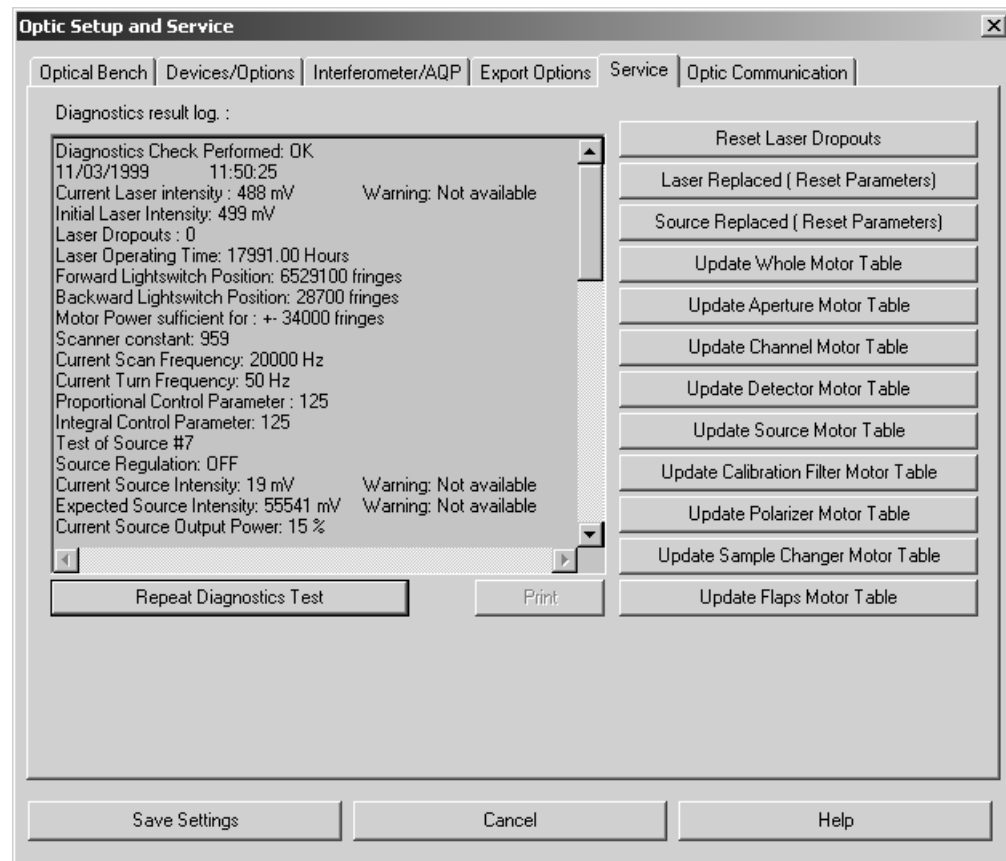


Figure 80: Optic Setup and Service - Service tab

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 when replacing 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 81). Check the *Auto Scroll* box if you want the list to automatically scroll.

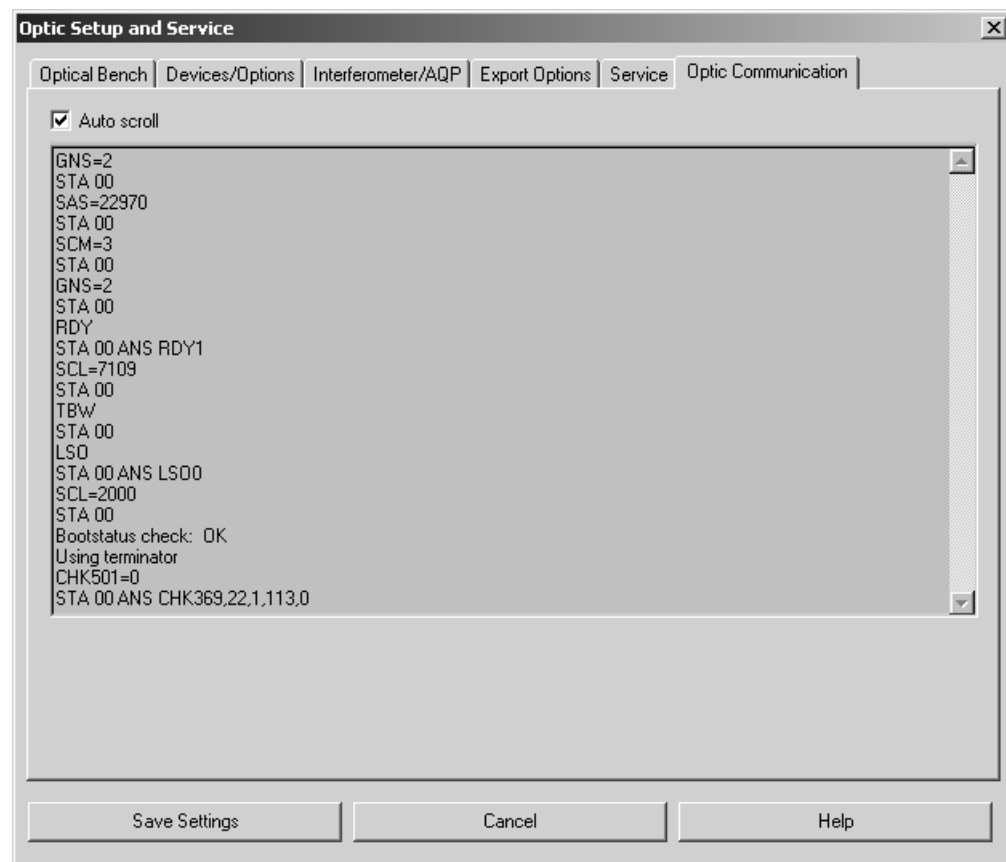


Figure 81: Optic Setup and Service - Optic Communication tab

In case of spectrometers connected by a network the *Optic Communication* tab includes the appropriate URLs.

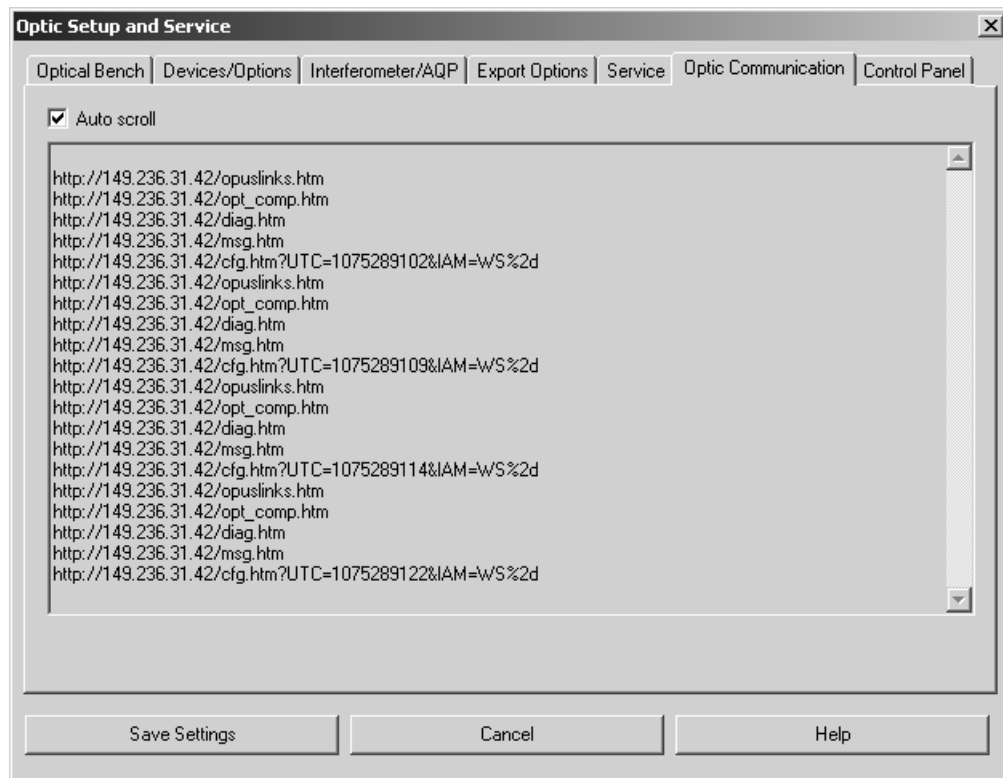


Figure 82: Optic Setup and Service - Optic Communication With URLs

7.1.7 Control Panel

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

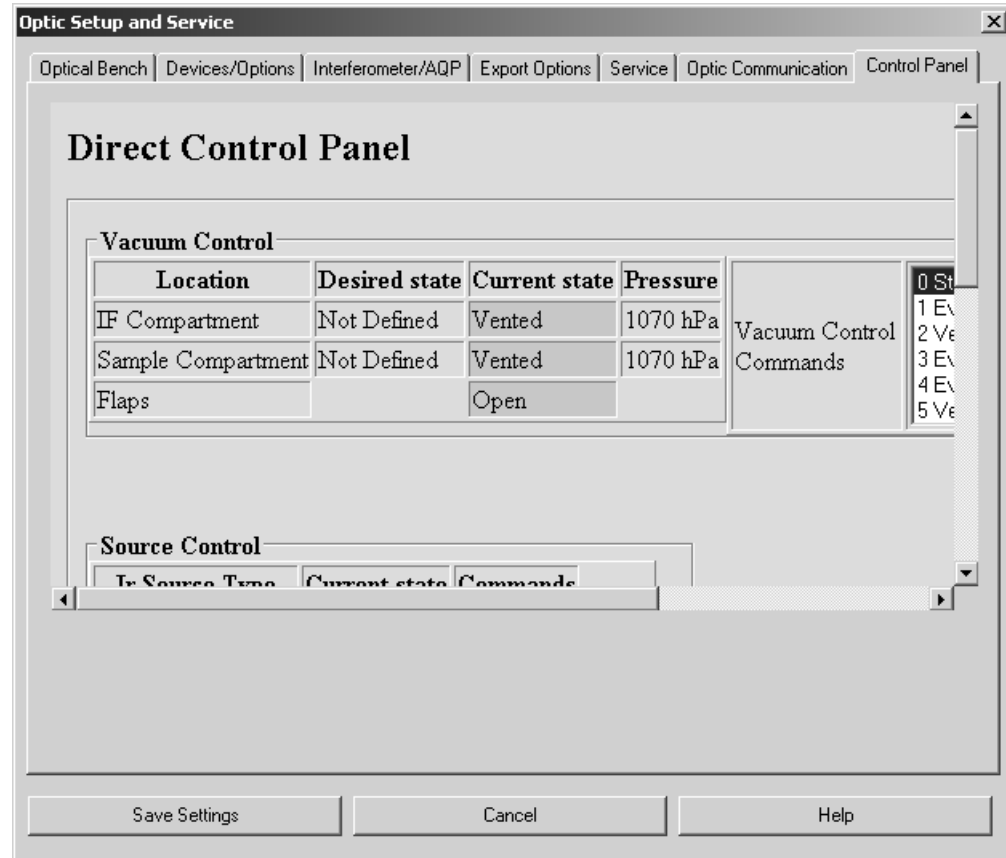


Figure 83: Optic Setup and Service - Control Panel tab

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 14.9), 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 7.2.12.

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 98). 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:

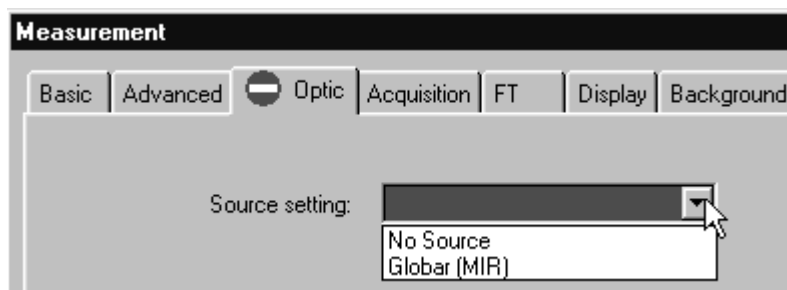



Figure 84: Error caused by wrong selection

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 *Global (MIR)*. This means, that *Global (MIR)* has been entered as source in the method, but the spectrometer is not equipped with a global. Open the *Source Setting* drop-down list to see the sources available. After correcting the entry, the warning symbol will disappear.

Example 2:

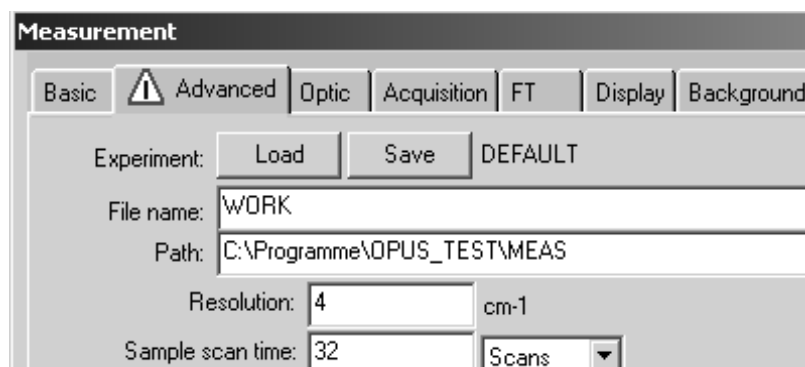



Figure 85: Error caused by wrong parameter

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 85 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

Wanted high frequency limit: 7899.00 cm-1

to

Wanted low frequency limit: 607.62 cm-1

Consequently, the  symbol will be displayed on the *Advanced* tab. Place the cursor on the respective entry field, to have the help text displayed.

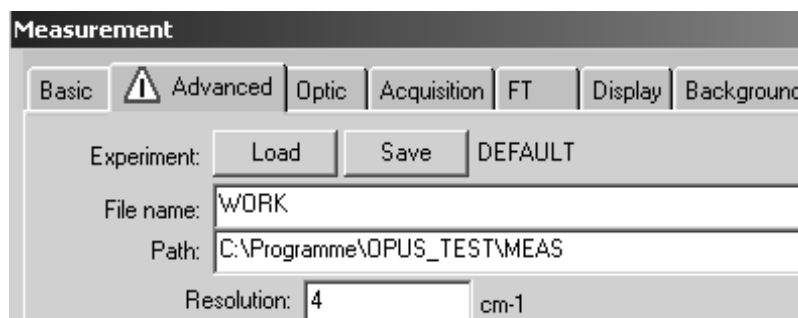


Figure 86: Error caused by wrong frequency limit

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.

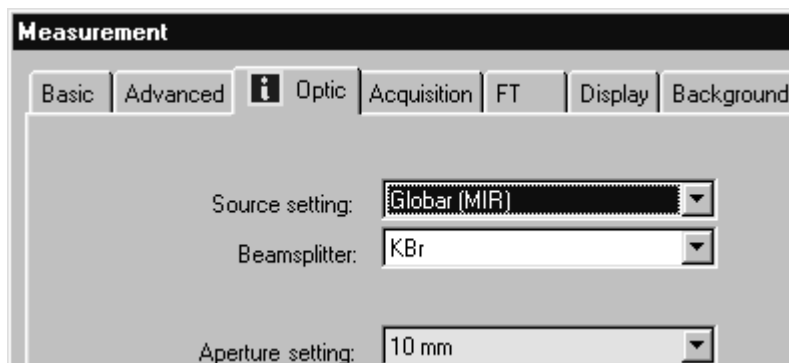





Figure 87: Information about restrictions on measurement

The measurement can be performed, but the resolution desired cannot be achieved above a wavenumber 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 the *User settings* command 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.

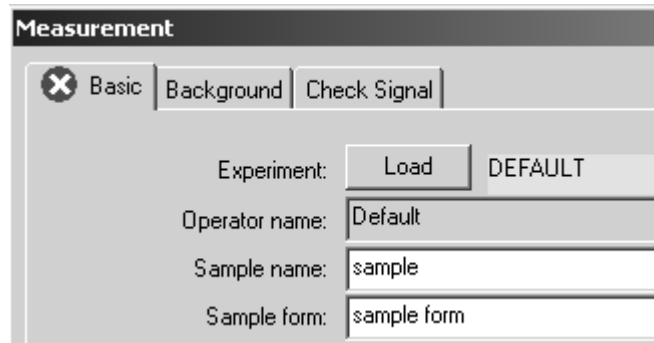


Figure 88: Error caused by limited user rights

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.

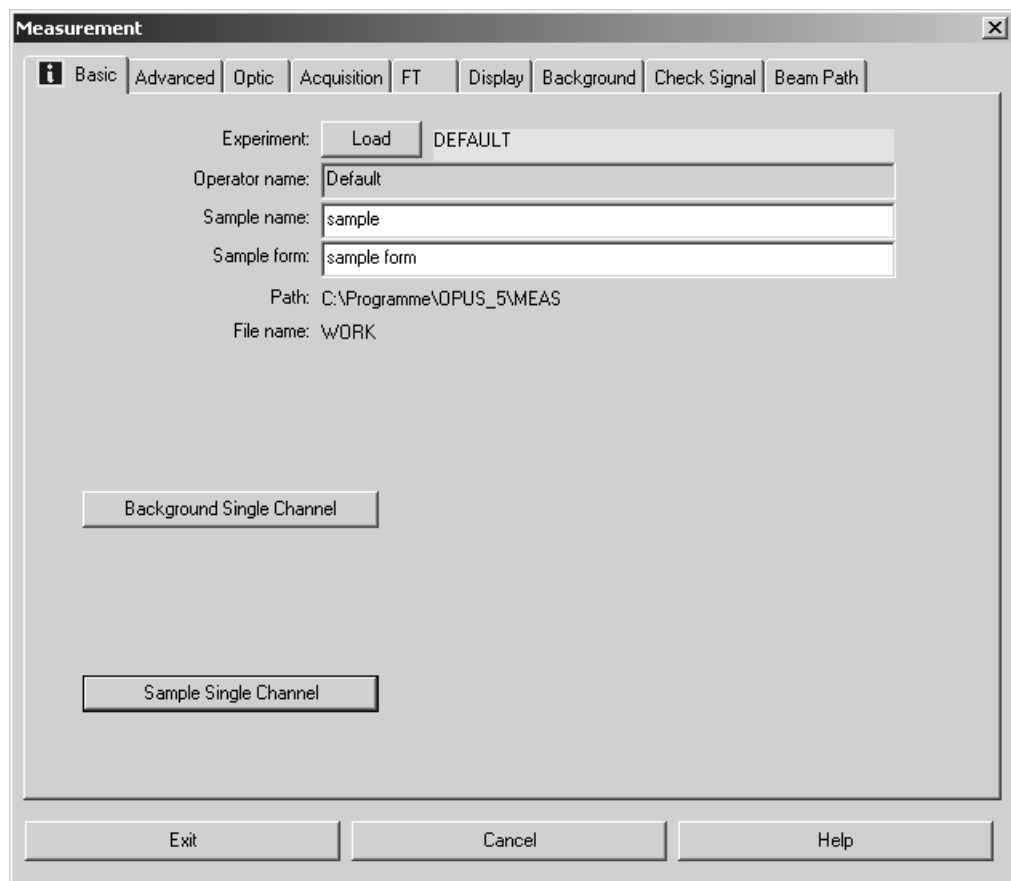


Figure 89: Measurement – Basic tab

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 commands.

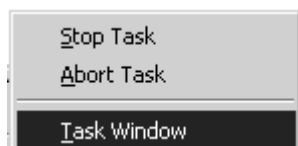


Figure 90: Pop-up menu to stop tasks

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

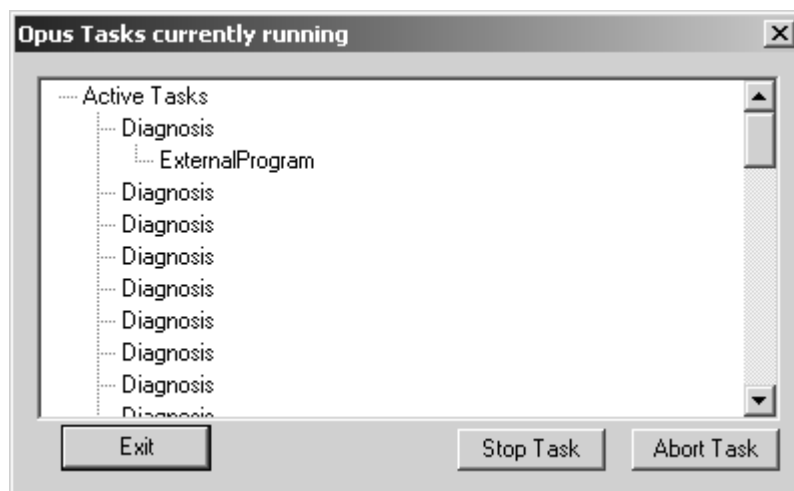


Figure 91: OPUS task list

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.

Note: When defining the file name you can also use information from the sample name. Enter the *<SNM>* parameter into the *File name* entry field. If you want to use several pieces of information from the sample name, you have to separate them by pointed brackets, e.g. *<SNM> <WSN>*. It is also possible to read only single characters from a particular entry field to define the file name, e.g. *<6SNM>* would indicate the first 6 characters of the sample name, *<2.4SNM>* the next 4 characters from position 2.

You can also use numbers, letters and characters for the file name. Below you find a list of possible formats. For details on OPUS parameters refer to appendix A:

a	Abbreviated weekday name
A	Full weekday name
b	Abbreviated month name
B	Full month name
c	Date and time representation appropriate for locale
d	Day of month as decimal number (01 – 31)
H	Hour in 24-hour format (00 – 23)
I	Hour in 12-hour format (01 – 12)
j	Day of year as decimal number (001 – 366)
m	Month as decimal number (01 – 12)
M	Minute as decimal number (00 – 59)
p	Current locale A.M./P.M. indicator for 12-hour clock
S	Second as decimal number (00 – 59)
U	Week of year as decimal number, with Sunday as first day of week (00 – 53)
w	Weekday as decimal number (0 – 6; Sunday is 0)
W	Week of year as decimal number, with Monday as first day of week (00 – 53)
x	Date representation for current locale
X	Time representation for current locale
y	Year without century, as decimal number (00 – 99)

Y
Year with century, as decimal number

z, Z
Either the time-zone name or time zone abbreviation, depending on registry settings; no characters if time zone is unknown

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.

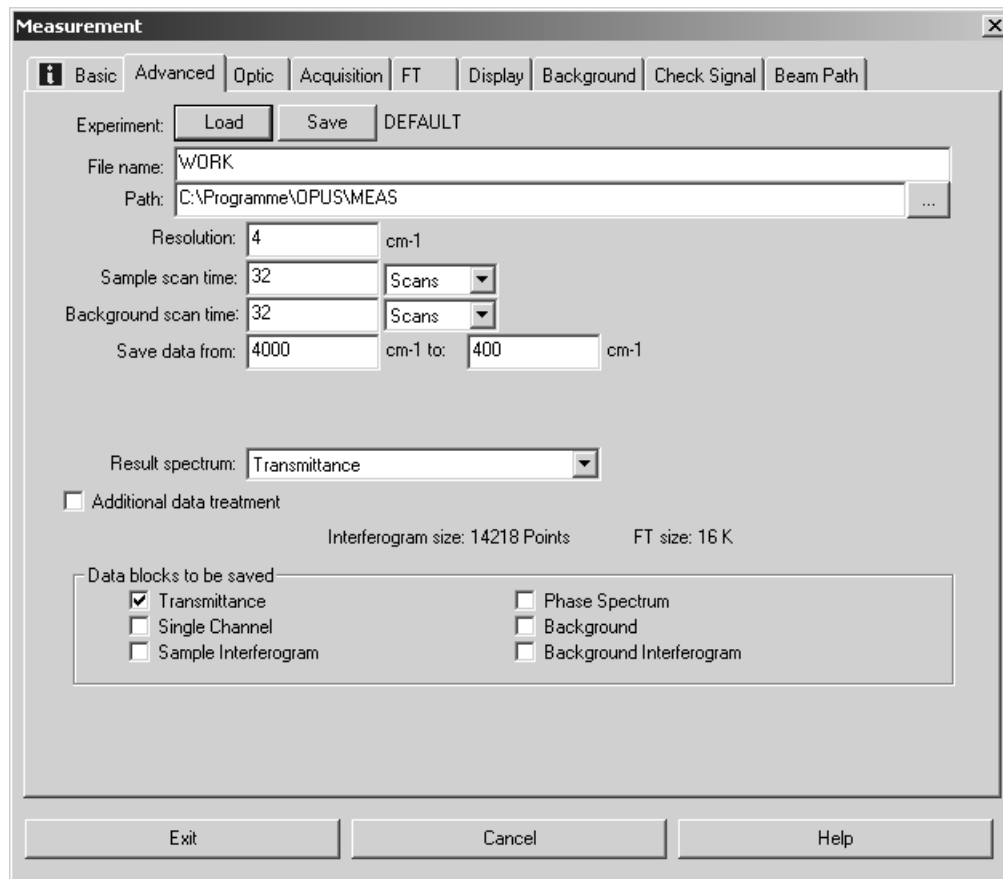


Figure 92: Measurement – Advanced tab

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 92 *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 93 may be different.

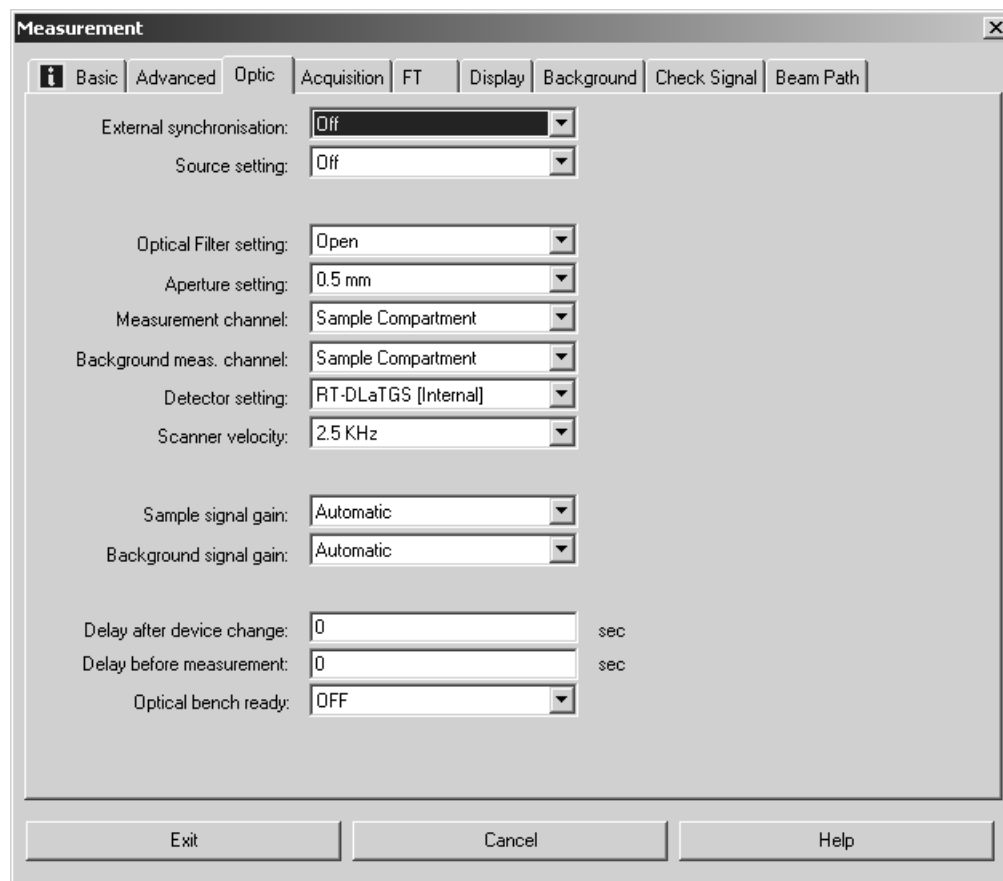


Figure 93: Measurement – Optics tab

Select an aperture setting from the *Aperture Setting* drop-down list. The aperture size defines the spectral resolution. An aperture diameter A causes a spectral peak broadening¹ $\delta\sigma$ at a wavenumber σ (provided a fixed focal length F of the collimated mirror in front of the interferometer is given):

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

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 photoacoustic 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.

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

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 intervals in 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 *Acquisition* 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 94).

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.

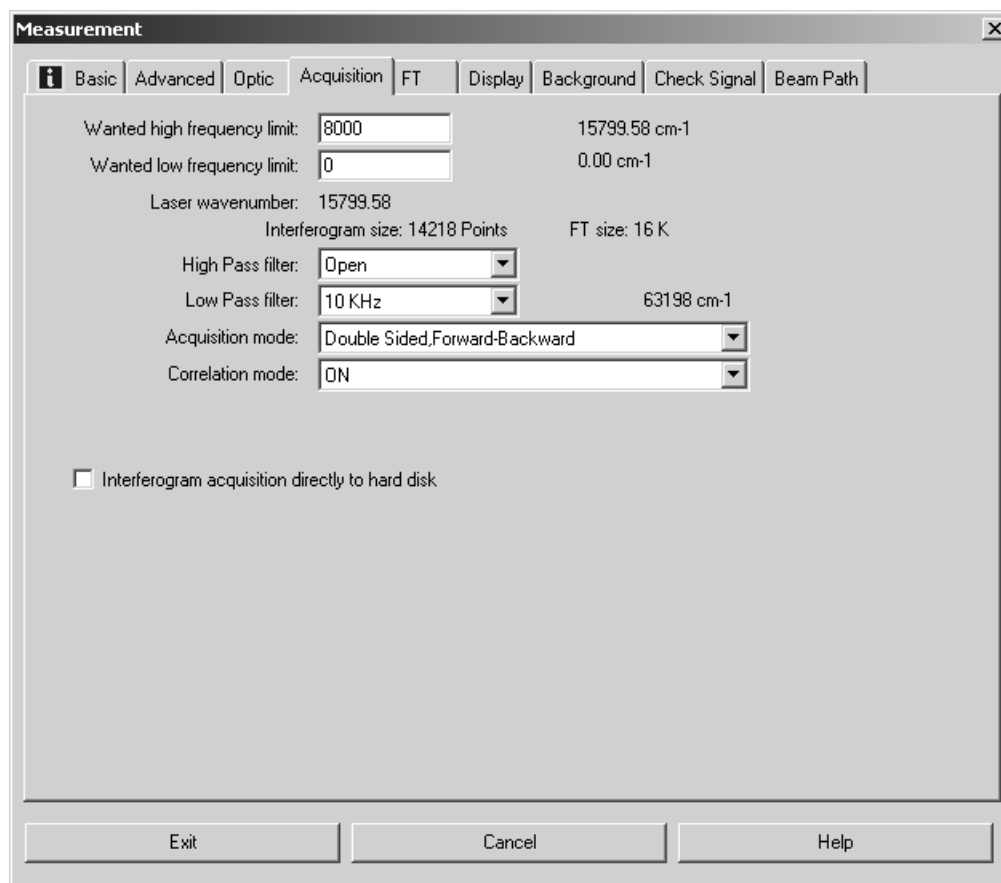


Figure 94: Measurement – Acquisition tab

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 wavenumbers 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 wavenumber σ which depends on v as follows:

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

In case of 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:

$$S/N (\text{no } \textit{Fast Return}) < S/N (\textit{Fast Return}) < S/N (\textit{Forward/Backward})$$

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 10 defective areas or if the number of defective points exceeds one eighth of the total number of interferogram points.
- *Reject Scans Exceeding ADC Limits*: if selected, two additional entry fields are available for defining the low and high ADC limit in this case. This means that scans with a signal amplitude above or below a fixed limit can be rejected. In contrast to *Around Peak Low* new interferograms do not depend on the first scan. Furthermore, there are three option buttons which allow to define when to finish the mea-

surement. By default, the first option button is activated. The other two allow manual input of up to 999 scans. This option is not supported by all types of spectrometer.

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.

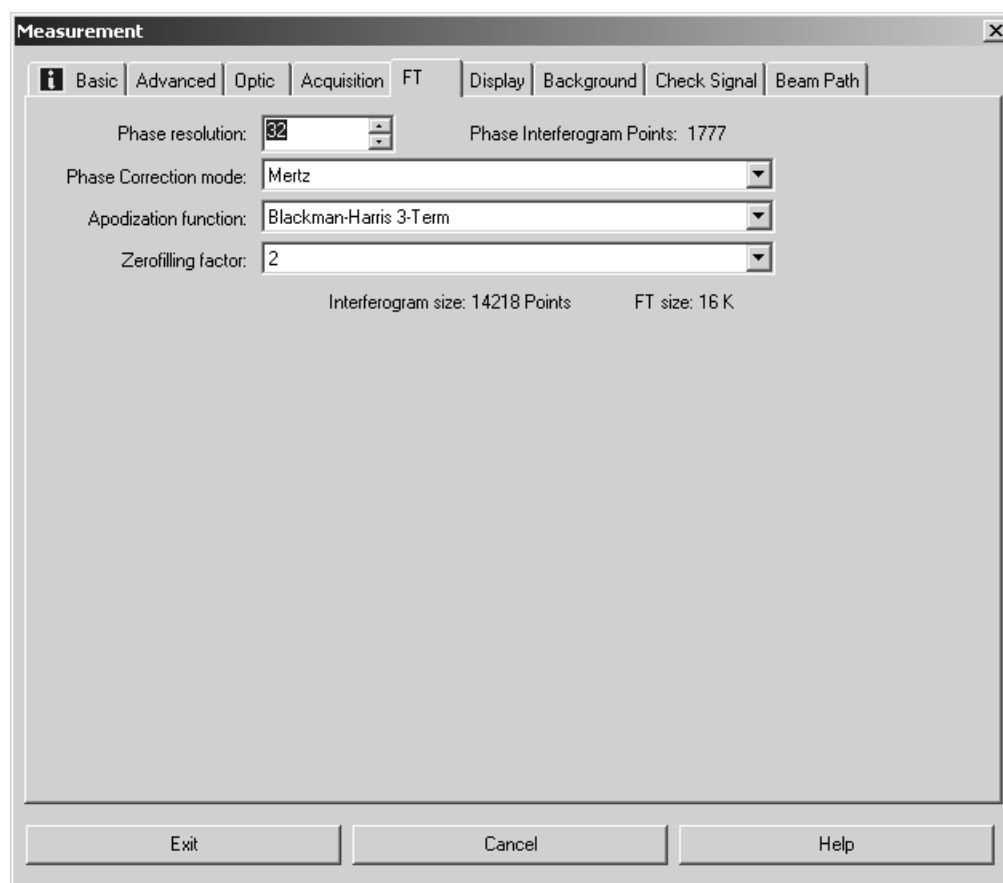


Figure 95: Measurement – FT tab

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.

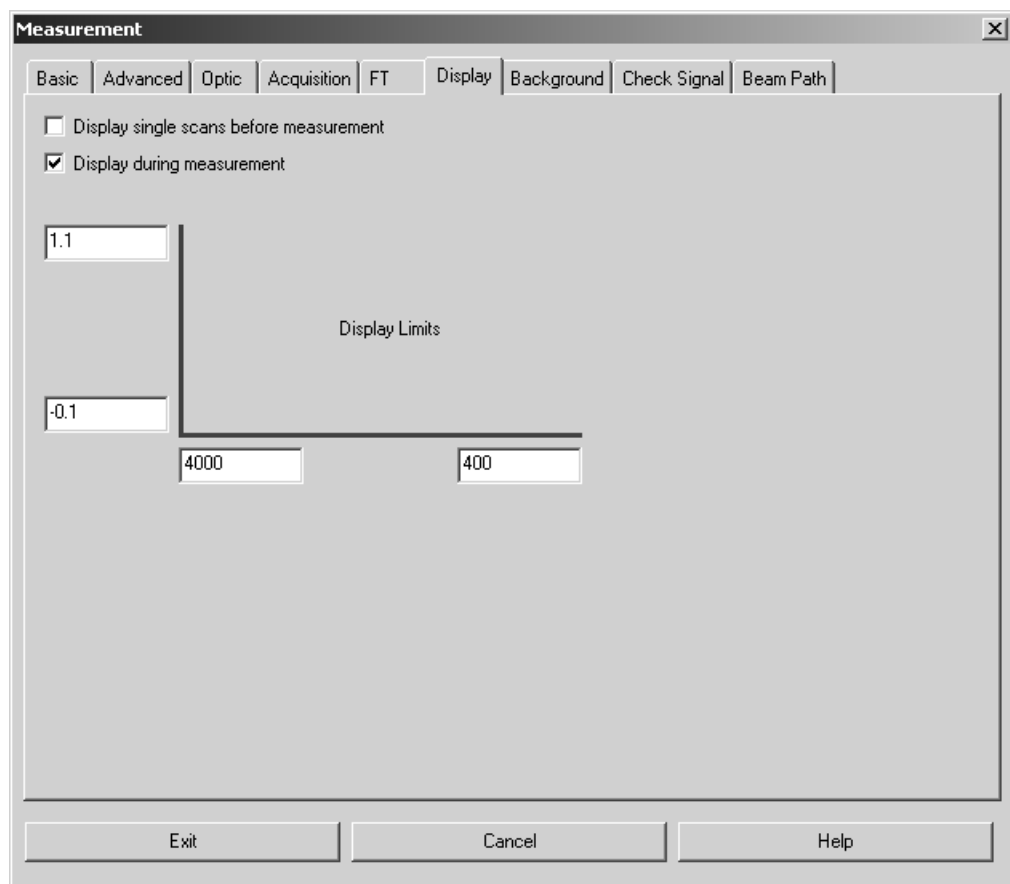


Figure 96: Measurement - Display tab

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.

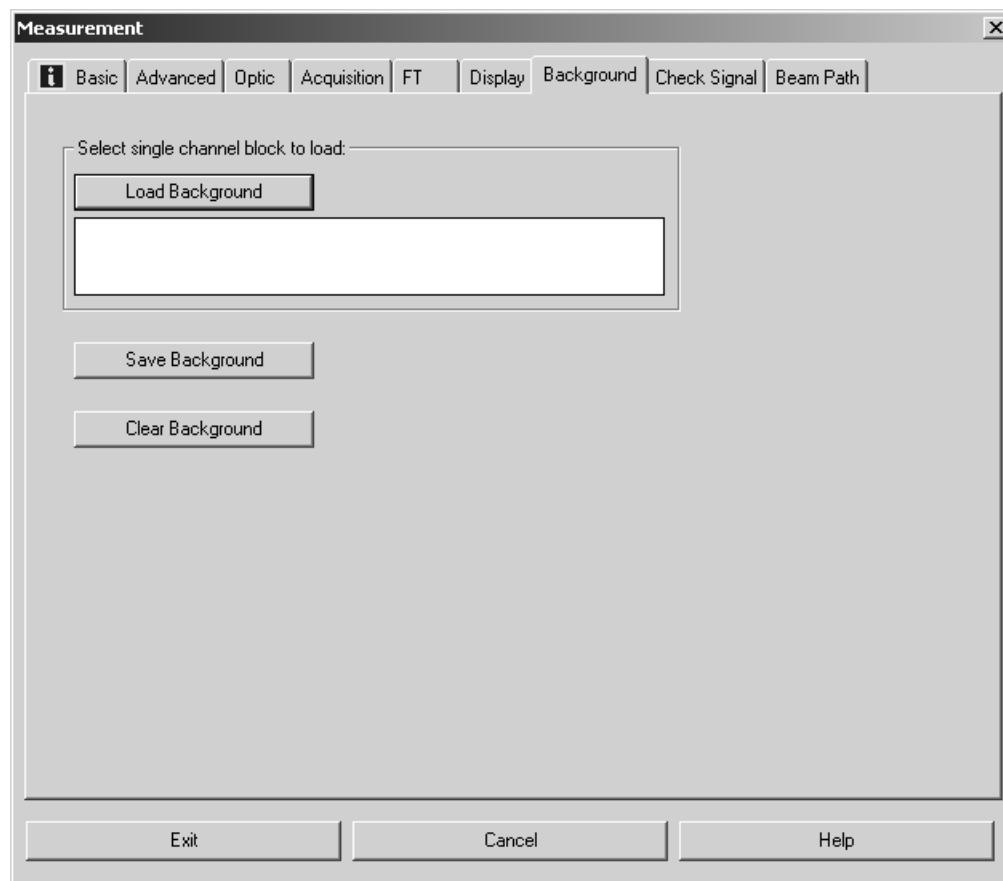


Figure 97: Measurement – Background tab

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 98 you may have additional functions available for your system.

To determine and save the exact interferogram peak position you 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.

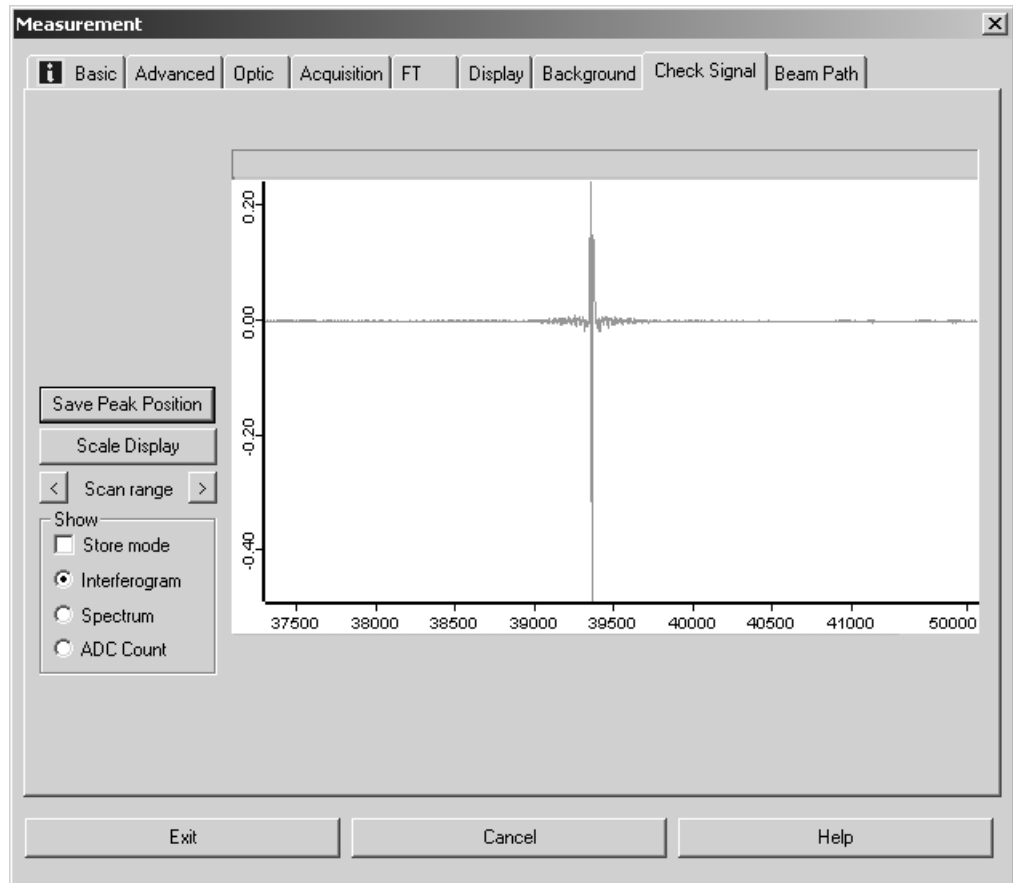


Figure 98: Measurement - Check Signal tab with interferogram

Similar to the spectrum display in the spectrum window you can also zoom in a particular section. The interferogram shown in figure 98 and 99 has been created by the AQP simulation mode. Therefore, the interferograms of your spectrometer used may be different.

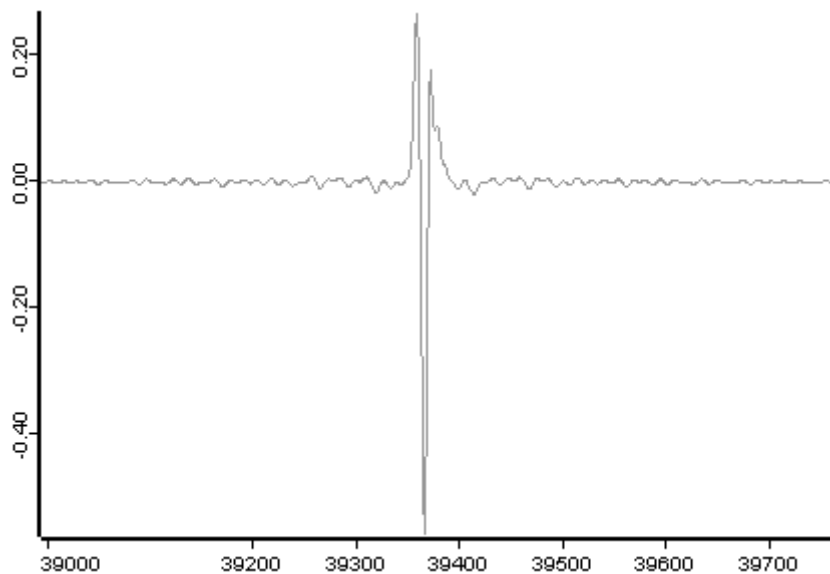




Figure 99: Interferogram zoomed-in

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 interferogram 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.

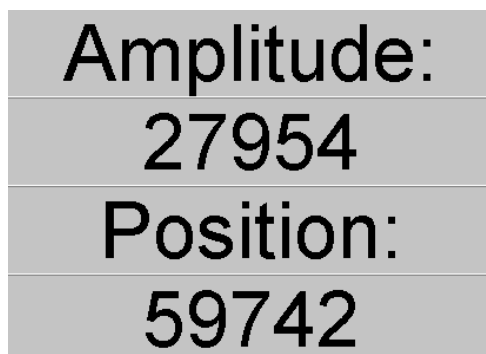


Figure 100: Numerical display of ADC count


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.



Figure 101: 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. To restore the motor position to 0 click on the *Restore* button.

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 graphically 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 102 shows a TENSOR 27 beam path. If an accessory is inserted in the spectrometer sample compartment, it is also graphically displayed.

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.

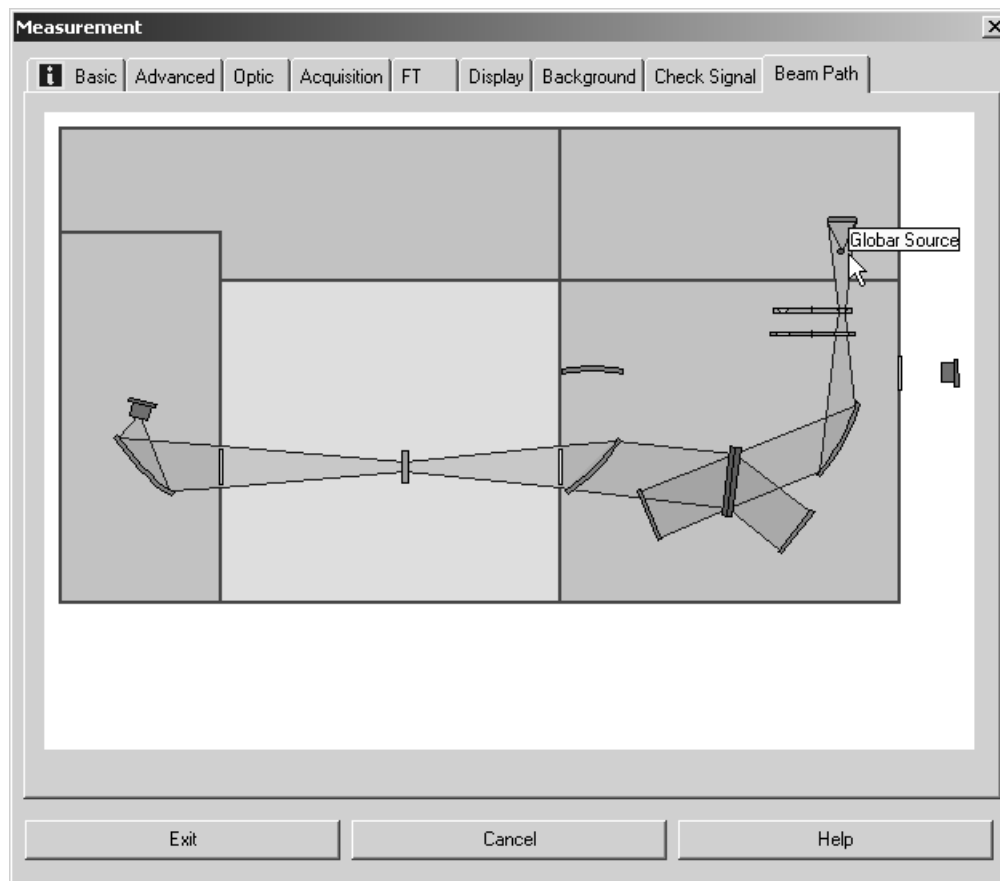


Figure 102: Measurement - Beam Path tab (TENSOR 27)

7.2.11 Spectral Range Selection

For spectrometers supporting the graphical beam path (e.g. TENSOR, VERTEX) the *Spectral Range Selection* tab allows to interactively select the frequency range for a measurement. The optical components are automatically selected and the measurement can be started immediately.

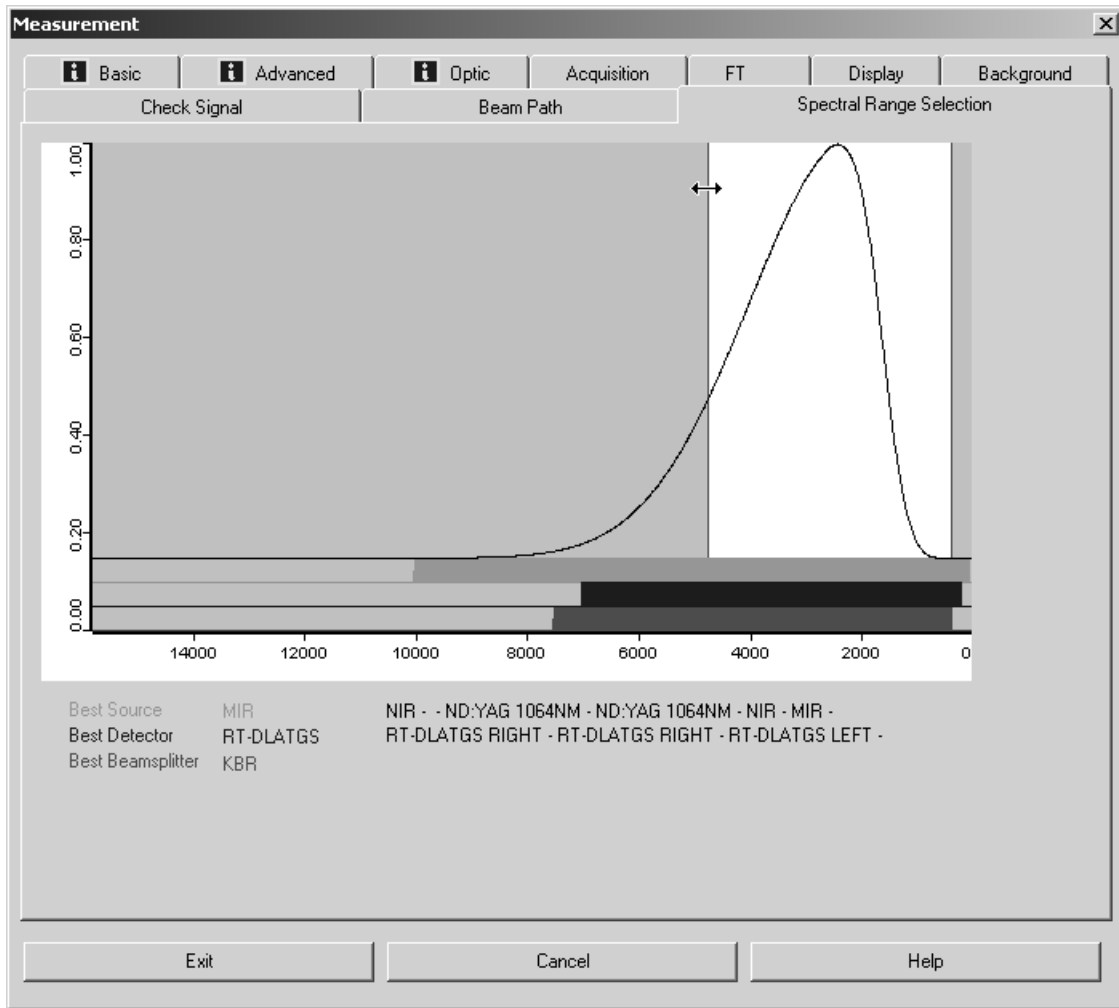


Figure 103: Spectral Range Selection tab - TENSOR 27

To select the frequency range position the cursor on the area edge, the cursor will change into . Now, you can move the frequency range to the position desired.

To enlarge a particular range right click onto the frequency range and select the *Zoom* command from the pop-up menu.

The best optical components for the spectrometer connected are indicated below the graphics.

Best Source	MIR	NIR - - ND:YAG 1064NM - ND:YAG 1064NM - NIR - MIR -
Best Detector	RT-DLATGS	RT-DLATGS RIGHT - RT-DLATGS RIGHT - RT-DLATGS LEFT -
Best Beamsplitter	KBR	

Figure 104: Exemplary best optical components for TENSOR 27

7.2.12 Raman Measurements

In case of Raman measurements you can also specify the laser power on the *Basic* tab (see figure 105).

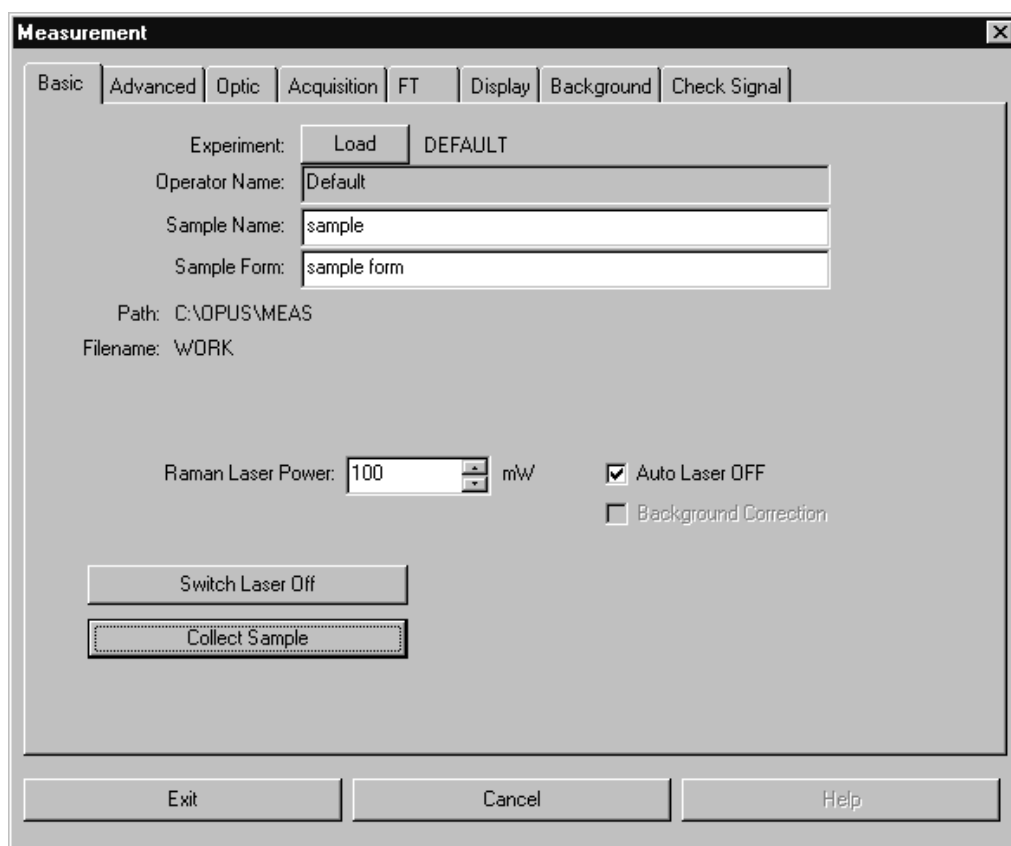


Figure 105: Raman Measurement - Basic tab

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.

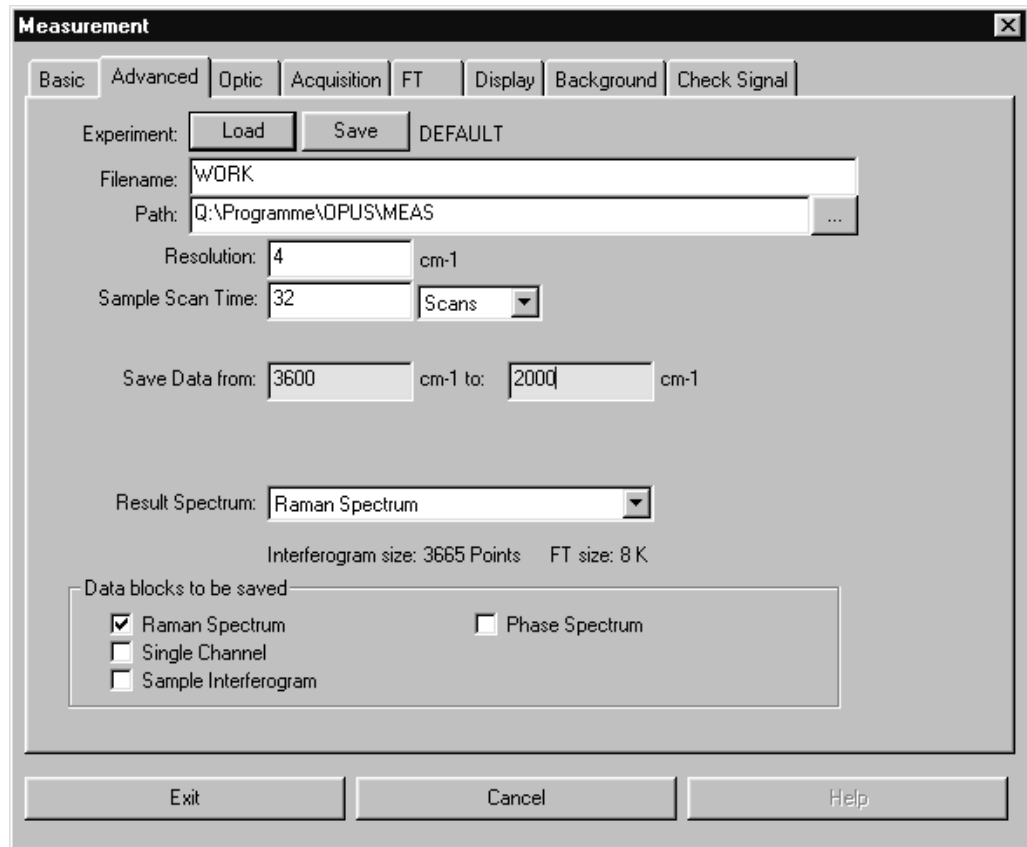


Figure 106: Raman Measurement – Advanced tab

On the *Acquisition* tab all frequencies are displayed in relation to the laser excitation energy.

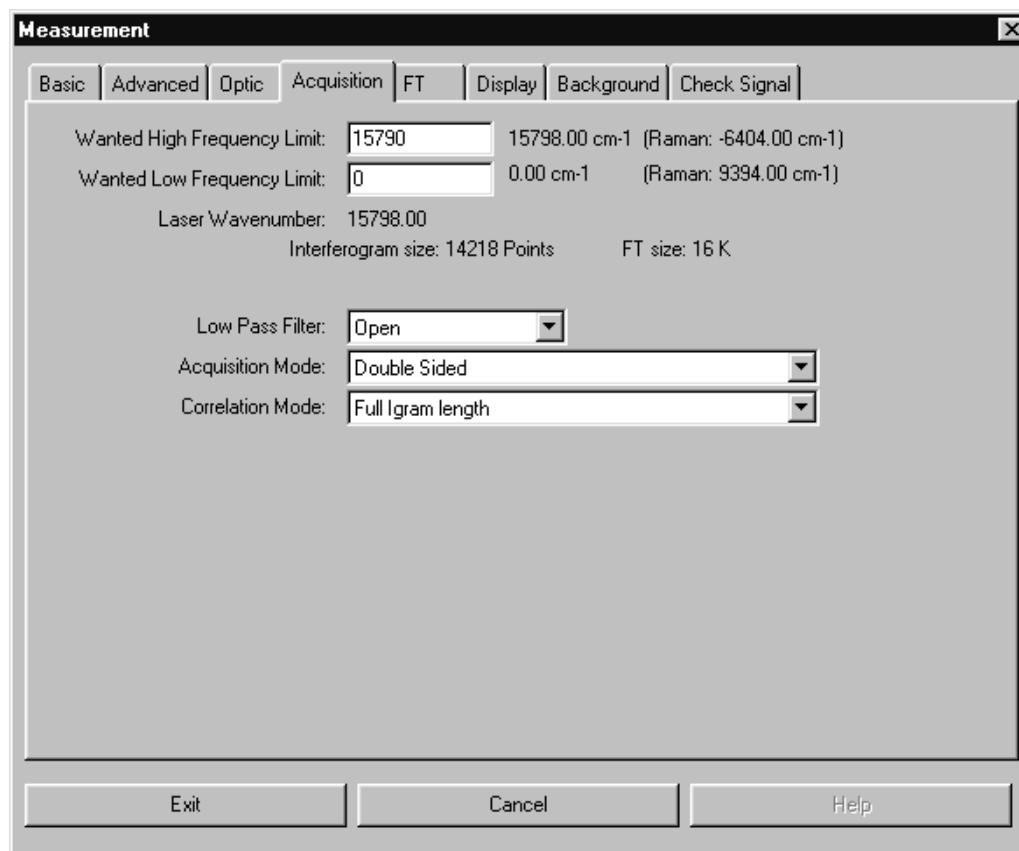


Figure 107: Raman Measurement – Acquisition tab

The laser power can be set using the slider on the *Check Signal* tab. The actual performance will be displayed.

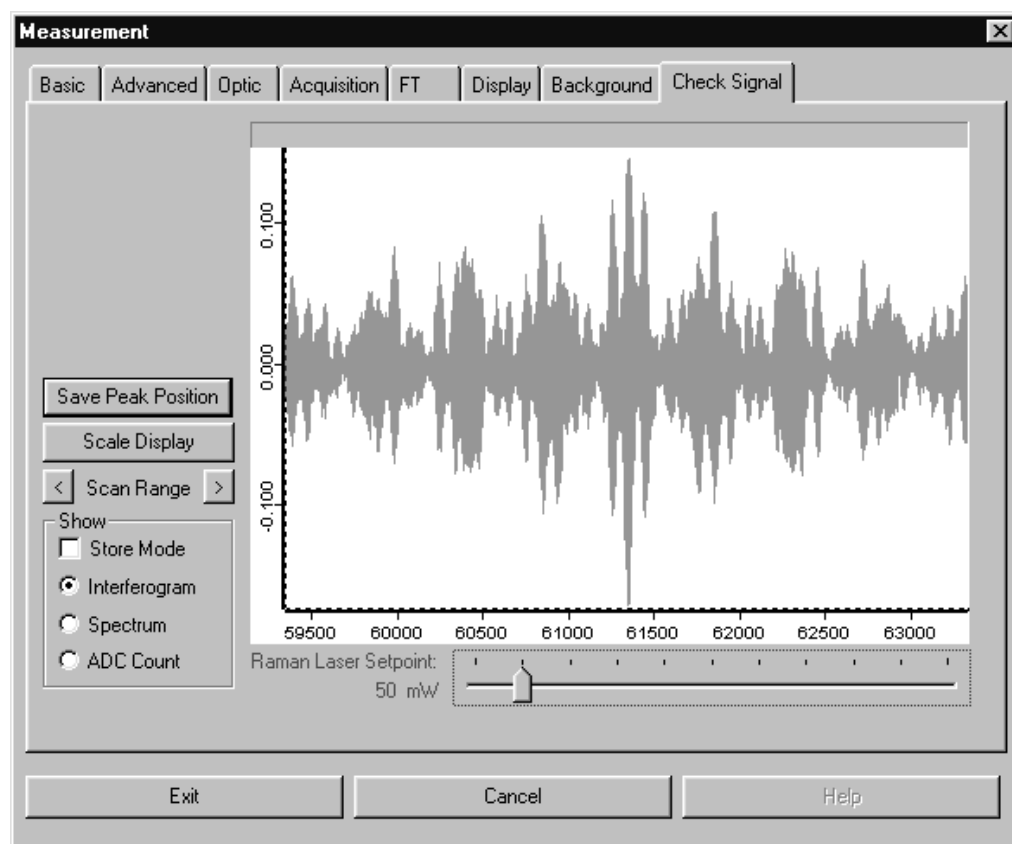


Figure 108: Raman Measurement - Check Signal tab

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.

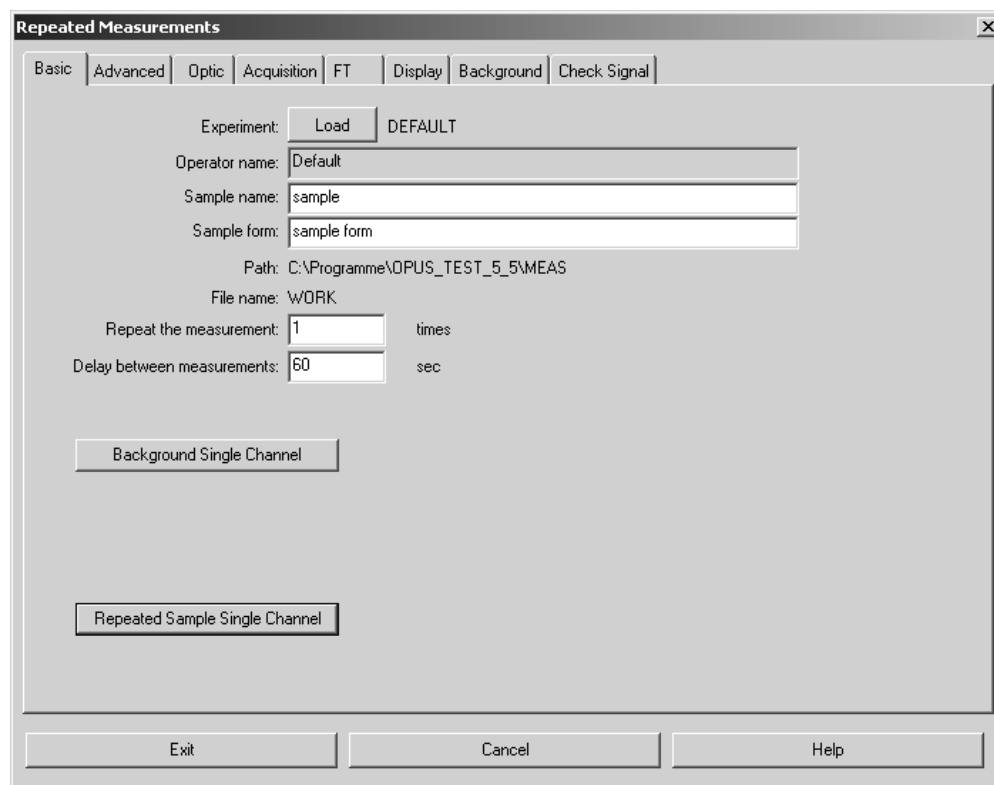


Figure 109: Repeated Measurements – Basic tab

7.4 Rapid Scan - Time Resolved Measurement

The *Rapid Scan Time Resolved Measurement* command allows 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 7900cm^{-1} and single-sided data acquisition:

AQP Memory	Max. Number of Interferograms (8cm ⁻¹)	Max. Number of Interferograms (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.

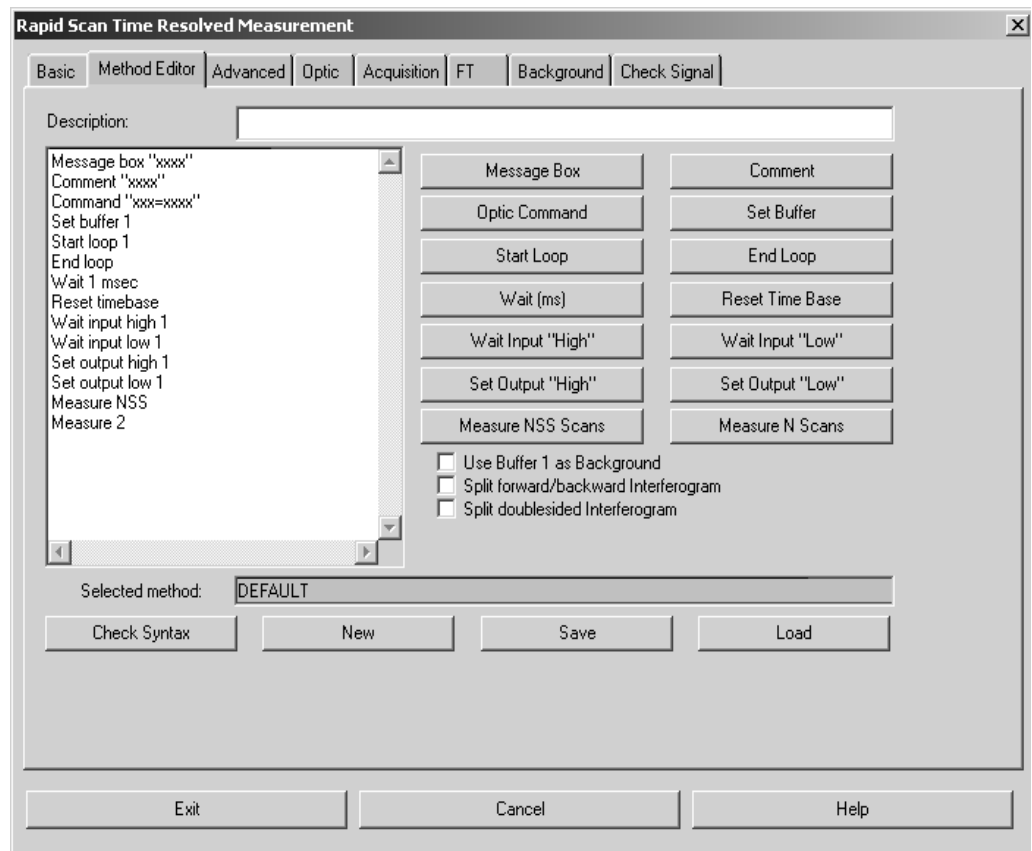


Figure 110: Rapid Scan Time Resolved Measurements – Method Editor tab

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 TTL¹ signal
- TTL signal output

1. Transistor-transistor-logic signal

- Optic commands output
- 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 110 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 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 110 shows the program code generated by these buttons. Below these buttons 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 110). 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 twice 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.

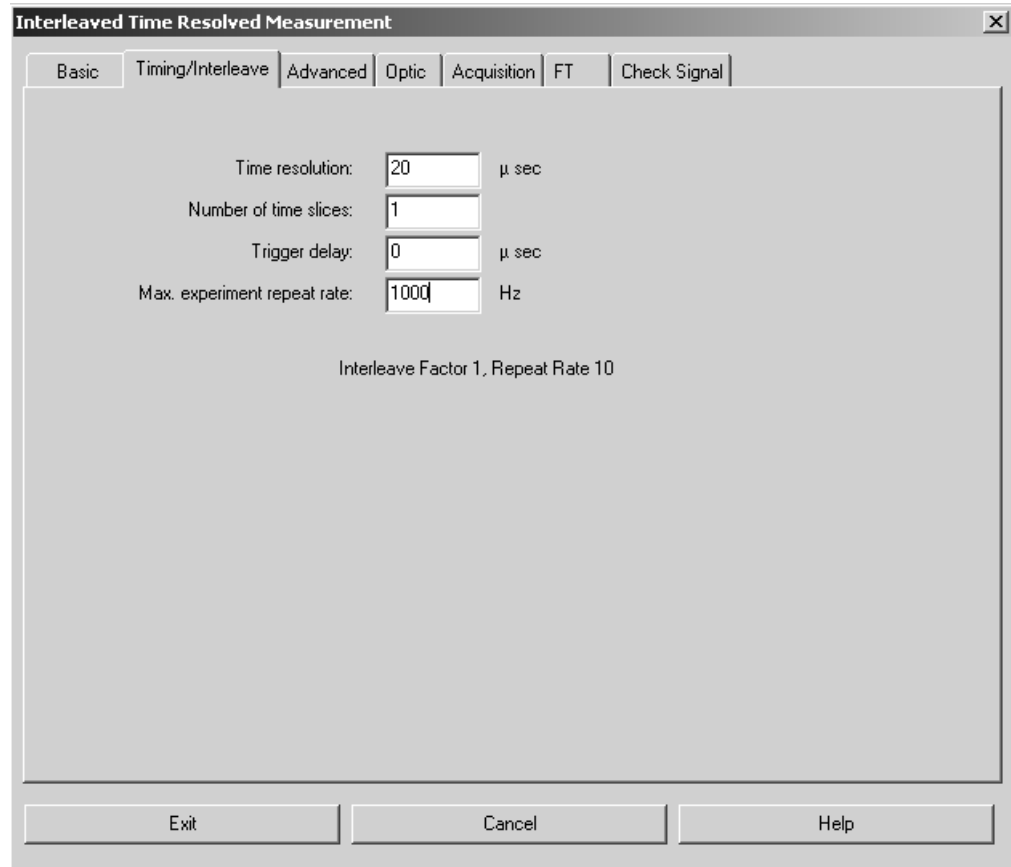


Figure 111: Interleaved Time Resolved Measurement - Timing/Interleave tab

- *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 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.

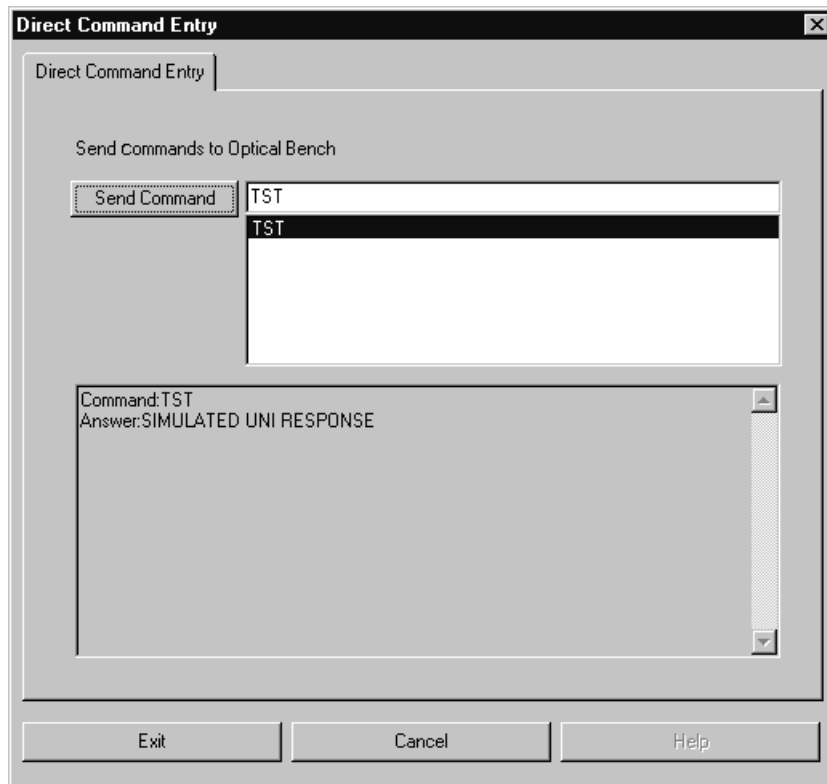


Figure 112: Direct Command Entry

7.7 Optics Diagnostics

The *Optics Diagnostics* command allows a quick check of the spectrometer components. The *Instrument Status* dialog will be described in the following.

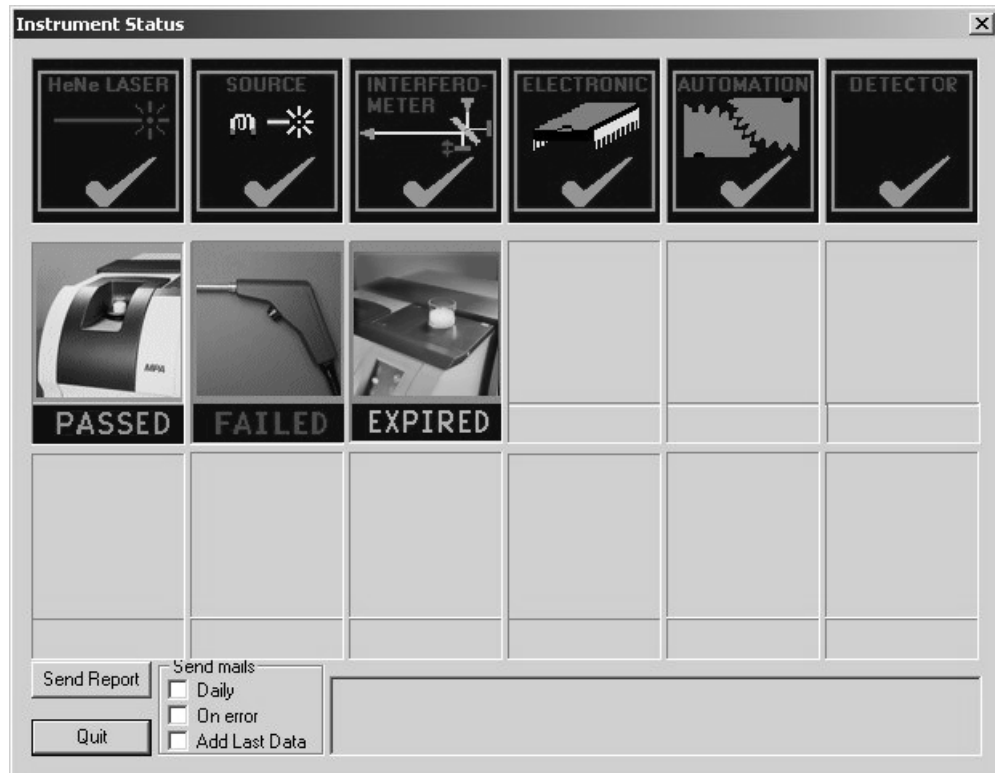


Figure 113: Optics Diagnostic - Instrument Status dialog

In OPUS there are two possibilities to have the instrument status indicated. By means of the status light (see also chapter 7.7.2) located in the bottom right corner of the OPUS interface, and by the icons displayed on the *Instrument Status* dialog.

There are two important distinctions to be considered: the status light indicates the status based on the currently active channel or measurement experiment loaded, whereas the icons in the *Instrument Status* dialog correspond to the respective test channel.

In the *Diagnose* dialog the hardware components, e.g. source, laser, interferometer etc. are displayed in the upper icon line. The status can be displayed as follows:

- **Green check mark:** component is okay
- **Yellow check mark:** lifetime of the component expires
- **Red check mark:** component defect

The second and third row of icons refer to the possible active test channels and indicate the result of the last instrument test performed. The results can be as follows:

- **PASSED** (green): test successfully performed and still valid
- **FAILED** (red): test failed or has not yet been performed
- **EXPIRED** (light-blue): test expired

The complete instrument status report can automatically be sent to Bruker Service by e-mail. Click on the *Send Report* button (figure 114). Different sending options are available.



Figure 114: Sending options for instrument report

You can define when the instrument report has to be sent, e.g. on a daily basis or as soon as errors occur in the report. For details on the diagnostics result log select the *Optic Setup and Service* command and click on the *Service* tab.

For details on how to define test channels in case of spectrometers which do not support OVP refer to chapter 14.9.1.

7.7.1 Diagnosis of Hardware Components

To perform a diagnosis of a particular hardware component click on the respective icon in the first icon row of the *Instrument Status* dialog. The following dialog opens:

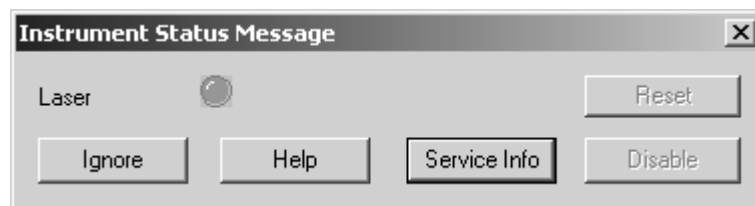


Figure 115: Instrument Status Message

Click on the *Service Info* button to have the status of the respective hardware component displayed. Figure 116 exemplifies a diagnosis page for the *Laser* hardware component.

Tensor 27 SN_MID0028 HeNe Laser Diagnostics Page

Back Refresh

Messages
No error

HeNe Laser

Current state	On		
Desired state	On	LSR=1	READY
Total run time	2 years, 49 days, 3 hours, 45 mn	since Wed, 21 Jan 2004 17:44:15	RESET

Page generated on Wed, 15 Mar 2006 10:03:03

Figure 116: Diagnosis page for HeNe laser

7.7.2 Status Light

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.

The color of the status light can be 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.

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 the IT channel positions defined in the *OVP Setup* dialog (see also chapter 13).

7.7.3 Status Light 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.

In this case you have to indicate an additional command using the *OPUS Properties* dialog, and to specify a time (in minutes) that OPUS should use to poll the current status of the active channel. Once during each interval, the particular status is polled, and the status light is updated. Right click on the *OPUS* icon of the *Windows Start* menu and select the *Properties* command. The following dialog opens:

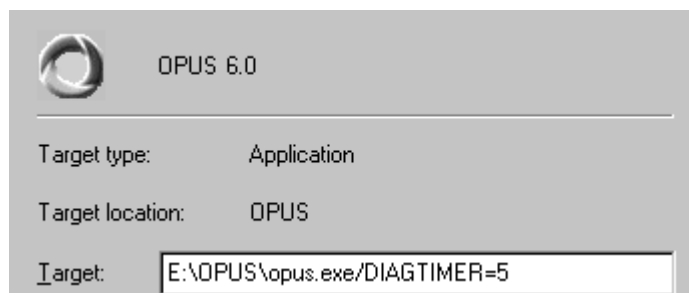


Figure 117: OPUS Property dialog

Enter the command line into the *Target* entry field. In figure 117 the */DIAGTIMER=5* command polls the status once every 5 minutes.

The status is not updated when loading an experiment file, it is only updated if the time interval has expired and the assigned program polled.

7.8 Temperature Control

The *Temperature Control* command allows the operation and control of external equipment, e.g. temperature-controlled stage.

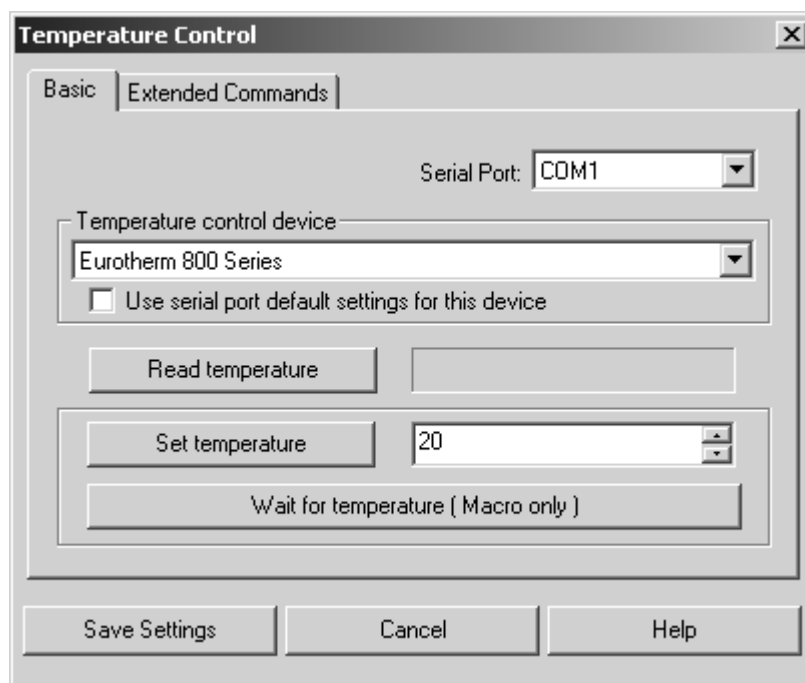


Figure 118: Temperature Control – Basic tab

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.

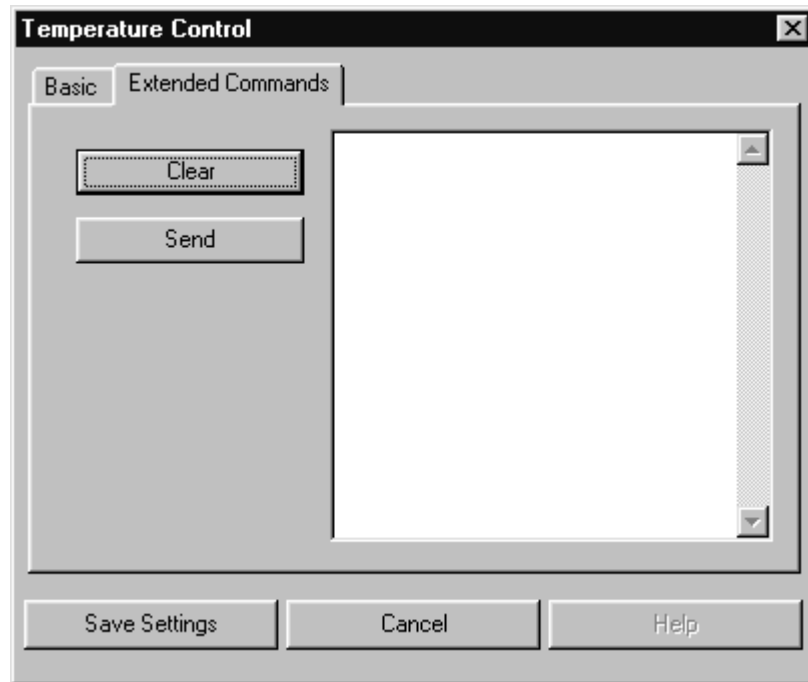


Figure 119: Temperature Control – Extended Commands tab

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. The *Clear* button provides a blank entry field. Save your command sequence using the *Save Settings* button.

7.9 Sample Wheel Measurement

This command can only be used in connection with spectrometers which are equipped with a sample wheel of 16 positions. If you select the *Sample Wheel Measurement* command, the following dialog opens:

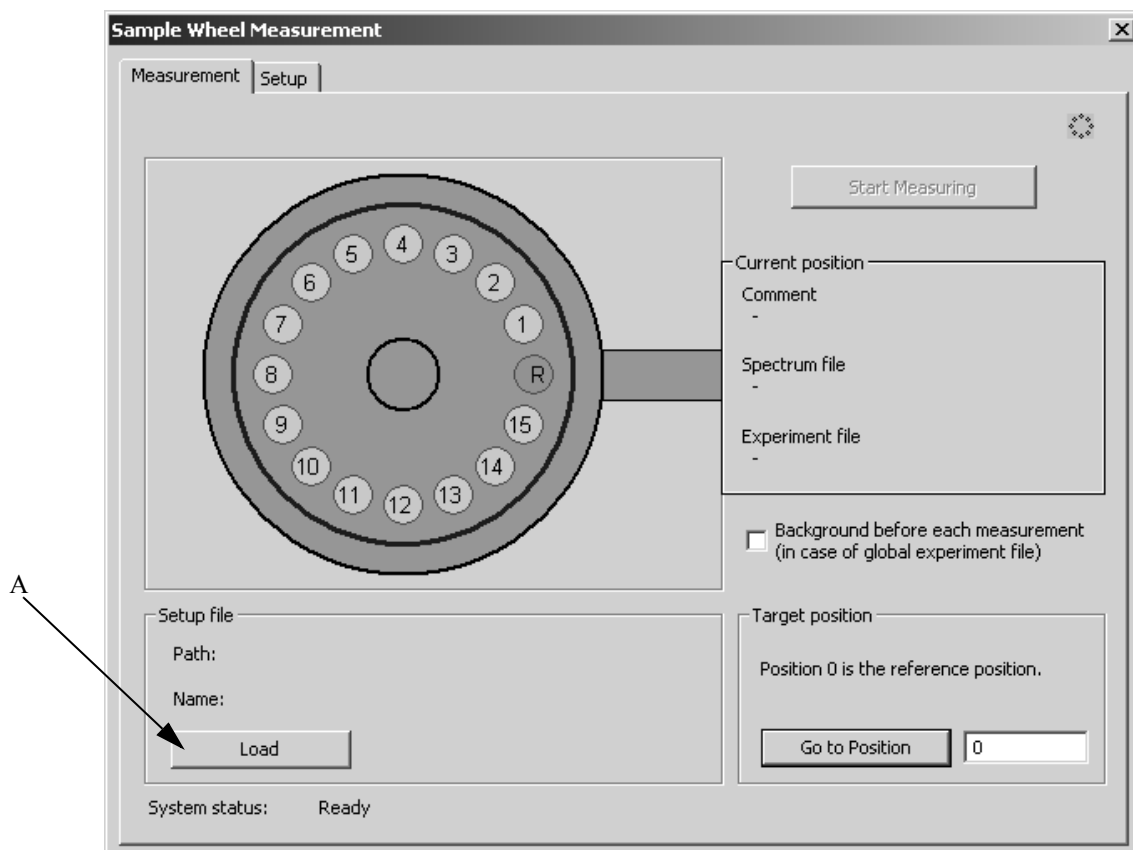


Figure 120: Sample Wheel Measurement - Measurement tab

First, you have to create a so-called setup file in which you define the single sample wheel positions. Click on the *Setup* tab.

7.9.1 Creating Setup File

For each position to be measured you can define a separate experiment method file, a user-defined file name and path to save the spectra files measured.

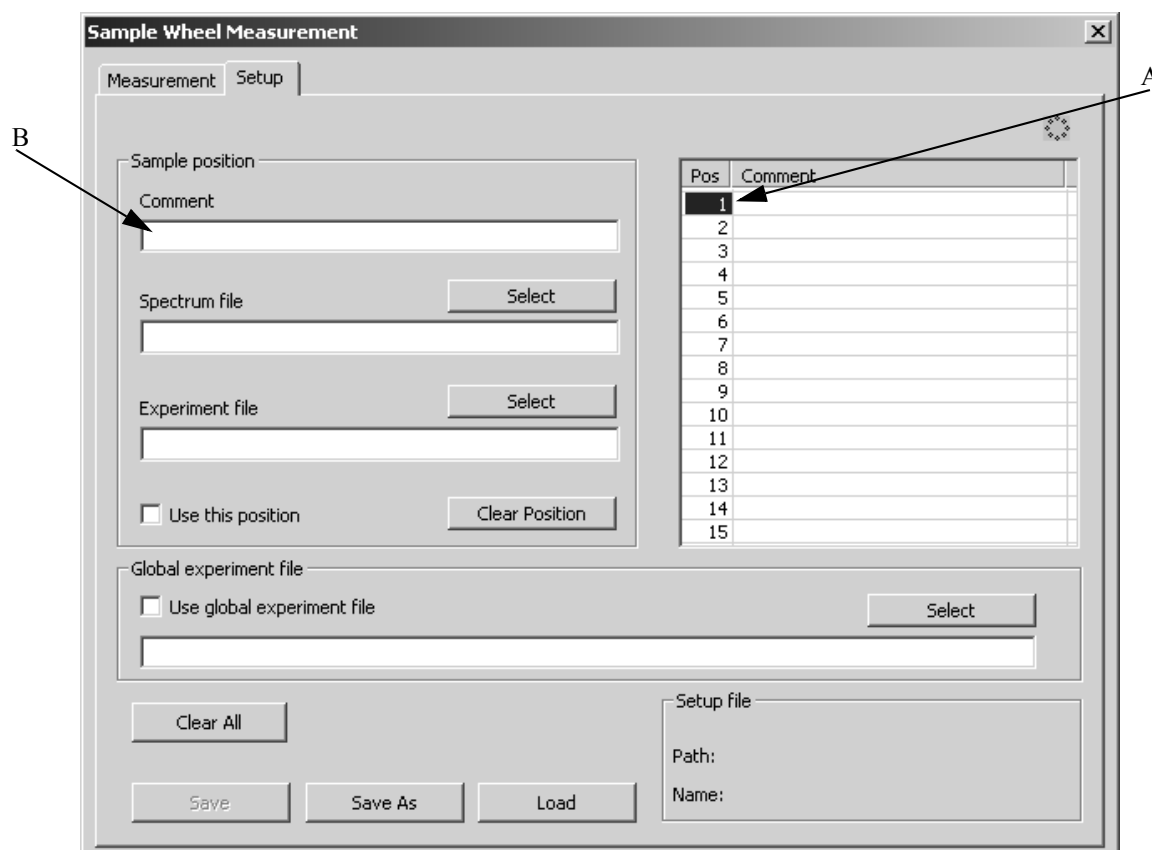


Figure 121: Sample Wheel Measurement - Setup tab

Define the sample wheel positions to be measured. Left click on any position (A in figure 121) on the. A selected position is displayed by a blue marking. It is not obligatory to consecutively fill in the sample positions, you can also skip positions.

Enter a comment for the position selected into the *Comment* entry field (B) and select a spectrum and experiment file.

- **Comment**

If you enter a comment for a specific sample wheel position, the comment is written to the sample name of the spectra saved during measurement.

- **Spectrum File**

Enter the path and name of the spectrum file which will be used for the sample position selected. Clicking on the *Select* button allows to select an already existing spectrum file. If you do not fill in this entry field, OPUS reads the path and file name of the spectrum file in the experiment.

- **Experiment File**

Either type in the path and file name manually or load them from the respective directory by clicking on the *Select* button. For details on how to create experiment files refer to chapter 13.1.

- **Use this Position**

If you activate this check box, the position selected is really used during measurement. Otherwise, the position is not used during measurement, the parameters set, however, will remain. If you click on the *Clear Position* button, only the sample position settings defined will be deleted. The position itself still remains.

Global Experiment File

A global experiment file applies to all sample wheel positions. In this case the experiment file individually assigned to each sample wheel position will not be considered to be valid.

Activate the *Use global experiment file* check box. Either type in the path and file name manually or load them from the respective directory by clicking on the *Select* button.

This kind of settings performs a single reference measurement which is used for all sample wheel positions. If you want to perform an additional reference measurement before each sample measurement, you have to activate the *Background before each measurement* check box on the *Measurement* tab as well.

7.9.2 Saving and Deleting Settings

Save the settings made by clicking either on the *Save* or *Save As* button. Click on the *Clear All* button to delete the settings made for all positions, and the global experiment file entry.

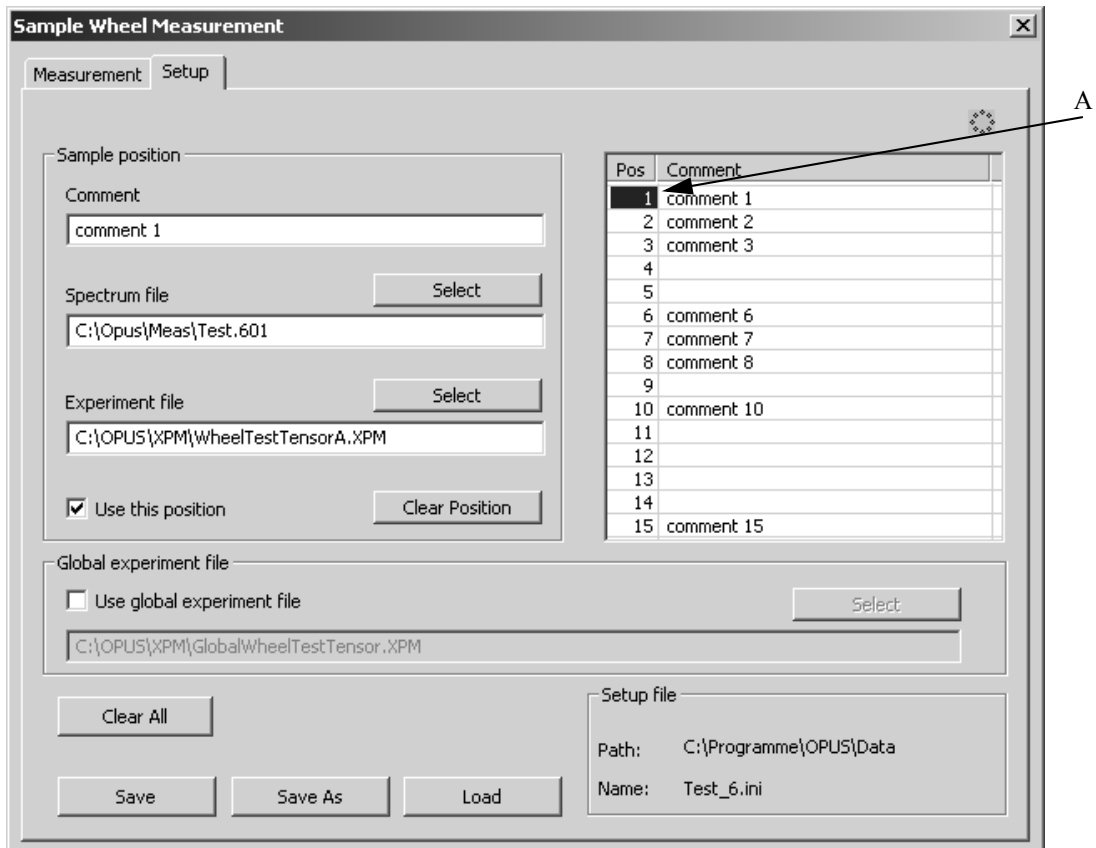


Figure 122: Sample Wheel Measurement - Example of a setup file

7.9.3 Loading and Editing Setup File

To load a previous configuration click on the *Load* button. To edit single sample wheel positions defined in the setup file left click on the corresponding position (A in figure 122). The settings defined for the position selected are displayed on the left. Edit these settings, as desired.

If you have edited a loaded setup file and you click on the *Measure* tab, you will be asked whether these changes made are to be stored. If you click on the *Yes* button, the changes will be stored and become effective during measurement.

7.9.4 Measurement/Background Measurement

First, load a previously created setup file (see chapter 7.9.1) which defines which sample wheel position is to be measured. Click on the *Load* button (A in figure 120) and select the correct setup file. A setup file for a sample wheel measurement always has the file extension **.ini*.

By default, the single sample wheel positions on the graphic display (see figure 120) are gray. If you have loaded a setup file, all positions defined in this file will turn to light-green.

The *Background before each measurement* check box is only available if you have activated the *Use global experiment file* check box on the *Setup* tab. If you activate the *Background before each measurement* check box, a background (reference) measurement will be performed before each single sample is measured.


Example: R - S - R - S - R - S; (R = reference measurement, S = sample measurement)

If you deactivate the check box, only one single background measurement will be performed before each sample measurement.

Example: R - S - S - S - S - S; (R = reference measurement, S = sample measurement)

Even if you do not use any global experiment file, a background measurement will always be performed before each sample measurement. This is due to the fact that the experiment file used may be different for each sample position.

7.9.5 Starting Measurement

If you have prepared the sample wheel, click on the *Start Measuring* button. During measurement the button becomes deactivated. First, OPUS moves the sample wheel to the reference position () and performs the reference measurement(s), either using the global experiment file or the experiment file defined for the first sample wheel position.

If the reference measurement(s) has been completed, OPUS moves the sample wheel to the position selected and measures the sample. Then, the remaining sample or background measurements are performed according to the settings in the setup file.

All spectra measured will be saved, using the file name and path indicated in the setup file. If the setup file does not contain any file name and path, OPUS reads the two parameters from the experiment.

7.9.6 Current Position/Target Position

During measurement the current sample wheel position is always displayed in the *Current Position* group field, as well as the spectrum file and experiment file defined for this particular position. If a comment has been defined, this comment will also be displayed.

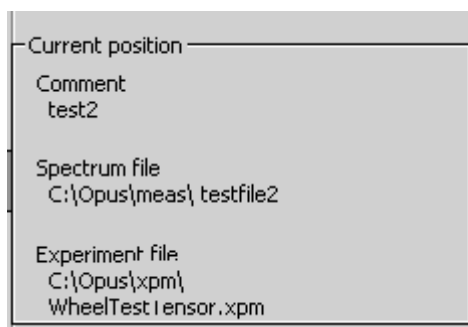


Figure 123: Example of current sample wheel position

It is possible to selectively move the sample wheel to any desired position when a sample run is not active. First, enter the number of the target position into the corresponding entry field, and then click on the *Go to Position* button to move to the position defined.

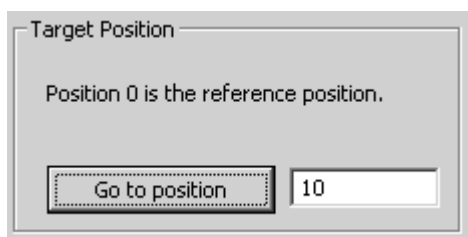


Figure 124: Example of target sample wheel position

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.

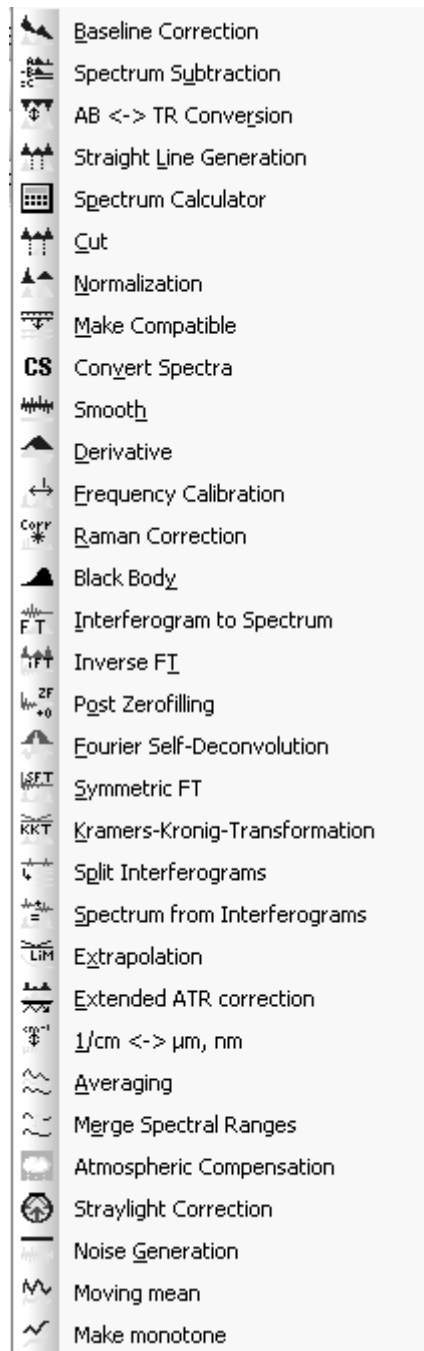


Figure 125: Manipulate menu

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

The baseline correction function allows to subtract baselines from spectra, which allows to get spectra with band edges of up to the theoretical baseline. In case of absorption spectra the theoretical baseline is 0 and 100% in case of transmission spectra.

Figure 126 shows the original spectrum with the calculated baseline and the corrected spectrum.

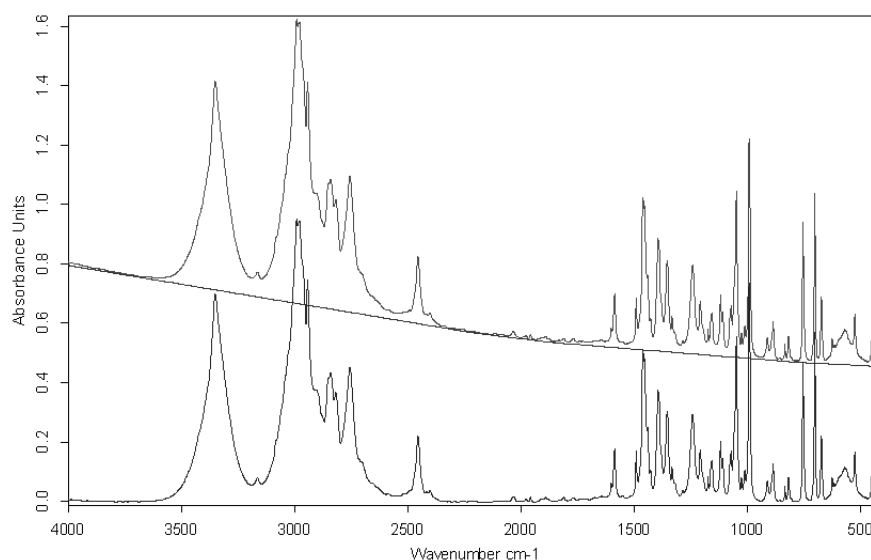


Figure 126: Top: original spectrum and baseline; Bottom: corrected spectrum

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.

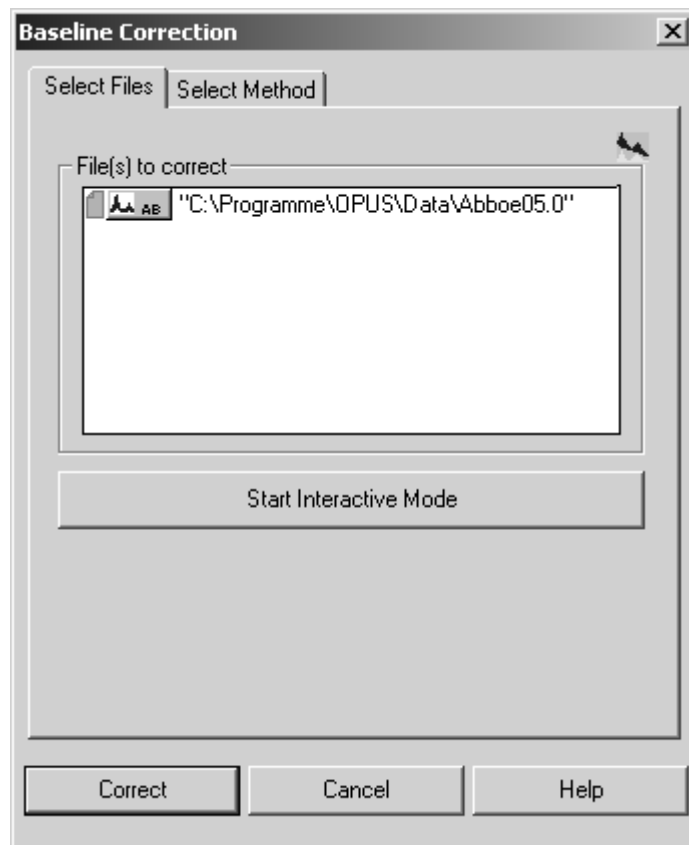


Figure 127: Baseline Correction – Select Files tab

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.

You can either define the baseline interactively by manually setting different baseline points, or have the baseline automatically calculated by OPUS.

8.1.1 Interactive Baseline Correction

Click on the *Start interactive mode* button (figure 127). A new window opens which shows the original spectrum on top and the result spectrum at the bottom.

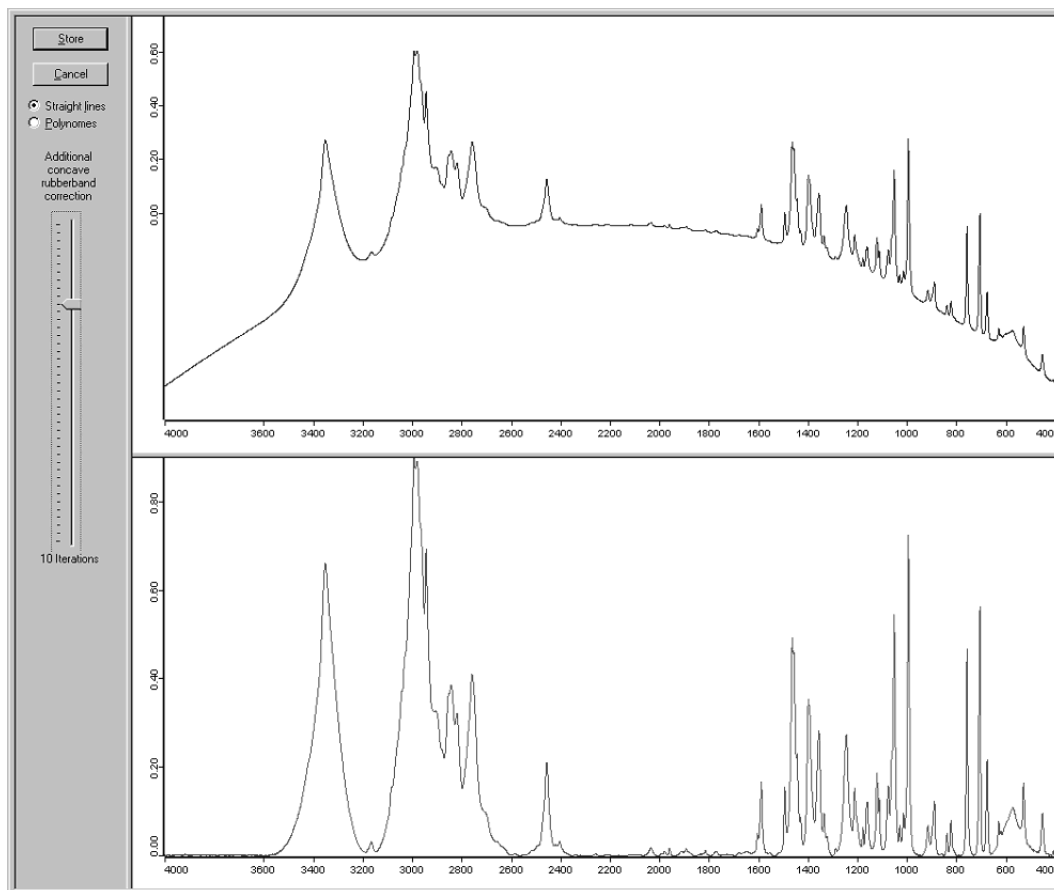


Figure 128: Baseline Correction – Interactive mode

Check the *Straight lines* or *Polynomes* option button to adjust straight lines or polynomes to the baseline.

Double click on the original spectrum to add baseline points. The result of this baseline 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 chapter 2.3.

Additionally, you can perform a concave rubberband correction (also see chapter 8.1.2). The slider position determines the number of iterations in the algorithm. Therefore, the result spectrum will be the original spectrum less the baseline points manually set (if they have been set at all) and a subsequent concave rubberband correction (if the number of iterations is greater than 0).

Click on the *Store* button to save the baseline correction results.

8.1.2 Automatic Baseline Correction

To automatically correct the baseline of your spectrum select the *Select Method* tab.

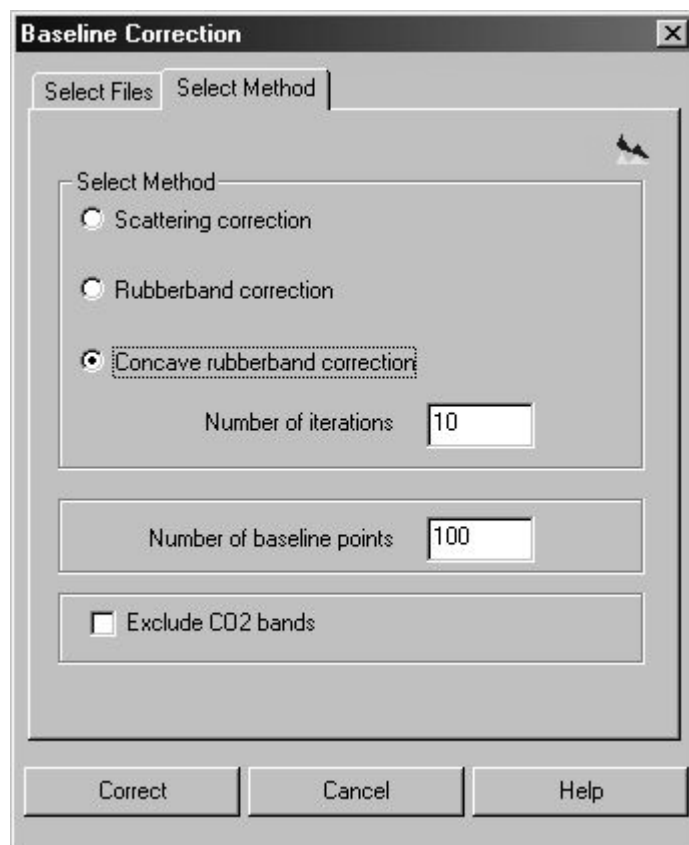


Figure 129: Baseline Correction – Select Method tab

There are three different baseline correction methods available:

a) Scattering Correction

In case of scattering correction the points are set such that the baseline shows monotonic decreasing and as small as possible negative increasing. This, of course, requires the baseline to touch the corresponding curve minima.

b) Rubberband Correction

This method uses - figuratively speaking - a *rubberband* which is stretched between the spectrum endpoints. The rubberband follows the spectrum minima.

c) Concave Rubberband Correction

This correction method is used in case of spectra whose baseline curvature has the same sign as the band peak, or whose baseline shows curvatures with different signs.

This method also uses a rubberband which is stretched from one spectrum end to the other, and the band is pressed onto the spectrum from the bottom up (in case of absorption spectra) with varying intensity. This

method performs iteratively, i.e. depending on the number of iterations the rubberband is pressed onto the spectrum with varying intensity. Enter the number of iterations into the corresponding entry field. Values greater than 50 are in most cases not reasonable. The effect caused by the number of iterations are shown in figure 130.

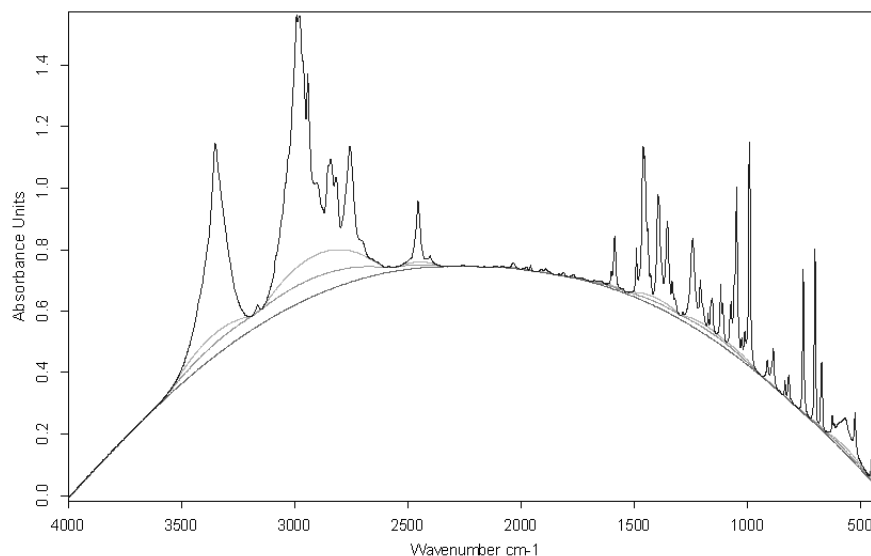


Figure 130: Concave rubberband correction method

In figure 130 the concave baseline has been calculated using 40, 15 and 8 iterations (top down). The result spectra are not displayed to avoid confusion.

All methods calculate the baseline as a frequency polygon, consisting of n baseline points. Define the number of baseline points in the corresponding entry field (figure 129). The values allowed are between 10 and 200. The greater the number of baseline points the more exactly the calculated baseline will follow the theoretical baseline, and the more calculation time is needed. The default values is 64.

Select the baseline correction method, e.g. scattering, rubberband or concave rubberband correction. It is also possible to exclude the spectral ranges which contain CO₂ bands (between 2400 ... 2275cm⁻¹ and 680 ... 660cm⁻¹). Activate the *Exclude CO₂ bands* check box (figure 129).

Start the baseline correction by clicking on the *Correct* button.

Baseline corrections can also be performed on transmittance spectra. The procedure is the same as in case of absorption spectra.

Figure 131 shows an original absorption spectrum and a baseline calculated by using the scattering correction (top) and rubberband method (bottom).

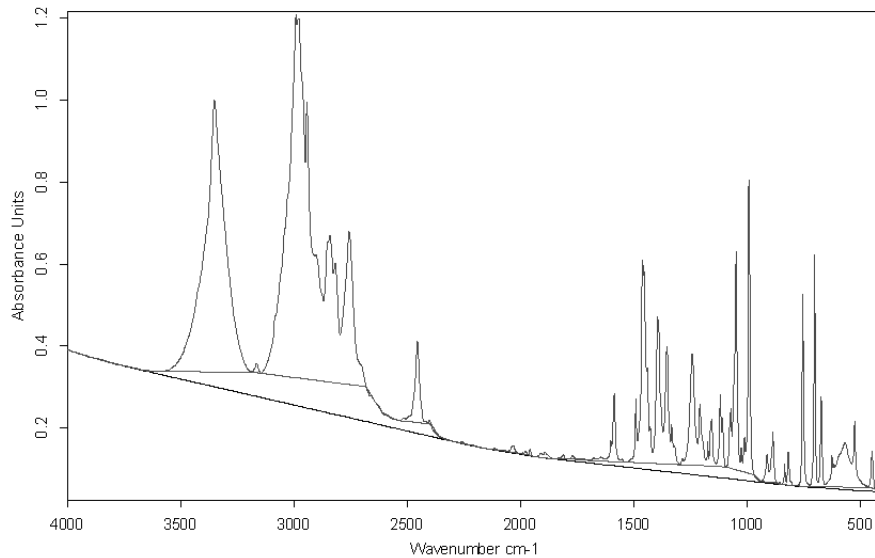


Figure 131: Original and corrected absorption spectrum

Figure 132 shows the original spectrum together with the result spectrum after the baseline correction has been performed. In this case the rubberband correction method has been used.

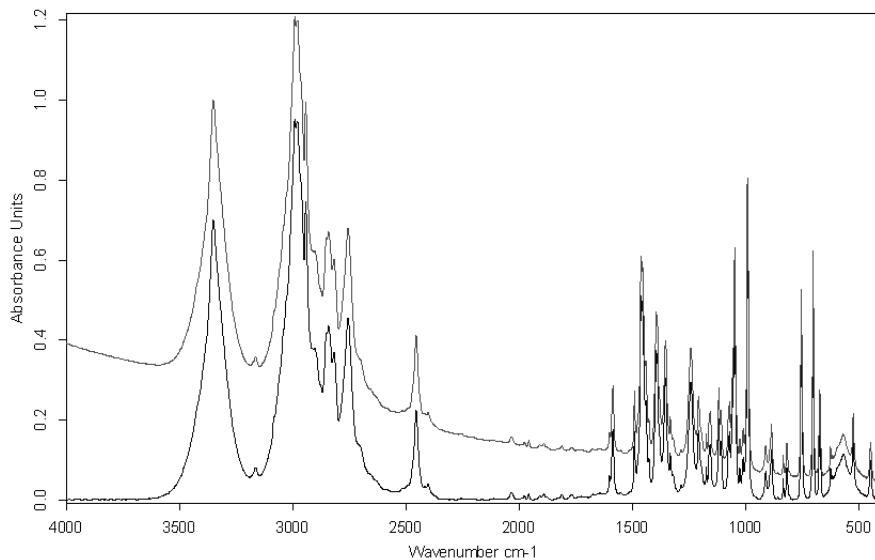


Figure 132: Original and result spectrum after baseline correction

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 133 and 134 show the *Spectrum Subtraction* dialogs:

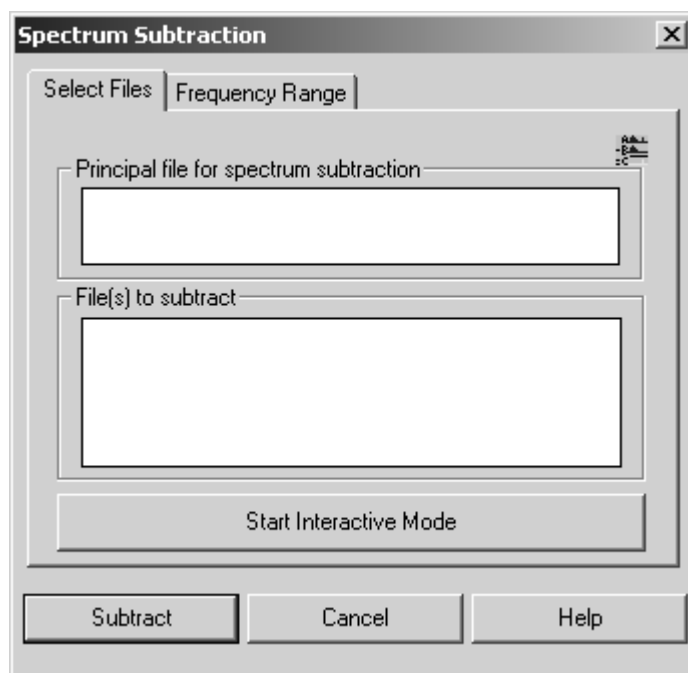


Figure 133: Spectrum Subtraction - Select Files tab

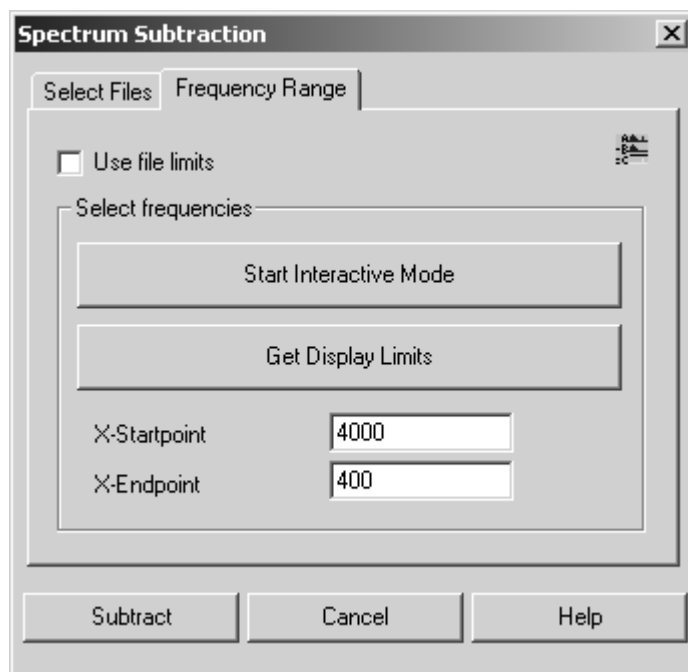


Figure 134: Spectrum Subtraction - Frequency Range tab

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

$$\begin{aligned} \text{Result spectrum (v)} = & \text{ multi-component spectrum(v)} \\ & - \text{ Factor1 * single-component spectrum (v)} \\ & - \text{ Factor2 * single-component spectrum (v)} \\ & \dots \\ & - \text{ Offset} \end{aligned}$$

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 on the *Select Files* tab, the following dialog box will be displayed:

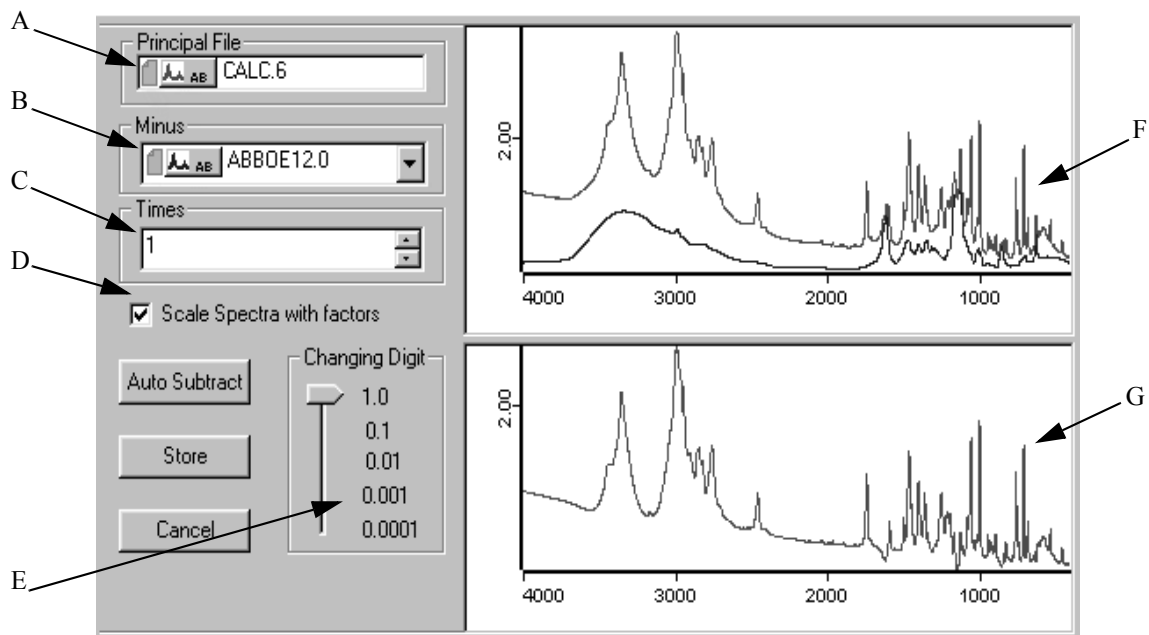


Figure 135: Interactive spectrum subtraction

- 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. This causes the factor values of (C) to be adapted.
- 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 SUBTR data block, the *Show Report* option pops up. Select this option to open the report window:

	Block	File	Path	Modified
1.000000	AB	CALC.6	Q:\PROGRAM\OPUS\WORK	x
-0.000250				
-0.699500	AB	ABBOE12.0	Q:\PROGRAM\OPUS\DATA	
-1.299462	AB	ABBOE08.0	Q:\PROGRAM\OPUS\DATA	
-2.300329	AB	ABBOE05.0	Q:\PROGRAM\OPUS\DATA	

Figure 136: 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.

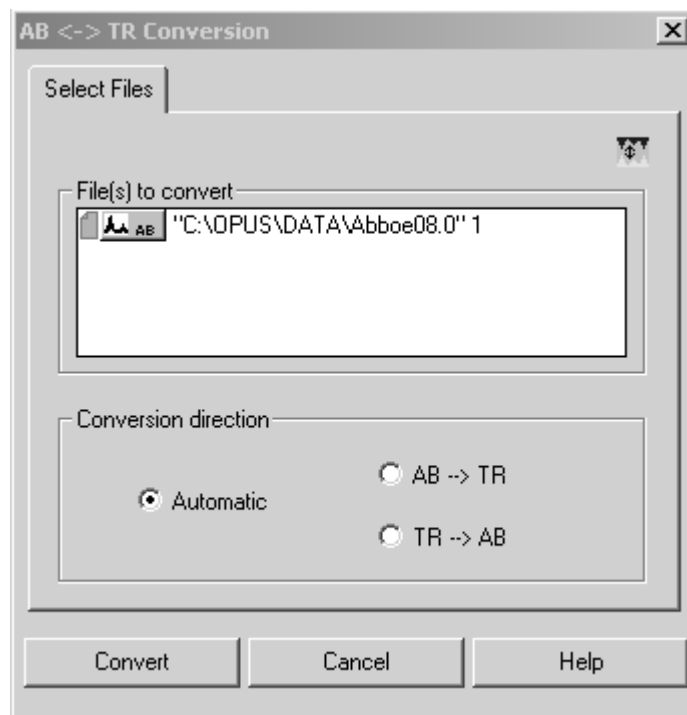


Figure 137: AB <-> TR Conversion - Select Files tab

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.

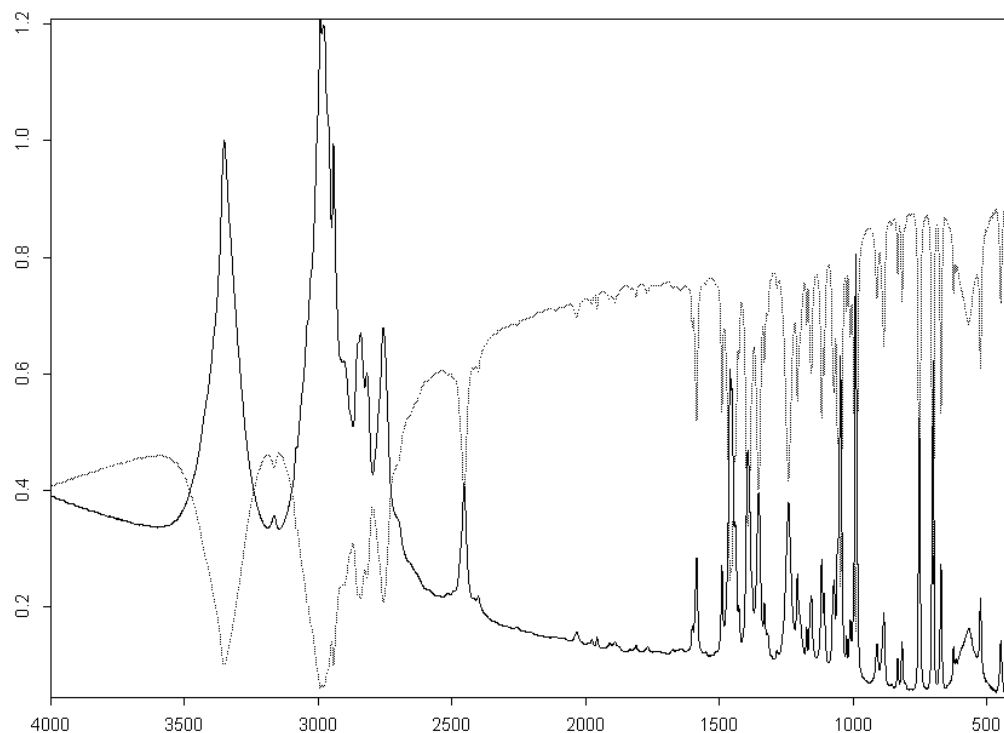


Figure 138: Absorbance spectrum converted into a transmittance spectrum

The spectrum displayed by a dotted line (figure 138) has to be generated by an AB \rightarrow TR conversion.

The equation required for an TR \rightarrow AB conversion is:

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

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

The equation required for an AB \rightarrow 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 139). 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.

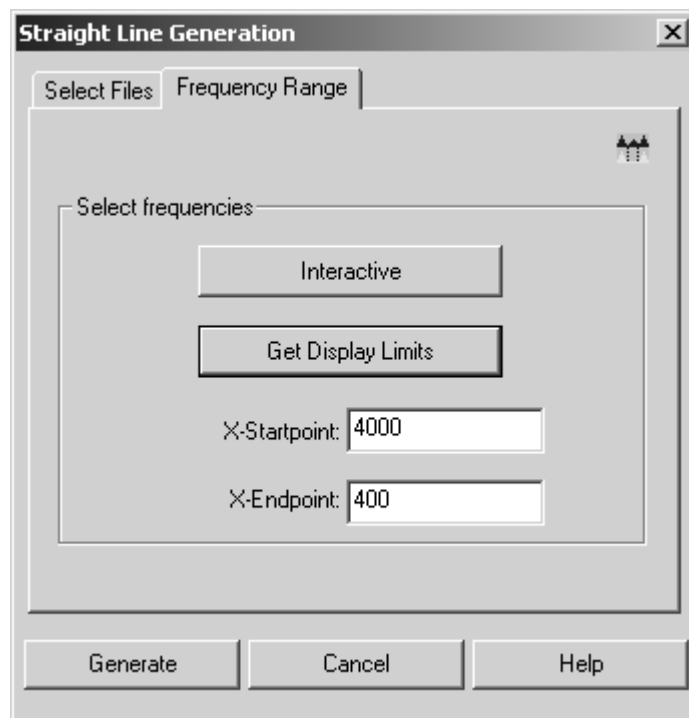


Figure 139: Straight Line Generation - Frequency Range tab

Figure 140 shows a straight line generated between 2,550 and 2,360 wavenumbers, which replaces the original peak (dotted line).

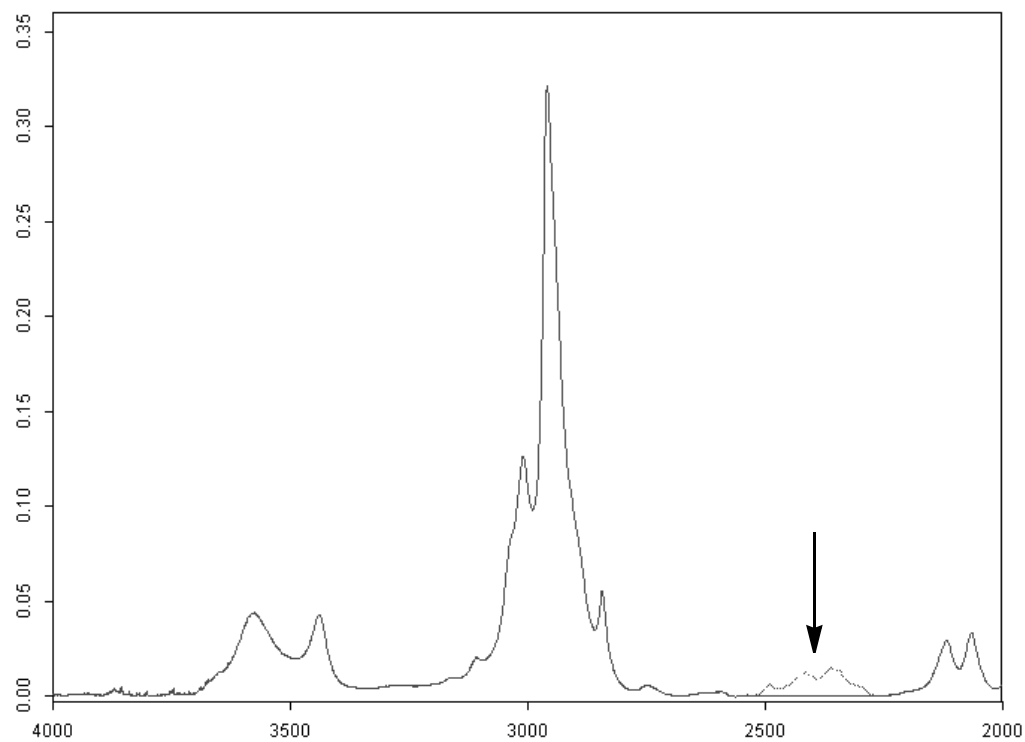


Figure 140: Spectrum before and after generating a straight line

8.5 Spectrum Calculator

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

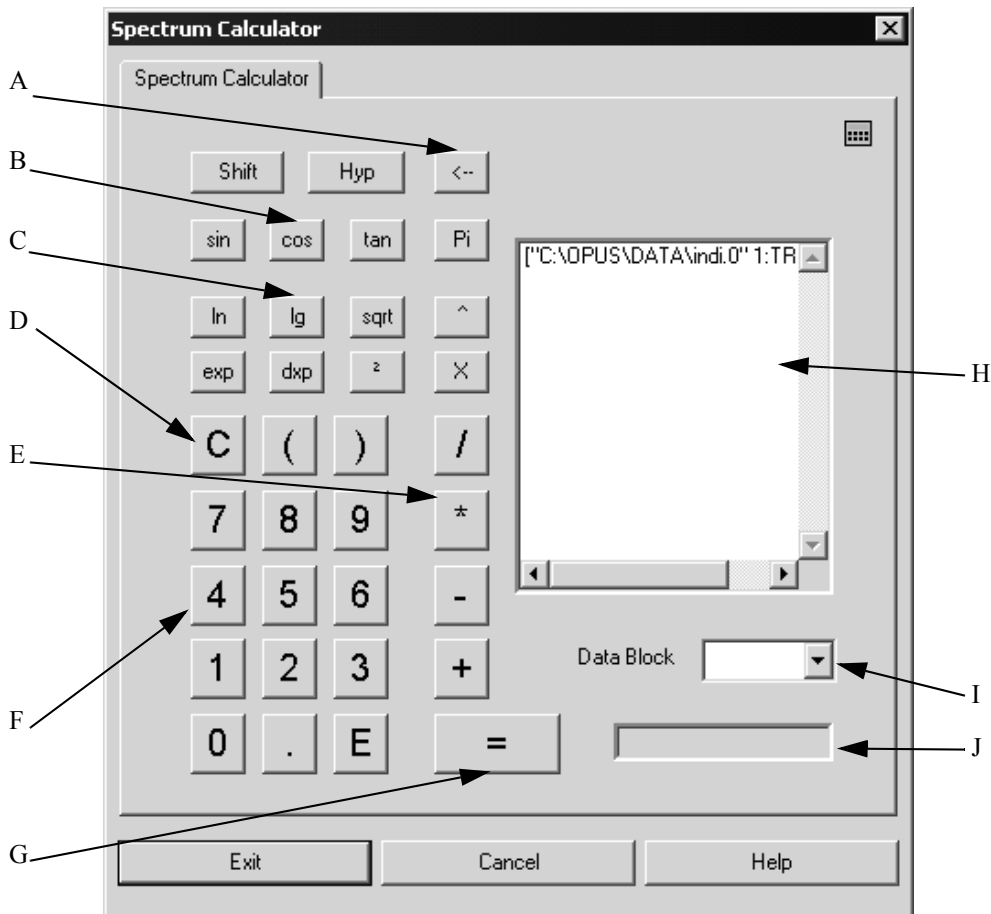



Figure 141: Spectrum Calculator

- 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 $^{\wedge}$, as well as π and special function **x** are made available.
sqrt is the square root function $\sqrt{\quad}$
ln is the natural logarithm
lg is the logarithm to the base 10
exp is the exponential function e
dpx takes the following entry to the power of x (i.e. 10^x)
- D) *C* clears the display in (H) and (I). You can use the brackets (\quad) 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 (G).
- H) You can drag & drop spectra from the OPUS browser window to the entry field (H). The spectra 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 $100\sqrt{\quad}$ into the pocket calculator you expect the result to be 10. The spectrum calculator, however, operates with algebraic formulae. Therefore, you need to enter $\text{sqrt}(100)$.

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 142 shows a frequency range (thicker curve line) generated by using the *Cut* command.

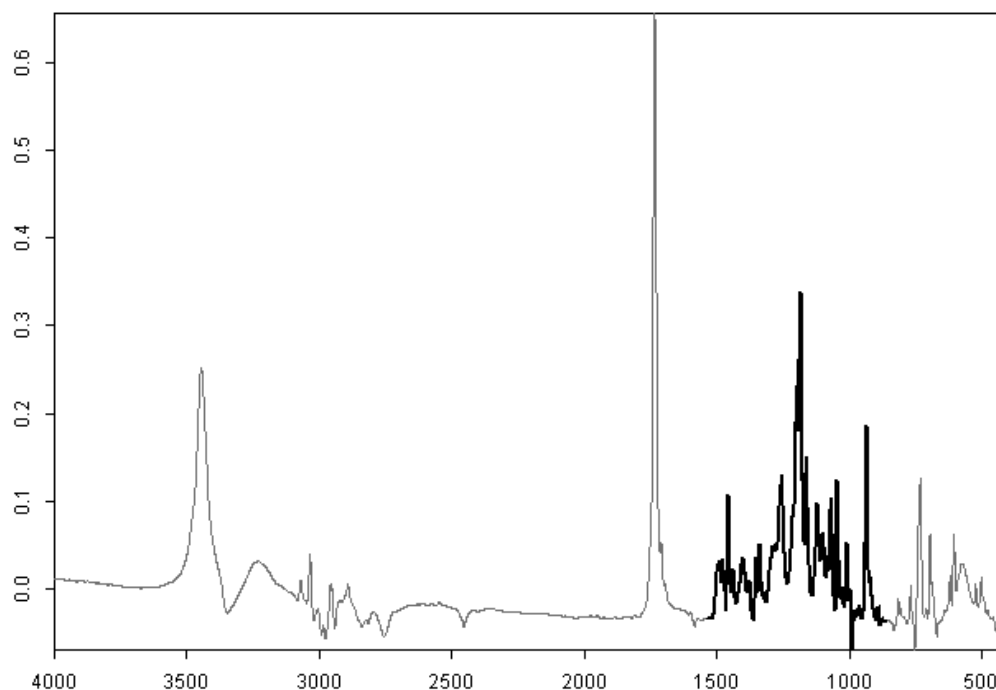


Figure 142: Original spectrum (thin line) and cut-out range (thick line)

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:

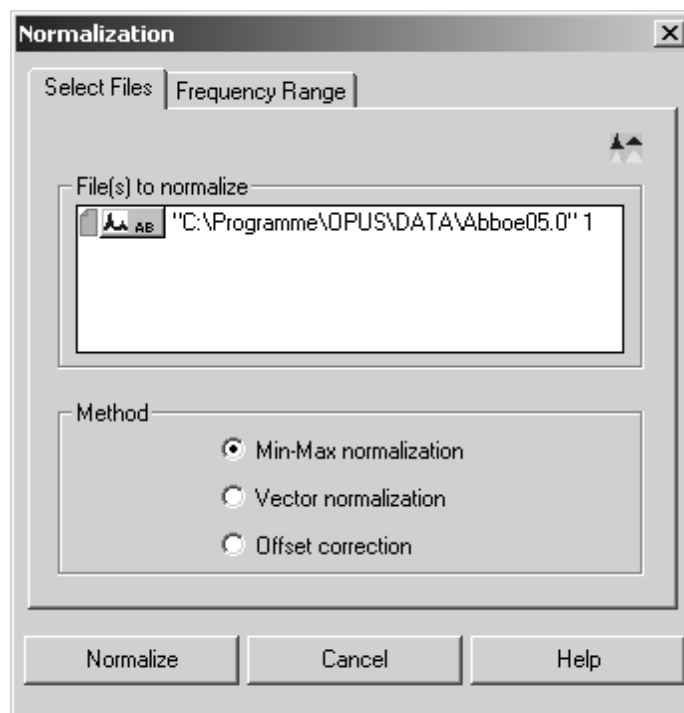


Figure 143: Normalization - Select Files tab

- **Min/Max normalization** – This method scales spectrum intensities to the effect that the minimum absorbance unit will be 0 and the maximum 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:
$$\sum_{i=1}^{NPT} (x_i)^2 = 1$$

with x_i being the spectral intensity of data point i .

- **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.

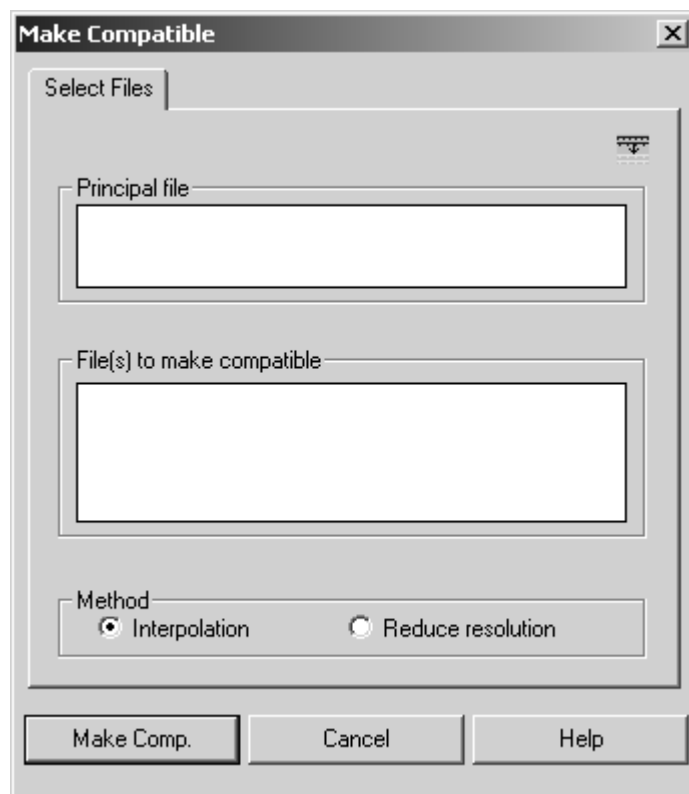


Figure 144: Make Compatible - Select Files tab

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 5,000 cm^{-1} . The number of data points is 4,001 (i.e. 1 cm^{-1} resolution). The frequency of the first point is 4,000.5, of the last 200.5 cm^{-1} . The number of data points is 1,901 data points (2 cm^{-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 1,000 cm^{-1} and the last one at 4,000 cm^{-1} . The number of data points is 3,001 (1 cm^{-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.

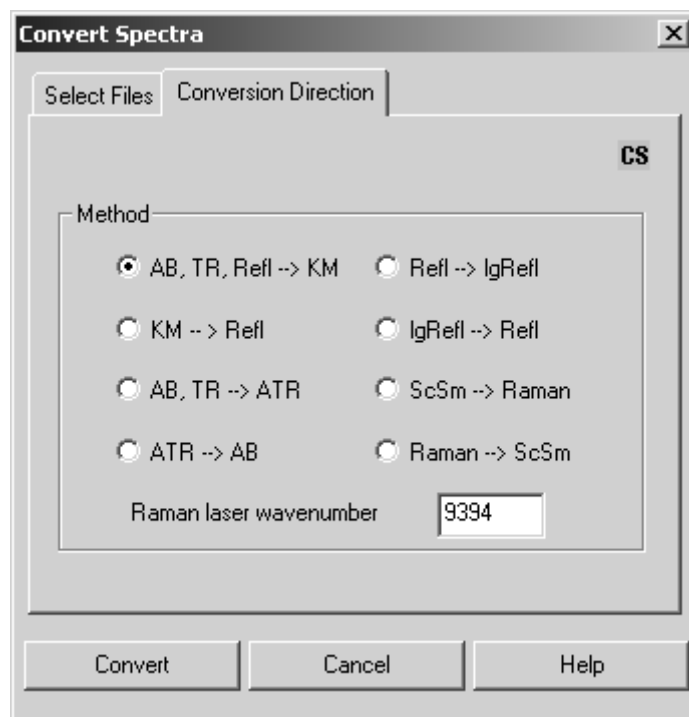


Figure 145: Convert Spectra – Conversion Direction tab

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

8.9.3 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.

8.9.4 Convert to Reflectance Spectra

The following conversion formula is applied:

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

8.9.5 Convert to ATR Spectra

The following conversion formula is applied:

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

X represents the wavenumber. Transmittance spectra are first converted to absorbance spectra. As in case of Attenuated Total Reflection measurements the penetration depth is inversely proportional to the wavenumber (frequency), the spectra are normalized to a constant penetration depth.

8.9.6 Convert to Absorbance Spectra

The following conversion formula is applied:

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

8.9.7 Logarithmize Reflectance Spectra

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

$$\log\text{Refl} = -\log(\text{Refl})$$

8.9.8 Convert Logarithmized Reflectance Spectra

The following conversion formula is applied:

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

8.9.9 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 **Raman Laser Wavenumber**. 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.

8.9.10 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.

8.9.11 Raman Laser Wavenumber

This value will be used for the *ScSm* → *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:

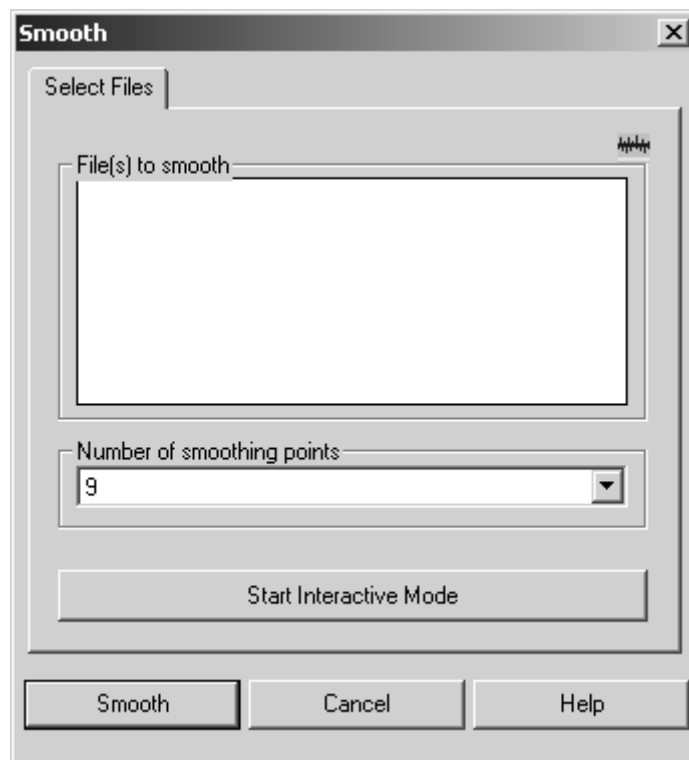


Figure 146: Smooth – Select Files tab

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:

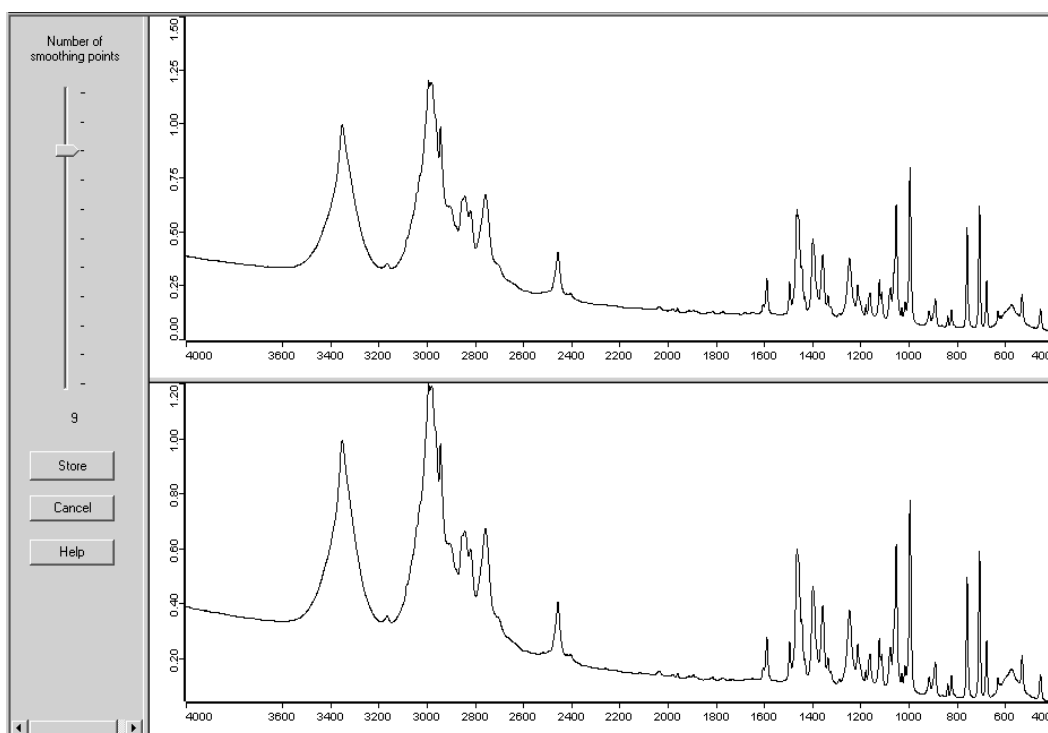


Figure 147: Interactive smoothing

Figure 147 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 the *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 148 directly compares the original spectrum with the smoothed one. The original spectrum band shows more pronounced peaks.

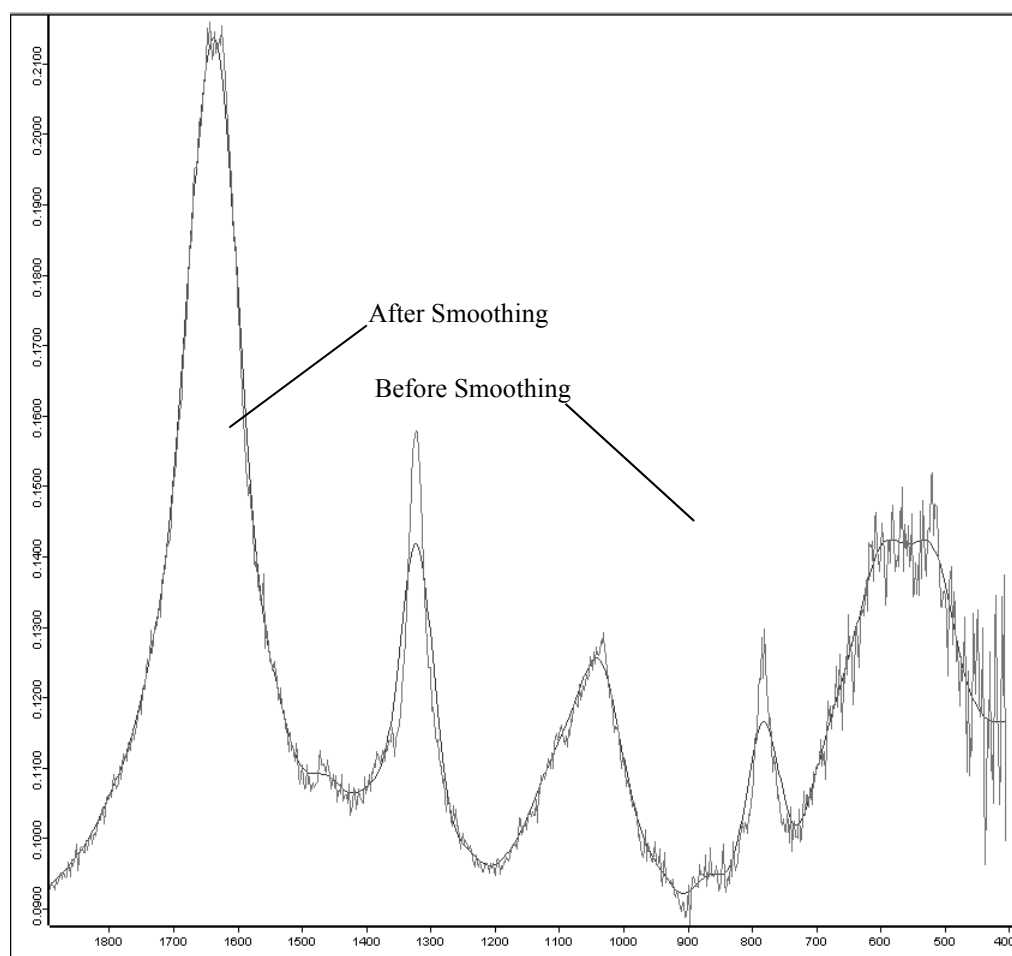


Figure 148: Smoothing effects on a spectrum

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.

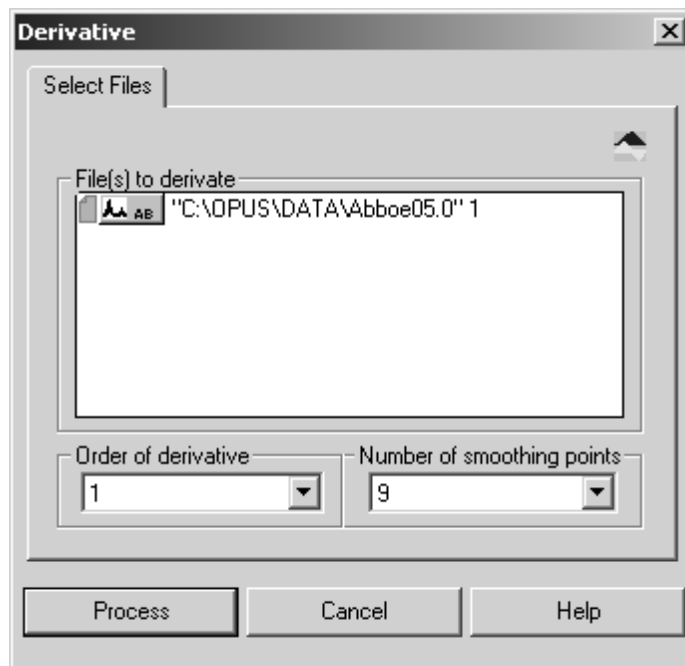


Figure 149: Derivative - Select Files tab

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 v_{old} x-values of the data points:

$$v_{new} = v_{old} \cdot M + A \quad (\text{or} \quad f_{new} = f_{old} \cdot M + A)$$

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

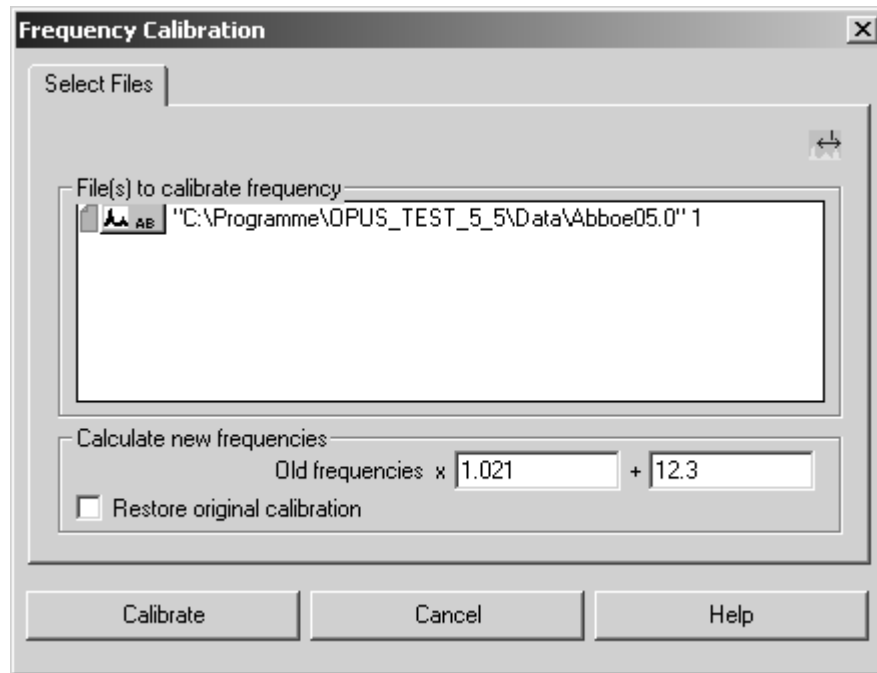


Figure 150: Frequency Calibration - Select Files tab

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

The original data set before the calibration looked as follows:

Data parameters AB	Values
Data Point Format	1
Number of Data Points	3735
Frequency of First Point	4000.146484
Frequency of Last Point	399.243164
Y - Scaling Factor	1.000000
Y - Maximum	0.748212
Y - Minimum	0.040979
X Units	Wavenumber cm-1
Y Units	Absorbance Units
Derivative	0
Date of Measurement	07/08/84
Time of Measurement	11:35:06

Figure 151: 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.

Data parameters: AB	Values
Data Point Format	1
Number of Data Points	3735
Frequency of First Point	4096.449561
Frequency of Last Point	419.927271
Y - Scaling Factor	1.000000
Y - Maximum	0.748212
Y - Minimum	0.040979
X Units	Wavenumber cm-1
Y Units	Absorbance Units
Derivative	0
Date of Measurement	07/08/84
Time of Measurement	11:35:06
Mult. for Freq.Calib	1.021000
Add for Freq.Calib	12.300000

Figure 152: Set of data parameters after frequency calibration

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

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

and later by

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

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:

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

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

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


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

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

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

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.

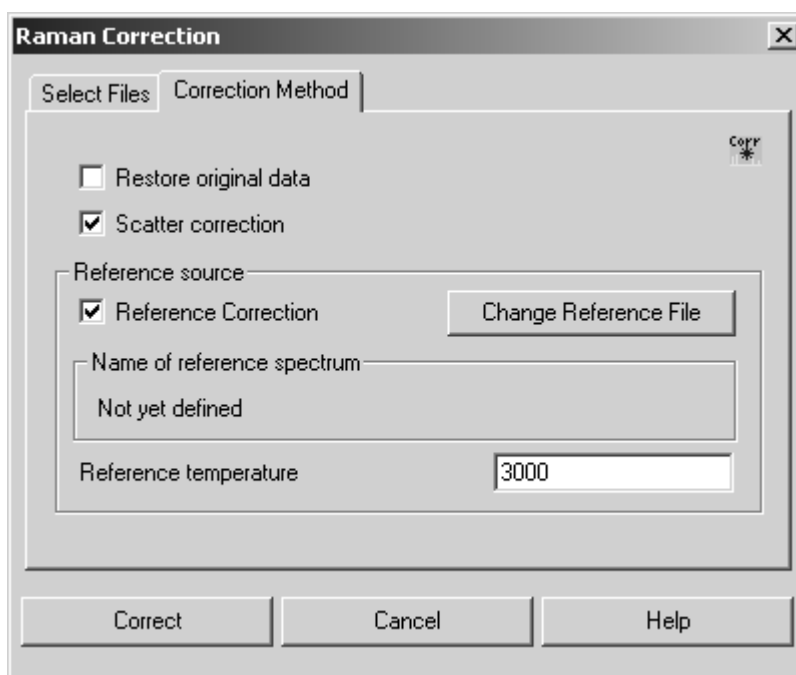


Figure 153: Raman Correction - Correction Method tab

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:

Instrument parameters	Values
Temperature	4000.000000
Raman Laser Wavenumber	9394.000000
Raman Background Corrected	YES
Raman Scattering Corrected	YES

Figure 154: Raman Correction Flags

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

8.13.1 Raman Correction Theory

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

$$\left(\frac{\nu_{Laser}}{\nu}\right)^4$$

In case of *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 wavenumber).

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 wavenumber) can be calculated.

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

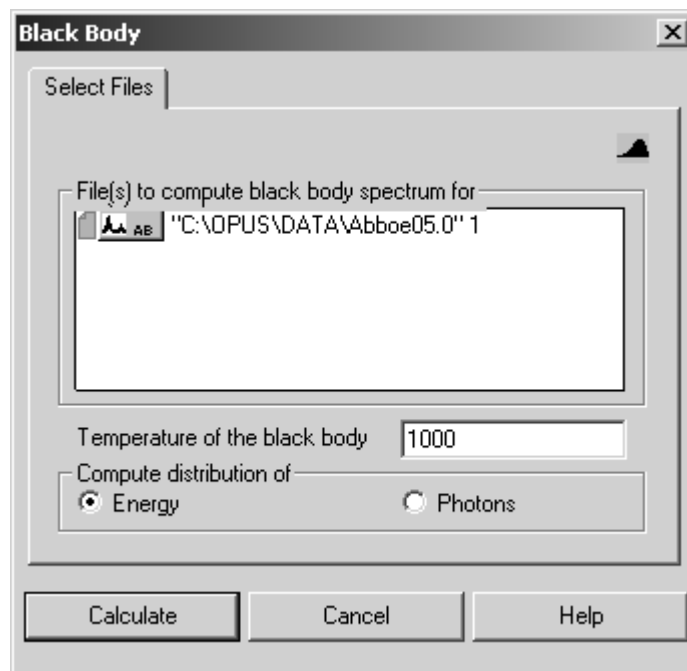


Figure 155: Black Body - Select Files tab

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 156 shows the radiation spectrum of a black body at a temperature of 1000K.

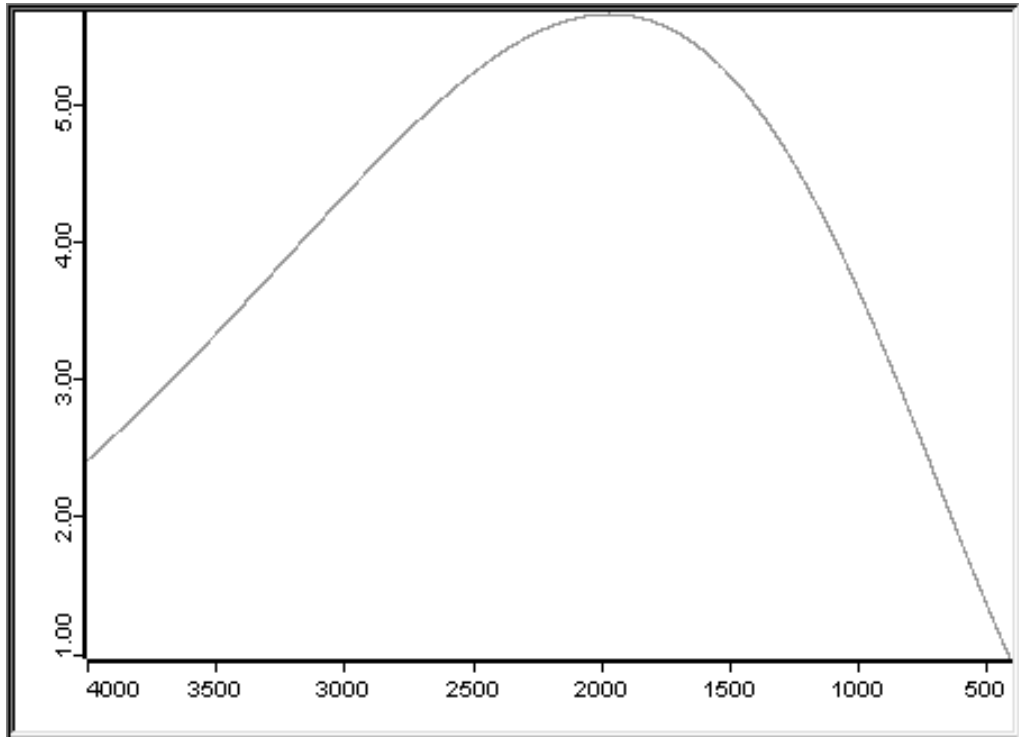


Figure 156: Radiation emitted by a black body at 1000K

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

$$\text{Energy per wavenumber: } y = \frac{2 \times 10^8 hc^2 \nu^3}{e^{\left(\frac{100\nu hc}{kT}\right)} - 1}$$

$$\text{Photon flux per wavenumber: } y = \frac{2 \times 10^{-15} c \nu^2}{e^{\left(\frac{100\nu hc}{kT}\right)} - 1}$$

where:

T = Temperature [K]

c = 2.99792458 · 10⁸ [ms⁻¹]

h = 6.626176 · 10⁻³⁴ [m²kgs⁻¹]

k = 1.380662 · 10⁻²³ [m²kgs⁻²K⁻¹]

ν = Wavenumber [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.

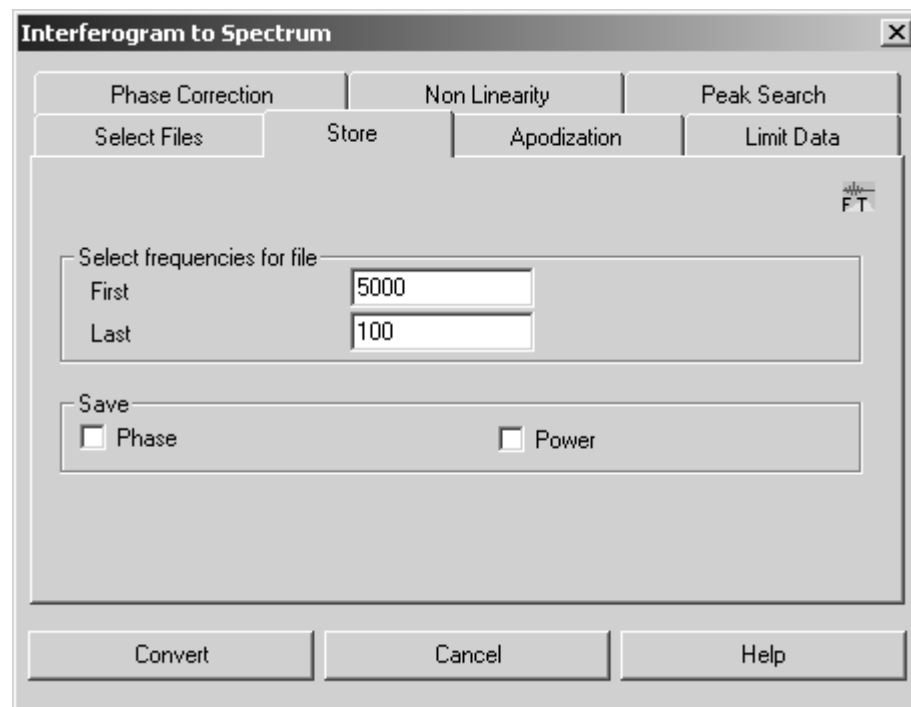


Figure 157: Interferogram to Spectrum – Store tab

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 which natural width is smaller than or comparable with the measured resolution. These side lobes can be suppressed, however at the expense of line broadening, by multiplying the interferogram by means of an apodization function.

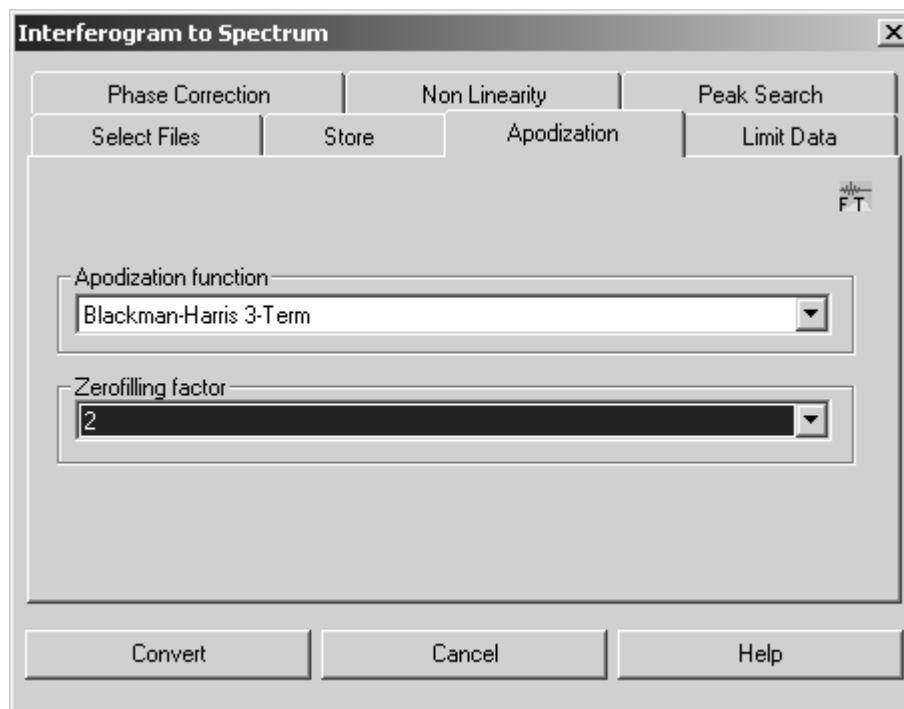


Figure 158: Interferogram to Spectrum – Apodization tab

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 2. If the number of data points has already been a power of 2, 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.

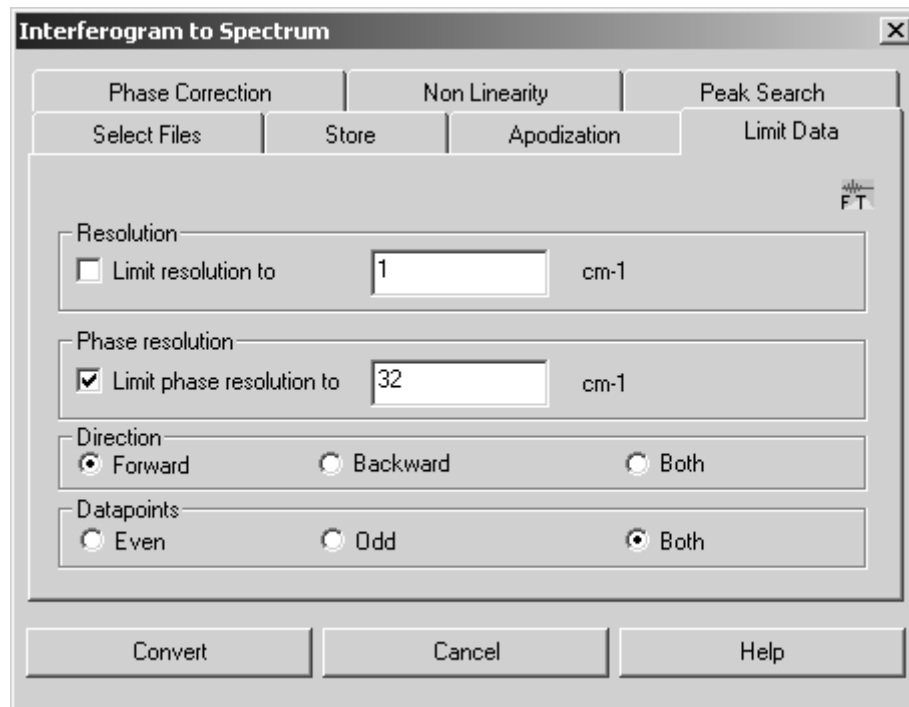


Figure 159: Interferogram to Spectrum – Limit Data tab

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

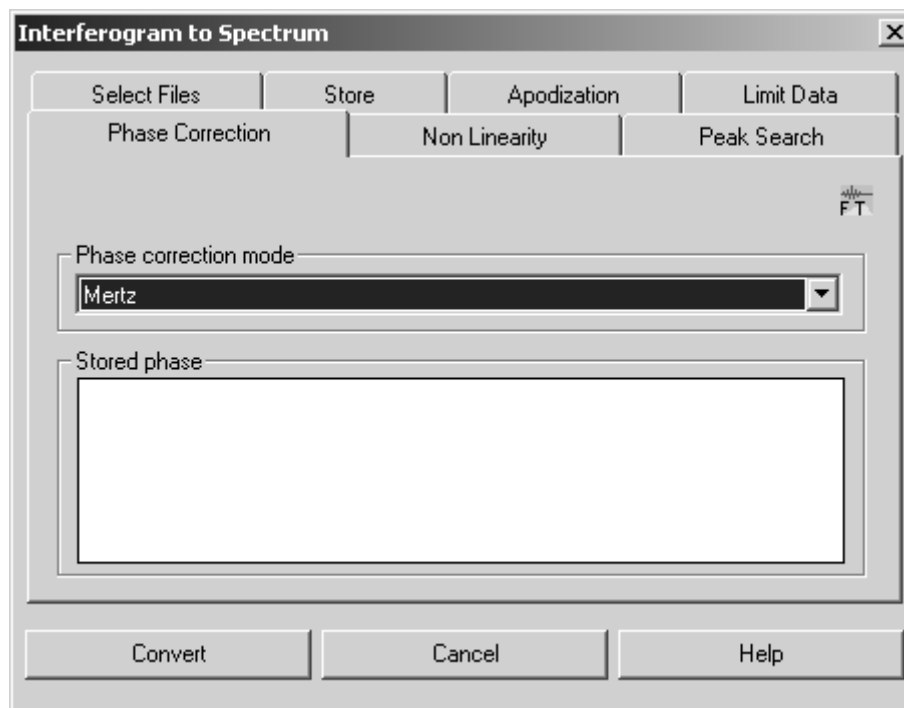


Figure 160: Interferogram to Spectrum – Phase Correction tab

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 which requires, however, higher a computational period.

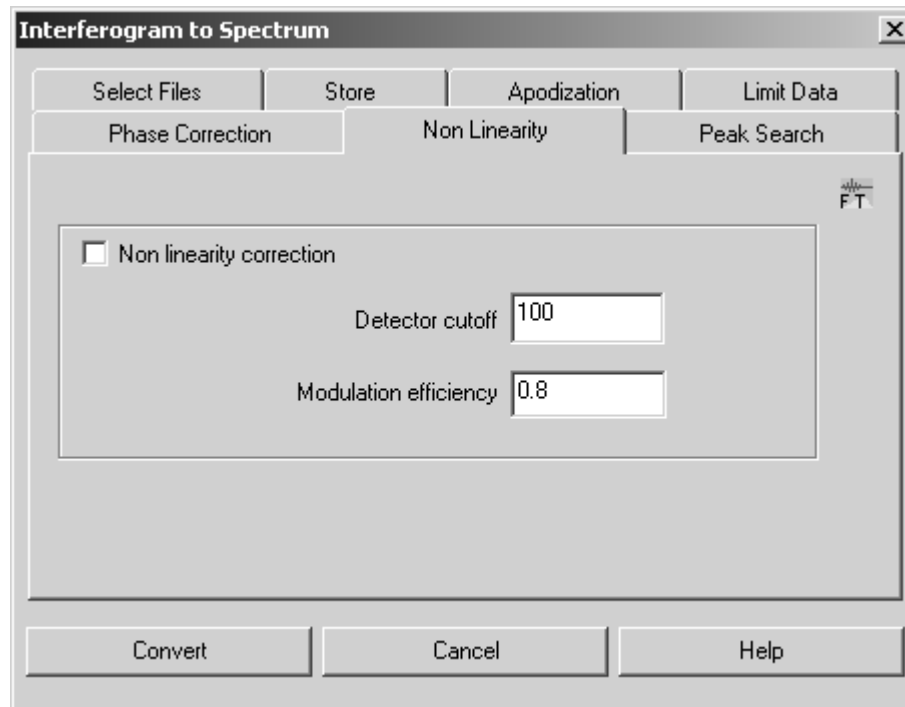


Figure 161: Interferogram to Spectrum - Non-linearity tab

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 0cm^{-1} up to the maximum wavenumber at which the detector can send a signal.
- Electronic filters must not be used. Spectra have to undergo a broadband 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):

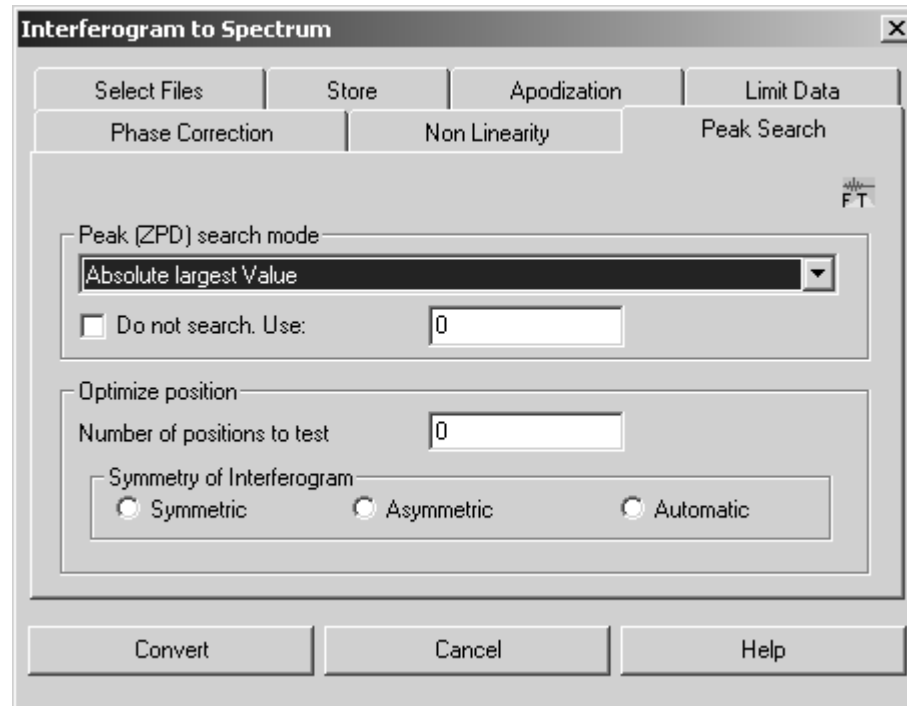


Figure 162: Interferogram to Spectrum - Peak Search tab

- *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.

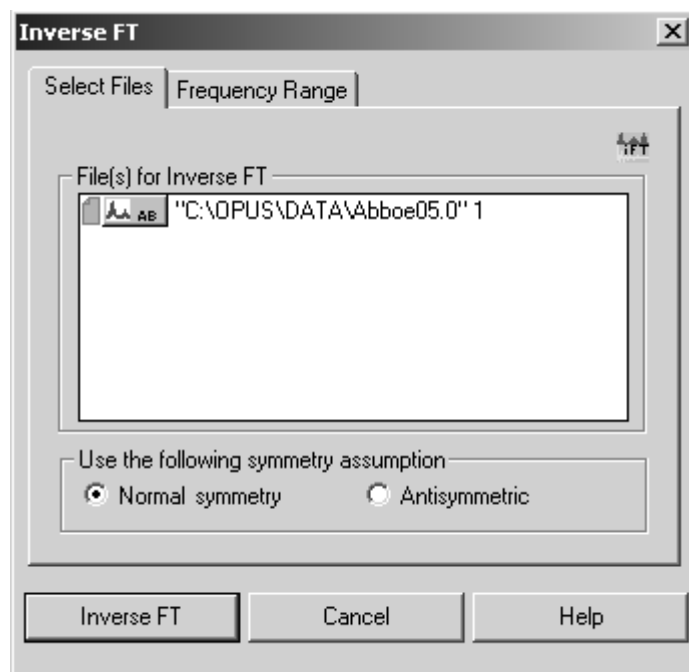


Figure 163: Inverse FT - Select Files tab

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 symmetrically 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 wavenumber. 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.

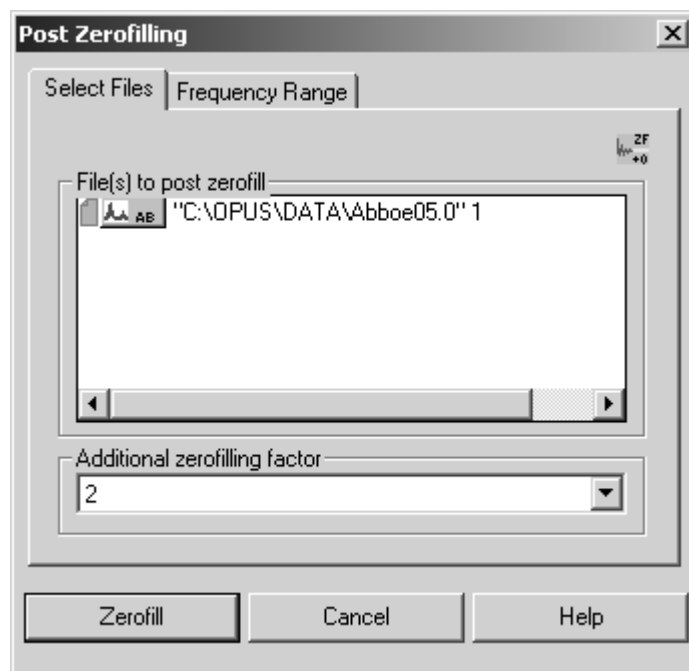


Figure 164: Post Zerofilling - Select Files tab

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 164), the spectra file(s) selected will be interpolated using the additional zerofilling factor specified.

Figure 165 exemplifies a post zerofilling factor of 4. The interpolated curve definitely includes more (quadruple) data points as the original data.

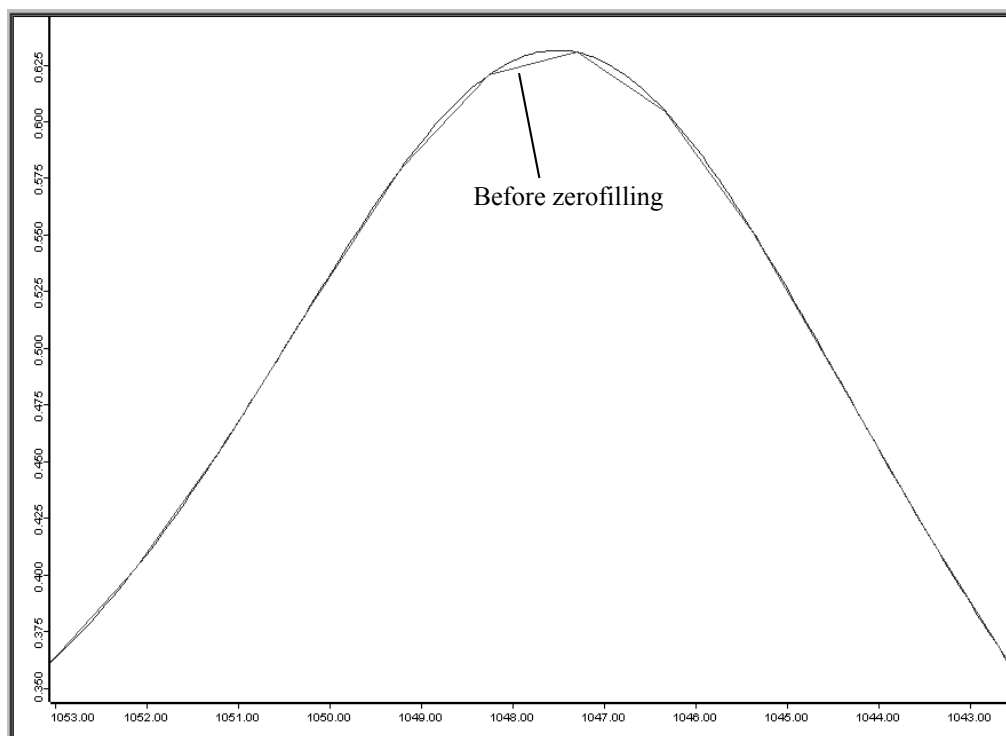


Figure 165: Digital resolution before and after post zerofilling

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 166: Fourier Self-Deconvolution - Adjust Parameter tab

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 recommended 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 $1/(\text{zerofilling factor})$ is recommended to reduce noise.

Figure 167 shows a spectrum before and after a deconvolution has been performed, using the parameters shown in figure 166. 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.

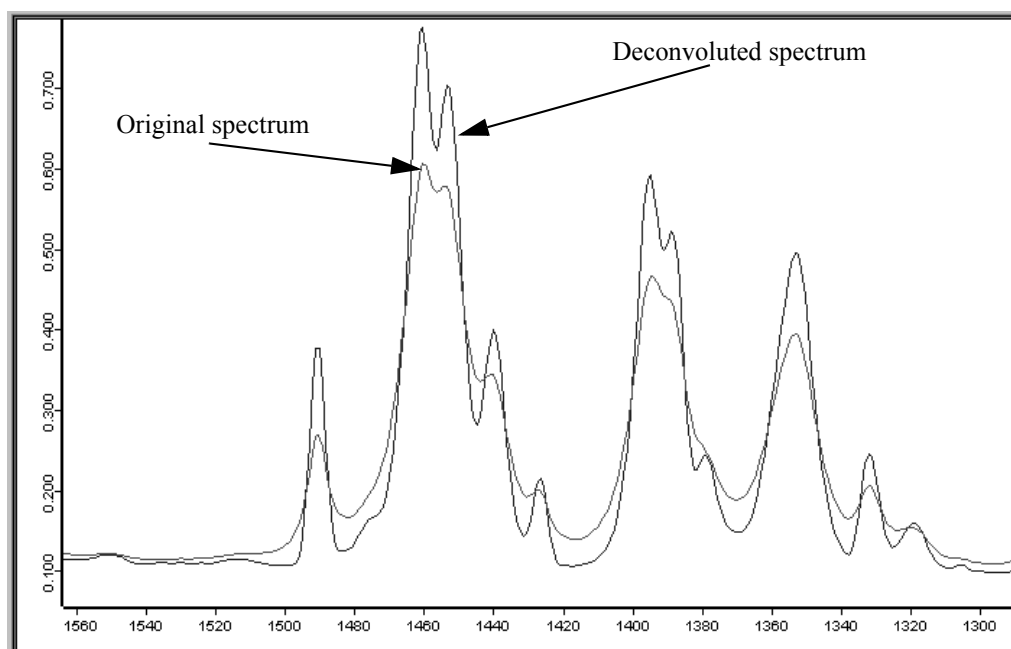


Figure 167: Spectrum before and after Fourier self-deconvolution

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.

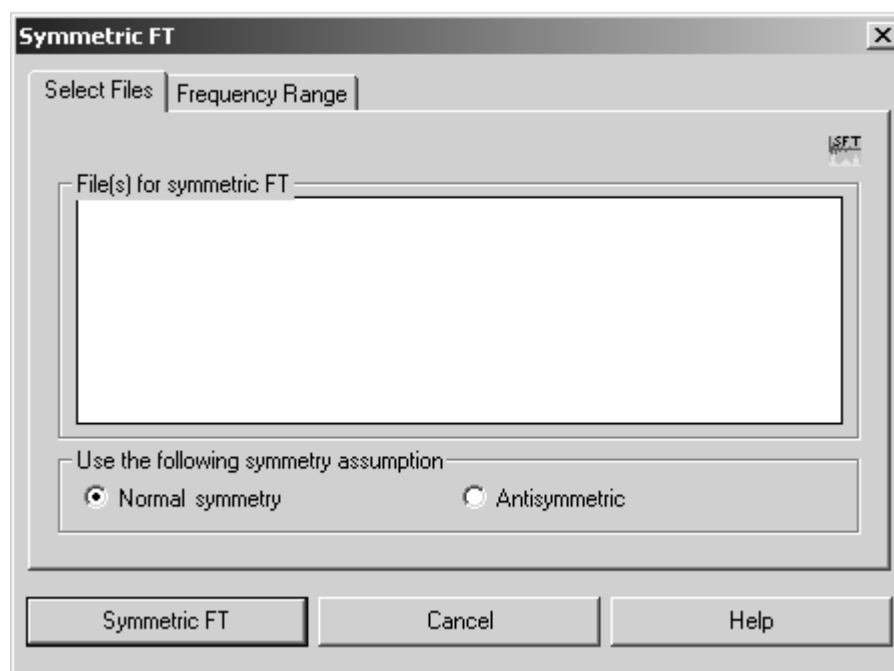


Figure 168: Symmetric FT - Select Files tab

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.

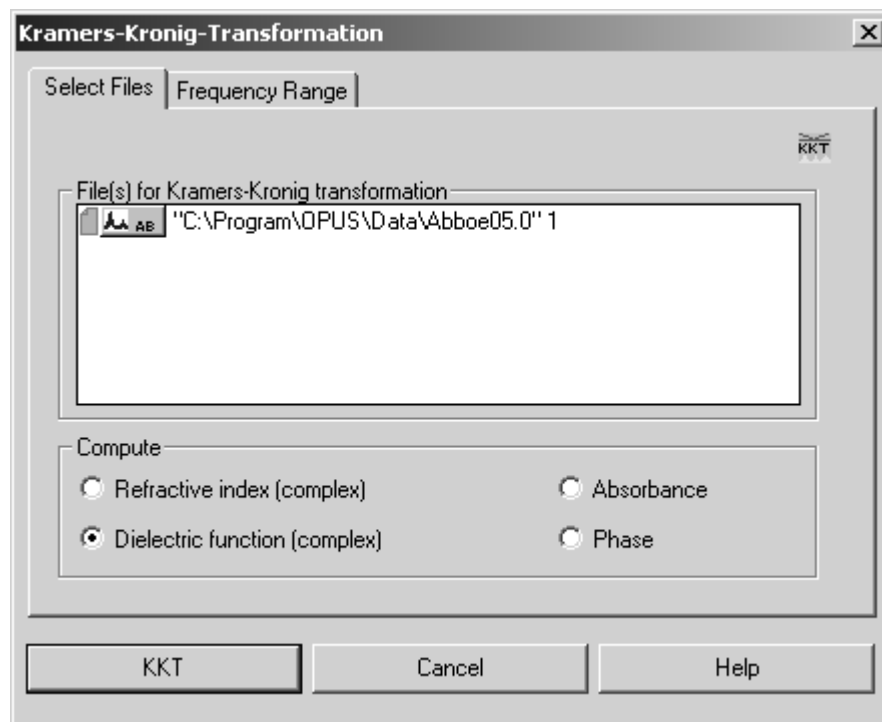


Figure 169: Kramers-Kronig Transformation - Select Files tab

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 $-2\lg(1 - [\text{Input} - \text{Reflectance spectrum}])$ using the OPUS spectrum calculator.

Note: For a separate description on how to use the KKT and some exemplary spectra refer to appendix B.

8.21 Split Interferograms

Due to measurement reasons interferograms are not continuously but selectively acquired. An efficient acquisition can be achieved by using rapidly scanning interferometers. Each interferogram can only be acquired up to a maximum limited path length difference, which is due to experimental

restrictions. Therefore, the spectral resolution is reciprocally proportional to the maximum path length difference.

Depending on the acquisition mode selected during measurement you can split interferograms. Splitting interferograms allows to increase the time resolution, in case of time-resolved measurements (TRS).

If you have selected the *Double Sided* acquisition mode, 2 interferogram will be generated during splitting. In case of a double-sided *Forward-Backward* acquisition mode, 4 interferograms will be generated during splitting. This yields to the maximum possible time resolution of single spectra at a given mirror velocity.

The spectra files used for the *Split Interferograms* command have to contain an interferogram data block. You can use single spectra files or 3D files. Drag and drop the interferogram data block into the *File(s) to split* entry field and click on the *Split Interferograms* button.

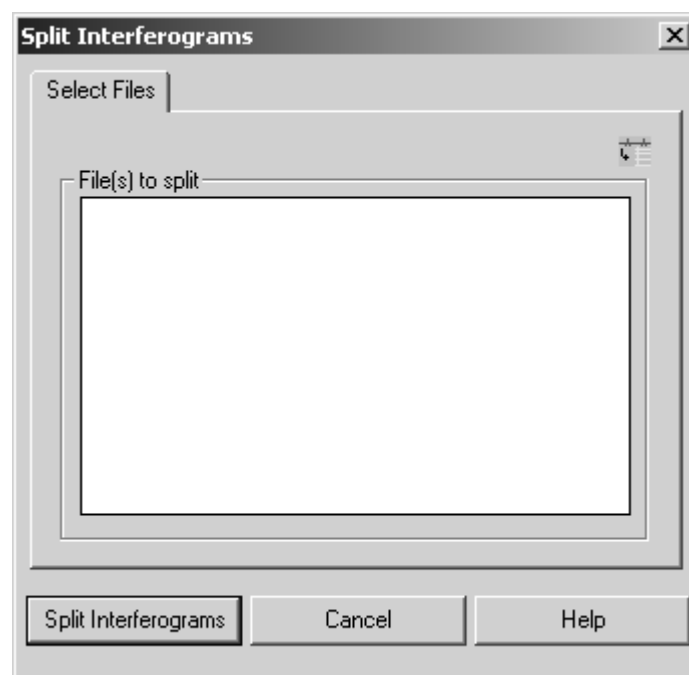


Figure 170: Split Interferograms - Select Files tab

8.22 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.

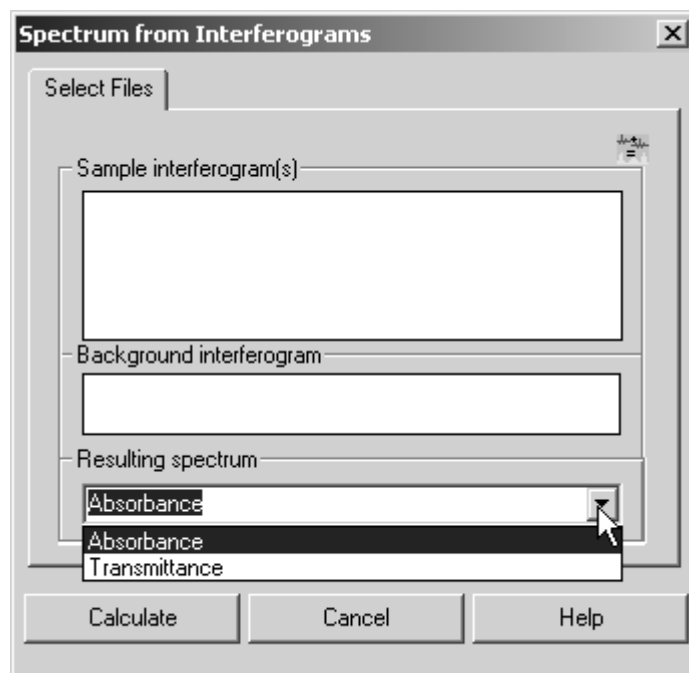


Figure 171: Spectrum from Interferograms - Select Files tab

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.

8.23 Extrapolation

You can extrapolate reflectance spectra to 0cm^{-1} or to an upper frequency limit selectable by the user. The previous wavenumber 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 I .

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.

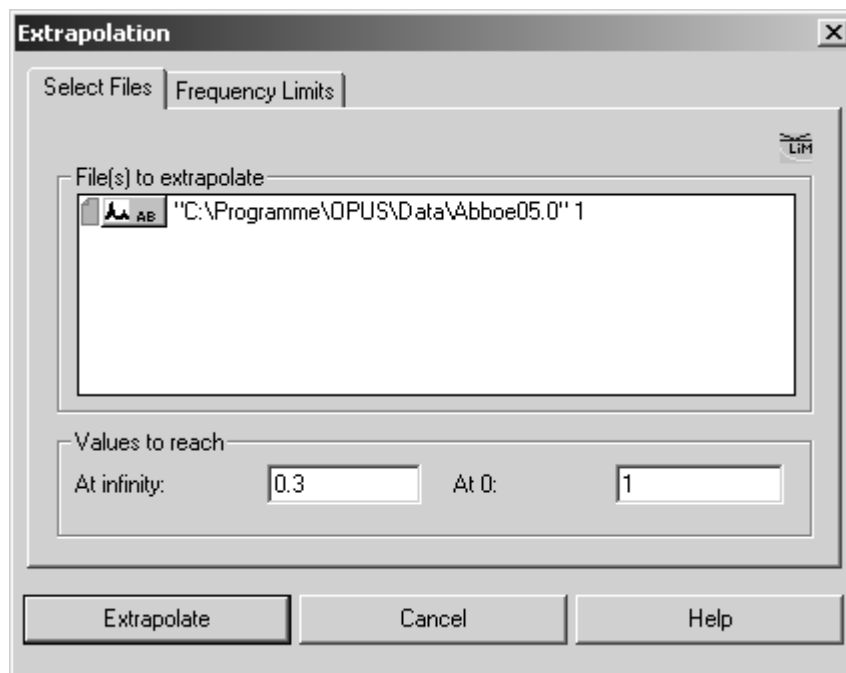


Figure 172: Extrapolation - Select Files tab

8.23.1 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 wavenumber 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 wavenumber smaller than the lower wavenumber 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.

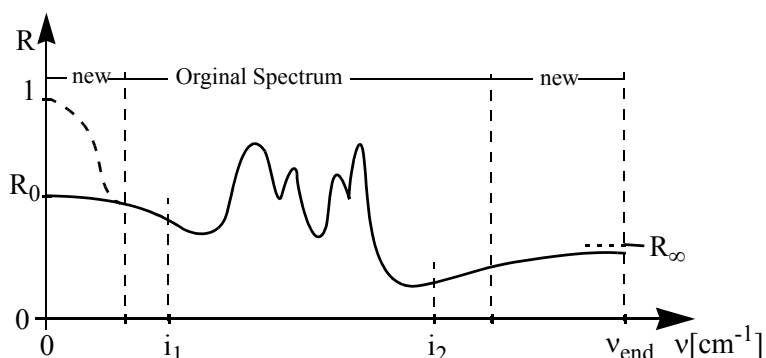


Figure 173: Parameters used for extrapolation

8.23.1.1 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 wavenumber 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.

8.23.1.2 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 wavenumber of the spectrum beginning), the a_2 coefficient can be eliminated:

$$R(s) = R(0) + a_1s^2 + a_2s^4$$

$$a_2 = \frac{R(s) - R(0) - a_1s^2}{s^4}$$

The remaining function is:

$$\Phi_1 = R(0) + a_1\nu^2 + (R(s) - R(0) - a_1s^2)\left(\frac{\nu}{s}\right)^4$$

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

8.23.2 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 wavenumber up to which the extrapolation has to be performed.

8.23.2.1 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 wavenumber 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:

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

8.24 Extended ATR correction

In case of the extended ATR (Attenuated Total Reflection) correction feature you have to use spectra which have been measured by an ATR unit. These spectra are corrected such that the position and intensity of the absorption bands are similar to those of a spectrum acquired in transmission mode.

The correction is based on the following physical effects:

- The penetration depth into the sample depends on the wavenumber in case of total absorption on the ATR crystal. This results in a modified band intensity, related to the frequency in the spectrum.

The correction of this effect is a simple spectra manipulation which has already been performed by the OPUS *Convert Spectra* command.

- In case of ATR measurement the absorption of the sample relates to the sample refraction index which depends on the wavenumber. Due

to the anomalous dispersion of the sample the band positions are erroneously shifted towards smaller wavenumbers. The correction of this effect is called extended ATR correction.

8.24.1 Theory of extended ATR correction¹

The extended ATR correction includes both effects mentioned above. When corrected, an AB (absorption) spectrum is modified according to the following equation:

$$ATR = AB \cdot \frac{1}{N} \cdot const \cdot \nu \cdot \frac{\sqrt{n_{12}^2 \cdot \sin^2(\Theta) - 1}}{E^2}$$

Where:

- ATR = result spectrum
- AB = uncorrected original spectrum
- N = number of ATR reflections
- ν = wavenumber
- n_{12} = ratio of refraction indexes between ATR crystal and sample, with the refraction index of the sample relating to the frequency in the spectrum
- Θ = angle of incidence
- E = middle electric field at the boundary

8.24.2 Performing extended ATR correction

Load the spectra measured by an ATR unit into the OPUS browser and select the *Extended ATR correction* command. The following dialog opens:

1. Literature: Francis M. Mirabella, jr (ed.); Internal Reflection Spectroscopy, Theory and Applications, Marcel Dekker, Inc., 1992, p 276ff.

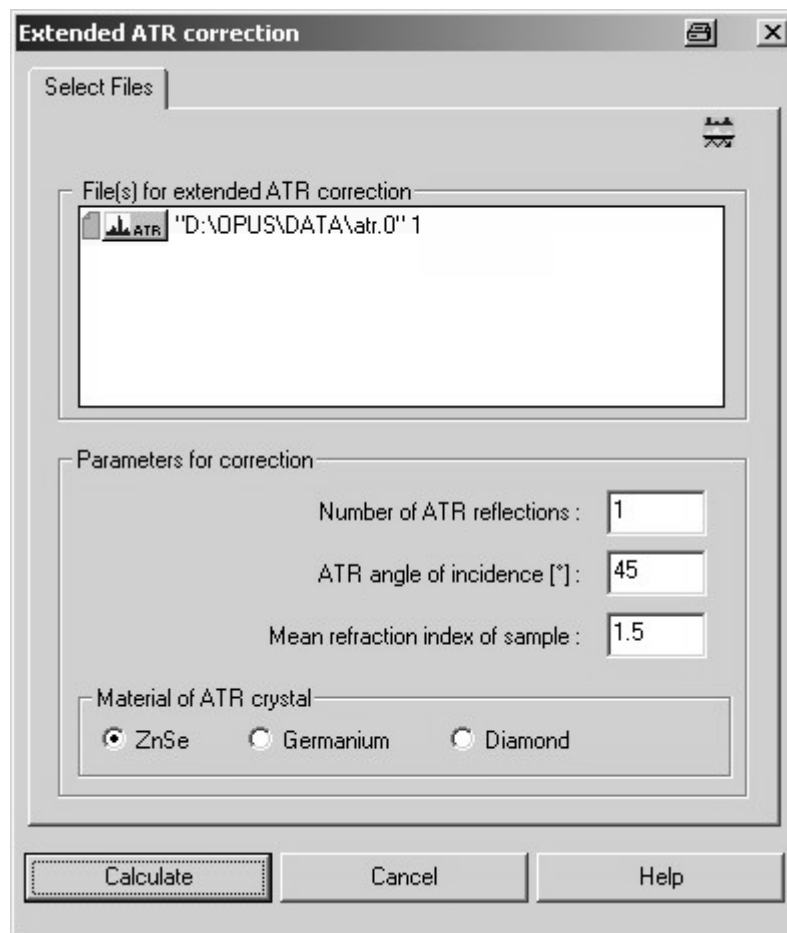


Figure 174: Extended ATR correction - Select Files tab

Drag and drop the data block from the OPUS browser to the *File(s) for extended ATR correction* selection field. Note that OPUS only accepts AB or ATR data blocks for ATR correction, either 2D or 3D spectra files. Using 3D files, however, requires the OPUS registry to contain a package which allows data manipulation of 3D files.

Define the following parameters:

- 1) Number of ATR reflections at the boundary between sample and ATR crystal
- 2) ATR angle of incidence with regard to the surface normal of the ATR crystal
- 3) Mean refraction index of the sample within the measured frequency range

Specify the material which the ATR crystal is made of. Activate the corresponding option button. Start the correction by clicking on the *Calculate* button.

The result is always stored in an ATR data block and overwrites the original spectrum stored in the AB or ATR data block.

8.25 1/cm <-> μm , nm

The $1/\text{cm} \leftrightarrow \mu\text{m}, \text{nm}$ command changes the x-axis (abscissa) unit of a spectrum. Wavenumbers 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.

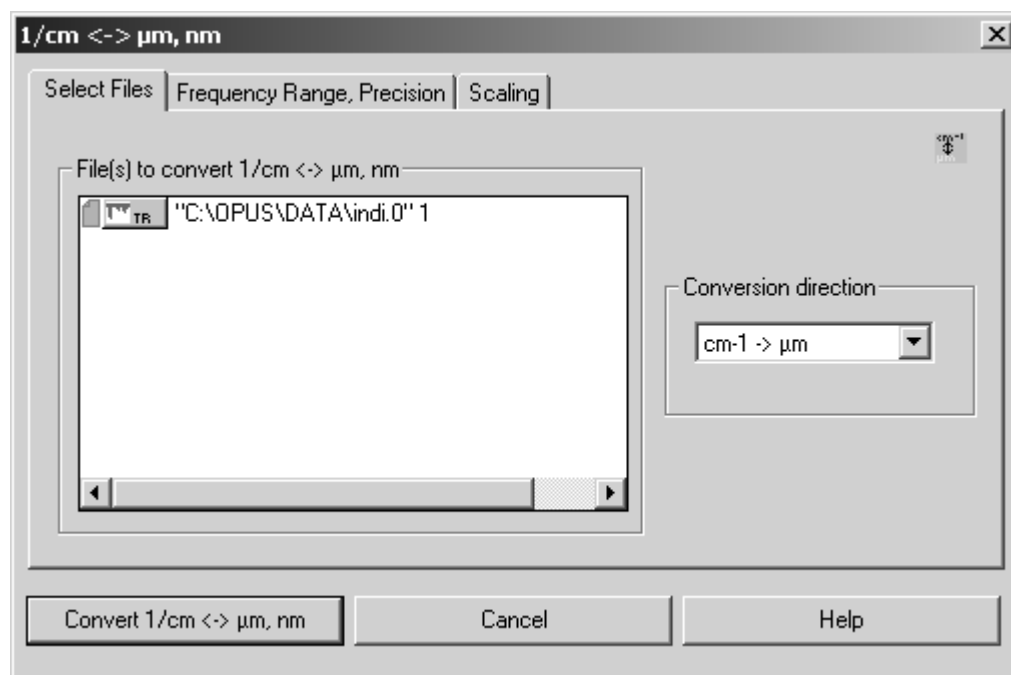


Figure 175: 1/cm <-> μm , nm – Select Files tab

On the *Frequency Range, Precision* tab you can individually define the frequency range or use it from the original spectrum.

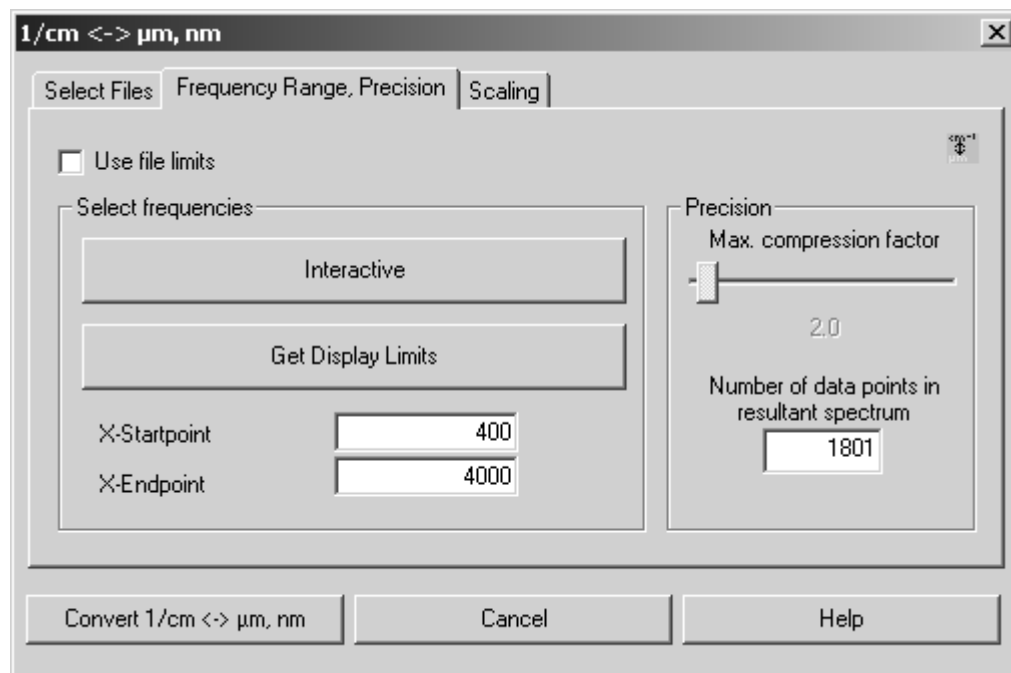


Figure 176: 1/cm <-> μm, nm – Frequency Range, Precision tab

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.

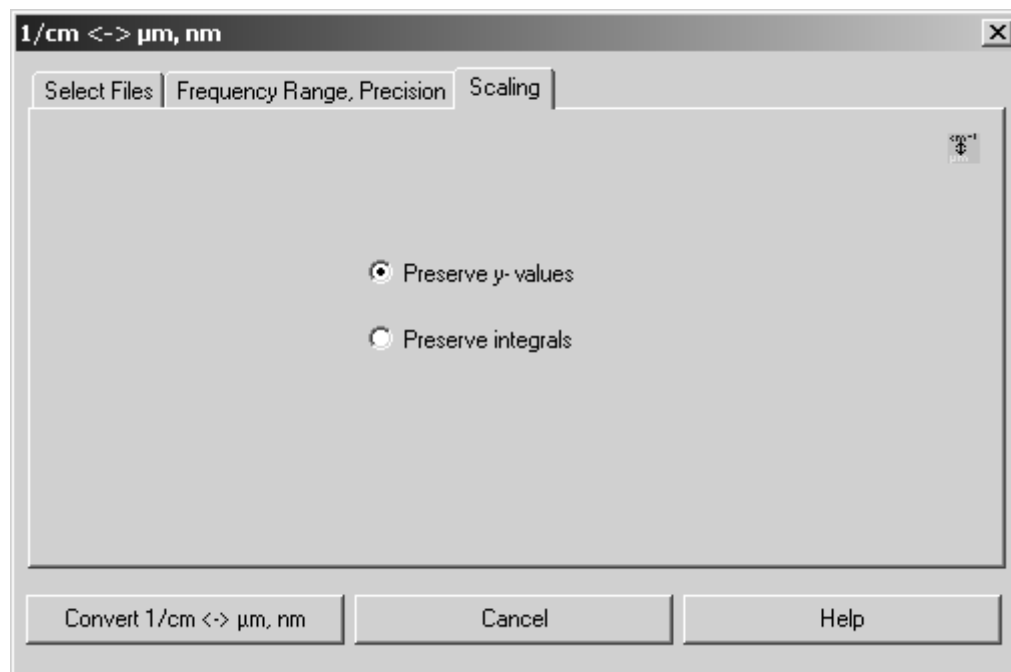


Figure 177: 1/cm <-> μm, nm – Scaling tab

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 wavenumber [cm^{-1}] and wavelength [μm] is based on the following formula:

$$\text{Wavelength } [\mu\text{m}] \times \text{wavenumber } [\text{cm}^{-1}] = 10000.$$

Each wavenumber 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 wavenumber. After the conversion, however, the data points are no longer equidistant.

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

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 wavenumber 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 wavenumbers (higher wavelenghts) 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 178 shows the original data scaled in wavenumbers. 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 wavenumbers 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.

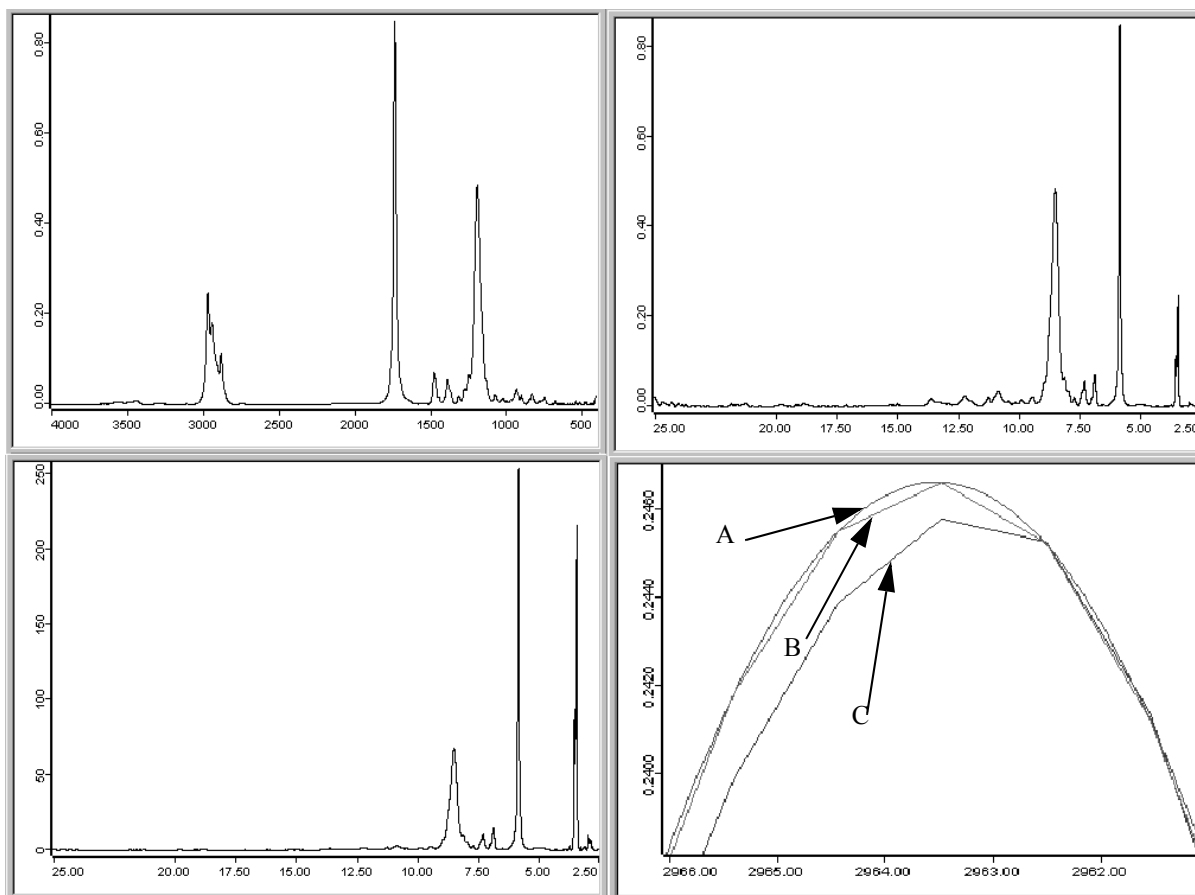


Figure 178: Original data and converted spectra after abscissa conversion

8.26 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.

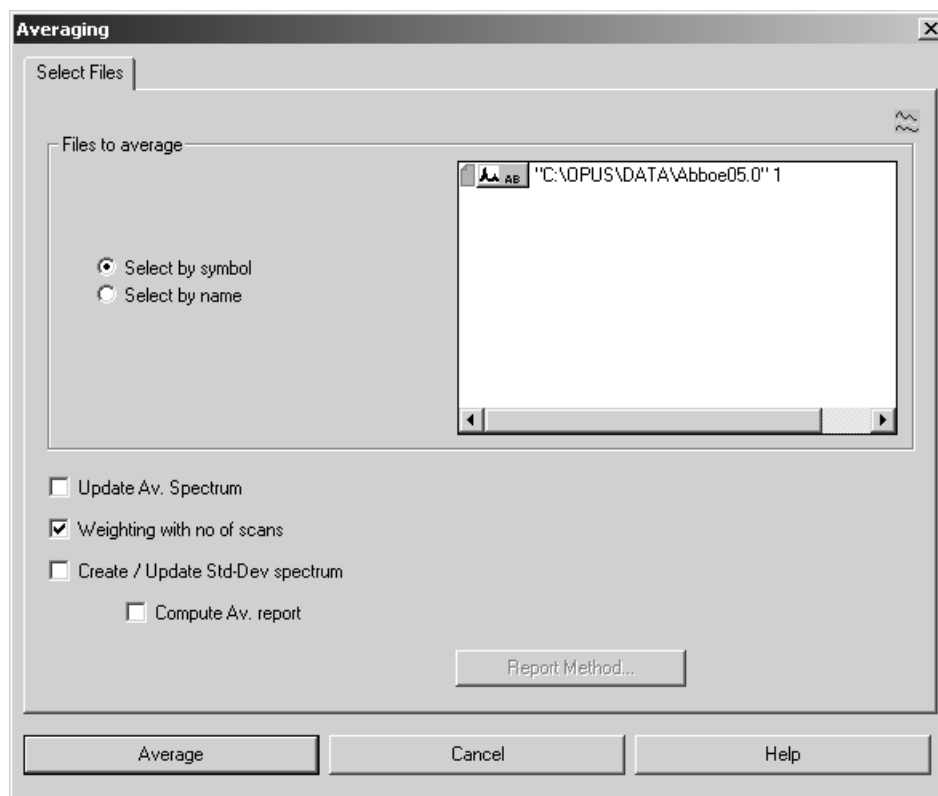


Figure 179: Averaging - Select Files tab (select by symbol)

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 180).

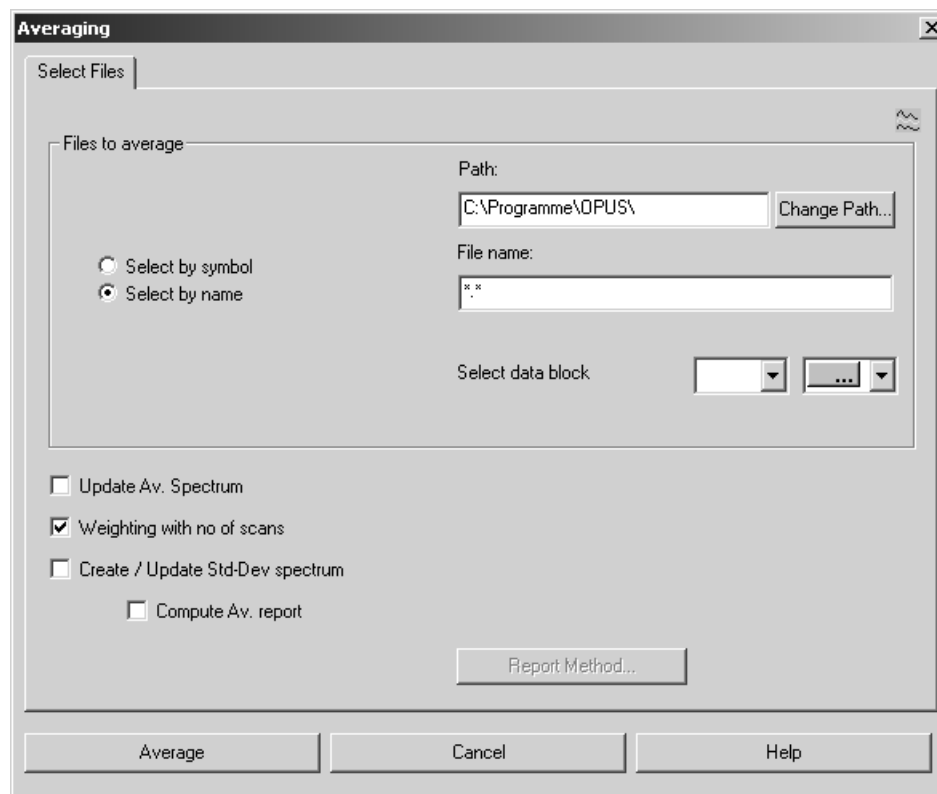


Figure 180: Averaging - Select Files tab (select by name)

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 drag & drop 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.

8.26.1 Averaging Theory

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

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

The σ standard deviation is:

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

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.

8.27 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.

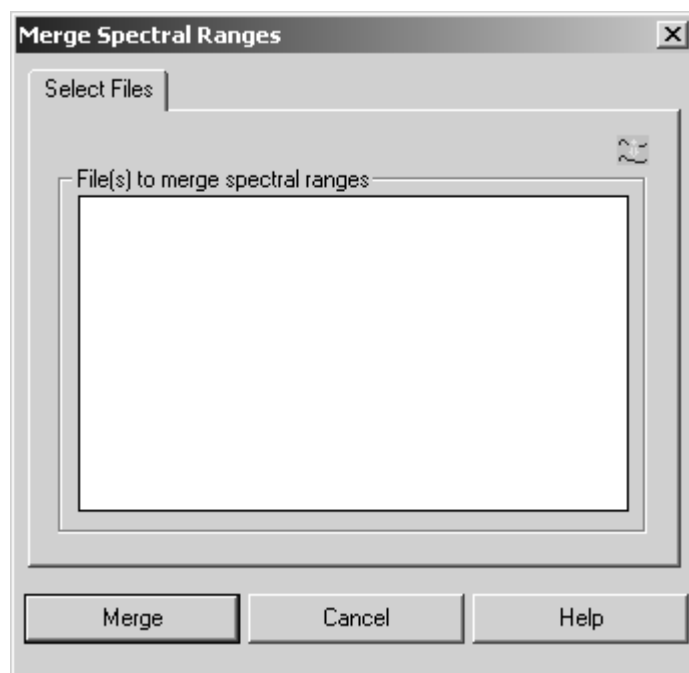


Figure 181: Merging Spectra Ranges

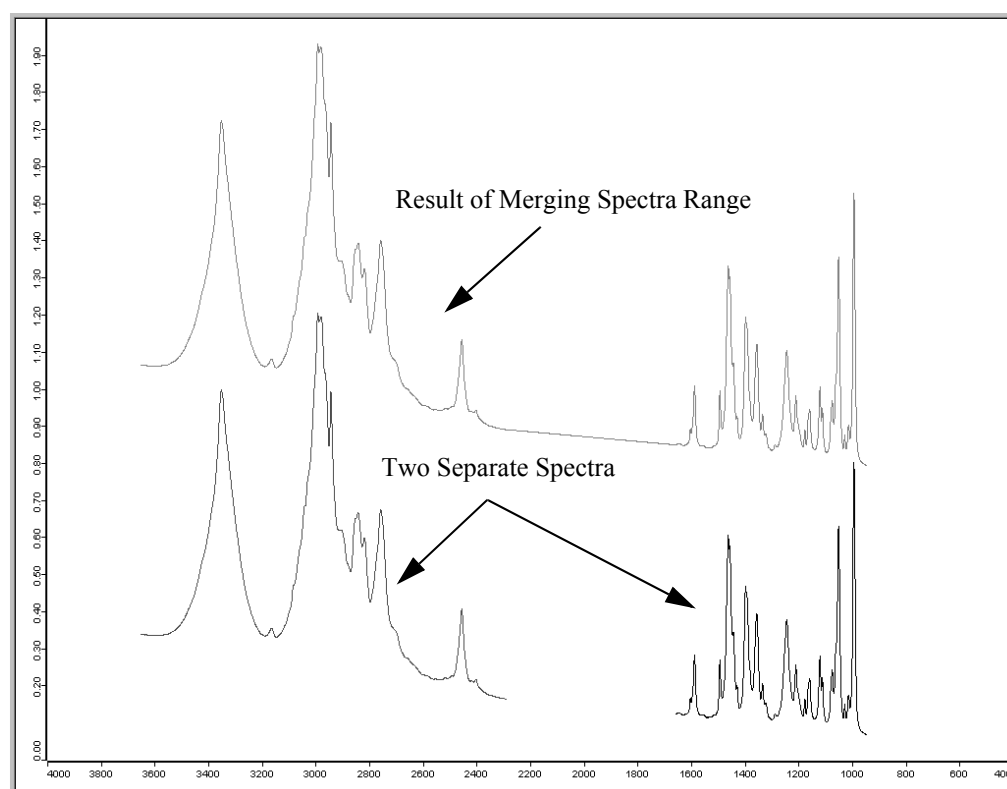


Figure 182: Original and merged spectra

8.28 Atmospheric Compensation

The *Atmospheric Compensation* command eliminates disturbing H₂O and/or CO₂ bands in ratio spectra. These bands arise due to different H₂O/CO₂ 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) H₂O and/or CO₂ bands. The algorithm has mainly been developed for MIR spectra. However, you can also use NIR spectra in connection with this algorithm.

If you select the *Atmospheric Compensation* command the following dialog box opens:

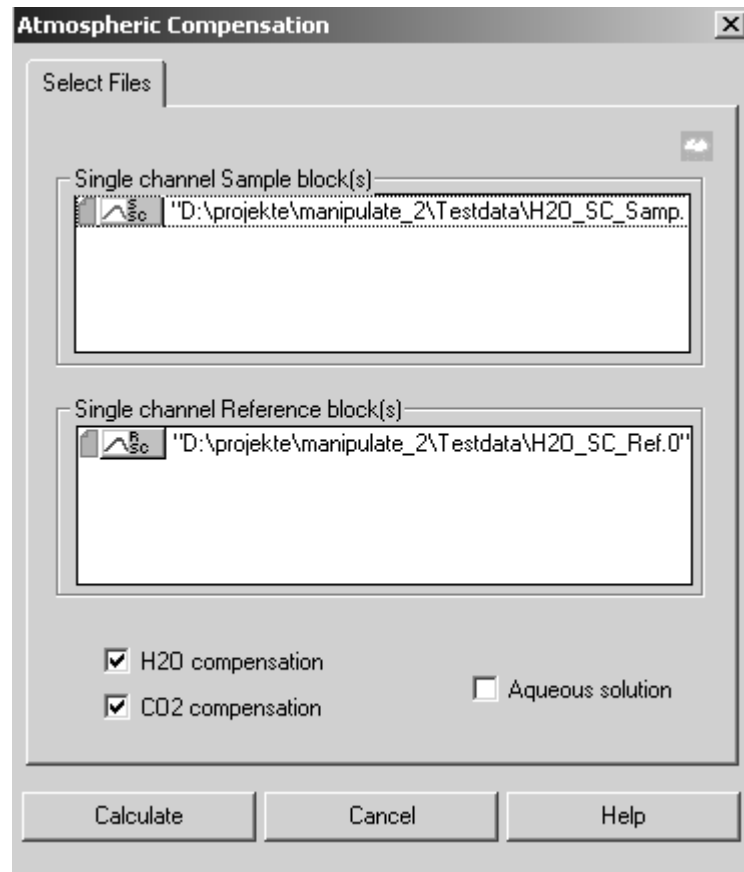


Figure 183: Atmospheric Compensation - Select Files tab

8.28.1 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:

8.28.1.1 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. If the file additionally contains a ratio spectrum, you can also drag and drop the ratio spectrum into the first selection field. Wrong data block types will automatically be ignored (see figure 183).

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

8.28.1.2 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 184.

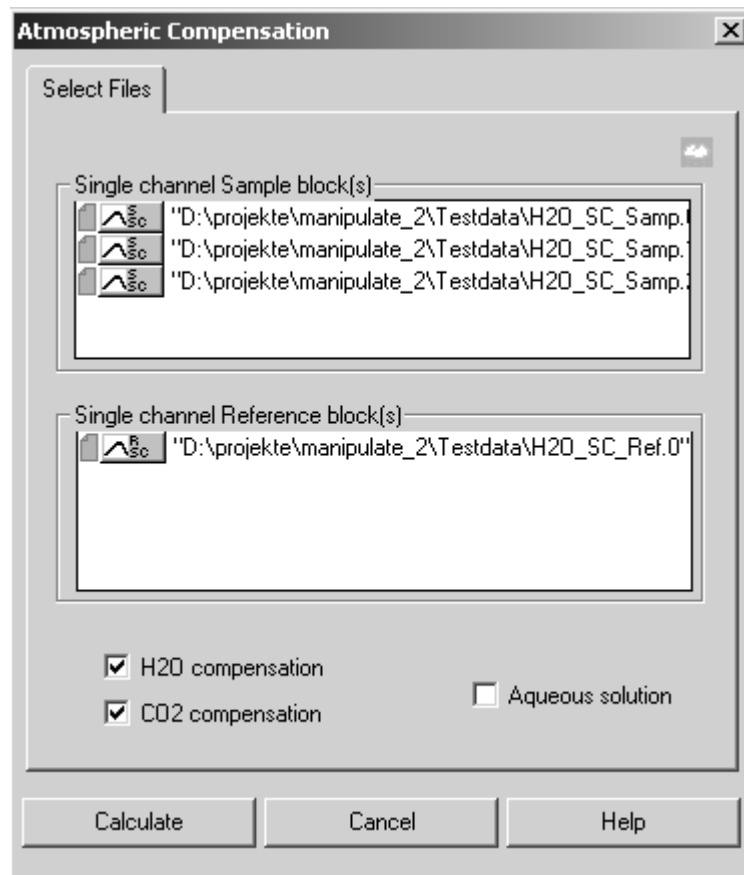


Figure 184: Atmospheric Compensation - single-channel spectra in different files

8.28.2 H₂O/CO₂ 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 184), 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.

8.28.3 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 185 shows *Atmospheric Compensation* effects.

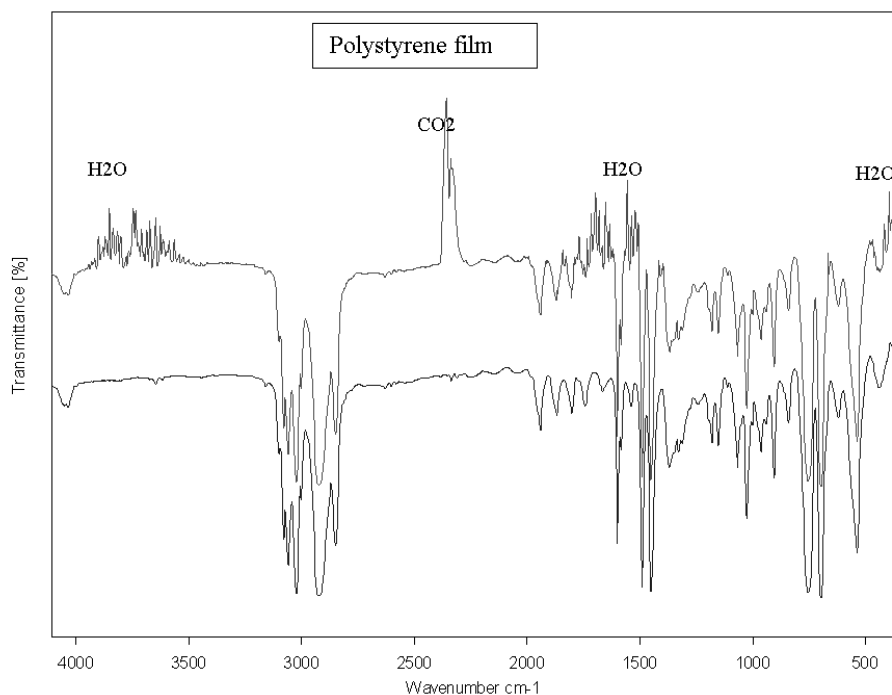


Figure 185: Atmospheric compensation effects

The upper curve is the transmission spectrum of a polystyrene film. H₂O and CO₂ bands can be clearly seen in several wavenumber ranges. The lower curve is the result of atmospheric compensation. Disturbing absorption lines of H₂O and CO₂ have nearly been eliminated.

8.28.4 Requirements

- Single-channel spectra have to contain wavenumber ranges starting from 3600 to 4000cm⁻¹ for H₂O compensation, and 2300 to 2400cm⁻¹ for CO₂ compensation. NIR spectra have to contain the wavenumber range from 5000 to 5600cm⁻¹ for H₂O compensation.
- Sample absorption within these wavenumber 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 wavenumber which shows strong absorption of atmospheric gases. To get a similar H₂O compensation (see figure 186), the lower wavenumber limit **must not** be around 1700cm⁻¹.


- For compensation in aqueous solutions the spectrum has to include wavenumber ranges of 2300-2400cm⁻¹ and 1800-1900cm⁻¹ for both CO₂ and H₂O.
- These wavenumber ranges must be free of sample absorption bands.

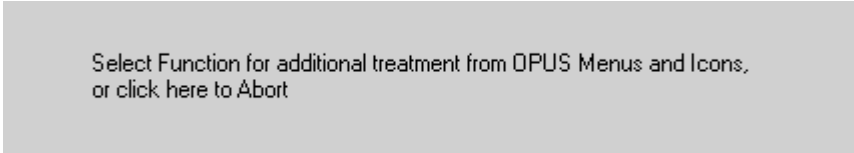
8.28.5 Limits

The *Atmospheric Compensation* command uses physical models to estimate the amount of atmospheric gases in the single-channel spectra and therefore compensates disturbing H₂O and/or CO₂ bands. *Atmospheric Compensation* is a kind of data manipulation and has to be used with due care.

8.28.6 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 186: Atmospheric Compensation - Select Files tab

- 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 187. If the sample measurement has been successful, *Atmospheric Compensation* will be performed immediately after the measurement.

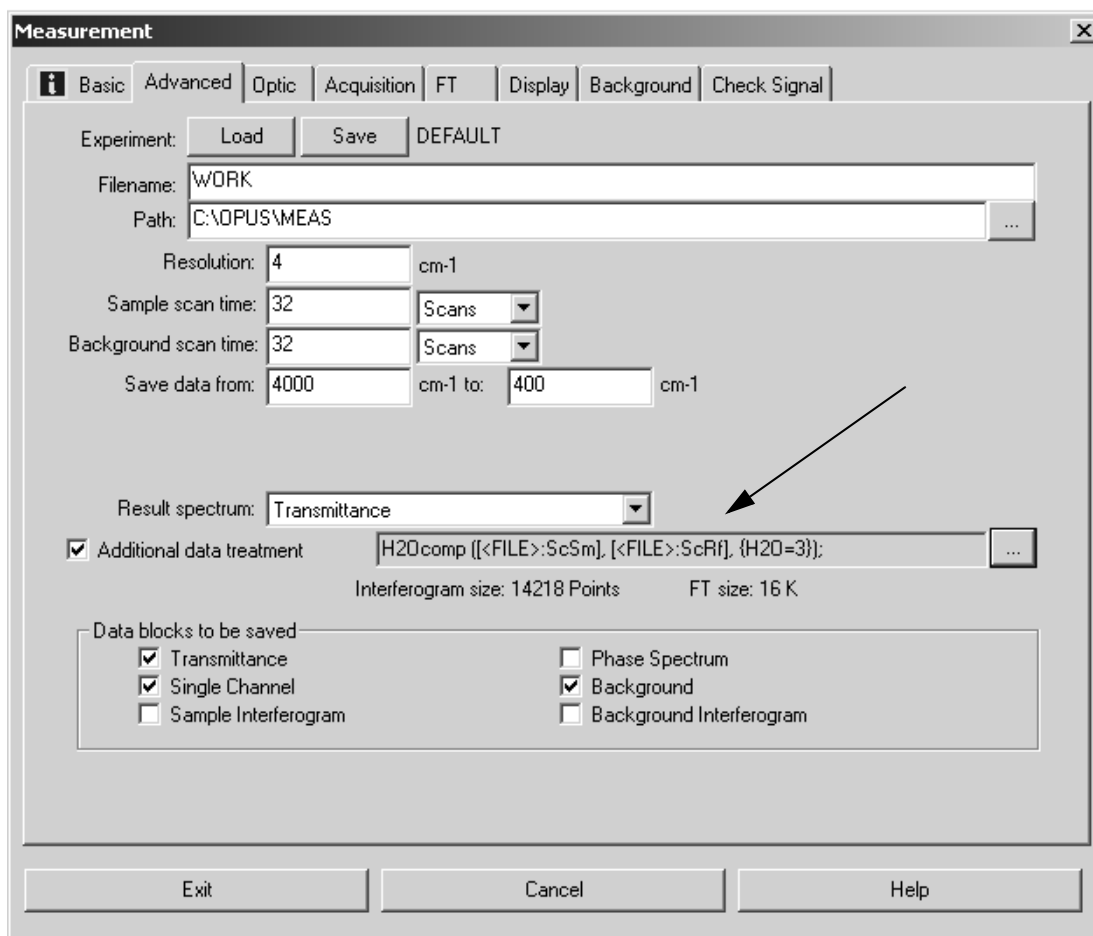


Figure 187: Measurement - activated post-measurement manipulation

8.29 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:

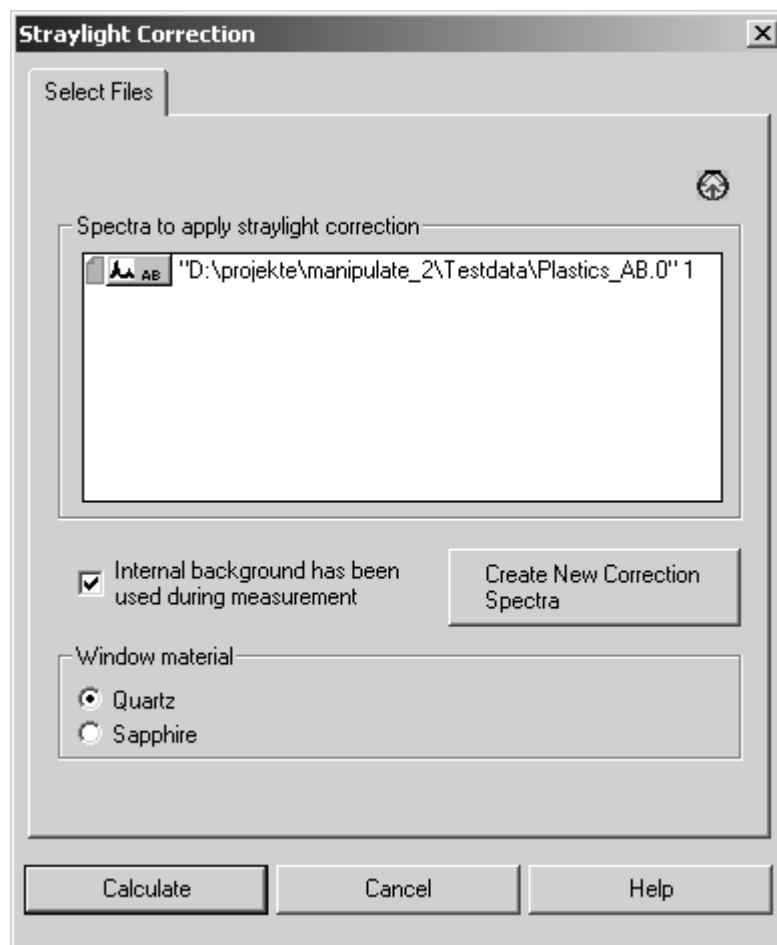


Figure 188: Straylight Correction - Select Files tab

8.29.1 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.

8.29.2 Internal Background

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

8.29.3 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.

8.29.4 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:

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

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

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:

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

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 189 shows straylight correction effects.

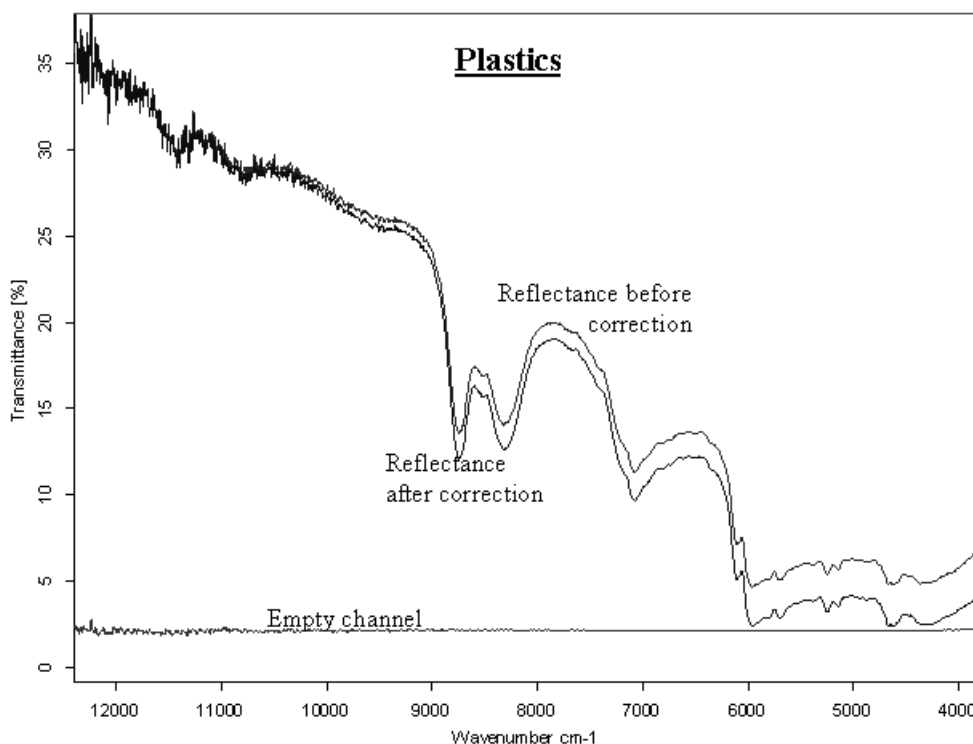


Figure 189: Straylight correction effects

8.29.5 Create new correction spectra

Before you start to use the *Straylight Correction* command you have to acquire correction spectra on the respective spectrometer. The nominal output of the different spectrometer components changes in the course of time, e.g. due to a decreasing laser or source lifetime etc. This will have effects on the entire instrument status. Therefore, to ensure a nearly 100% comparison to the respective instrument status, you should regularly acquire new correction spectra.

To proceed successfully you need a standard material, e.g. gold standard or certified Labsphere standard (99%). It is also possible to create correction spectra even if no standard is available. This is, however not reasonable, as the measurement may be falsified when applying straylight correction. The correction algorithm assumes that the standard used has a diffuse reflection of about 100% within a wavenumber range of 12,500 to 3,600 cm^{-1} .

Click on the *Create new correction spectra* button. A new dialog opens.

Note: The latest gold standards have a serial number and are supplied by an accompanied data sheet. This data sheet includes the averaged reflectance of the gold standard. Enter this numerical value as a figure between 0.8 and 1.2 into the entry field provided. If you use different types of standard or do not know the exact reflectance value, you should not change the default setting of 1.0.

Follow the on-screen instructions. If you have finished, the new correction spectra will automatically be stored on hard disk.

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 optional *Sphere Microsample* channel.

The following ratio spectra are calculated from these 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.

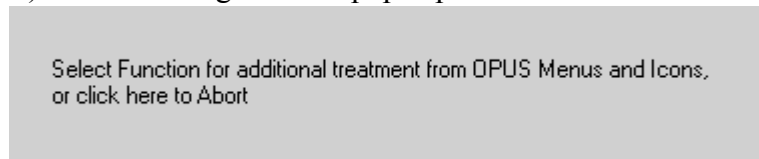
The *Straylight Correction* command always uses the latest correction spectra measured, i.e. correction spectra which have the biggest file name extension in the *(OPUS-Dir)/StrayCorr* directory.

8.29.6 Using straylight correction as part of the measurement process

If you want to use the *Straylight Correction* command 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:



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

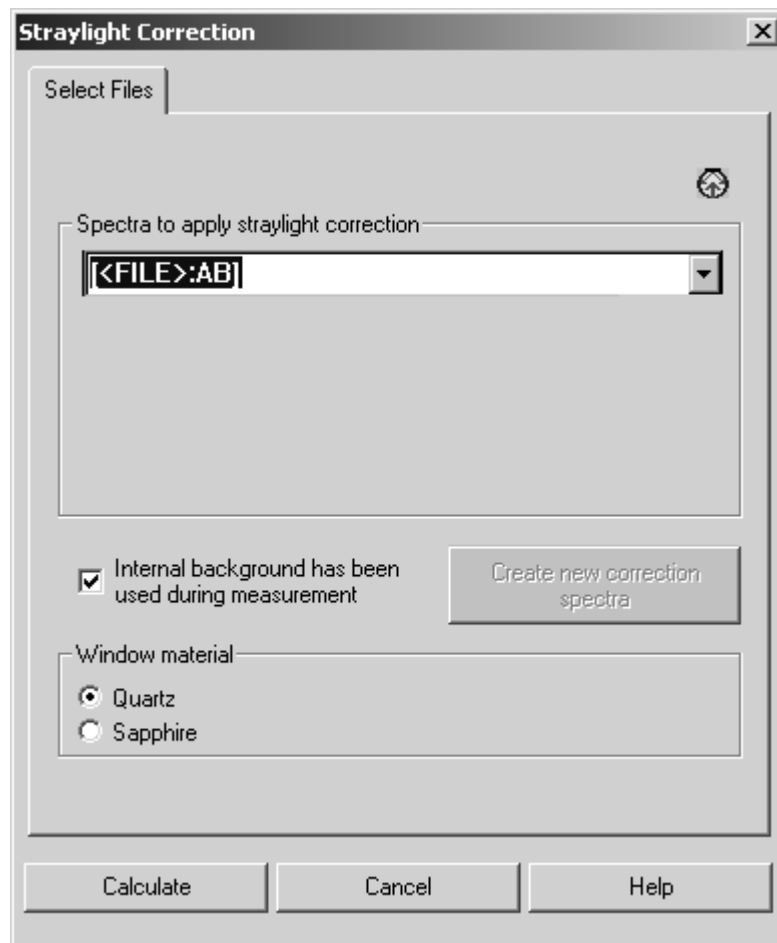


Figure 190: Straylight Correction - Select Files tab

- 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 191. If the sample measurement has been successful, additional spectra manipulation, e.g. *Straylight Correction* will be performed immediately.

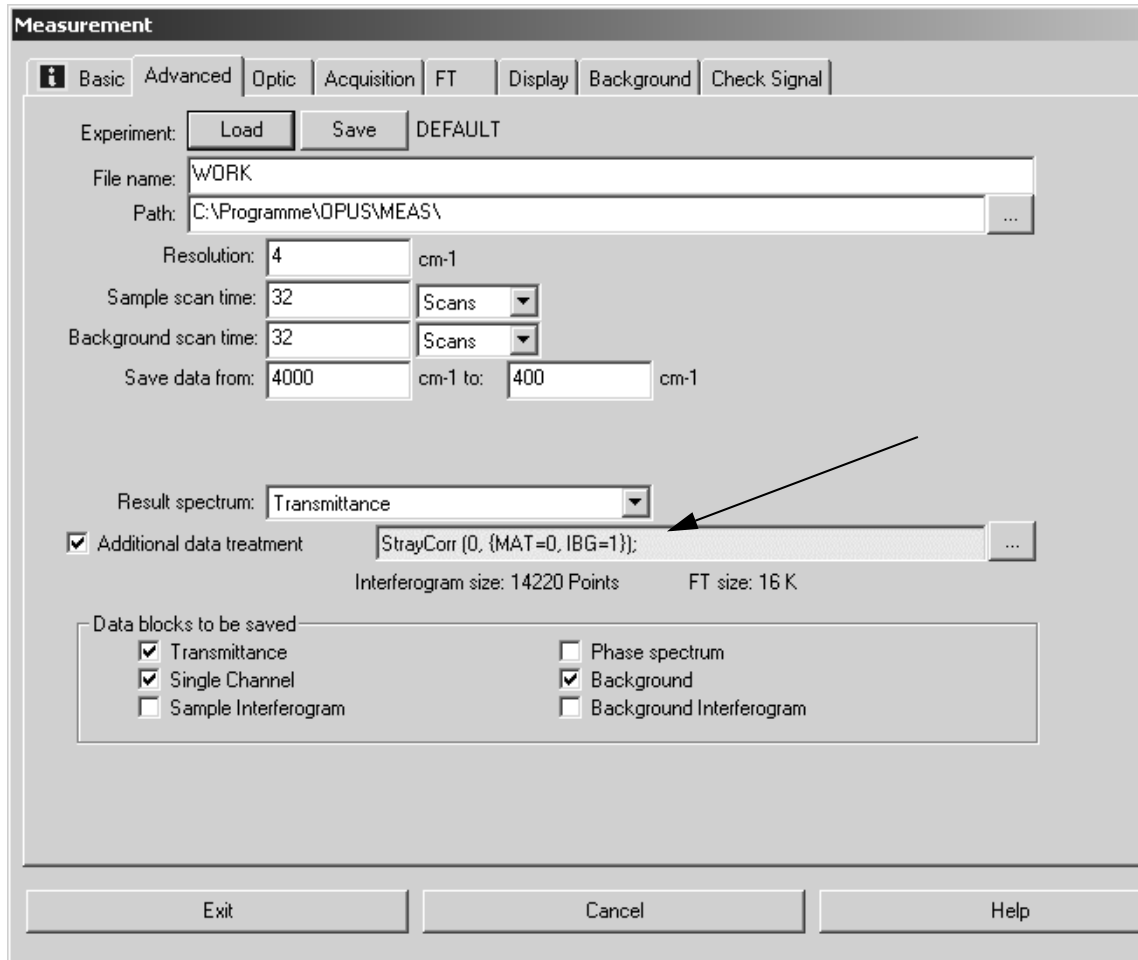


Figure 191: Measurement with activated post-measurement manipulation

8.30 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:

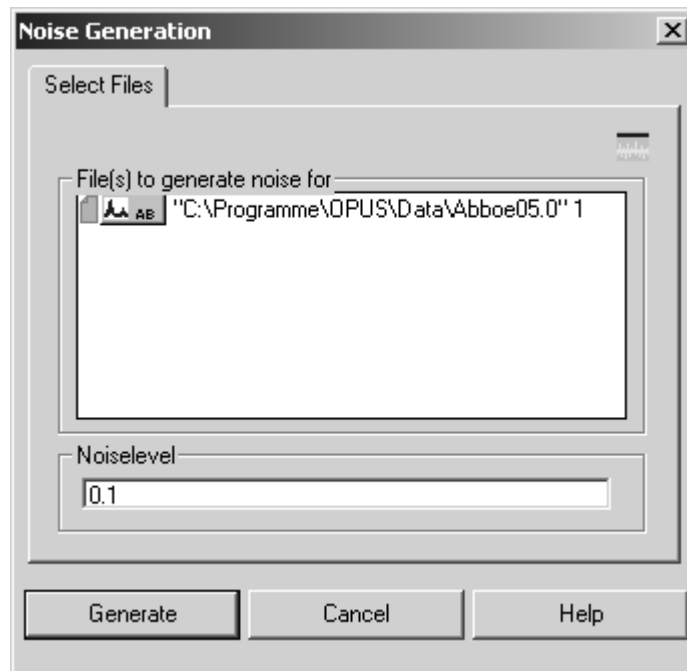


Figure 192: Noise Generation - Select Files tab

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

8.31 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:

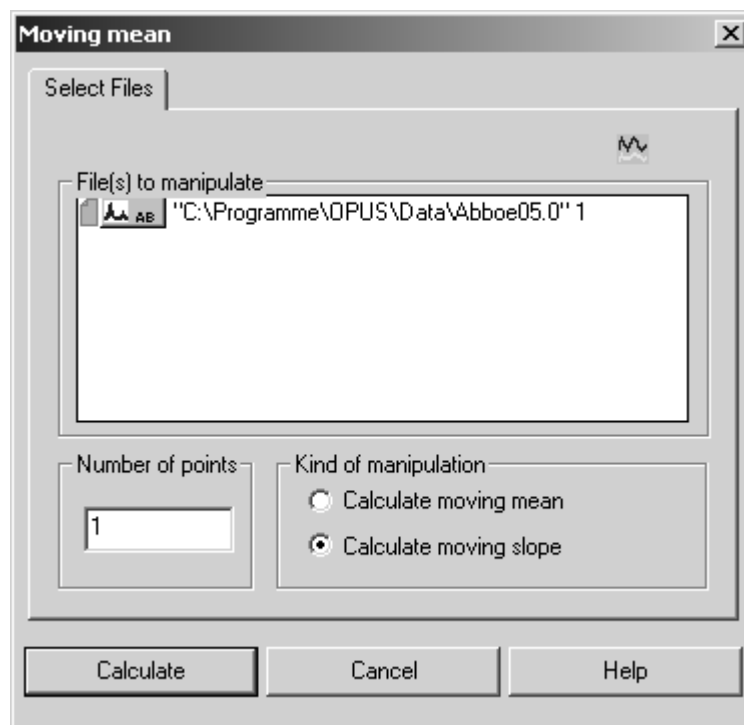


Figure 193: Moving Mean - Select Files tab

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 activate the *Calculate moving slope* check box, 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.

8.32 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:

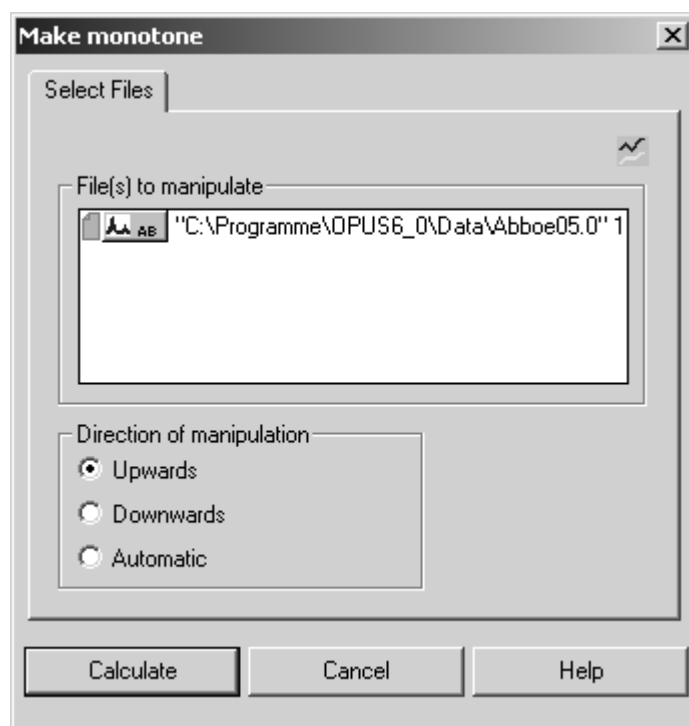


Figure 194: Make Monotone - Select Files tab

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

9 Evaluate

The commands 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.

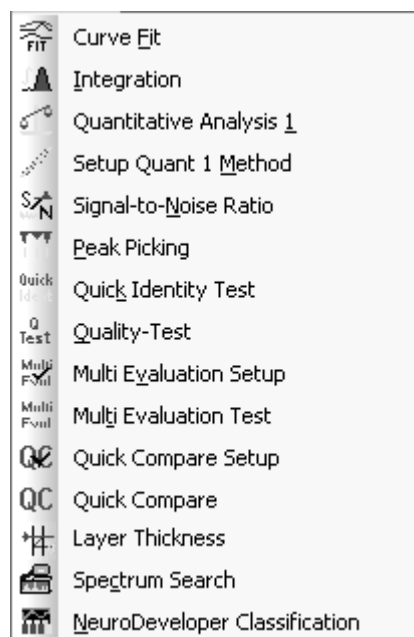


Figure 195: Evaluate menu

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.

9.1.1 Setup Model

Select the *Curve Fit* command and a dialog box opens which you use to specify the spectrum to be fitted and the frequency range.

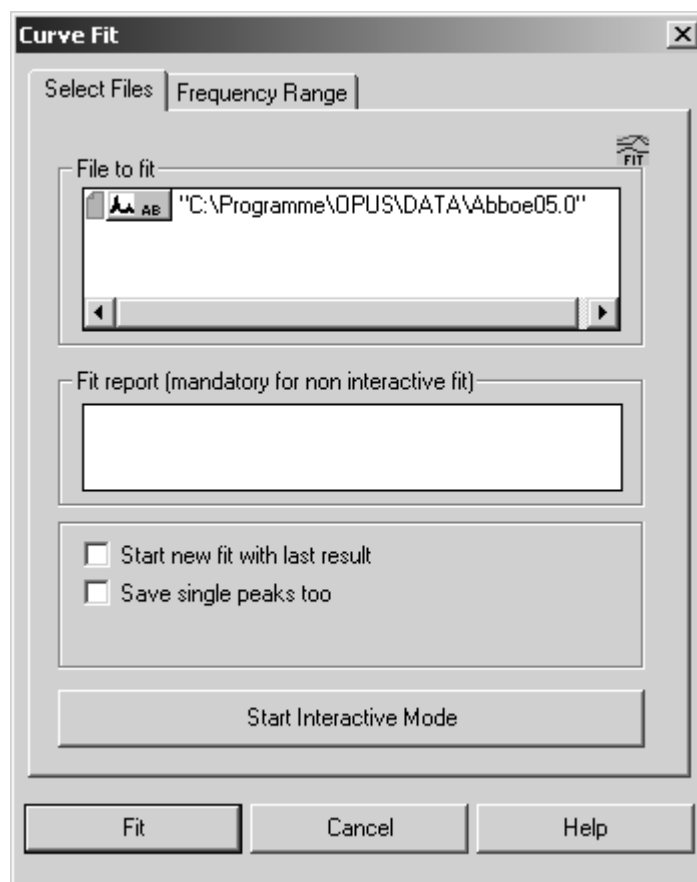


Figure 196: Curve Fit - Select Spectrum to Fit tab

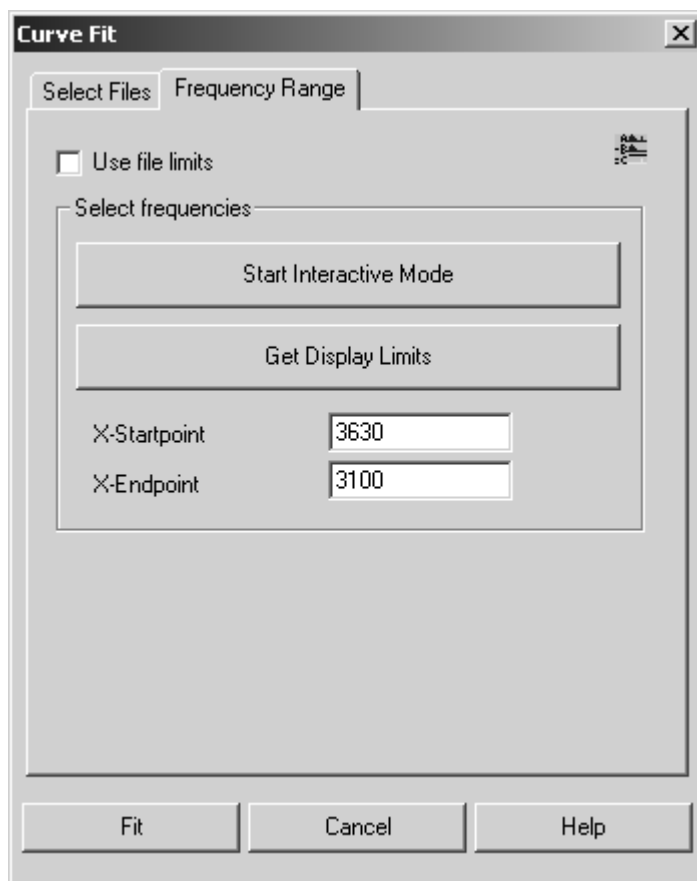
Drag & drop the spectrum to be fitted from the OPUS browser window into the *File to fit* selection field on the *Select Files* tab. Make sure that the spectrum is of absorbance type and baseline corrected.


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.

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.

On the *Frequency Range* tab (see figure 197) you define the frequency range of the spectrum you want to fit. Click on the *Set Interactive Mode* button and define the area to be fitted.

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 use the original frequency range of the file. In this case the options included in the *Select frequencies* group field are disabled.



Drag the FIT.REP block () of the already fitted spectrum into the *Fit report* entry field on the *Select Files* tab.

To perform a curve fit you first have to create a method. Click on the *Start Interactive Mode* button, and the spectrum selected will be opened in the curve fit setup window (see figure 198).

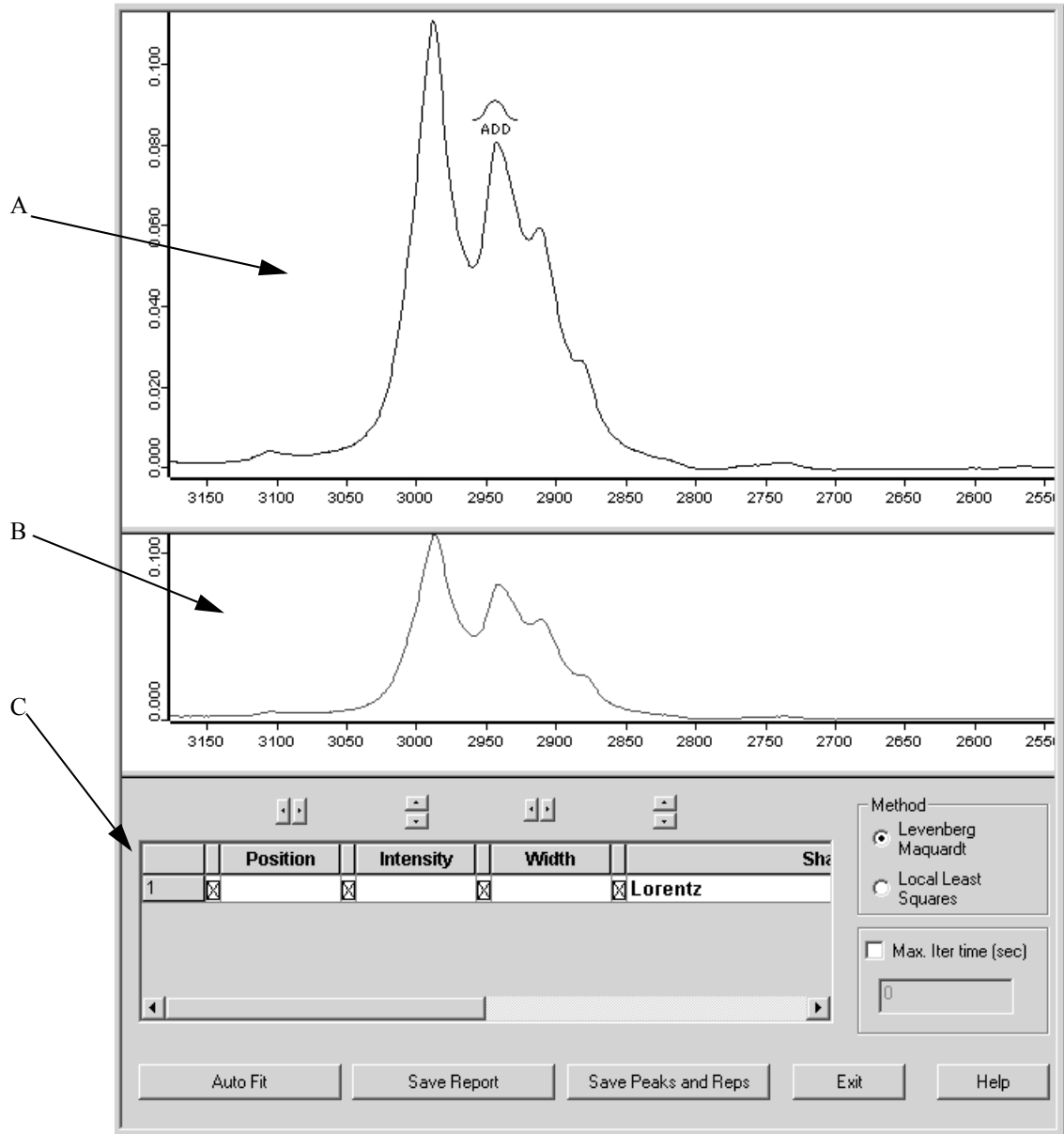





Figure 198: Curve Fit window before fit

In the upper window (A in figure 198) the spectrum to be fitted is displayed, whereas in the bottom window (B in figure 198) the difference between the original spectrum and the fitted spectrum is shown.

To create a curve fit model place the cursor into the top window. The cursor changes from an arrow to the  symbol. As soon as you click onto the peak, a curve will appear close to the selected peak.

If you position the cursor on top of the peak, the  symbol 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 dragging to the left, the curve will become wider, whereas dragging to the right reduces the curve width.

9.1.2 Peak Parameters

In the bottom half of the window (C in figure 198) various parameters can be edited. *Position*, *Intensity* and *Width* can be specified more precisely than by using the cursor. To change the values of a curve, click into one of the entry fields and directly type in the values or use the arrow buttons above the respective entry field. If certain peak parameters are not to be considered during automatic curve fit, deactivate the checkbox in front of the respective parameter(s).

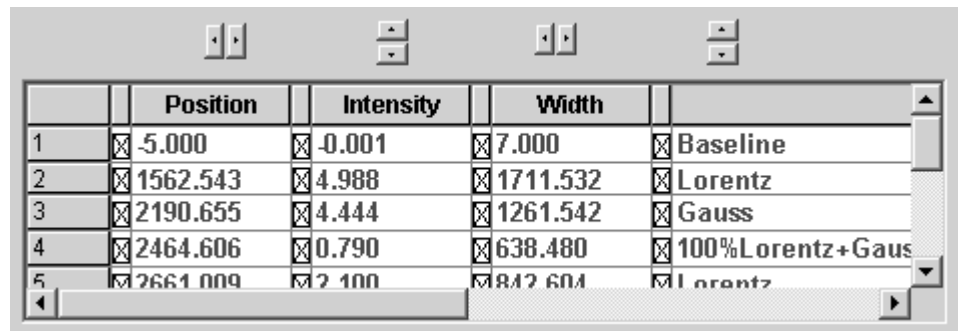
Each peak is shown in one line of the peak list including all peak parameters. The lines with non-selected peaks are green and the currently selected peak is marked in violet. The peaks in the list are always sorted by peak position.

9.1.3 Peak Shape

Several different options exist for the peak shape:

- Lorentz
- Gauss
- Baseline
- Lorentz + Gauss

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*.



	Position	Intensity	Width	
1	<input checked="" type="checkbox"/> 5.000	<input checked="" type="checkbox"/> -0.001	<input checked="" type="checkbox"/> 7.000	<input checked="" type="checkbox"/> Baseline
2	<input checked="" type="checkbox"/> 1562.543	<input checked="" type="checkbox"/> 4.988	<input checked="" type="checkbox"/> 1711.532	<input checked="" type="checkbox"/> Lorentz
3	<input checked="" type="checkbox"/> 2190.655	<input checked="" type="checkbox"/> 4.444	<input checked="" type="checkbox"/> 1261.542	<input checked="" type="checkbox"/> Gauss
4	<input checked="" type="checkbox"/> 2464.606	<input checked="" type="checkbox"/> 0.790	<input checked="" type="checkbox"/> 638.480	<input checked="" type="checkbox"/> 100%Lorentz+Gaus
5	<input checked="" type="checkbox"/> 2664.000	<input checked="" type="checkbox"/> 2.100	<input checked="" type="checkbox"/> 842.604	<input checked="" type="checkbox"/> Lorentz

Figure 199: Curve Fit parameters

Clicking again on the down arrow button and based on the Lorentz type, the peak shape changes to *100%Lorentz + Gauss*. In principle, the peak shape simulated is a pure Lorentzian function but it represents the special case of a mixture between 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.

9.1.4 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 *Width* parameter is replaced by the *Slope* parameter in the peak list. Baseline parameters can be set interactively by using the mouse, or directly entered into the peak table.

The baseline parameters are automatically modified, not until the *Levenberg-Marquardt* algorithm is used. If the *Local Least Squares* algorithm has been selected, the parameters are set manually.

9.1.5 Algorithm

Two different algorithms are available to optimize the model:



Figure 200: Curve Fit algorithms

Before starting calculation, select the appropriate algorithm which can also be changed during calculation. The principle of the two algorithms is described in the following.

9.1.6 Status Line

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

Example: 2sec: Residual RMS error 0.095696

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

Message: * Bad Fitting Model! *

If the **Bad Fitting Model!** message is displayed in the status line, the program has not been able to fit one or more peaks. These peaks can be found at the left or right end of the frequency range and usually have a very small intensity.

Delete these bands before you continue with the calculation. To delete a band click on the band number (left row) to select the band and press the *Delete* key on your keyboard. Confirm the dialog displayed by clicking on the *Yes* button.

9.1.7 Max Iter. Time (sec)

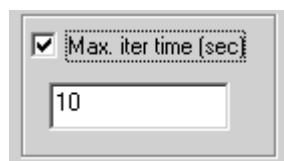


Figure 201: Maximum iteration time

First, activate the check box and define the maximum iteration time in seconds for the calculation.

9.1.8 Auto Fit

The *Auto Fit* button is used to start the calculation. If the calculation starts, the button text changes to *Stop*.

During the iteration the newly calculated peaks are shown on the screen in real time. The calculation can be interrupted at any time by clicking on the *Stop* button.

9.1.9 Save Report

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

9.1.10 Save Peaks and Reps

If you click on the *Save Peaks and Reps* button, the fit report is added to the original spectrum.

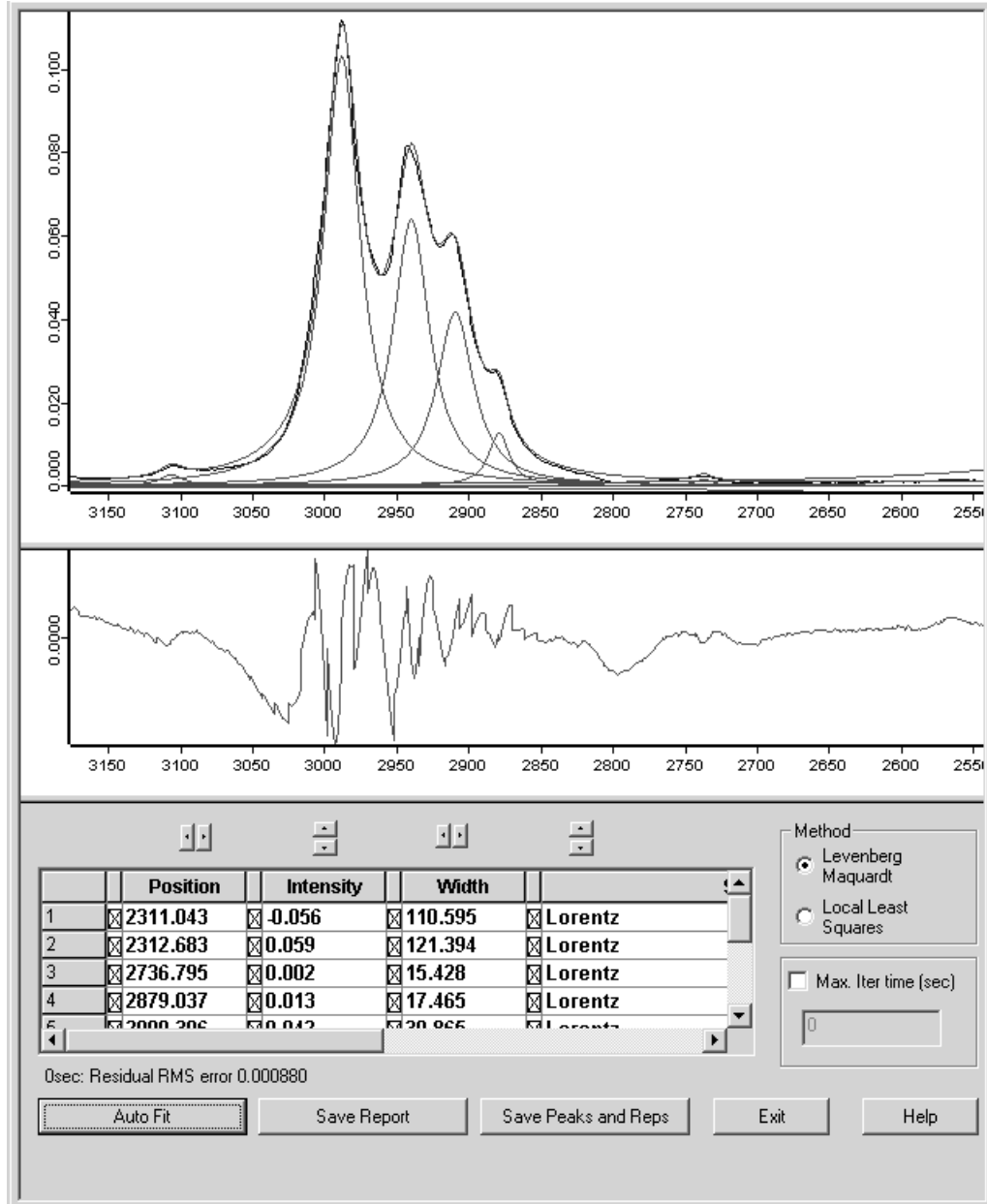


Figure 202: Curve Fit window after fit

9.1.11 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

9.1.11.1 Levenberg-Marquardt Algorithm

The quadratic equation for the deviation between the 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 have to be within the specified frequency range.
- The width of a peak must not be greater than the specified frequency range.
- Peak intensities have to be positive.
- The contribution of Lorentz- and Gauss functions for mixtures has to be within the range 0% to 100%.
- The sum of both parts has always to be 100%.

9.1.11.2 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 substantially reduces the amount of data required for the calculation. Compared to the *Levenberg-Marquardt* method the speed increases, but this is accompanied by some loss of precision.

The *Local Least Squares* algorithm has some conditions:

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

The given model can be seen as an area in an 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 model selected, i.e. the calculation either yields to the absolute minimum or is around the local minima. The latter case can be detected by a relatively large error and a visually obvious poor fit. In this case, start the calculation again by using a new optimized model.

9.1.11.3 Criteria for the selection of an algorithm

In most cases the *Levenberg-Marquardt* algorithm results in a better fit compared to the *Local Least Squares* algorithm, but needs significantly more calculation time. If the number of points in the selected range 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:

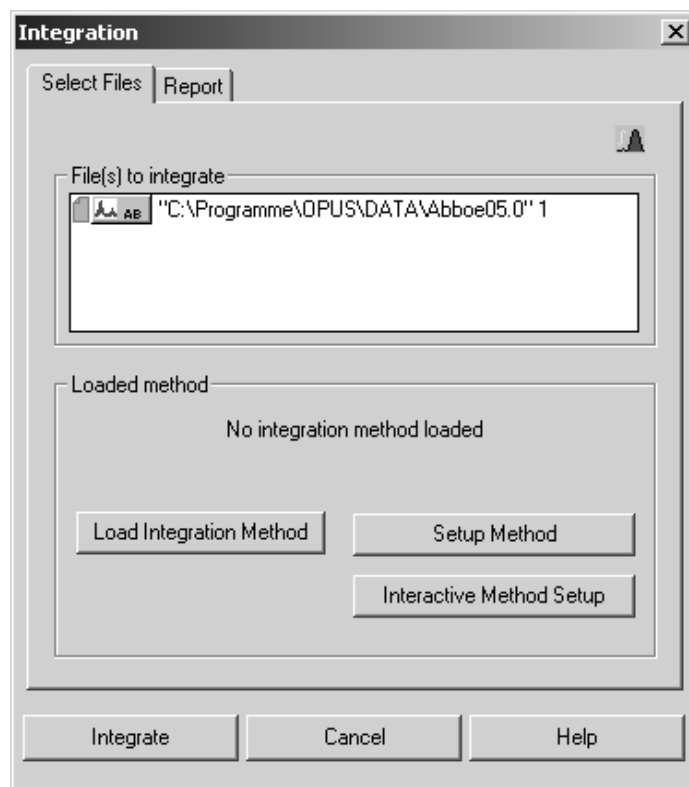



Figure 203: Integration - Select Files tab

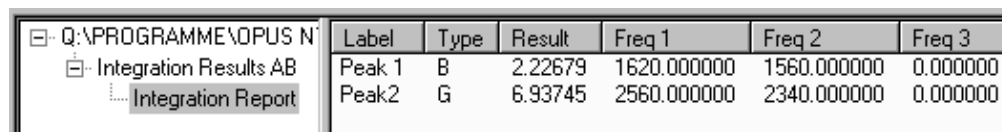
Drag & drop the file(s) to be integrated from the OPUS browser window into the *File(s) to integrate* selection field. Before you can start an integration you have to load a method previously created, or set up a new one.

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.

As soon as you click on the *Integrate* button the spectrum and the integration result will be displayed in the spectrum window. If you want to delete the integration result view, select the INTEG data block () in the OPUS browser. This data block stores the integration result. Right click on the data block and select the *Remove from Display* command from the pop-up menu. To have the integration result displayed again click on the INTEG data block and drag & drop it into the spectrum window. The color of the integration area displayed is exactly the same as of the spectrum.

By means of the *Show Report* command from the pop-up menu you can have the integration result displayed in the form of a report. This report includes the frequency limits as well as the integration method used.



The screenshot shows a file explorer window with a tree view on the left and a table on the right. The tree view shows a folder structure: Q:\PROGRAMME\OPUS N, Integration Results AB, and Integration Report. The table has the following data:

Label	Type	Result	Freq 1	Freq 2	Freq 3
Peak 1	B	2.22679	1620.000000	1560.000000	0.000000
Peak 2	G	6.93745	2560.000000	2340.000000	0.000000

Figure 204: Integration report

The integration report displayed in figure 204 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.

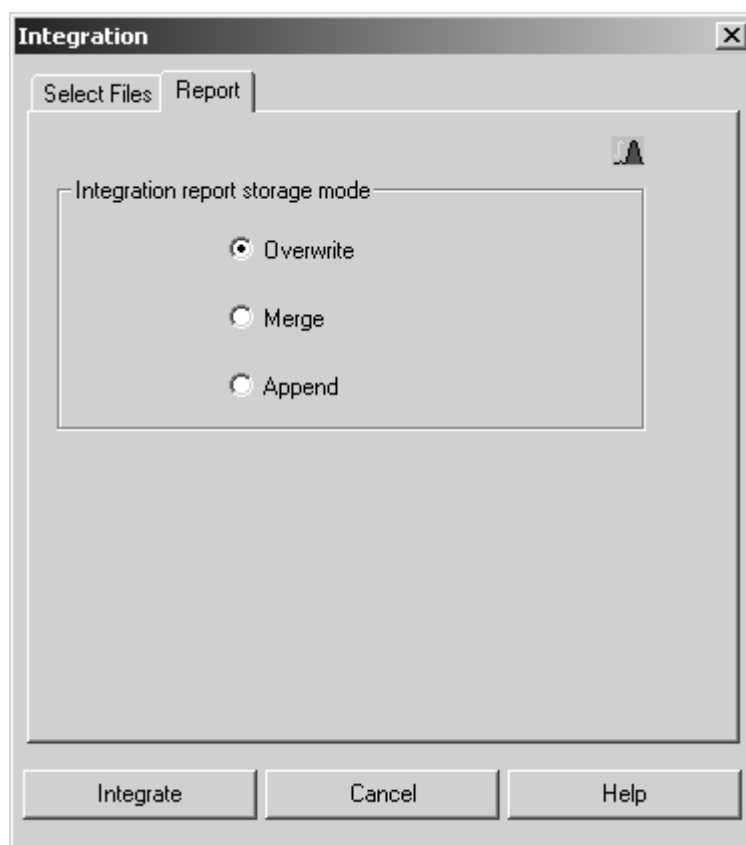


Figure 205: Integration – Report tab

- 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.

Label	Type	Result	Freq 1	Freq 2	Freq 3
Peak 1	B	2.22679	1620.000000	1560.000000	0.000000
Peak 2	G	6.93745	2560.000000	2340.000000	0.000000

Figure 206: Appending a new integration report to an existing one

The integration areas and modes used for the integration can be printed together with the spectrum. Click on the *Print Spectra* command in the *Print* menu and select a layout which contains a spectral frame. Then, *drag & drop* the spectral data block as well as the respective integration data block (INTEG) into the appropriate selection field. To get a preview of the spectrum and the integration areas click on the *Show preview* button.

Figure 207 shows a spectrum with two integration areas and the integration modes A and B (see chapter 9.2.1).

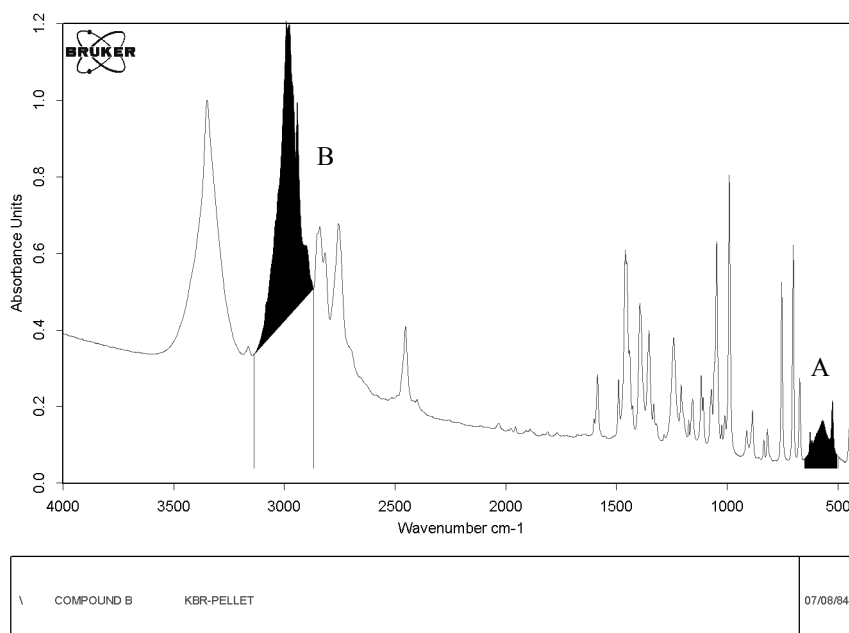


Figure 207: Preview window with integration area

A spectrum file evaluated by integration can also be used to create a new layout. For further details on the spectral frame layout refer to chapter 11.5.8.4.

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.

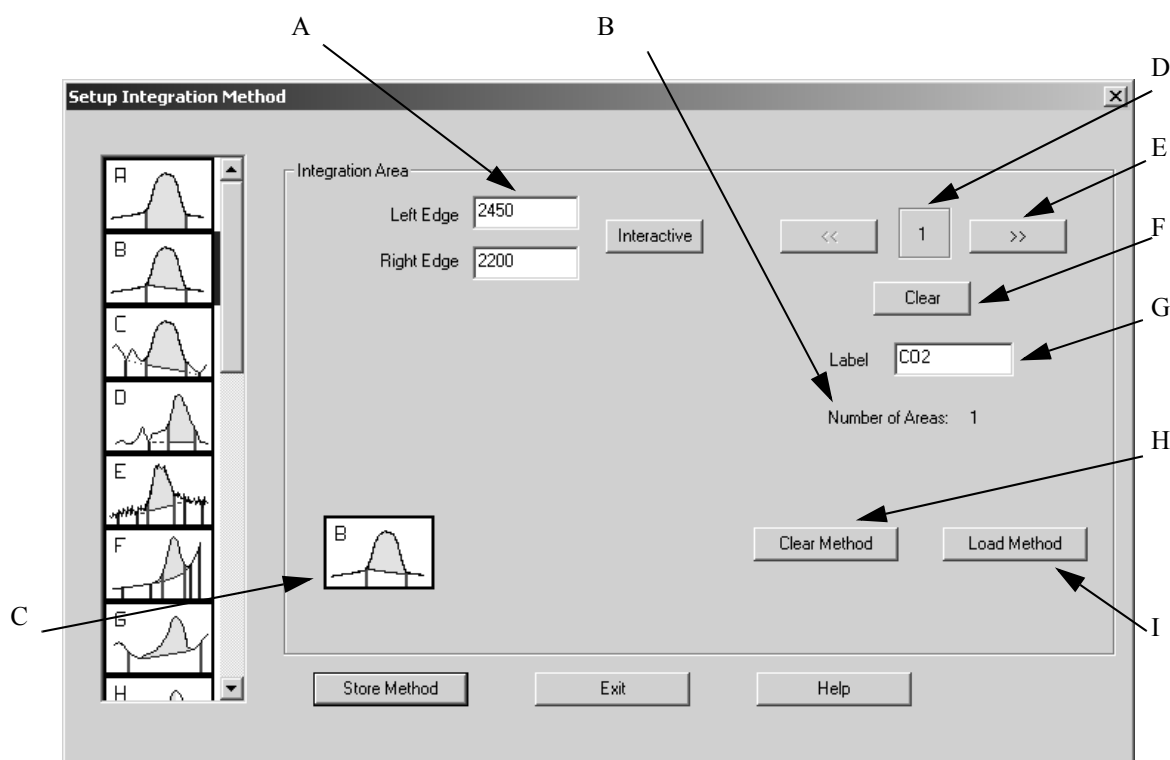


Figure 208: Setup Integration Method

- 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.

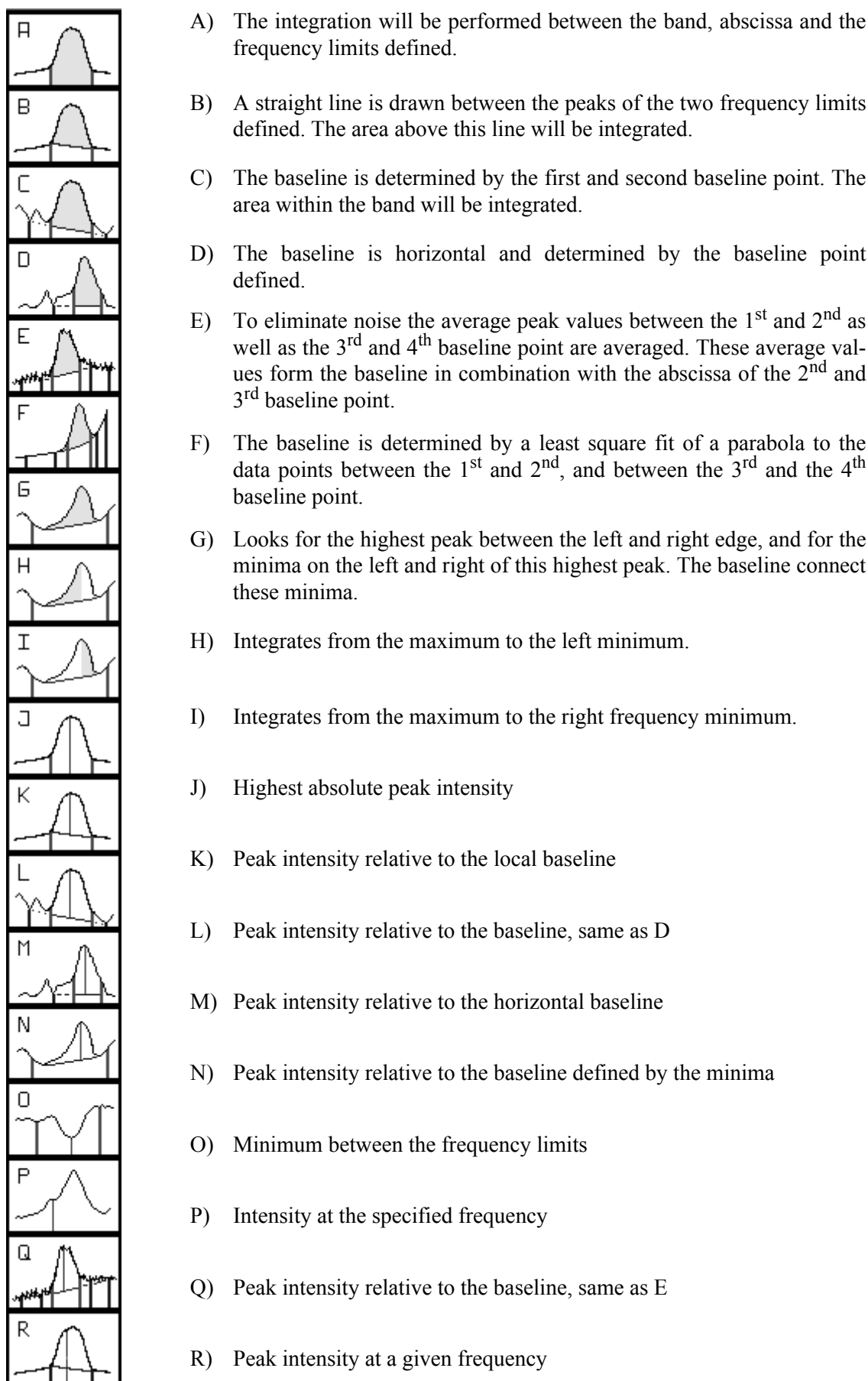


Figure 209: Integration modes

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.

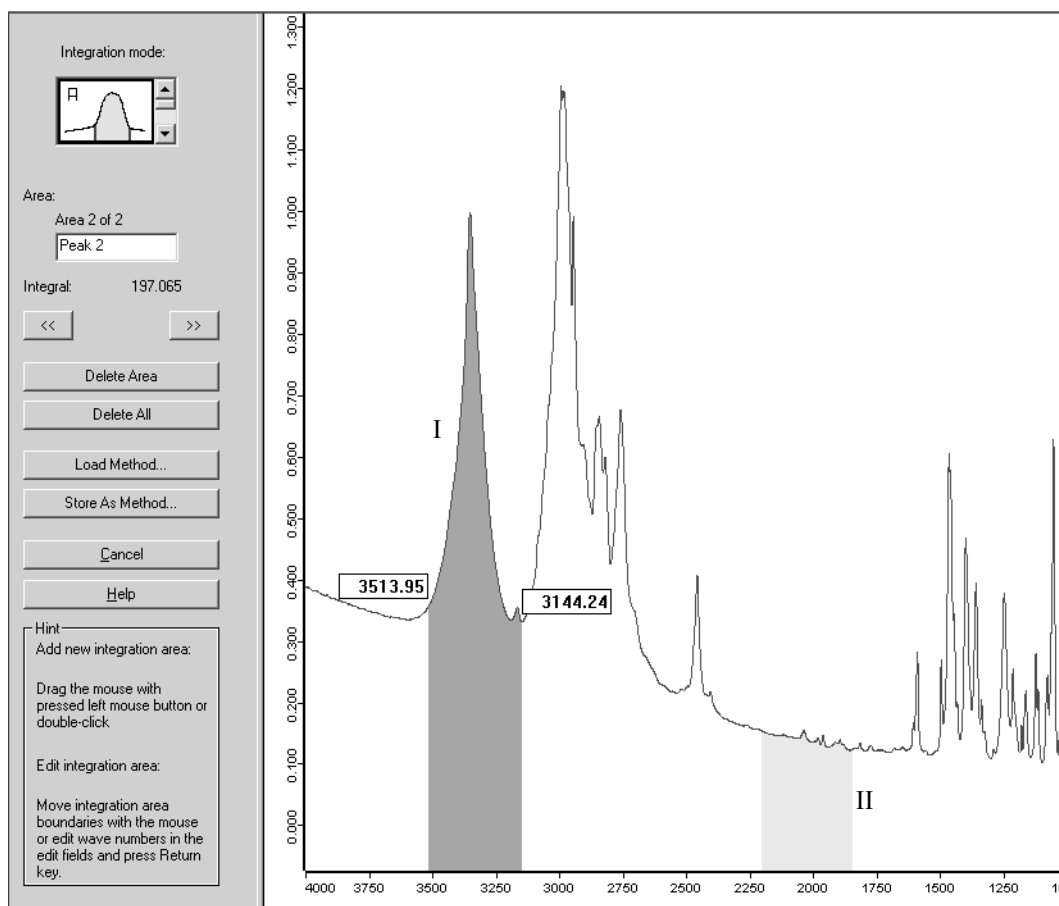





Figure 210: Integration - Interactive Method Setup

The integration modes *A*, *B*, *J* and *K* (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 integration mode *J* yields to the highest absolute peak position, and in case of mode *K* the peak intensity is relative to the local baseline.

The limits are exactly defined by the frequency range set. There will be no minimum. To define a new integration area click on a certain frequency limit, press the left mouse button and move the mouse to the second limit. The frequency limits of the activated integration area will be indicated by the exact wavenumber (see figure 210).

It is also possible to left click somewhere below the spectrum, draw a line and release the mouse button. The area selected will then be highlighted. To edit the wavenumber displayed, click into the respective entry field.

To change between the different integration areas use either the forward () and backward () arrow buttons, or left click on the respective integration area. 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 of mode *A* and *B* is displayed in red (I in figure 210), non-activated areas are displayed in light red (II in figure 210). In case of mode *J* and *K* the limits and maximum spectrum value are displayed by black vertical lines.

To change the limit of an integration area you first have to select the area. If you position the cursor on the area edge, the cursor will change into . Now, you can move the limit 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 an existing method by clicking on the *Load Method* button, or store current settings as integration method. In the latter case click on the *Store As Method* button.

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 overlapping it is recommended to use QUANT 2.

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 and can be determined e.g. 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 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:

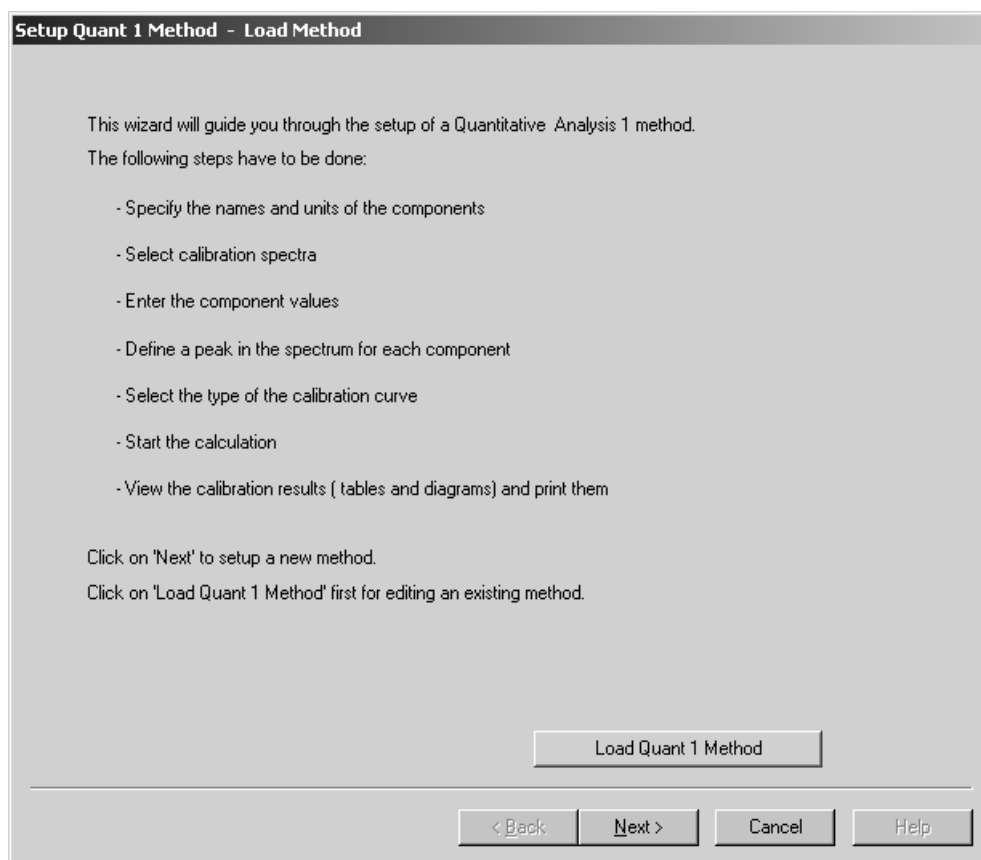


Figure 211: Setup Quant 1

Continue with the next page. Here you can enter the name of the components and their units. Start by clicking on the *Add Component* button.

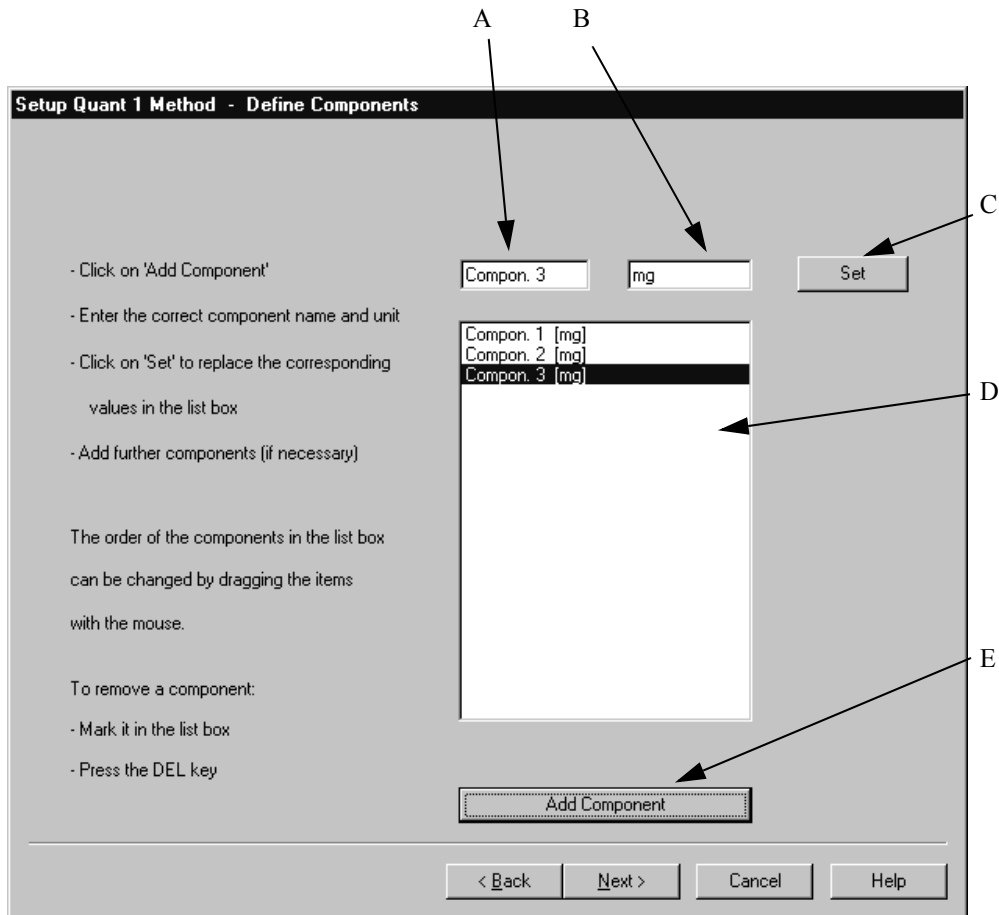


Figure 212: Define components

The default name of the first component and the *mg* unit appears in the entry fields (A) and (B). Select a name which is representative of the compounds you use and save the name by clicking on the *Set* button (C). To include additional compounds use the *Add Component* button (E). The selection list (D) displays all components and units. To remove a component, select it by using the mouse and press the *Del* 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 2 components.

Setup Quant 1 Method - Enter Component Values

	Filename	Compon. 1	Compon. 2	Compon. 3
1	ST100.0	4.5	2.3	0.9
2	ST101.0	1	0.5	3.6
3	ST102.0	2.4	4.1	4.5
4	ST103.0	3.6	0.6	1.2
5	ST104.0	2.5	1.7	0.8
6	ST105.0	1.6	2.3	3.2
7	ST106.0	0.6	3.8	2.7
8	ST107.0	1.6	2.5	4.2
9	ST108.0	3.5	1.2	2.7
10	ST109.0	1.9	0.8	3.8
11	ST110.0	3.9	1.6	0.8
12	ST111.0	3.6	2.7	2.3
13	ST112.0	4.2	0.8	1.9
14	ST113.0	2.7	4	1.8
15	ST114.0	1.8	3.5	3.4
16	ST115.0	1.4	2.9	2.2
17	ST116.0	2.6	3.9	3.1
18	ST117.0	0.6	2.4	3.4
19	ST118.0	2.5	3.1	0.9
20	ST119.0	3	2.7	1.5
21	ST120.0	1.2	1.8	3.9
22	ST121.0	0.9	2.4	2.7

Add Spectra Change Path Remove Selected Spectra Print

< Back Next > Cancel Help

Figure 213: Component list – component value input

Using the *Add Spectra* button you can add spectra to the list. Navigate to the directory holding the spectra by clicking on the *Change Path* button. If you want to exclude a spectrum, select the spectrum and click on the *Remove Selected Spectra* button. You can also print this table for your records by clicking on 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, which peak height or integral is to be used for calibration.

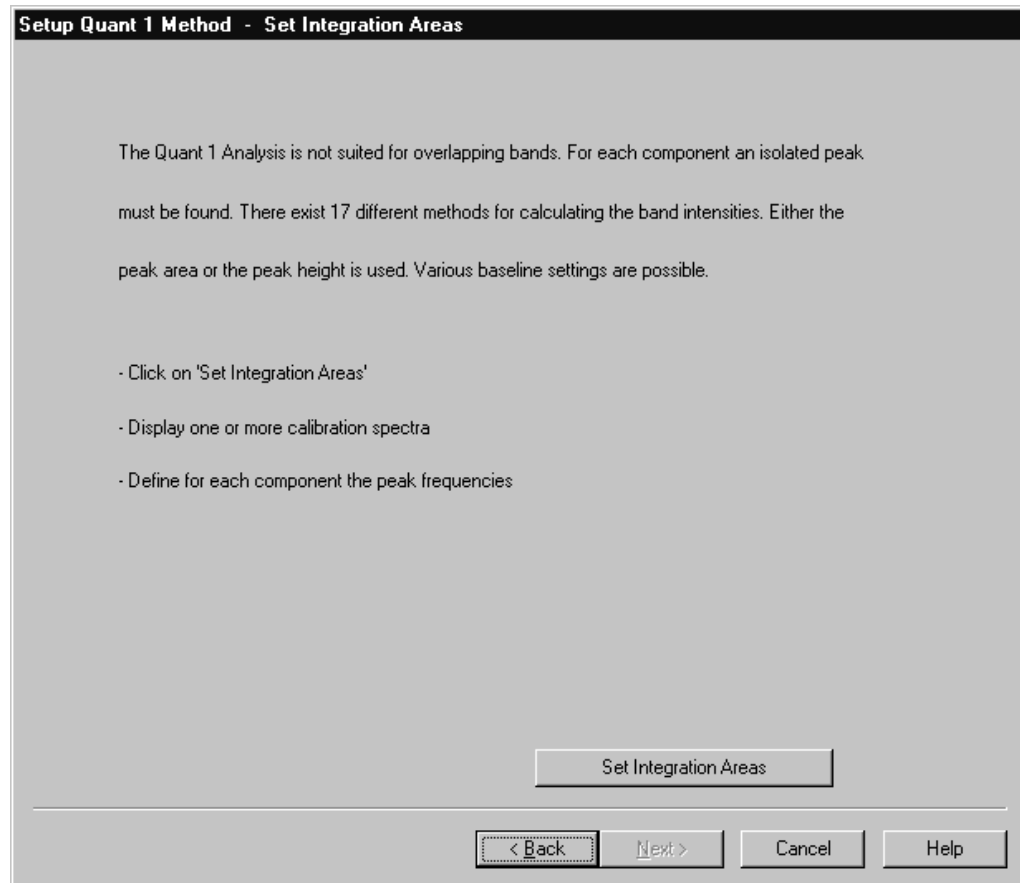


Figure 214: Setup integration method

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.

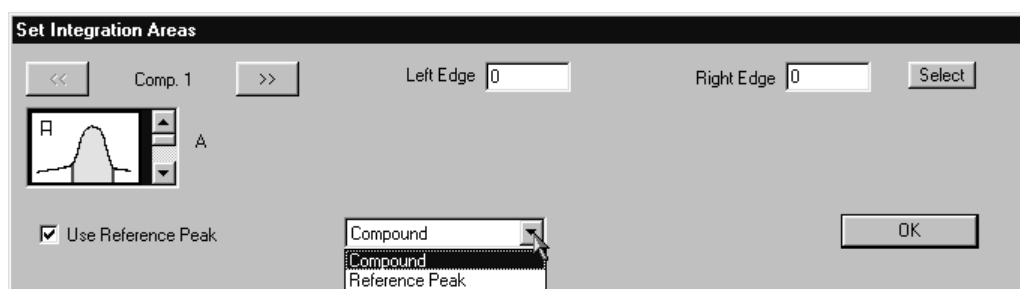


Figure 215: Define integration method

In addition, you have the possibility to define a reference peak by activating the *Use Reference Peak* check box. Select an integration method and frequency region for this peak as you would for any other peak. Make sure that you select *Reference Peak* from the drop-down list. This reference peak will be used to normalize the spectrum.

Finally, you have to 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.

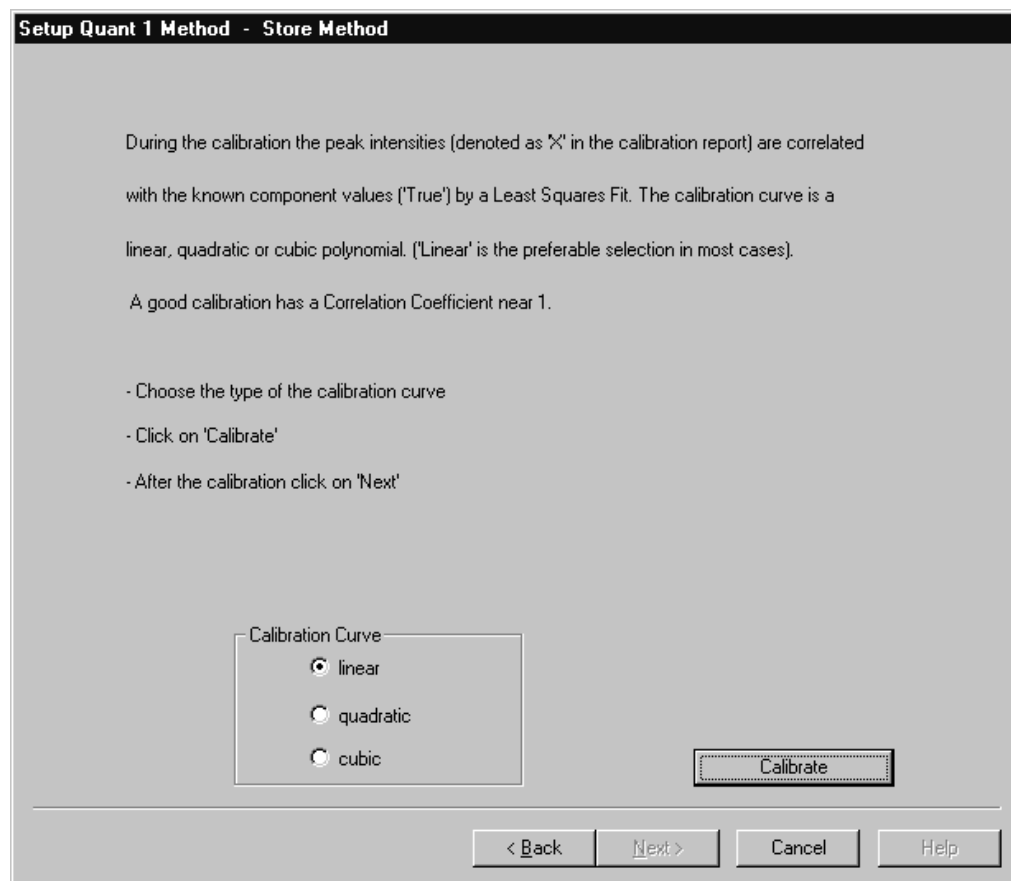


Figure 216: Choose calibration curve

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. 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 the *Next* button 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 displayed 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.

Setup Quant 1 Method - View Calibration Reports

	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

Calibration Report Compon. 1 << >> Print

< Back Next > Cancel Help

Figure 217: Calibration results

You can change between the result pages for each component using the arrow button. Change between the tabular view and a report view of the results by activating the *Calibration Report* check box. The report view displays a printable version of the report.

If you click on the *Next* button, a graph of the calibration result will be created. The graph allows to easily recognize data with poor correlations, e.g. incorrect values caused by typographical errors during data entry.

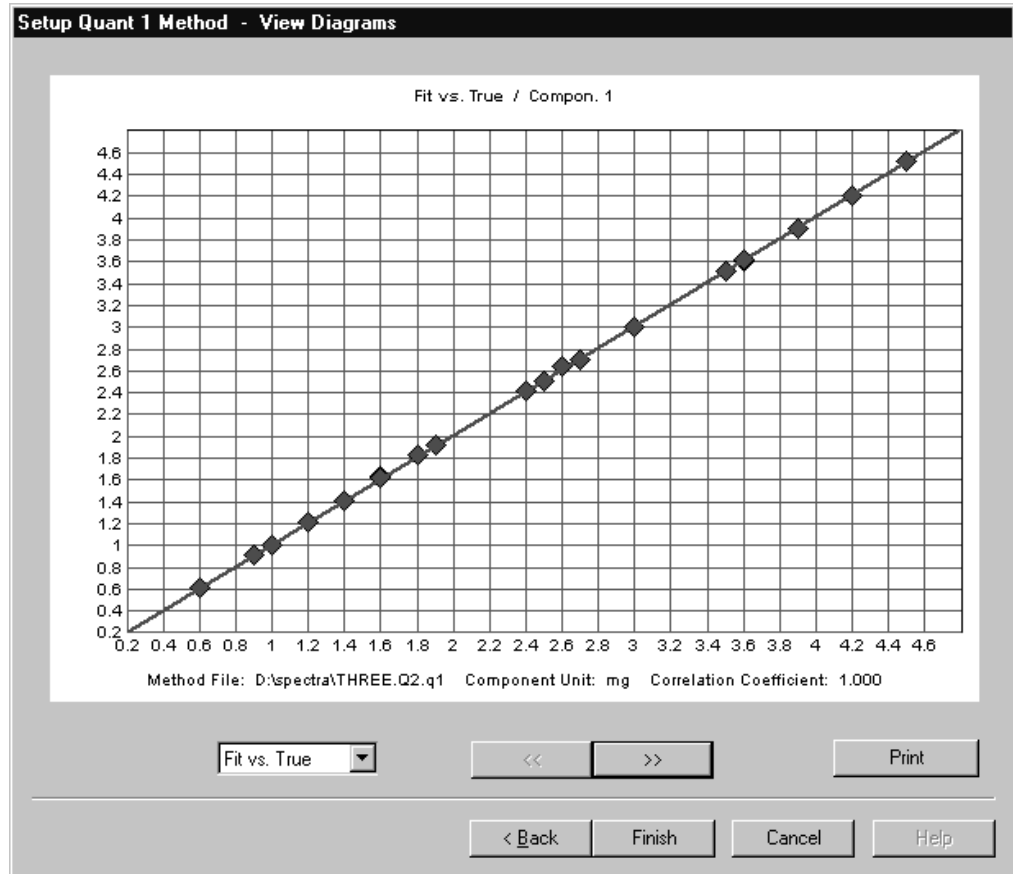


Figure 218: Calibration results – Fit vs. True

Below the graphics, the method file, correlation coefficient and calibration equation are indicated.

Using the drop-down list at the bottom of the graph you can change 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*.

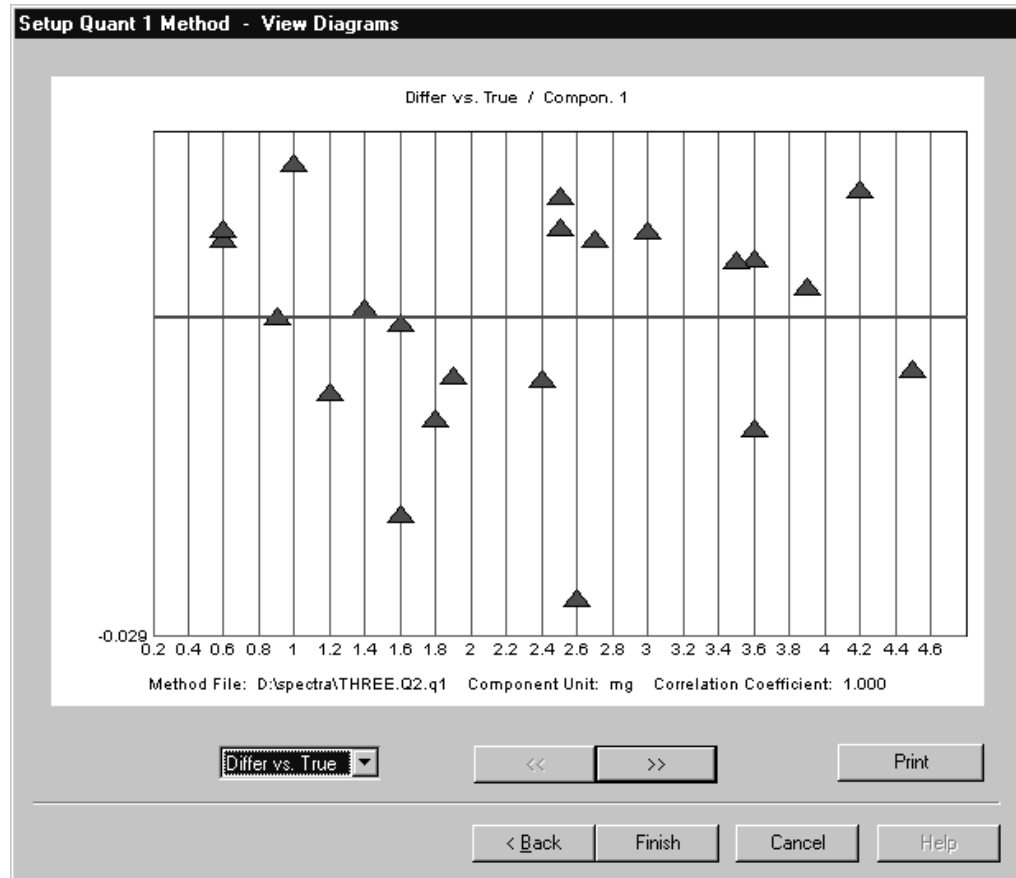


Figure 219: Calibration results – Difference vs. True

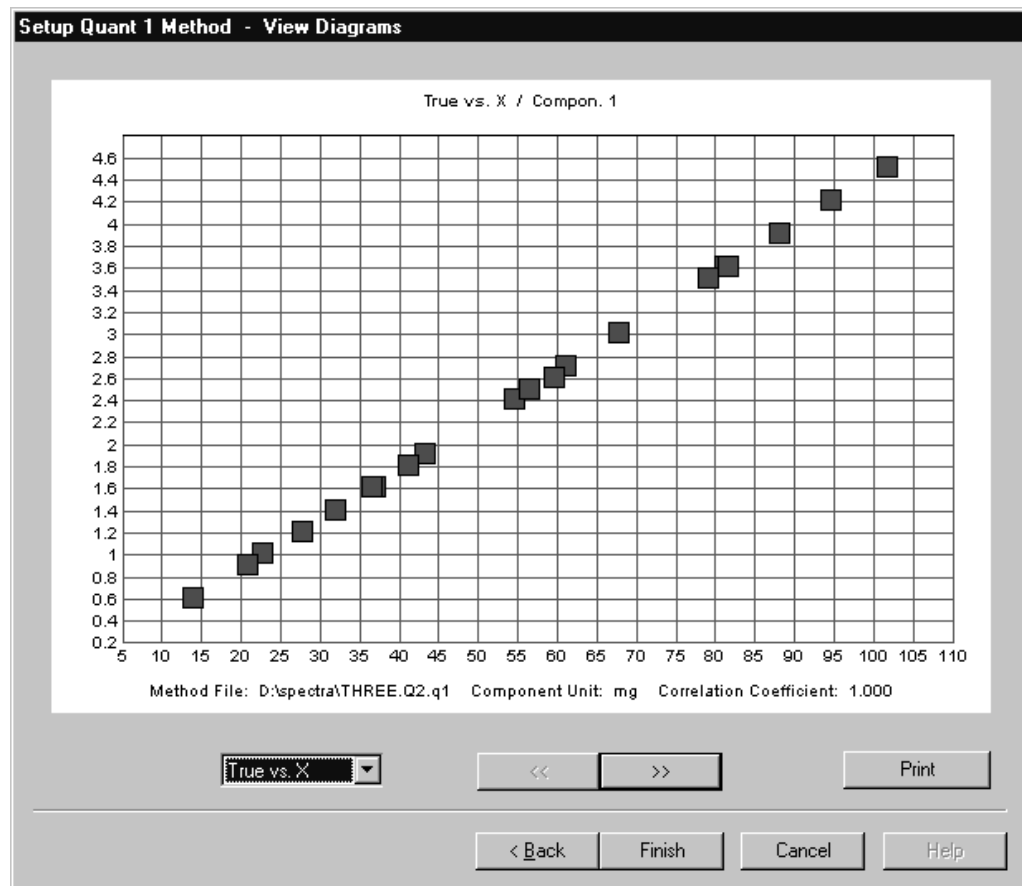


Figure 220: Calibration results – True vs X

You can print the results, figures as well as data tables by 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 the *Finish* button.

9.3.2 Quantitative Analysis 1

If you have created a calibration set, you can now start to analyze your samples. Keep in mind that the concentration of the samples should be 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.

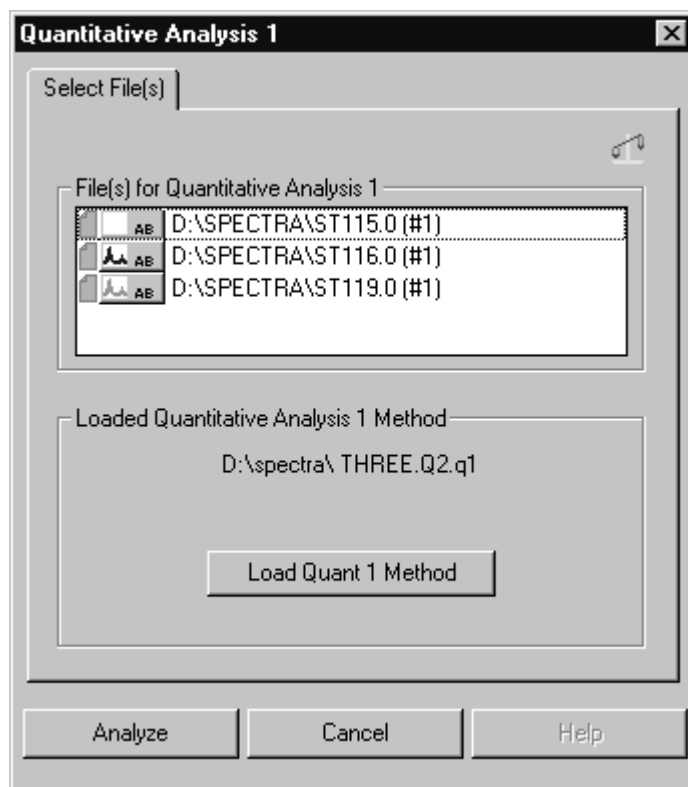


Figure 221: Quantitative Analysis - Select Files tab

Select the spectra you wish to analyze and load the appropriate QUANT 1 method. If a method has been created or loaded before, it will automatically be available for the analysis.

Click on the *Analyze* button 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 by a red flag in the browser.

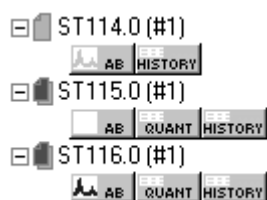


Figure 222: QUANT data block

Like every other report, QUANT reports can be displayed in a report window. The header includes the name of the QUANT method used for the analysis and the date when the method has been 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.

D:\SPECTRA\ST119.0 (#1)		Quantitative Analysis 1 Report		Values		
Quant Report AB		Method File:		THREE.Q2.q1 (07/28/98 1		
Quantitative Analysis 1 Report		Component	Prediction	Sigma	Unit	Integr. Result
		Compon. 1	2.992	0.0103	mg	67.72
		Compon. 2	2.7	0.00955	mg	77.62

Figure 223: 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. Change between the different reports by clicking on the report name of the tree.

9.3.3 Theory

The functions used for the calibration will be saved in the calibration record as $Y = f(X)$, with Y being the value obtained by the fit, and X being the peak size obtained from the spectra.

Sigma is a parameter representing the difference between the 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 :

$$r = \frac{\sum((Z_i - Z_m)(Y_i - Y_m))}{\sqrt{\sum(Z_i - Z_m)^2 \sum(Y_i - Y_m)^2}}$$

In this case Z represents the true concentration 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 (SN) of a spectrum within a given spectral range. The results can be stored with the spectrum. Some spectrum types (e.g. absorption, emission) have a baseline close to zero. In this case indicating the output of noise can be reasonable.

Two values are calculated for the noise output:

- RMS (Root Mean Square) - this value is the square root of the sum resulting from the squared deviations for all data points within the range selected, divided by the number of data points. The following equation applies:

$$\text{RMS} = \sqrt{\frac{\sum (y_i - y_{iFit})^2}{N}}$$

- PP (Peak to Peak) - this value is the difference of the minimal and maximal bands within a spectral range. The following equation applies:

$$\text{PP} = y_{Maximum} - y_{Minimum}$$

In both cases a curve is fitted to the spectrum in the spectral range of interest. This curve is either a straight line or (optionally) a quadratic parabola, and defines the (nominal) signal. The SN applies to both noise amplitudes (RMS and PP). The following equations apply:

- $\text{SN (RMS)} = \frac{\text{Signal}}{\text{RMS}}$
- $\text{SN (PP)} = \frac{\text{Signal}}{\text{PP(Noise)}}$

RMS and PP are divided by the average intensity. The (mean) nominal signal is divided by the calculated noise values and yields the SN. The result for the PP SN is normally less (*worse*) than that for the RMS SN value.

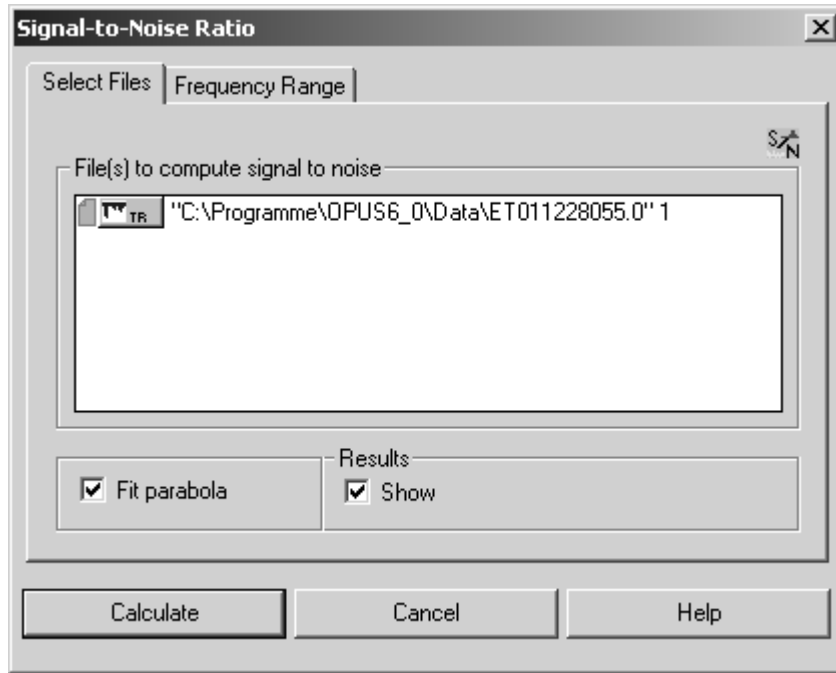


Figure 224: Signal-To-Noise Ratio - Select Files tab

You can choose the parabolic fit function by activating the *Fit Parabola* check box, otherwise a linear function is automatically fit to the data. If you activate the *Show* check box, the results of the fit will be displayed.

On the *Frequency Range* tab you can select between different frequency ranges which have been pre-defined.

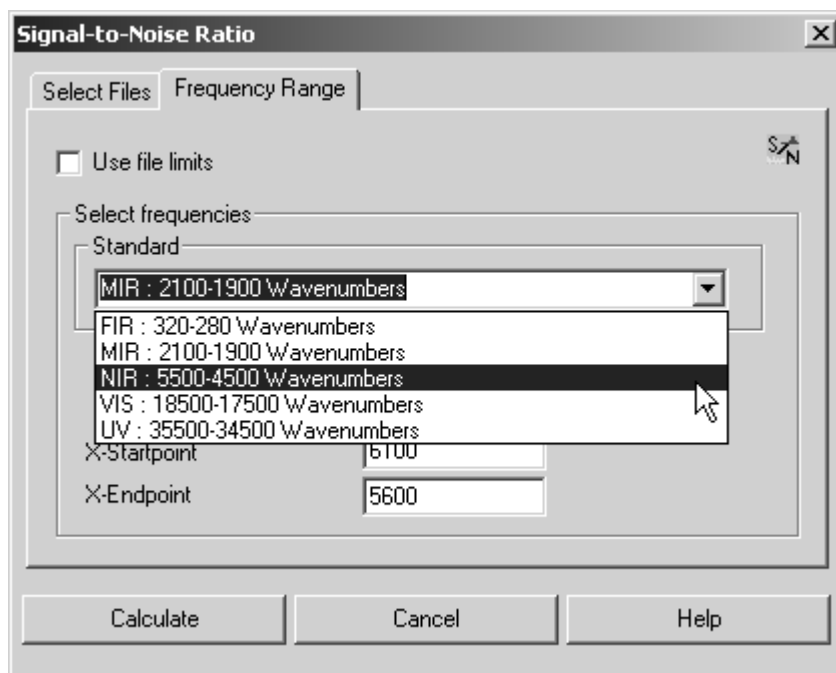


Figure 225: Signal-To-Noise-Ratio - Frequency Range tab

You can also interactively select the frequency range or use the current file limits. If you click on the *Calculate* button, the signal-to-noise ratio will be determined.

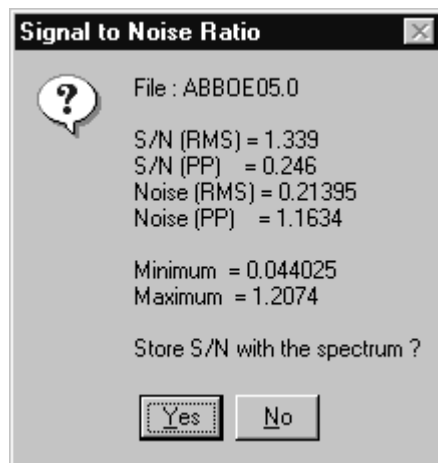


Figure 226: Calculated SN result

Minimum and *Maximum* gives the extrema of the ordinate values of the evaluated range. If desired, you can store the results by clicking on the *Yes* button. The OPUS spectrum window displays the spectrum with the calculated SN ratio.

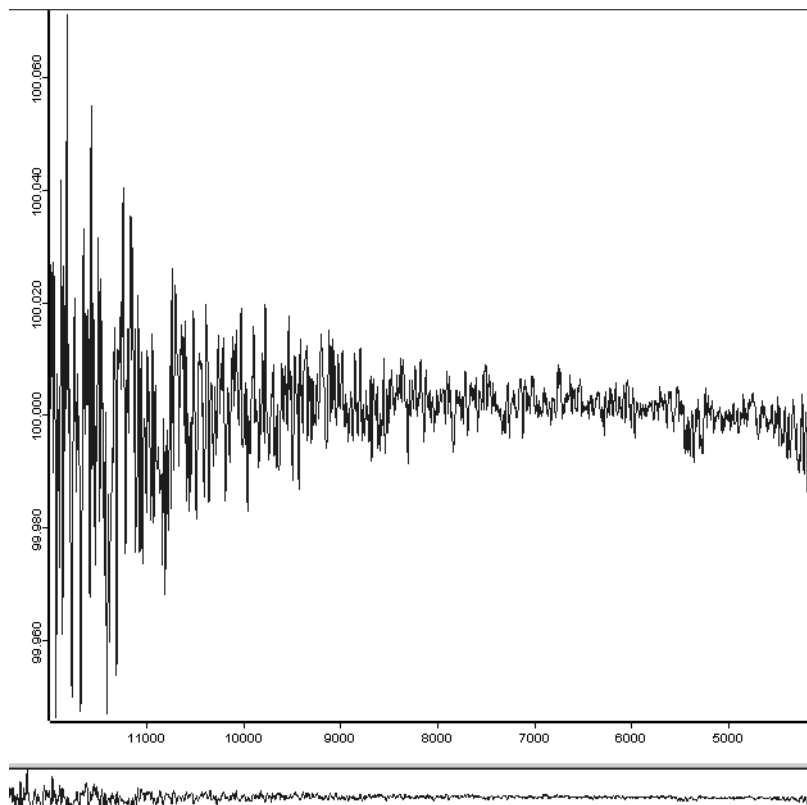


Figure 227: Spectrum with SN

If the result of an SN analysis is stored together with the spectrum, the corresponding parameters can be obtained from the *Data Parameters...* list. To open the report view right click on the spectrum file name in the OPUS browser window and select the *Show Parameters* command from the pop-up menu.

Data parameters TR	Values
Data Point Format	1
Number of Data Points	2048
Frequency of First Point	11994.494019
Frequency of Last Point	4099.725769
Y - Scaling Factor	1.000000
Y - Maximum	1.000714
Y - Minimum	0.999466
Date of Measurement	28/12/2001
Time of Measurement	10:49:30
X Units	Wavenumber cm-1
S/N (RMS)	55193.501249
S/N (Peak-to-Peak)	10072.190023
Max. Ordinate in S/N region	1.000065
Min. Ordinate in S/N region	0.999963
First S/N Frequency Limit	6101.379272
Second S/N Frequency Limit	5600.001709
Noise (RMS)	0.000018
Noise (Peak-to-Peak)	0.000099

Figure 228: Report with SN data parameters

9.5 Peak Picking

The *Peak Picking* command helps 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.

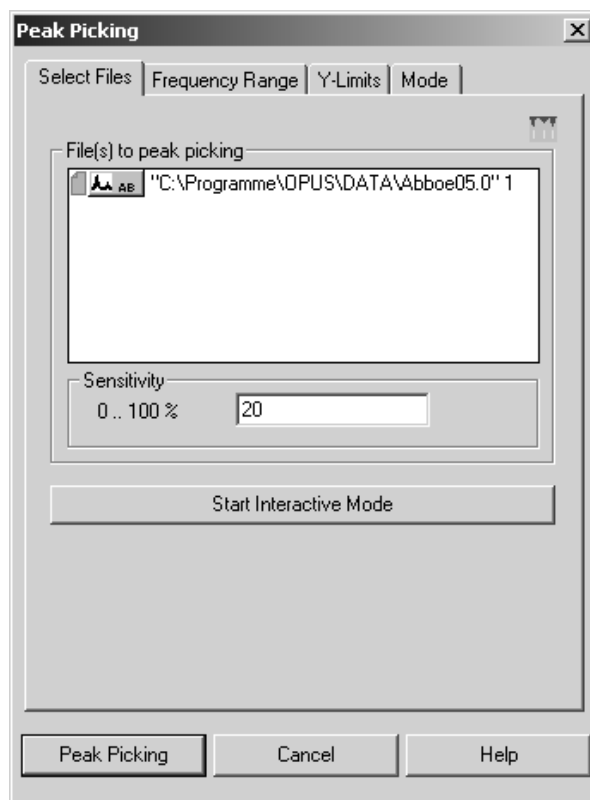


Figure 229: Peak Picking – Select Files tab

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 230).

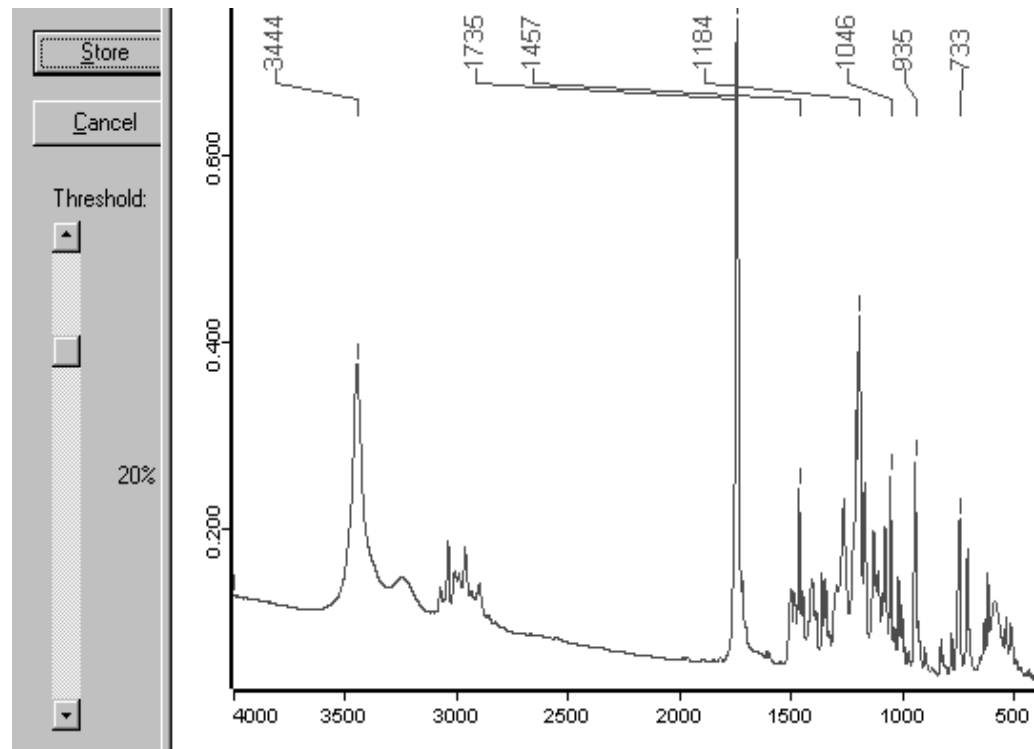


Figure 230: Peak Picking – Interactive mode

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.

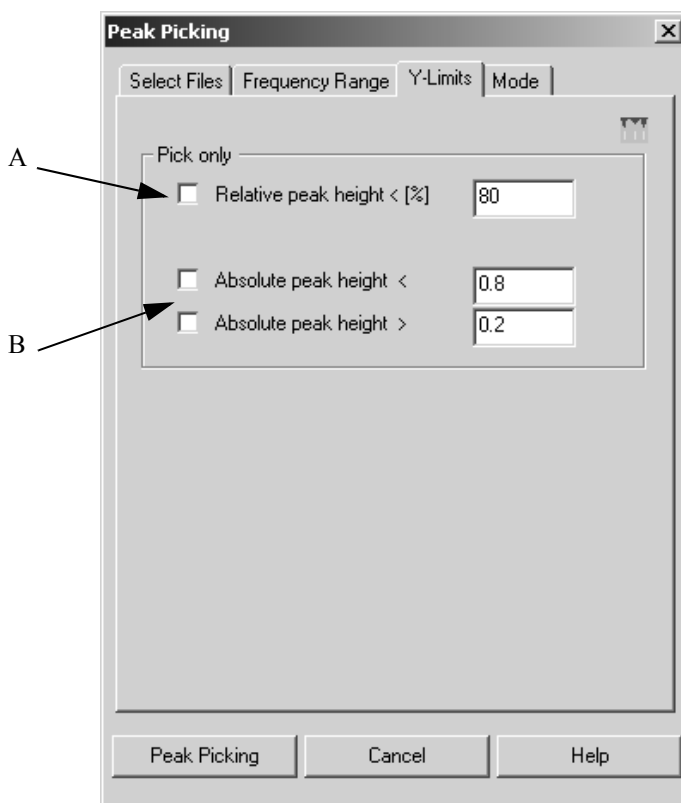


Figure 231: Peak Picking – Y-Limits tab

The relative peak height (A in figure 231) 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 231).

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).

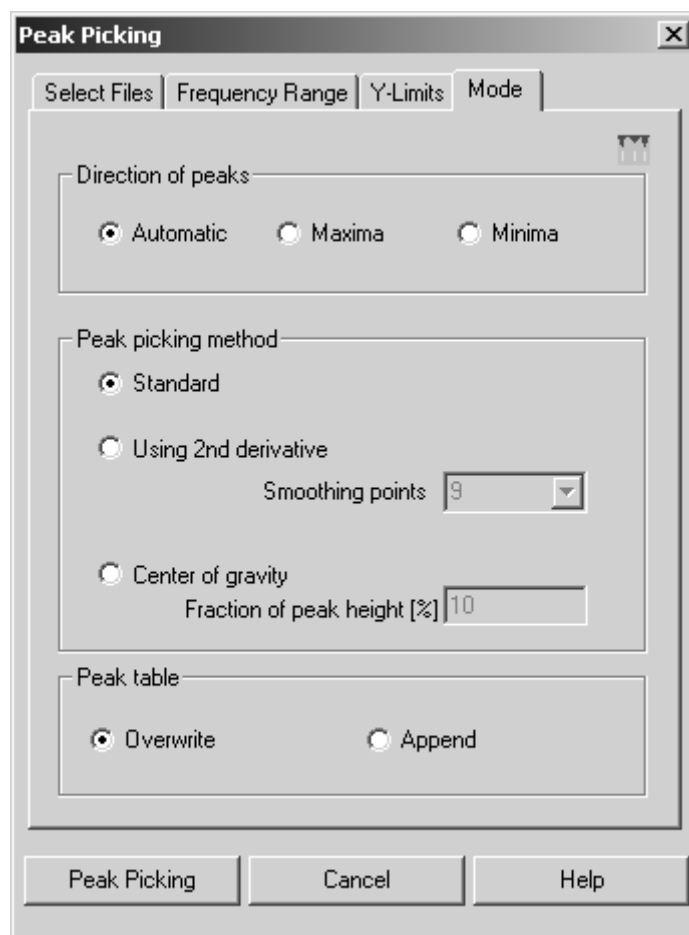


Figure 232: Peak Picking – Mode tab

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 the 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 wavenumber units is:

$PeakPos_{COG}(v) = PeakPos_{COG} \cdot \Delta v + v_{min}$ and Δv being the wavenumber distance between two measuring points and v_{min} being the wavenumber of the first data point.

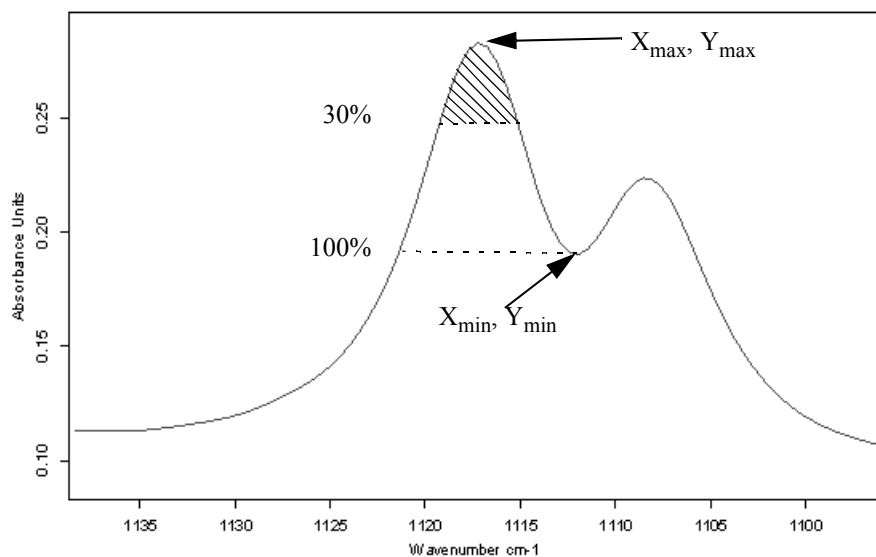


Figure 233: Band edge

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.

9.5.1 Theory

The standard method is used for peaks with small or no overlapping 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).

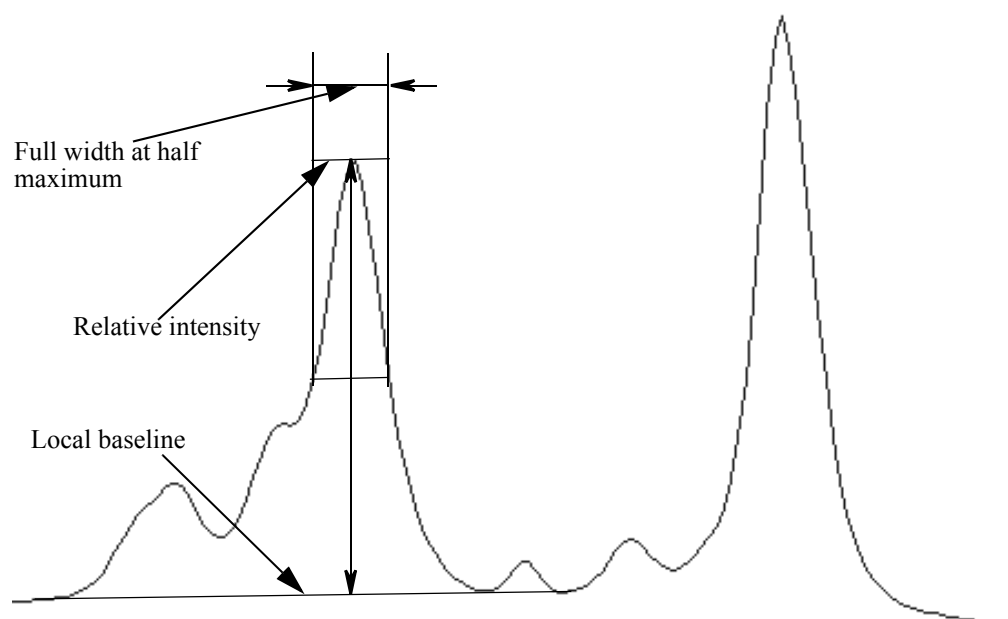


Figure 234: Spectrum with line width, relative intensity and baseline indicated

The lateral extremes are searched, starting from the x-position of the band, until a different band (or the end of the spectrum is reached), which is at least as strong as the first one, has been found. The lowest point within this interval is then used as a lateral minimum (or maximum).

To determine the line width, a line parallel is drawn to the local baseline which intersects the middle of a vertical line connecting the maximum (or minimum) of the band and the local baseline.

Peaks will be included into the peak pick table if their relative intensity is within the interval defined on the *Y-Limits* tab. This interval has been 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.

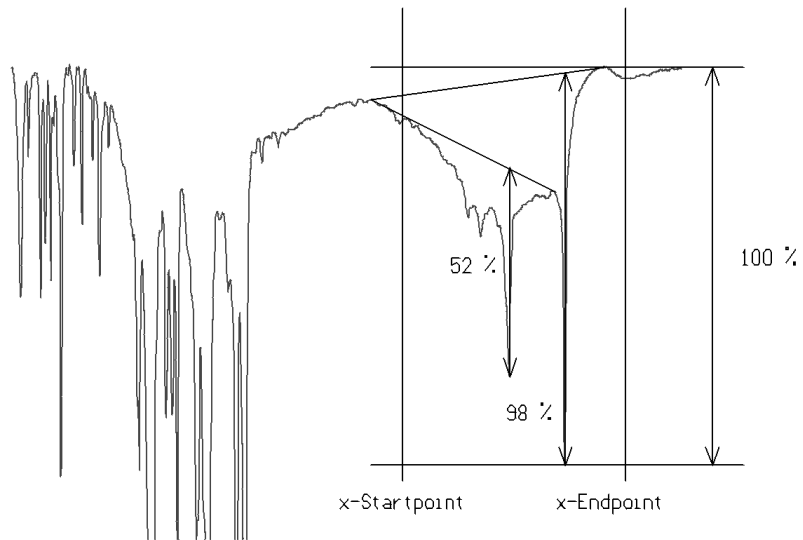


Figure 235: Calculation with baseline reference

The peak search using the second derivative method is recommended for high resolution spectra only.

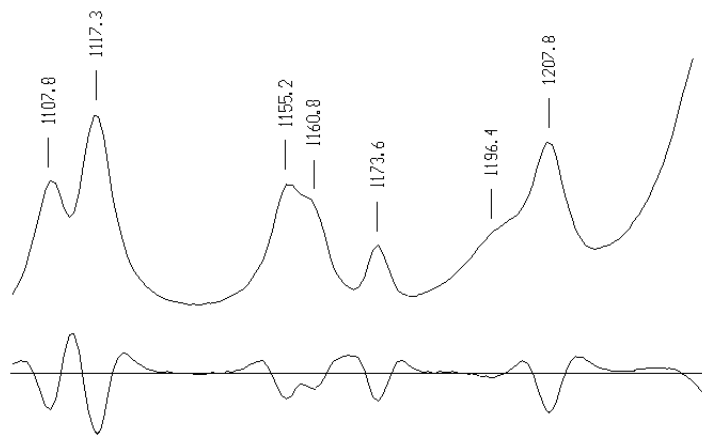


Figure 236: Absorption spectrum and second derivative

The x-positions are the x-values of the minima (or maxima) second derivative spectrum which has been smoothed. 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:

$[v_{-1}, 0]$ (zero-point)

$[v_0, I''_0]$ (minimum)

$[v_1, 0]$ (zero-point)

In figure 237 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.

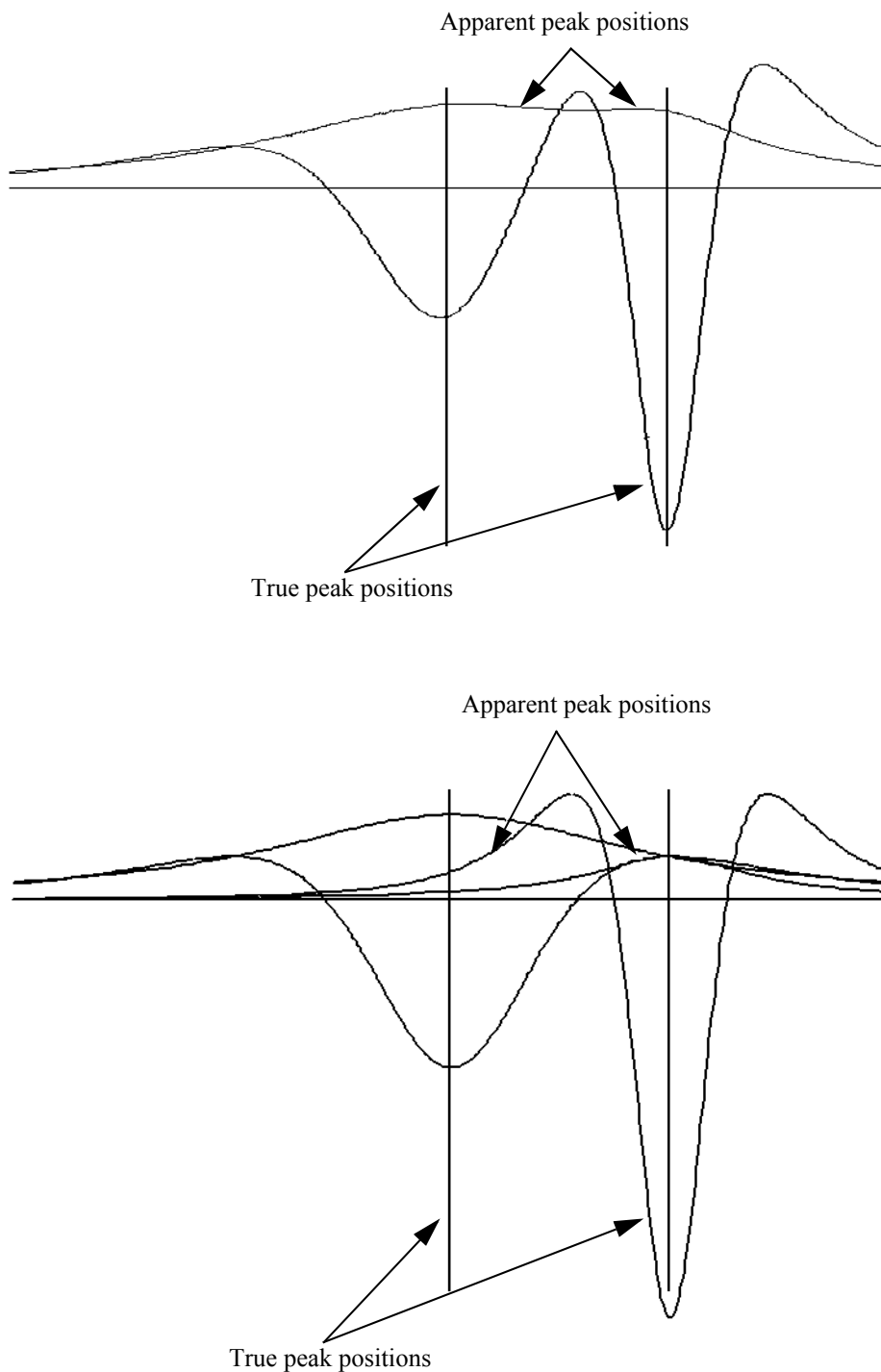

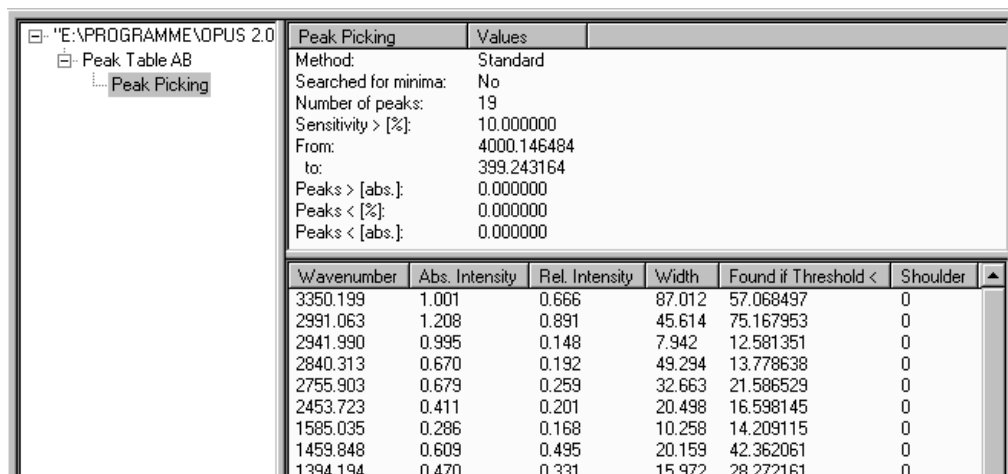


Figure 237: Apparent and true peak positions

To access the peak table, right-click on the PEAKS data 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 be as follows:



Peak Picking		Values				
Method:		Standard				
Searched for minima:		No				
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 238: Peak Search result

9.6 Quick Identity Test

The quick identity test offers a user-friendly method to evaluate 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.

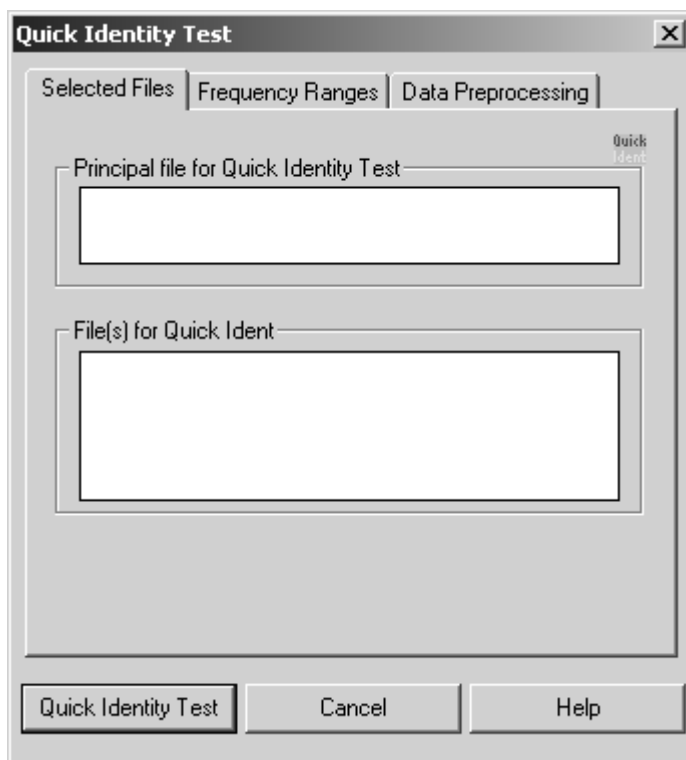


Figure 239: Quick Identity Test – Selected Files tab

Enter the reference spectrum into the *Principal file for Quick Identity Test* selection field, and the files to be tested into *File(s) for Quick Ident* selection field.

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.

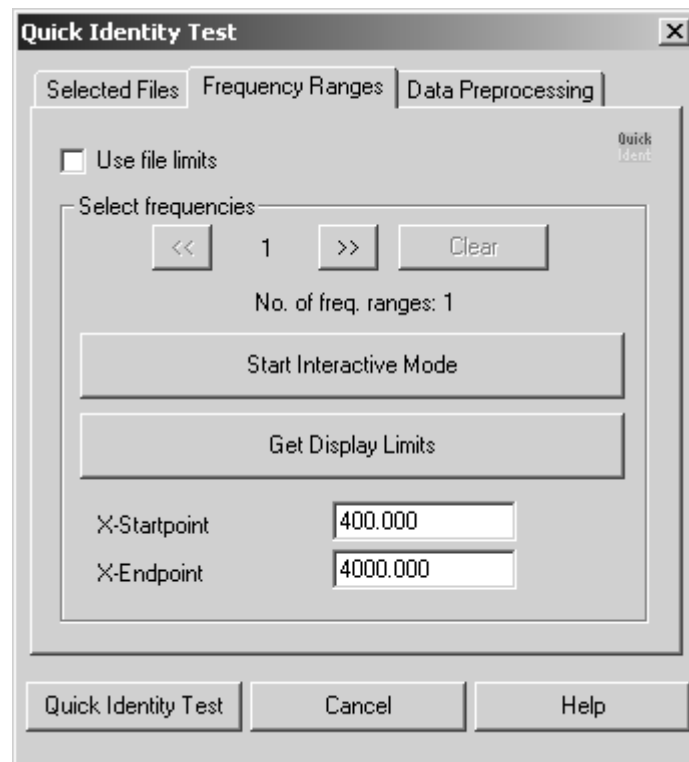


Figure 240: Quick Identity Test – Frequency Ranges tab

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.

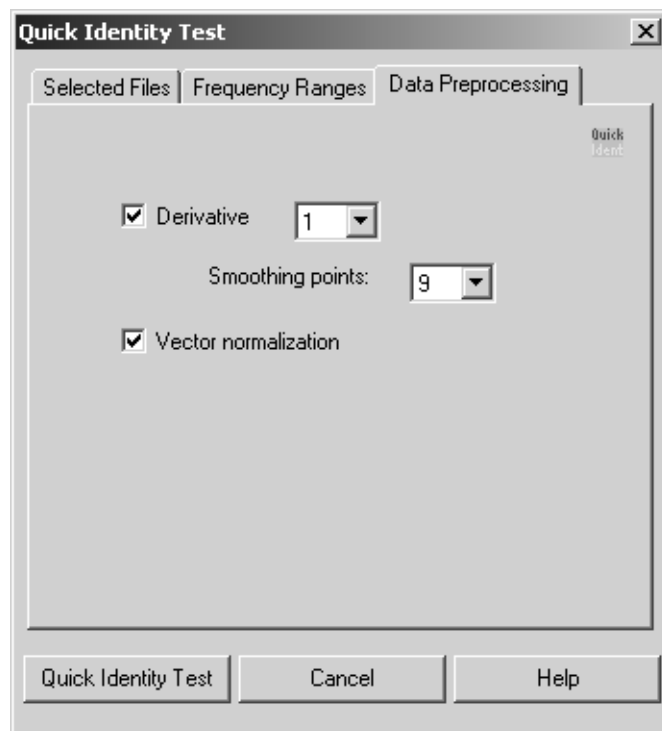


Figure 241: Quick Identity Test - Data Preprocessing tab

A report block will be appended to every spectrum which has been 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 spectrum, *Hit Quality* and 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.

Report of Correlation Search		Values	
Method file:	Quick Identity Test\		
from (date):			
(time):			
Expected Reference:	Probe 2 YP428Y02.12		
IDENTITY NOT CHECKED:	0		
Hit quality with expected reference:	0.000000		
No Threshold avail:	0.000000		
Threshold calculation:			
Algorithm:	Standard		
Vector normalizes spectra:	Yes		
Order of Derivative:	0		
Smoothing points:	1		
No. of used factor sp.:	0		
2 hits of 2			
X-Ranges:	1		
From:	3799.969360		
to:	14999.269922		
Class Name:			
Class Test NOT PERFORMED:	0		
Using residuals:	No		
Order of Internal Derivation:	0		
Smoothing Points for Internal Derivation:	1		
Reduction Factor:	1		
Hit No.	Hit Quality	Sample Name	File Name
1	0.025327	Probe 2	\YP428Y02.11

Figure 242: 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 normalizes spectra**
Indicates that vector normalization has been 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 by 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 243) opens:

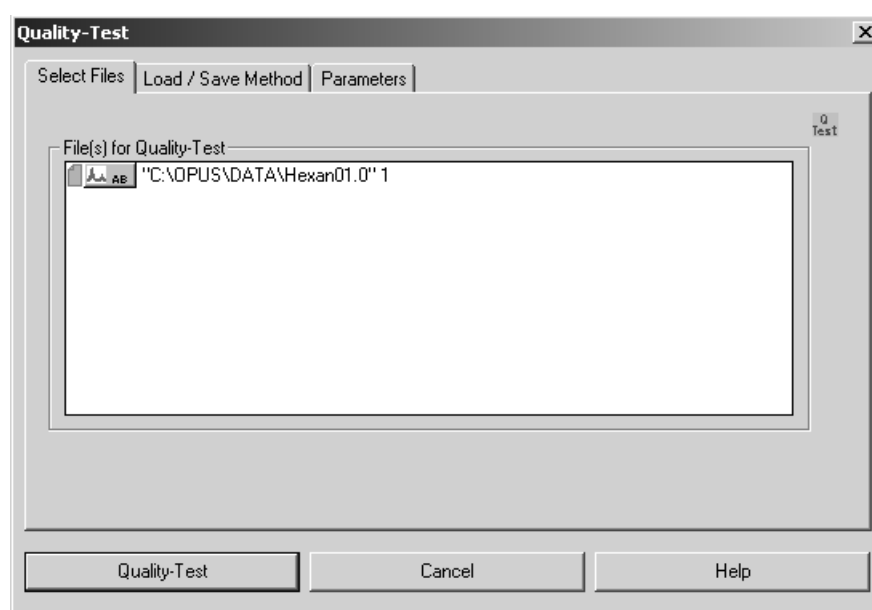


Figure 243: Quality Test - Select Files tab

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.

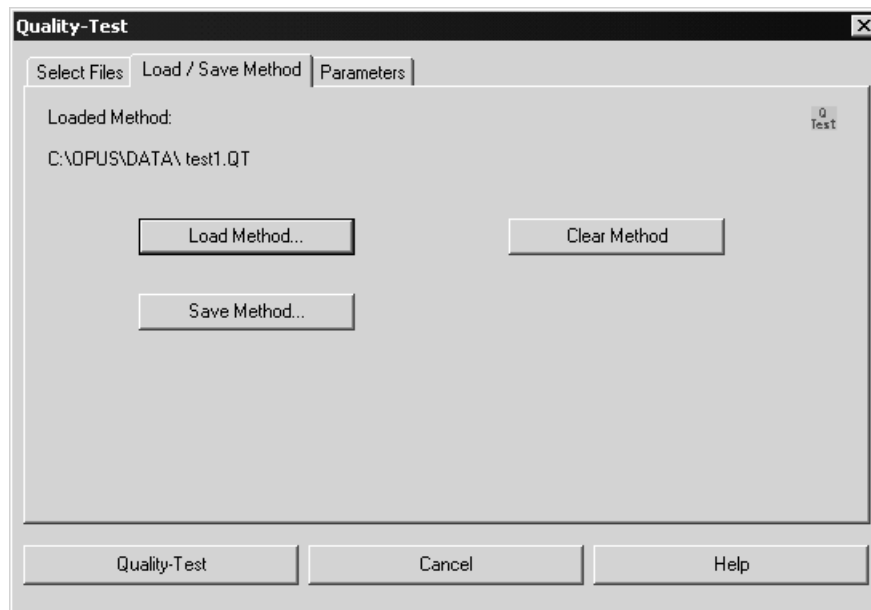



Figure 244: Quality Test - Load/Save Method tab

The quality test results are stored in the *Quality-Test Report* data block () 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 245 shows an example of a *Quality-Test Report*.

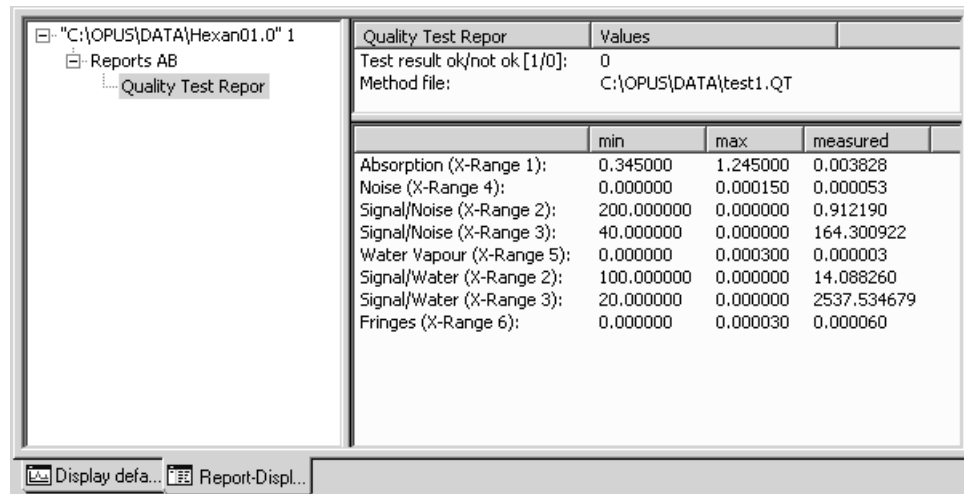


Figure 245: Quality Test report

The first line of the report indicates the test result. A value of *1* means *test passed*, whereas *0* means *test 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.

	X-Range 1	X-Range 2	X-Range 3	X-Range 4	X-Range 5	X-Range 6	Q Test
x-Start:	2100	1700	1200	2100	1847	2300	
x-End:	1600	1600	960	2000	1837	2000	
Delta y min:	0.345						
Delta y max:	1.245						
Noise max:				0.00015			
Signal/Noise:		200	40				
Water max:					0.0003		
Signal/Water:		100	20				
Fringes:						3e-005	

Figure 246: Quality Test - Parameters tab

9.7.1 Parameters

Some parameters and their limit values are explained in the following:

x-Range 1

The range defined in the first column (2100 - 1600 cm^{-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 - 1600 cm^{-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 $S_1/\text{Noise-ratio}$ 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 $S_1/\text{WaterVapor-ratio}$ 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 $960 - 1260\text{cm}^{-1}$). 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 $S_2/\text{Noise-ratio}$ 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 $S_2/\text{WaterVapor-ratio}$ 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: $2000 - 2100\text{cm}^{-1}$).

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: $1847 - 1837\text{cm}^{-1}$). 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: $2200 - 2000\text{cm}^{-1}$). 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. For further details see the OPUS STATISTICS manual.

9.9 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 9.9.2) 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 14.9.

9.9.1 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:

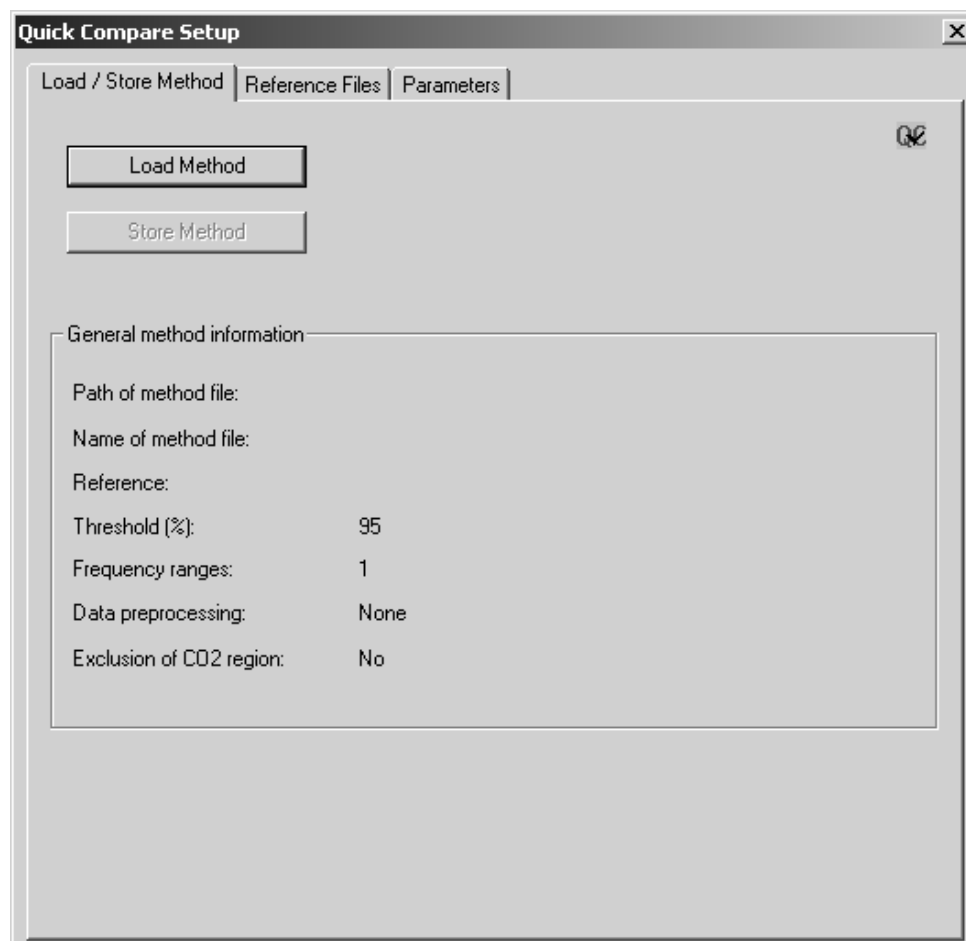


Figure 247: Quick Compare Setup - Load/Store Method tab

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.

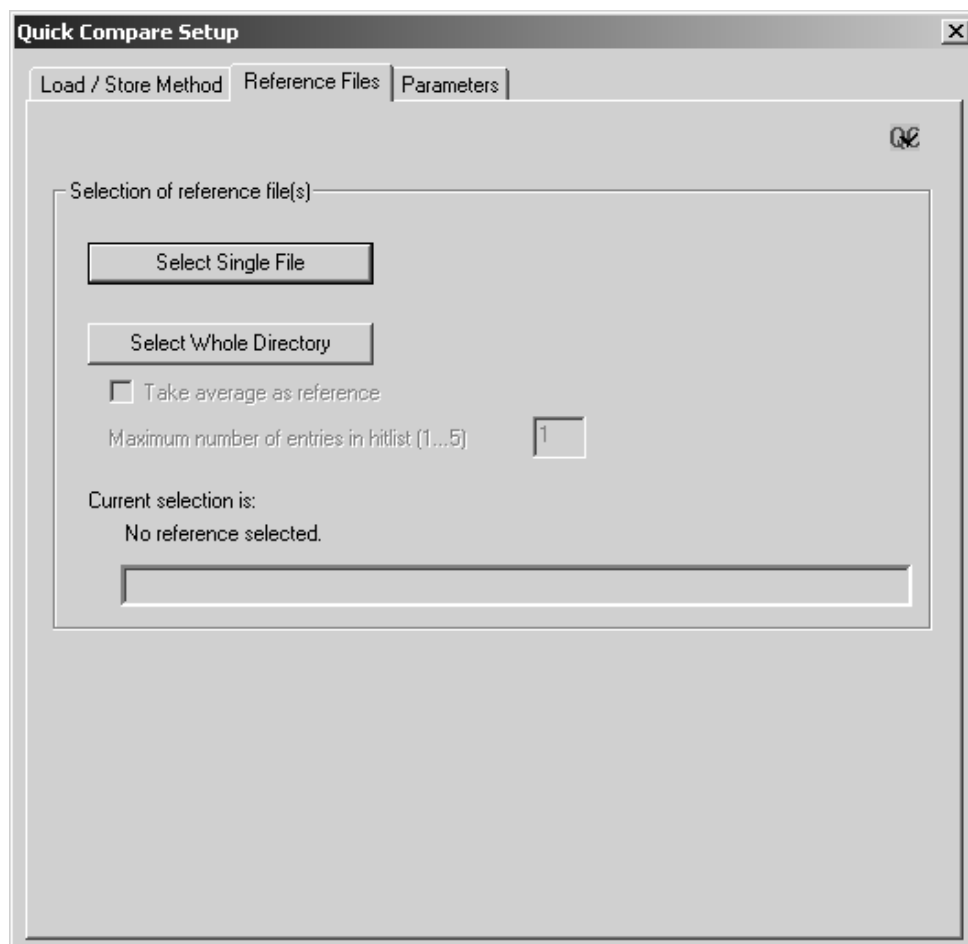


Figure 248: Quick Compare Setup - Reference Files tab

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.

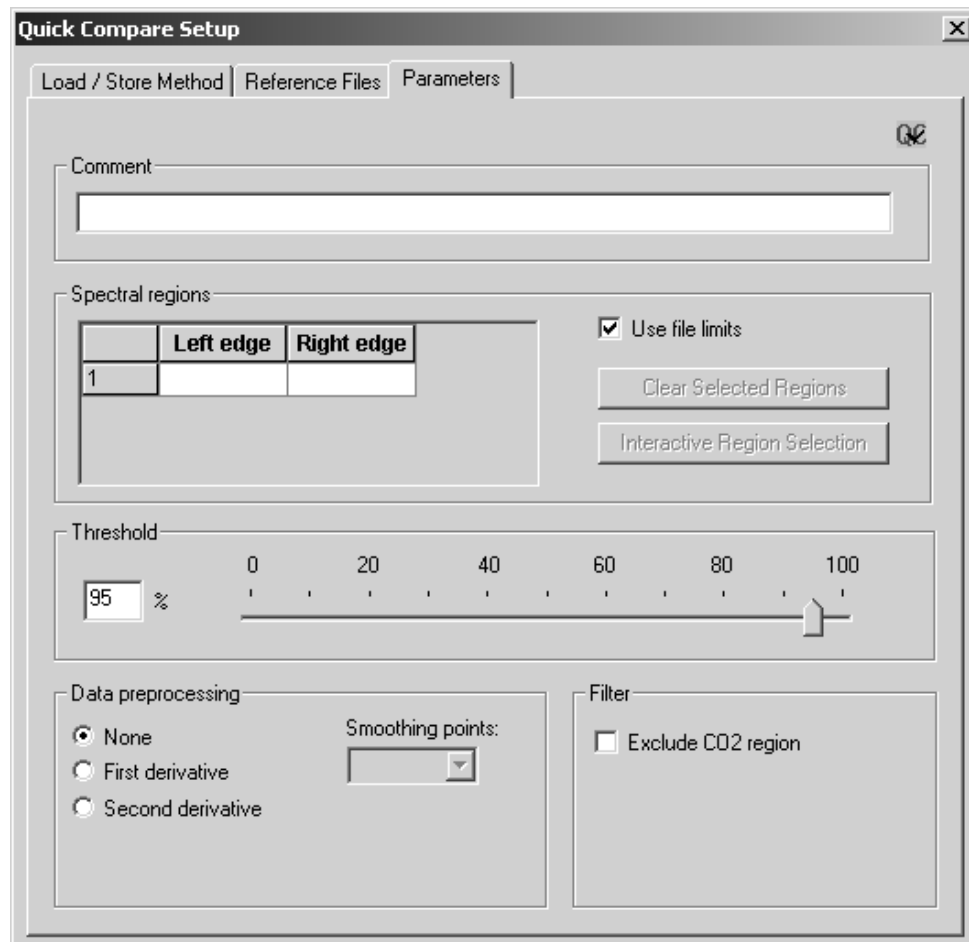


Figure 249: Quick Compare Setup - Parameters tab

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 wavenumber 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 CO₂ bands from the calculation. If you activate this check box, the wavenumber regions of 660 to 680cm⁻¹ and 2,275 to 2,400cm⁻¹ are excluded when calculating the correlation coefficient (see chapter 9.9.2).

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 wavenumber range.

9.9.2 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} :

$$r = \frac{\text{Cov}(y_1(k), y_2(k))}{\sigma_{y_1} \cdot \sigma_{y_2}}$$

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 $-1 \leq r < 0$ range is mapped to 0%, and the $0 < r \leq 1$ range is mapped linearly to 0% ...100%.

9.9.3 Quick Compare

Start the comparison by clicking on the *Quick Compare* command. The following dialog opens:

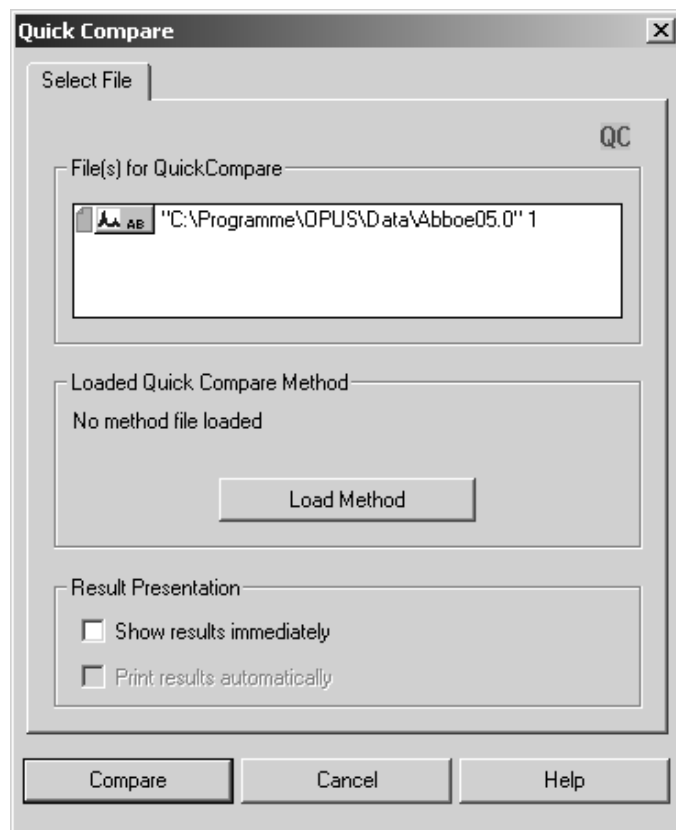



Figure 250: Quick Compare - Select File tab

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 wavenumber 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 251 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.

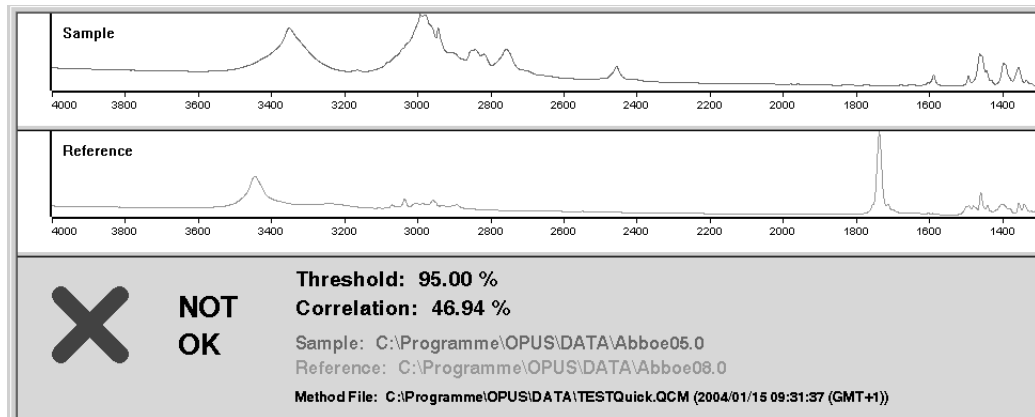


Figure 251: QC Results-Display - result not OK

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.

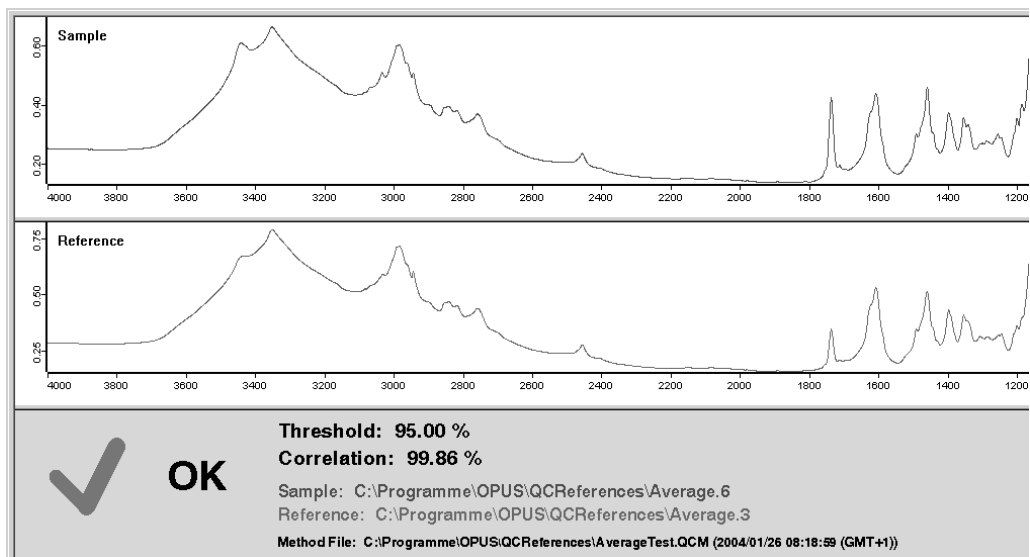


Figure 252: QC Results-Display - result OK

Figure 252 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.

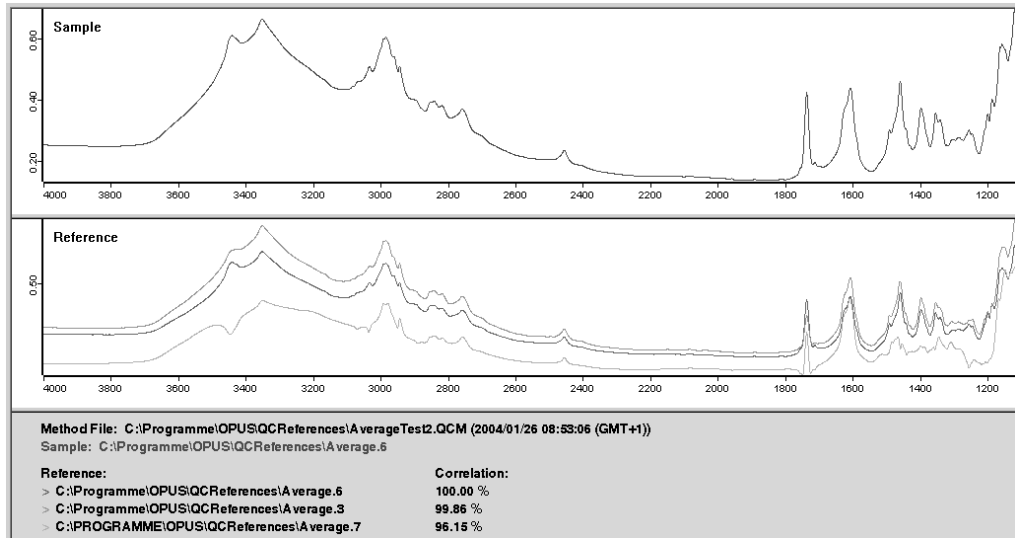


Figure 253: QC Results-Display - several single spectra

If a sample spectrum is compared with the average value of several reference spectra, the *QC Results-Display* can be as follows:

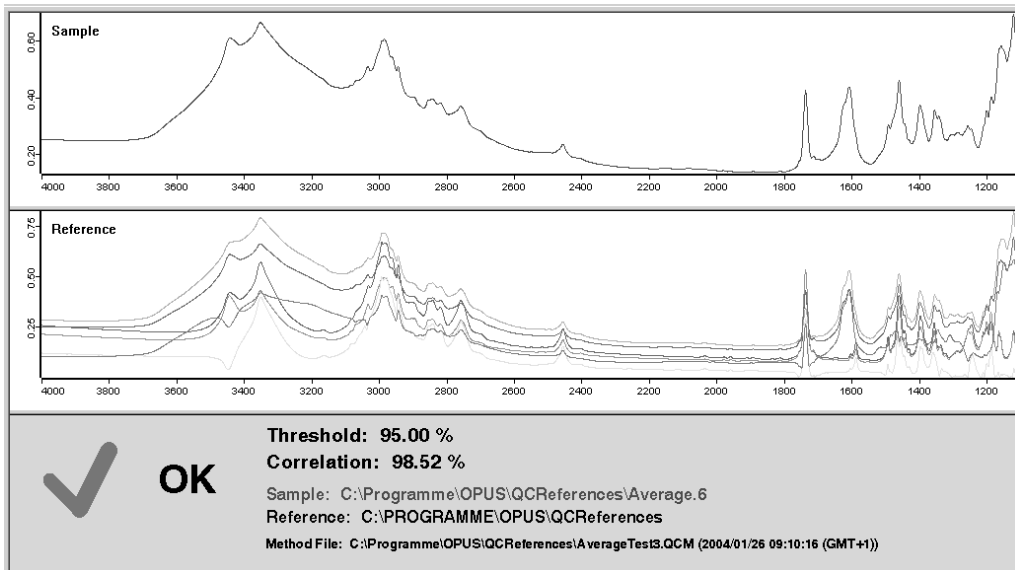



Figure 254: QC Results-Display - average as reference

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 255.

Quick Compare Report	Values
Operator	Default
Date and Time	2004/01/15 10:32:41 (GMT+1)
Method File	C:\Programme\OPUS5\DATA\TESTQuick.QCM (2004/01/15 09:31:37 (GMT+1))
Comment	
CO2 Region	Not Excluded
Preprocessing	None
Threshold	95.000000
Reference Mode	Single File
Entries in Result View Hit List	1
Number of Reference Files	1
<hr/>	
Reference:	Correlation:
C:\Programme\OPUS5\DATA\Abboe08.0	46.939225

Figure 255: Quick Compare report

9.10 Layer Thickness

Based on interferences which have been caused by multiple reflection this command allows to determine the layer thickness ranging from sub- μm to mm. The actually available thickness range depends on the spectral resolution, the spectral range as well as the kind of sample used. You can determine the layer thickness for both homogenous samples (films, semi-conductor, glass plates etc.) as well as coated samples, provided the reflection or transmission spectrum contains meaningful interferences.

The algorithm determines the thickness d from the mean distance Δf of the interference maxima within the selected frequency range, and from the refraction index n of the measured layer: $d = 1/(2 \cdot n \cdot \Delta f)$.

This physical context reveals that the distance of the interference maxima decreases all the more, the thicker the layer and the greater the refraction index is.

Apart from the presence of meaningful layer thickness interferences a precise determination especially depends on the value used for the refraction index which you have to define as parameter. As the refraction index depends on the frequency, in general, the value defined is to be consistent with the frequency range selected.

Select a spectrum file and click on the *Layer Thickness* command to open the following dialog:

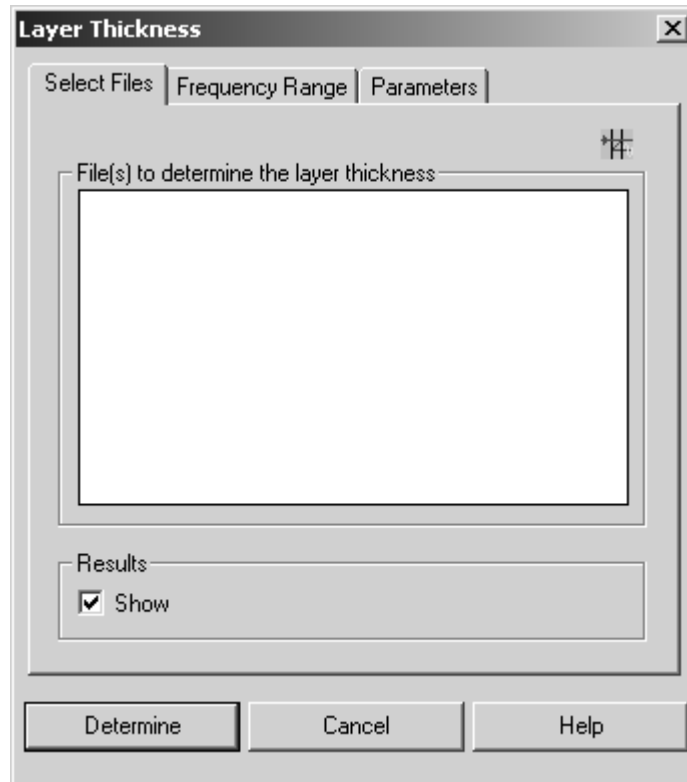


Figure 256: Layer Thickness - Select Files

Drag & drop the data block (transmission or reflection) into the *File(s) to determine the layer thickness* selection field. Select a frequency range (see also chapter 2.7) which contains meaningful layer thickness interferences.

Additional important parameters can be defined on the *Parameters* tab.

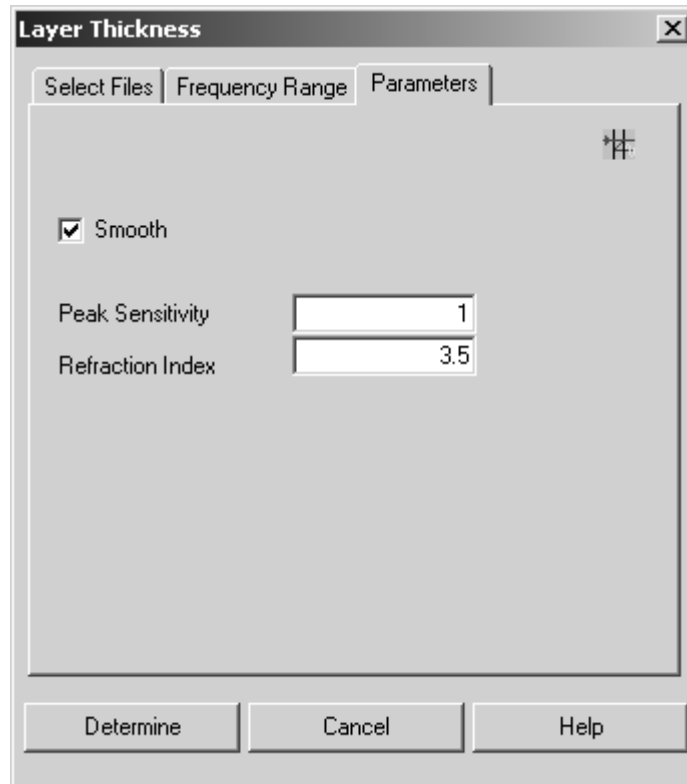


Figure 257: Layer Thickness - Parameters

Activate the *Smooth* check box only if the spectral range to be evaluated contains significant noise. Define the refraction index which depends on the type of material used and the frequency selected.

The peak sensitivity has to be defined as well. It determines how meaningful the maxima and minima have at least to be, to be considered by the algorithm (in many cases the default value of 1 yields positive results).

If the layer thickness has been determined, you have to check whether the defined peak sensitivity has produced a reasonable result. Check the maxima and minima found which are graphically selected in the spectrum window. If maxima/minima had been ignored or if noise had mistakenly be interpreted as maxima/minima, this would result in an erroneous layer thickness. In this case undo the determination by means of the *Undo changes* command in the *File* menu, and perform the determination once again using an appropriate peak intensity.

If you activate the *Show* check box (see figure 256), a dialog opens (see figure 258) which contains the results of the layer thickness determination. You will be asked whether you want to save these results together with the spectrum.

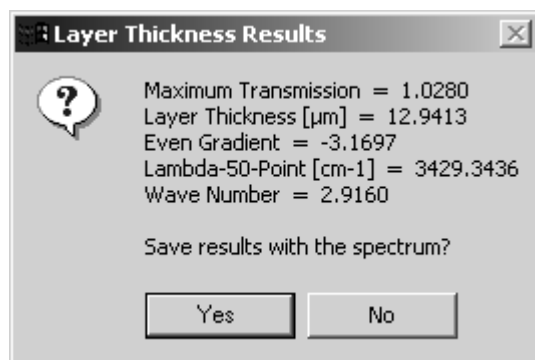


Figure 258: Layer thickness results

If the results are to be saved with the spectrum, click on the *Yes* button. The results are displayed in the parameter list. To open this list right click on the file name in the browser window and select *Show Parameters* from the pop up menu.

Data Parameters AB	Values
Data Point Format	1
Number of Data Points	3735
Frequency of First Point	4000.146484
Frequency of Last Point	399.243164
Y - Scaling Factor	1.000000
Y - Maximum	1.205080
Y - Minimum	0.045331
X Units	Wavenumber cm-1
Y Units	Absorbance Units
Derivative	0
Date of Measurement	07/08/84
Time of Measurement	11:32:34
Derivative	0
Smoothing points for der.	9
Smoothing points	9
Maximum Transmission	1.027952
Layer Thickness	12.941311
Even Gradient	-3.169740
Lambda 50	3429.343568
Wave Number	2.916010

Figure 259: Layer thickness results in report view

9.11 Spectrum Search

OPUS offers several library search commands. For details, e.g. *Library Editor* see the OPUS SEARCH manual which is 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.

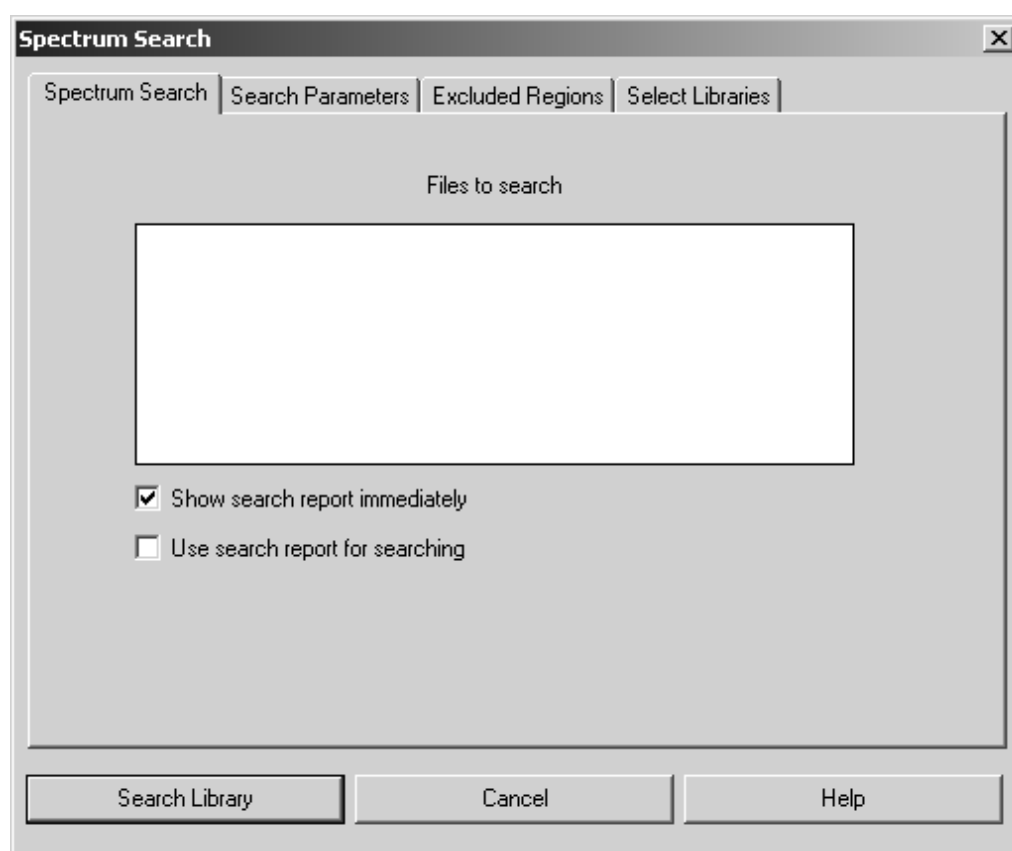


Figure 260: Spectrum Search - Spectrum Search tab

On the *Search Parameter* tab you define the desired search parameters.

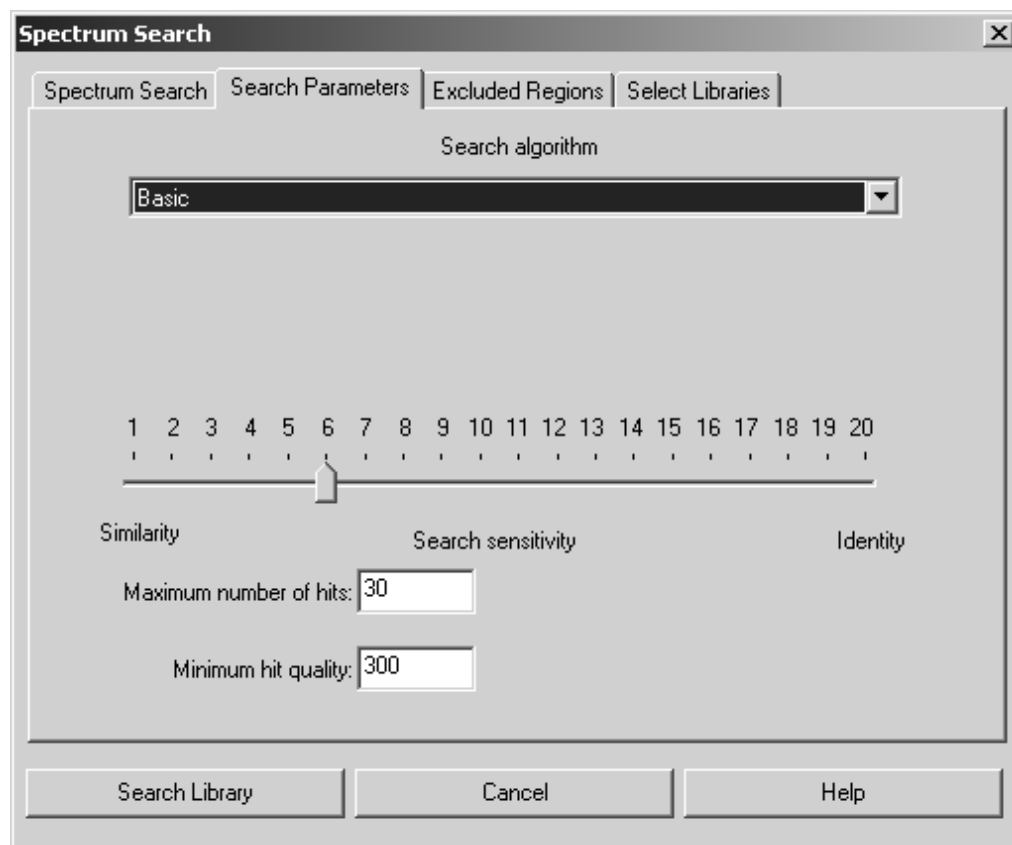


Figure 261: Spectrum Search – Search Parameters tab

- *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, e.g. 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, as the search result highly depends on the type of spectra recorded. 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 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 fit 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.

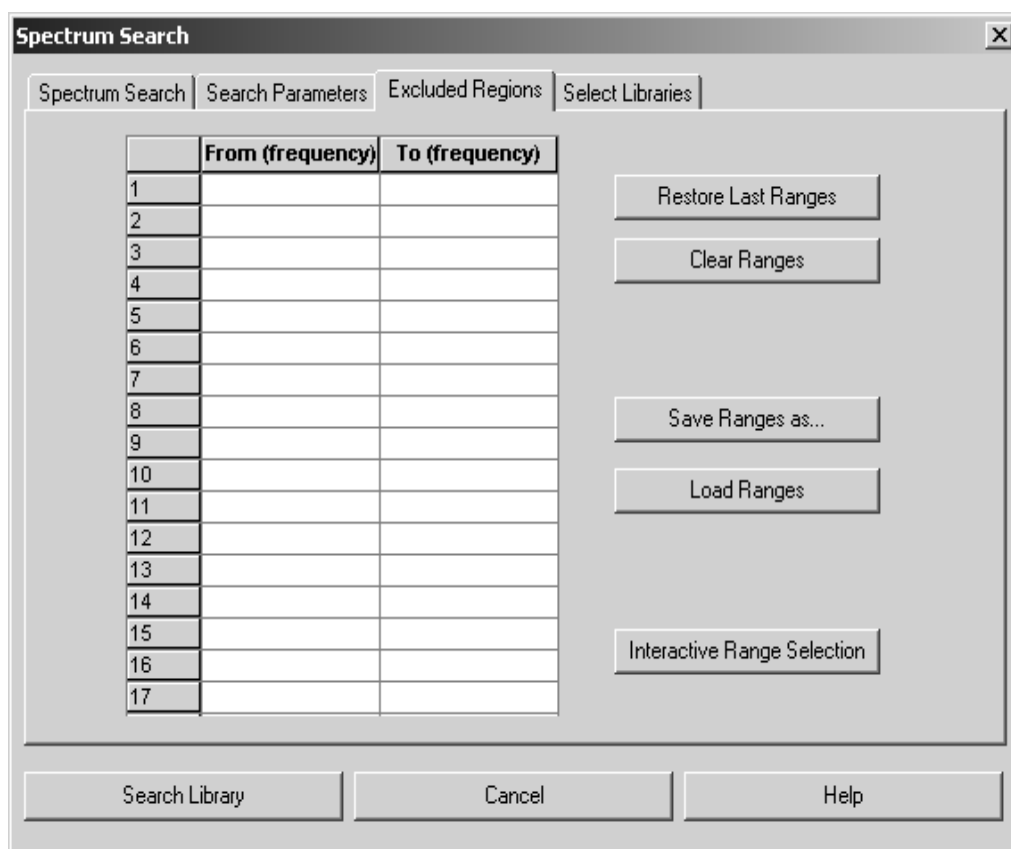


Figure 262: Spectrum Search – Exclude Frequency Regions tab

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.

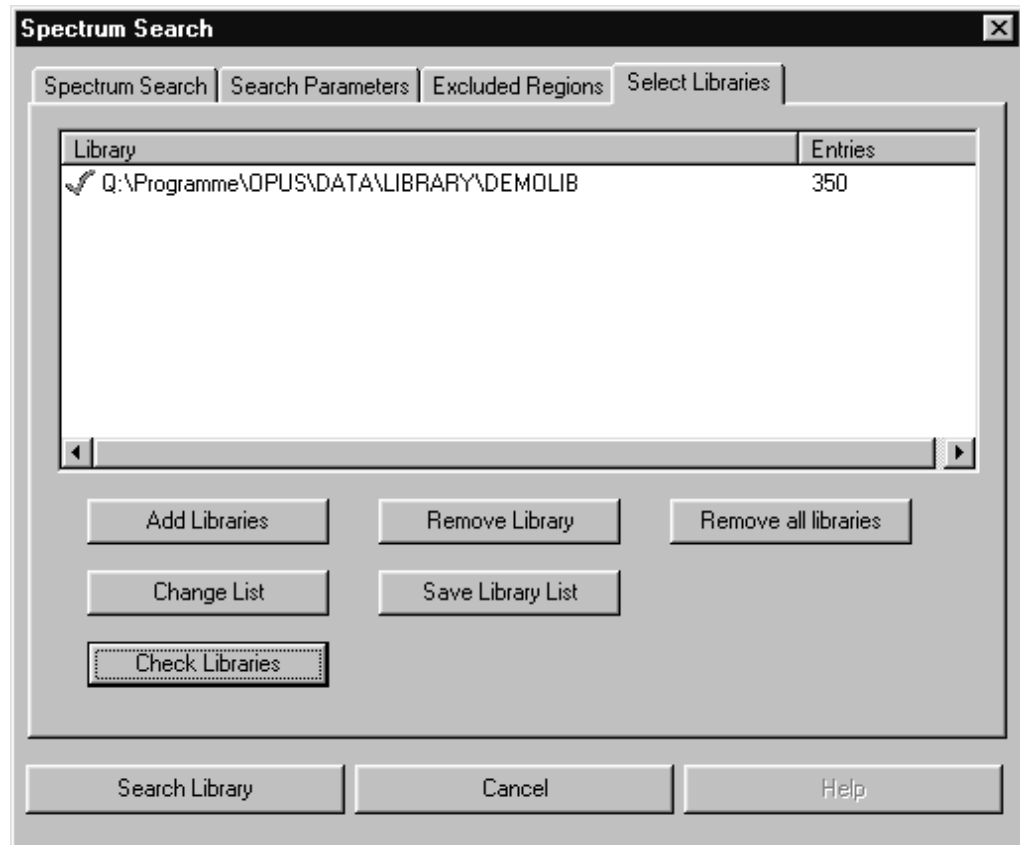


Figure 263: Spectrum Search – Select Library tab

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.

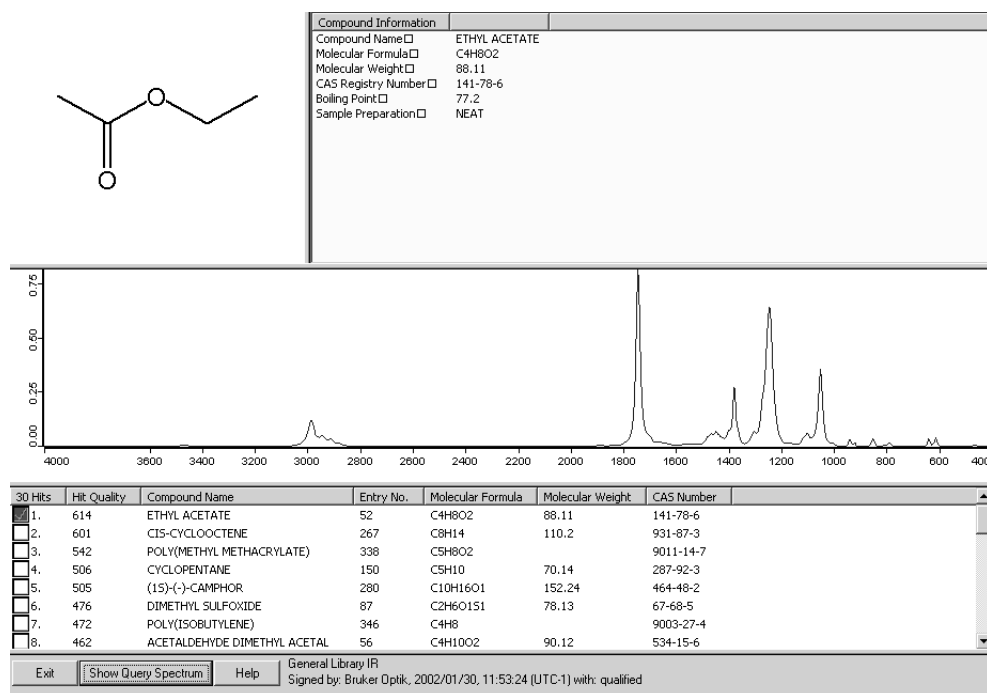


Figure 264: Search Report – results

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 in this menu allow to modify the display of the current spectrum window. You can zoom in certain areas of the spectrum window and restore the original display size. The availability of the commands substantially depends on the steps performed. For example, the *Forward* and *Back* commands are only enabled if you have zoomed in the current display before.

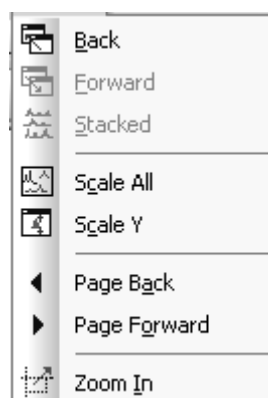


Figure 265: Display menu

10.1 Forward, Back

The *Back* command allows to restore the original display size of the spectrum window after you have zoomed in part of the spectrum displayed. *Forward* will display the zoomed-in area again.

10.2 Stacked

If more than one spectrum have been loaded into the same spectrum window, you have the option of a stacked display, i.e. the spectra will not overlap. The overview window is, however, not affected by this command.

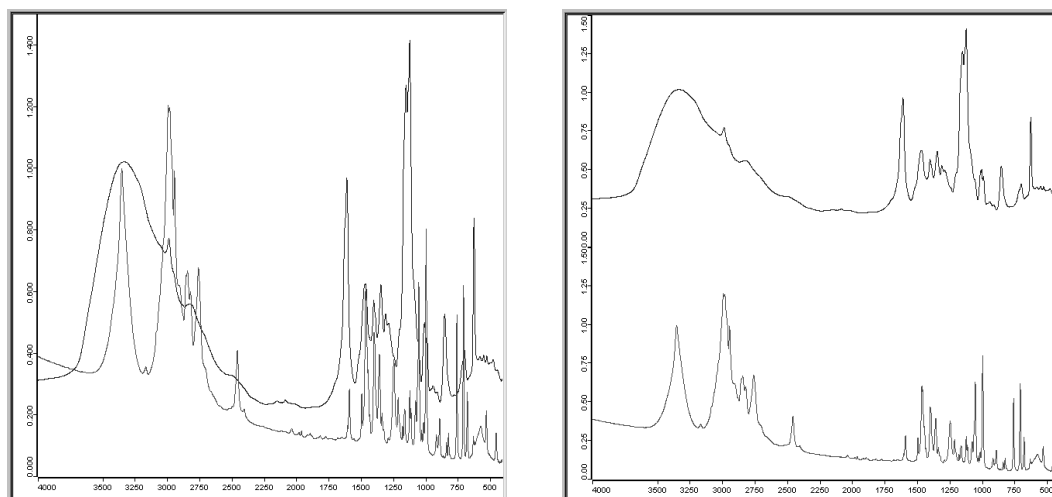


Figure 266: Spectrum window with overlapping and stacked display

The ordinate will automatically be duplicated when displaying several spectra in stacked mode (right spectrum window in figure 266). You can have separate axes displayed for each spectrum by right clicking onto the spectrum window and selecting the *Properties* command from the pop-up menu. Activate the corresponding check box on the *Axes* tab.

Figure 267 shows two spectra with separate axes for each spectrum.

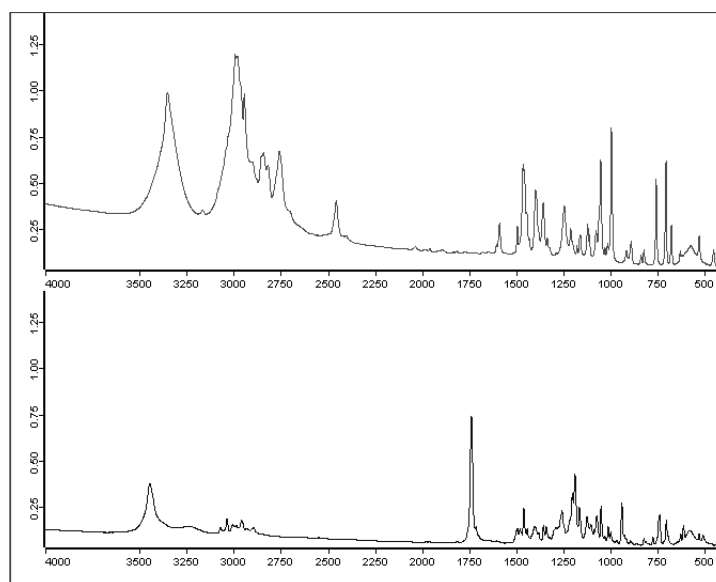


Figure 267: Spectra display with separate axes

If you zoom in a particular area of a spectrum displayed in stacked mode, all the other spectra displayed in the spectrum window will automatically be affected. To undo the stacked display, click on the *Stacked* command again.

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, select the *Scale Y* command.

10.4 Page Forward, Page Backward

If you have selected only a particular frequency range in the spectrum window, this range will be displayed on a white background in the overview window, while the rest appears on a gray background. The frequency range selected can be moved 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 range the same.

10.5 Zoom In

The *Zoom* command allows to enlarge particular spectral ranges. If you select this command, a cross-hair cursor will be displayed. Use the left mouse button to draw a frame around the range you would like to expand. If you click on the mouse button again, the cross-hair cursor disappears and you can reposition the frame. Now, left click again and the area marked by the frame will be resized to the spectrum window. The cross-hair cursor reappears and can be removed by a right click.

11 Print

The printing functions in the *Print* menu allow to print spectra, create new printing templates or layouts, and load existing layouts. 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 to the current OPUS version.

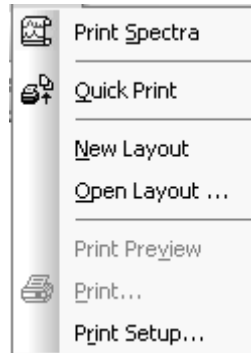


Figure 268: Print menu

Before being able to print 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 the 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, the new printer appears in the *Printer* dialog.
- 4) To check whether the new 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, e.g. paper size and print quality. Clicking on the *Properties* button opens a different dialog. The settings shown will depend on the printer configuration.

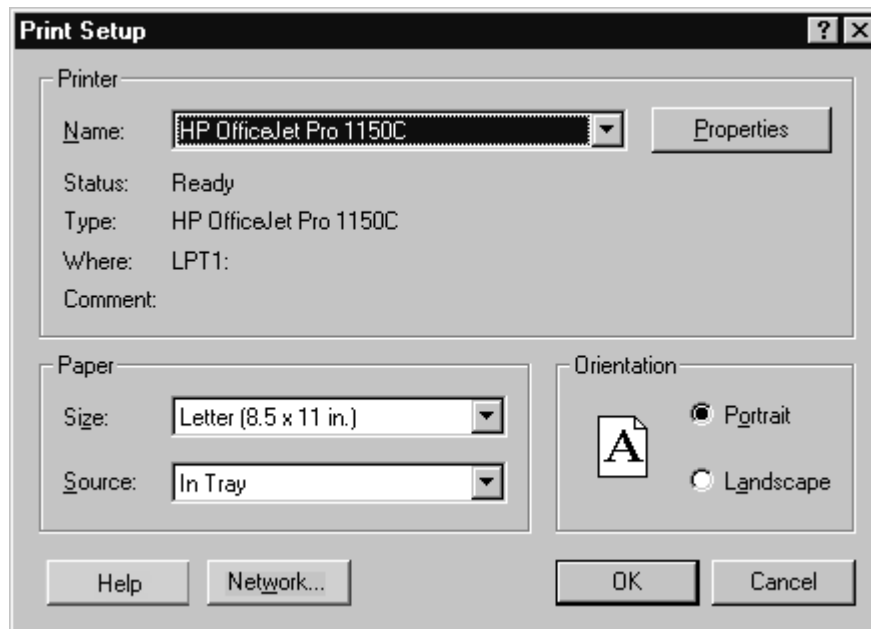


Figure 269: Print Setup

11.3 Print Spectra

Select the *Print Spectra* command to directly print spectra. The following dialog opens:

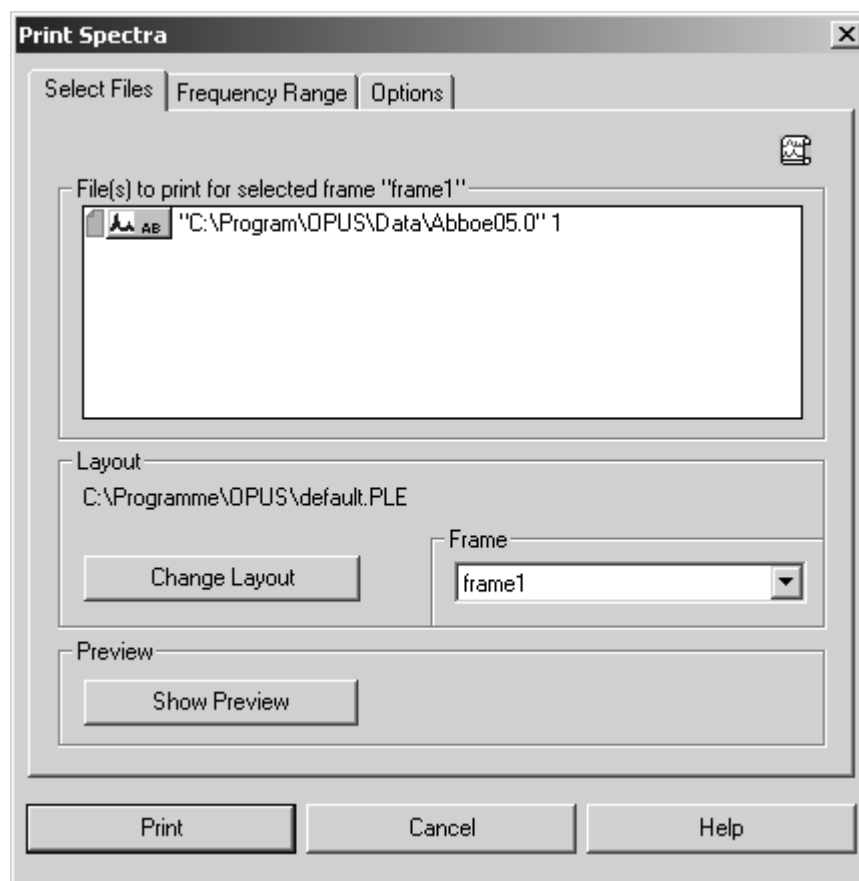


Figure 270: Print Spectra - Select Files tab

Drag & drop the respective spectrum from the OPUS browser window into the *File(s) to print...* selection field. Click on the *Change Layout* button to select the appropriate plot layout from the dialog that opens. The layout selected will be displayed in a preview window as exemplified in figure 271.

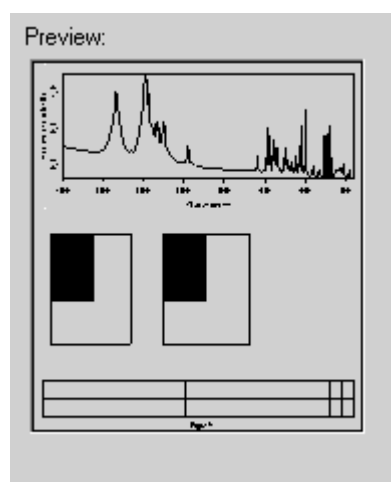


Figure 271: Example of PLE layout previewed

If the plot layout selected consists of more than one spectrum or report frame, you can use the *Frame* drop-down list (figure 270) to see which frame is assigned to what particular data block.

The *New Layout* and *Edit Layout* button below the preview window both allow to switch to the PLE workspace. If you close the PLE workspace, the *Print Spectra* dialog will be displayed again.

To display a preview of the plot click on the *Show Preview* (figure 270) 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.

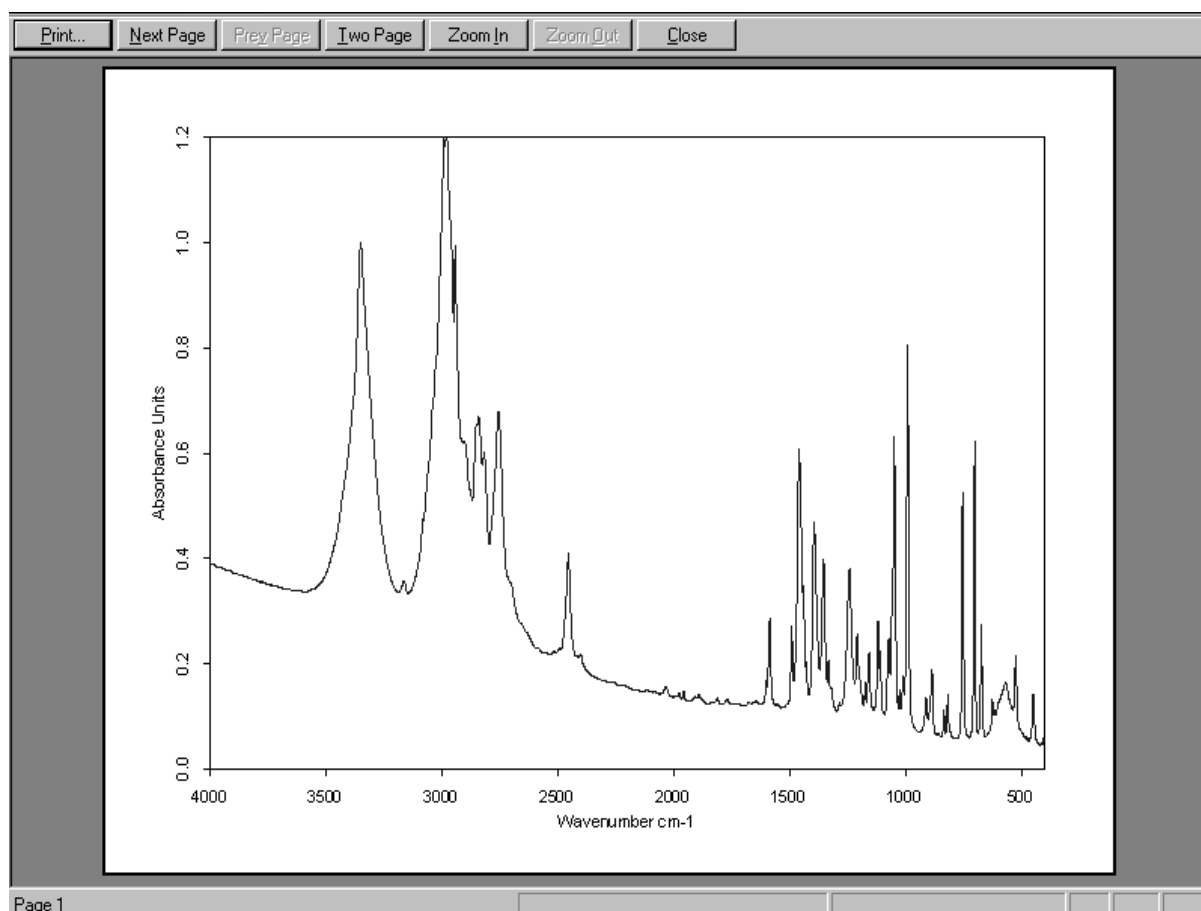


Figure 272: Print Preview

Click on the *Frequency Range* tab to define the limit values. You can select between several options.

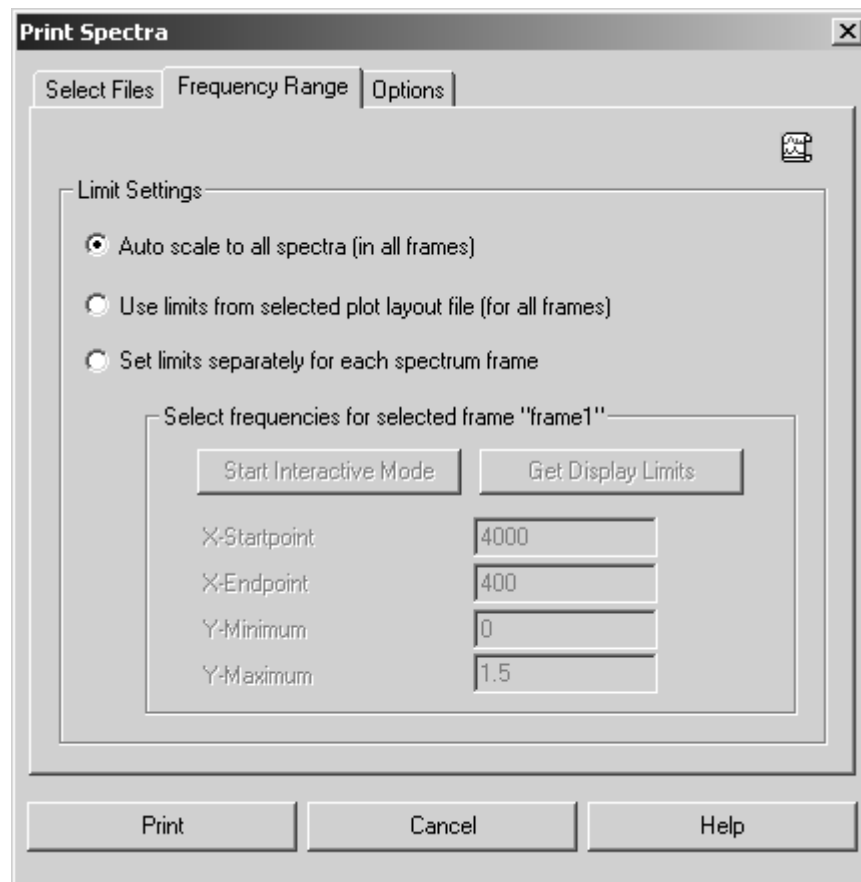


Figure 273: Print Spectra - Frequency Range tab

If you activate the *Auto scale to all spectra* option button, the axis of all spectra frames will be linearly scaled. If you activate the second option button, the frequency limits of the plot layout selected before will be used.

As soon as you activate the *Set limits separately for each spectrum frame* option button, the *Select frequencies for selected frame* group field will be enabled. Either type the limit values manually or define them interactively. If you click on the *Get Display Limits* button, the current limits displayed in the spectrum window are automatically set in the appropriate entry field.

On the *Options* tab you can define the number of peaks which are to be labelled as well as the printout format.

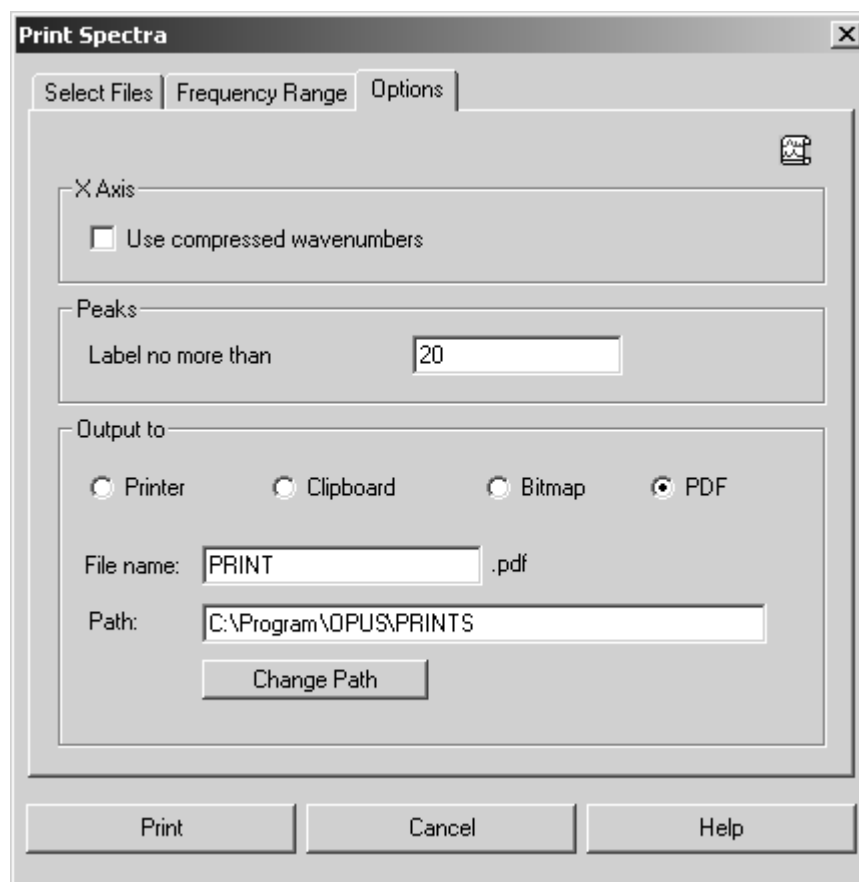


Figure 274: Print Spectra – Options tab

The *Use Compressed Wavenumbers* check box allows to plot compressed wavenumbers, i.e. the wavenumbers above 2000cm^{-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. If you activate the *Bitmap* or *PDF* option button, the *File* name and *Path* entry fields are enabled. To save the printing define the file name and path or edit the path by means of the *Change Path* button. Click on the *Print* 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. An appropriate default template 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
CHROMPOSTRUN.PLE	CHROM post-run window
CLUSTERANALY- SIS.PLE	Cluster analysis window
CORRELCHART.PLE	Band assignment chart window
3D.PLE	3D Window
3D+.PLE	3D+ Window
DEFAULT.PLE	Display (spectrum) window
EVALRESULTS.PLE	IDENT result window
FACTOR3D.PLE	Score plot window (part of IDENT factor- ization)
GRIDREPORT.PLE	Grid report 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
PROCESSCON- TROL.PLE	Trend view (OPUS PROCESS)
REPORT.PLE	Report window
SEARCHRESULTS.PLE	Search report window
SINGLEREPORT.PLE	Report window
STRUCTURE.PLE	Structure window
QCCOMPRESULT.PLE	Quick Compare result window
VIDEOPOSTRUN.PLE	Video postrun window
TEXTVIEW.PLE	Text View window

The *Quick Print* command generates a printout which shows the OPUS window as 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

The Plot Layout Editor (PLE) can be used to create templates, and allows to label peaks in a spectrum, plot details of a spectrum, print parameters and peak tables. The templates created can be saved using the *Save as* command from the *File* menu.

To create new templates select the *New Layout* command from the *Print* menu. A new PLE window will be displayed including the PLE tool bar.

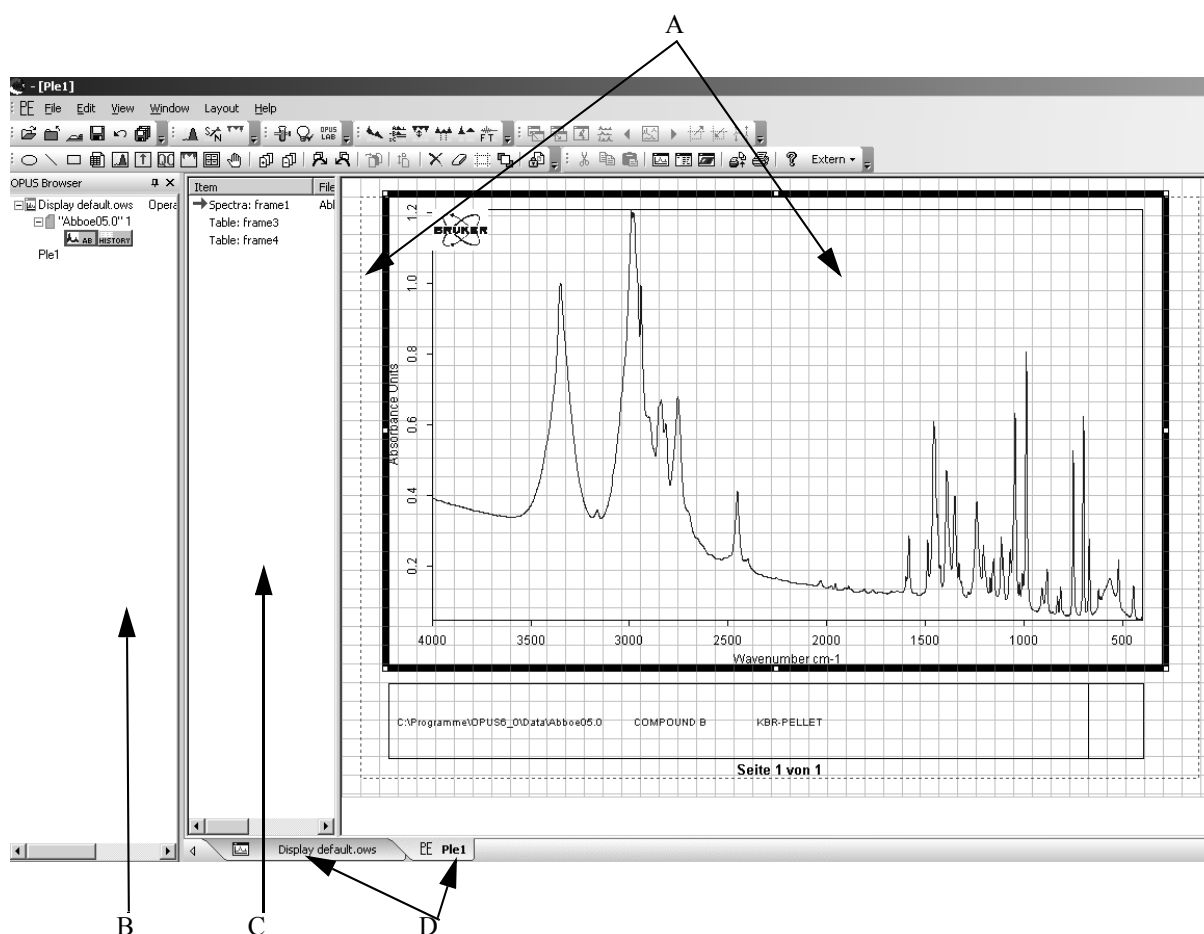


Figure 275: PLE user interface

The PLE drawing area (A) consists of a black grid and a red broken-line frame. This frame represents the available print area of the printer. Directly to the left there is the browser (B) and PLE item window (C). To switch between PLE and the OPUS spectrum window use the *Display* or *PE* (D) tab.

As the available drawing area depends on the printer setup you first have to configure the particular printer settings.

- 1) Select the *New Layout* command from the *Print* menu.
- 2) Select the *Print Setup* command from the *File* menu.
- 3) Click on the *Properties* button and set the appropriate paper size and format.
- 4) Confirm the settings by clicking on the *OK* button.

11.5.1 OPUS Browser

The OPUS browser window (B in figure 275) shows all windows currently open, including spectrum windows and PLE displays. You can switch between the spectrum windows and PLE displays by clicking on the appropriate icon in the browser window.



Figure 276: Icons in the browser window

11.5.2 PLE Item Window

The PLE item window (C in figure 275) shows all items displayed on the PLE drawing area. Frames will be referred to by the type of data included (table, spectrum etc.). The active frame is indicated by a red arrow in the item window and marked by a thick line on the PLE drawing area. Each new frame created is named *frame_x*, with *x* being automatically incremented. To activate a particular frame just click on it.

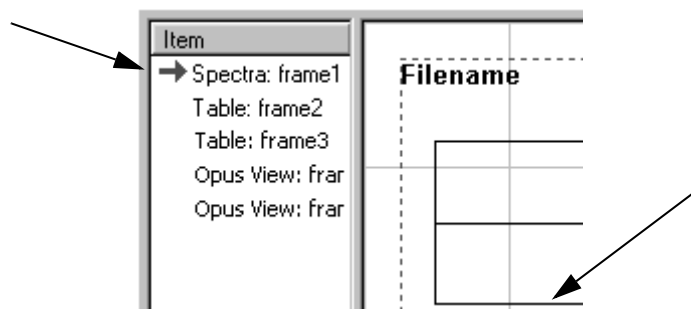


Figure 277: PLE item window

If you right click on an *OPUS View* frame item and select the *Properties* command from the pop-up menu, the following dialog opens:

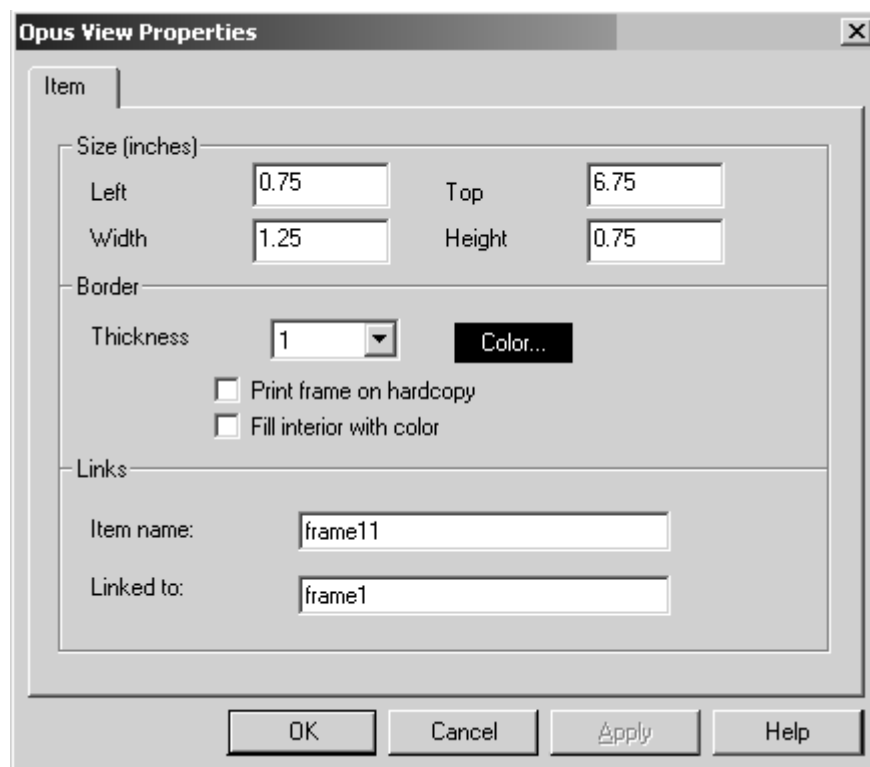


Figure 278: OPUS View Properties - Item tab

The *Item* tab enables to change different properties. Report frames, e.g. integration, QUANT, QC, peak picking, or standard parameter tables will automatically be linked to *frame1* (spectrum frame).

If you use a layout with report frames to print a spectrum, OPUS automatically searches the appropriate frame for the data blocks included in the spectrum file.

11.5.3 PLE Drawing Area

The PLE drawing area (A in figure 275) visually represents the plot view of the current template, containing all the frames. Each frame can be scaled and positioned individually. Below the drawing area two coordinates are displayed (figure 279).

The left display indicates the exact position of the activated frame on the drawing area, the right display indicates the frame size. Even if you resize the frame the current size is always shown in the corresponding display.

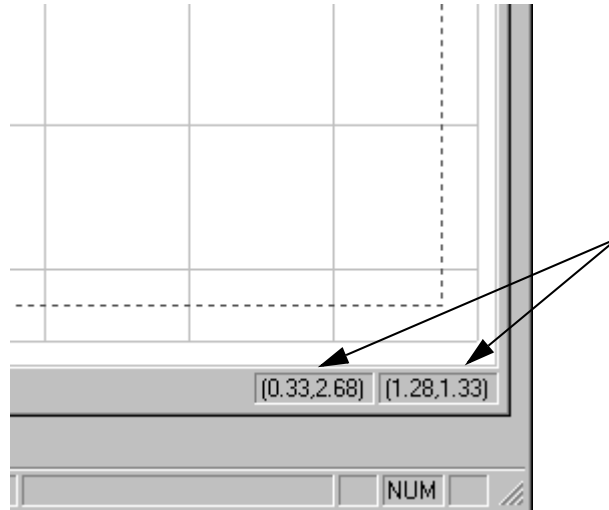


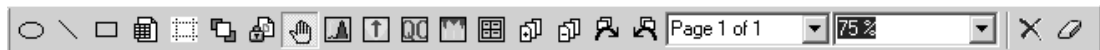
Figure 279: Coordinates of the drawing area




To change a frame right click on the respective frame. A pop-up menu opens which you select the *Properties* command from. To configure the frame individually use the different functions included in the tabs.

It is also possible to change the drawing area. Right clicking on an empty section opens the *Plot Page* dialog which can be used to individually configure the drawing area (see also chapter 11.5.6.1).

11.5.4 PLE Commands

The *Layout* menu contains different commands to be used to create a PLE plot. To get quick access to the most frequently-used PLE commands you can have the command icons displayed in an additional toolbar. Right click onto a free position of the available toolbar and select the *Customize* button in the dialog that pops up. For further details on how to configure toolbars refer to chapter 14.7.



-  Drawing a circle or ellipse
-  Drawing a line or an arrow
-  Drawing a frame



Drawing a table frame



Opening the *Ple Page* properties dialog (also see chapter 11.5.6)



Opening the *Spectral Frame Properties* dialog (also see chapter 11.5.8)



Anchoring an object



Selecting and moving items



Assigning integration report frame; the report frame will automatically be linked to the spectrum frame (*frame 1*).



Assigning QUANT report frame; the report frame will automatically be linked to the spectrum frame (*frame 1*).



Assigning QC (quick compare) report frame; the report frame will automatically be linked to the spectrum frame (*frame 1*).



Assigning peak report frame; the report frame will automatically be linked to the spectrum frame (*frame 1*).



Drawing a standard parameter table; the table frame will automatically be linked to the spectrum frame (*frame 1*).



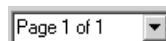
Adding or removing a page (in case of templates with several pages)



Selecting next page (in case of templates with several pages)



Selecting previous page (in case of templates with several pages)



Selecting page numbers (in case of templates with several pages)



Zooming in or out screen views. The zoom factor does not affect the actual template size. The drop-down list also includes the *Fit whole page* and *Fit page width* options.



Removing items



Clearing item contents

11.5.5 Pop-up Menu

If you right click on a frame, the PLE pop-up menu opens. This menu allows to individually configure the frame.

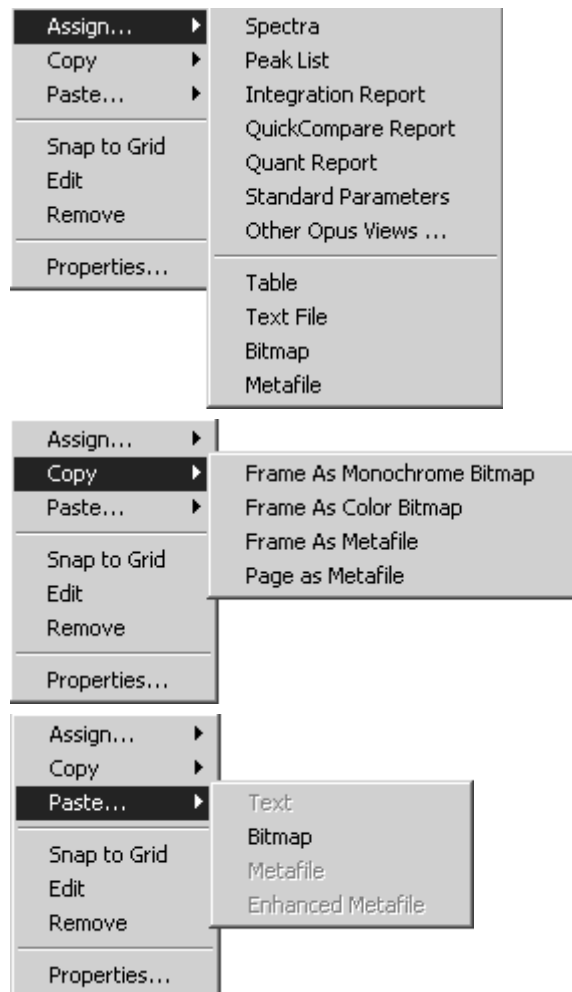


Figure 280: PLE pop-up menu

To change the contents of a frame use the *Assign* command. You can assign spectra, peak lists, standard parameters and other OPUS views (e.g. 3D, correlation chart etc.) as well as integration, quick compare and QUANT reports to a frame.

The *Copy* command duplicates the content of a frame as monochrome bitmap, color bitmap or meta file. The content of a page can be copied as metafile.

By means of the *Paste* command you can insert text, a bitmap, meta file or text from the clipboard into the active frame.

The *Remove* command deletes the frame from the drawing area, while the *Snap to Grid* command aligns this frame exactly on the closest grid lines. The *Edit* command allows to manipulate the frame contents. This command is only available for text and table frames.

If you select the *Properties* command, the *Properties* dialog of the selected frame opens.

11.5.6 PLE Page Properties

Similar to all PLE objects the drawing area also has an individual *Property* dialog. This dialog allows to define general settings of the PLE drawing area. Right click on any free spot within the drawing area.

The *PLE Page* dialog consists of several tabs which will be described in the following.

11.5.6.1 Page

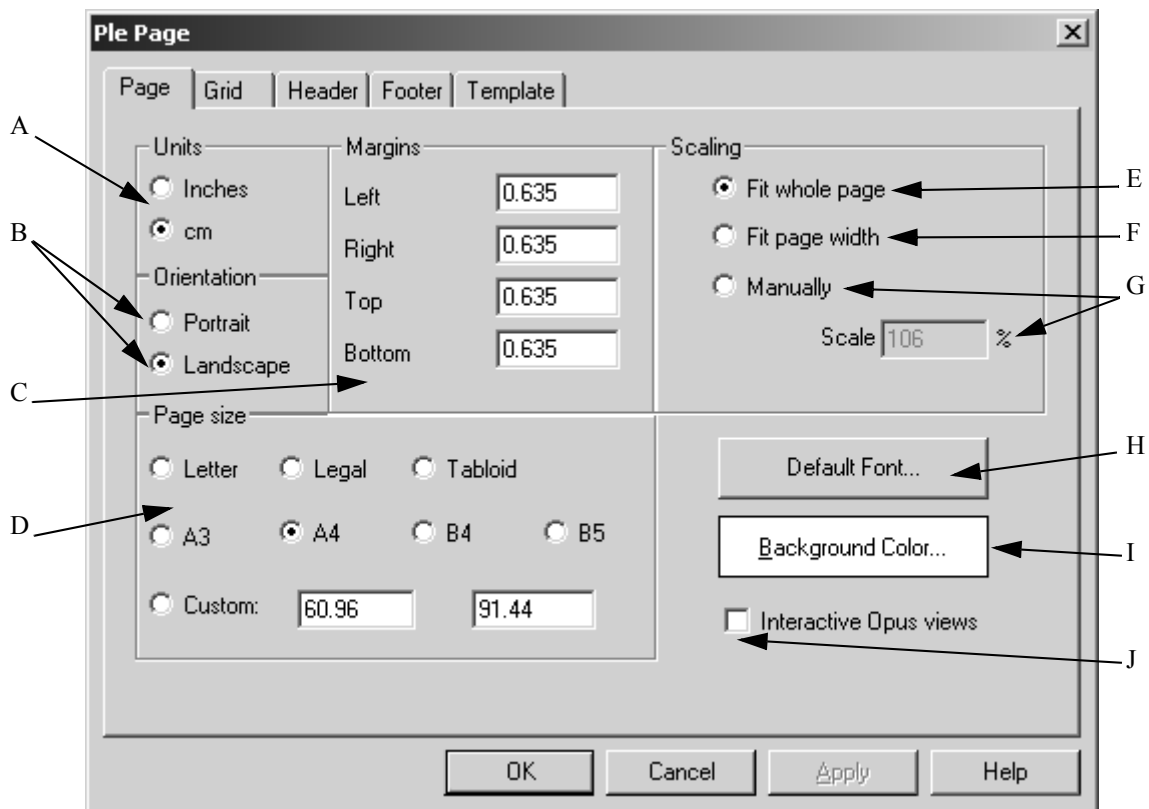


Figure 281: PLE Page - Page tab

- A) Specify the unit that you want to work with (inches or centimeters).
- B) You can print either in landscape or portrait.
- C) Define the maximum print area. Each printer has a particular margin used for paper feed, and which will not be printed on. These default settings are suitable for all common printers and has to be rarely adjusted. The maximum print area is represented by a dotted red line on the PLE document.

- D) Define the paper size. The corresponding unit has been defined by (A).
- E) Check this option button to extend the drawing area up to the size of the whole page.
- F) Check this option button to extend the drawing area up to the page width.
- G) If you check this option button to enter the scale factor manually, the entry field will be enabled. The scale factor required to view the PLE pages is indicated in per cent. Most computer screens are not large enough to allow viewing the entire page at 100% scale. In case of landscape orientation it is advisable to use a scale factor of 75%, in case of portrait orientation a scale factor of 50%.
- H) Specify the default font used when creating a frame within a document. If a frame includes data, the font can be changed no matter what kind of default setting you use.
- I) Define the background color of the view.
- J) Assign the desired OPUS view type to the frame using the *Assign* command from the pop-up menu. If you have selected a structure view, you can drag & drop a structure data block into the frame. To save the PLE page as a template remove the data block again, and the frame will only include the view type assigned to.
- If you have activated the *Interactive OPUS view* check box, 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 onto the frame to open the pop-up menu. Select the *Assign* → *OPUS View* command. The drop-down list includes all OPUS views available.

11.5.6.2 Grid

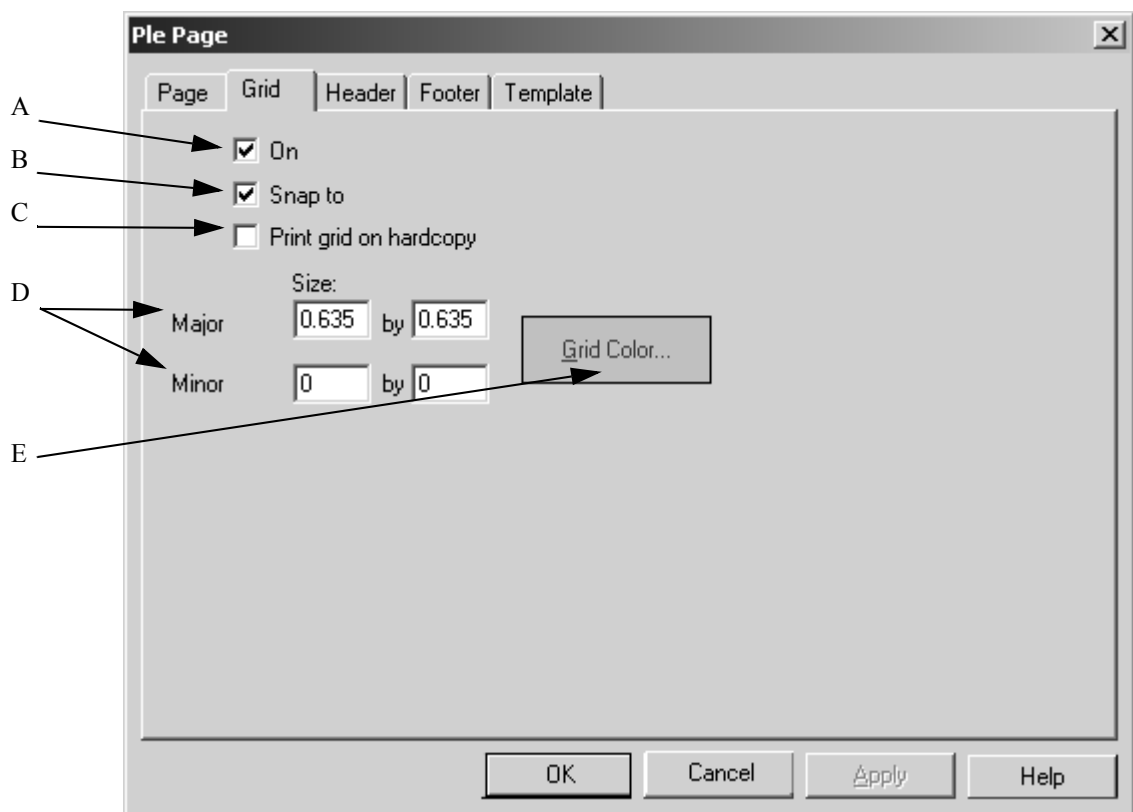


Figure 282: PLE Page - Grid tab

- A) If you activate the *On* check box, the grid will be visible. The grid can be useful to align objects on the drawing area.
- B) If you activate the *Snap To* check box, new objects created are automatically positioned and sized to line up with the closest major grid lines.

- C) Usually, the grid is only displayed on the screen to simplify object alignment. Activate the check box if you want to have the grid printed on paper.
- D) The *Major* and *Minor* settings define the grid size in the unit specified on the *Page* tab. Figure 282 exemplifies a grid size of 1 x 1 inch. The grid can be further divided by filling in the *Minor* entry fields.
- E) Define the color for the grid lines by the *Grid Color* button.

11.5.6.3 Header

The header and footer are printed on every page. The *Header* and *Footer* tabs are identical, therefore only the *Header* tab will be described in the following.

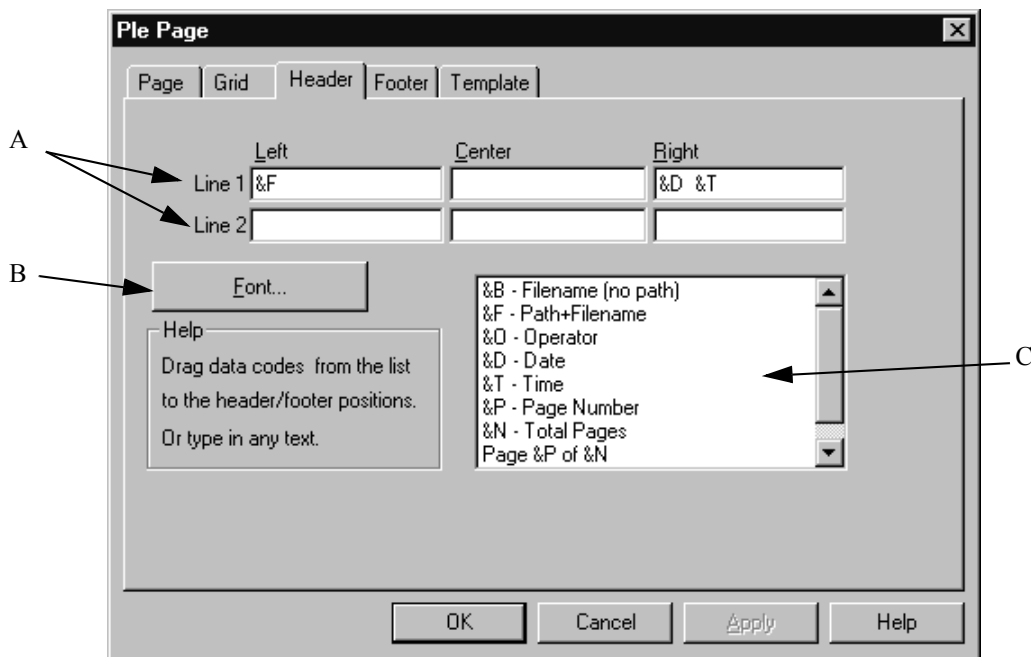


Figure 283: PLE Page - Header tab

- A) The header (or footer) can consist of up to 6 fields (2 rows on the left, middle and right). The entries in the fields consist of meta strings (also see chapter 11.5.9.1). You can either enter these meta strings manually or drag & drop them using the drop-down list (C). It is also possible to enter plain text for the header or footer.
- B) Click on the *Font* button to define the header font.
- C) The drop-down list includes special meta strings. PLE automatically converts these meta strings into readable text in the preview. You can drag & drop these commands from the list to the particular entry field which you want to have the information printed in. It is also possible to manually enter the commands into the particular entry field.

11.5.6.4 Template

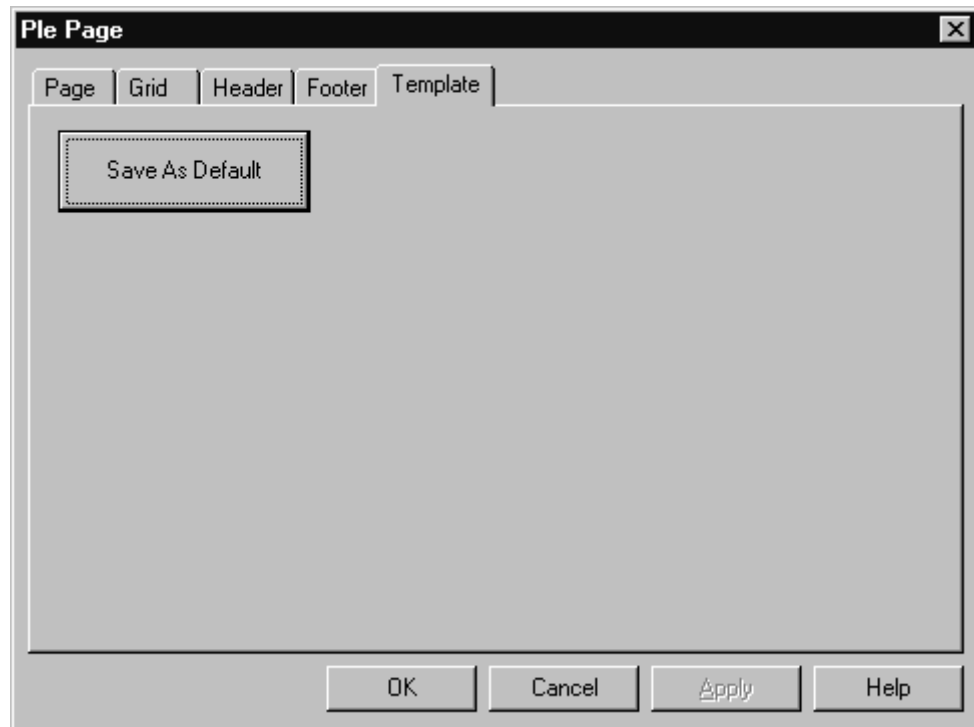



Figure 284: PLE Page - Template tab

You can also save a particular template as default. When creating new PLE documents the settings of this particular template will be used. The default template automatically has the extension *default.ple* and is located in the same directory as the OPUS program. The *Save As* command in the *File* menu allows to save templates, using any file name and directory (preferably the *Scripts* directory). To load these templates use the *Load File* command from the *File* menu.

11.5.7 Loading and displaying a spectrum

To load a spectrum drag & drop it from the browser window to the drawing area. Alternatively, draw a frame by selecting the  icon and assign the spectrum to this frame. Right click on the drawing area and select the *Assign → Spectra* command from the pop-up menu. Select the particular spectrum from the dialog displayed.

The spectrum will appear within the particular frame, including axes and possible annotations. To delete the spectrum from the frame, right click into the spectrum and select the *Remove* command from the pop-up menu.

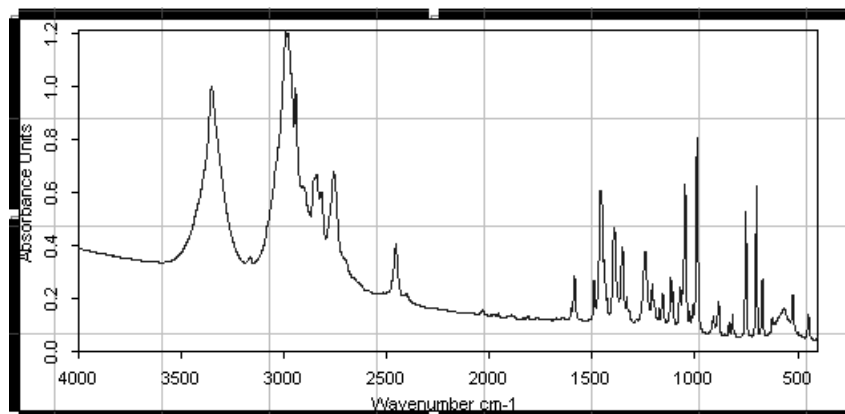



Figure 285: Spectrum frame

To display the standard spectrum parameters select the  icon from the toolbar. Click on the left mouse button and draw a frame onto the drawing area. This frame includes a table which consists of rows and columns, by default.

If you want to change these default settings, right click on the table and select the *Properties* command from the pop-up menu. The thickness of the dividing lines between the cells, and the colors as well as the font can also be changed.

Sample Name	^SNM	Aperture Setting	^APT
Sample Form	^SFM	Beamsplitter Setting	^BMS
Operator Name	^CNM	Detector Setting	^DTC
Resolution	^RES	Source Setting	^SRC
Scantime or Scans	^SOS	Measurement Channel	^CHN
Sample Scans	^NSS	Acquisition Mode	^AQM
Start Frequency Limit for F	^LFQ	Phase Correction Mode	^PH2
End Frequency Limit for Fil	^HFQ	Apodization Function	^AF2

Figure 286: Table frame including standard spectrum parameters

Text can be included using text frames, i.e. either enter text manually into, or import an existing text file to a frame. For manual text input draw a frame and right click on the frame. Select the *Edit* command from the pop-up menu. This will transform the frame into a text frame. Now, enter text into the entry field displayed. Close this entry field by left-clicking anywhere outside the field.

It is also possible to re-size the text frame. Left click into the frame and scale it up or down using the marker positions. Editing text is only possible by using the *Edit* command from the pop-up menu.

To import a text file, first draw a frame and select the *Assign → Text File* command from the pop-up menu. Specify the particular text file from the dialog displayed. Normally, only files with the extension **.txt* can be imported.

11.5.8 PLE Spectral Frame Properties

Similar to all PLE objects the spectral frame also has an individual *Property* dialog. This dialog allows to define general settings. Right click onto the spectral frame and select the *Properties* command from the pop-up menu.

The *Spectral Frame Properties* dialog consists of several tabs which will be described in the following.

11.5.8.1 Item

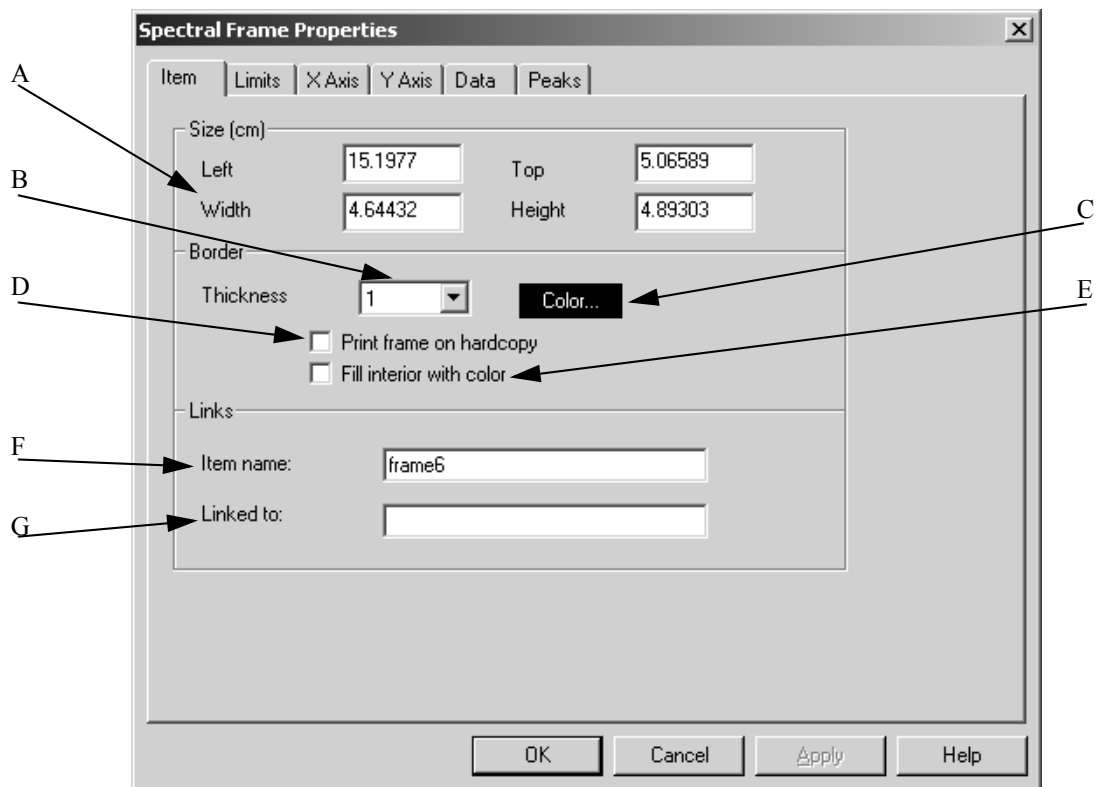


Figure 287: Spectral Frame Properties – Item tab

- A) To change the size and position of the frame on the drawing area use these entry fields. The unit (cm or inch) has been specified by the *PLE Page* dialog on the *Page* tab.
- B) The line thickness used for the frame is indicated in pixels in the drop-down list.
- C) The *Color* button defines the color used to draw the frame. If you click on the *Color* button, a color palette is displayed from which you can either pick a color or define your own color.
- D) Normally, the border lines of the frame are not printed. If you activate this check box, the frame will also be printed on hard copy.
- E) If you activate the *Fill Interior with Color* check box, the frame will be filled by the color specified in (C).
- F) You can assign a name to every object. Naming all the objects in your template simplifies their identification in complex layouts, and assignment of spectrum frames to printed data. You can use these names to link tables and text frames to spectrum frames.
- G) This entry field includes the name of a particular link. This option is only reasonable in case of tables, report frames and texts. If, e.g., you want to include data from a particular

spectrum frame into a table, enter the name of the spectrum frame into the *Linked To* entry field. This entry has to be adjusted as soon as the name of the respective spectrum name has been changed by the operator. Otherwise the link between the different frames cannot be ensured.

11.5.8.2 Limits

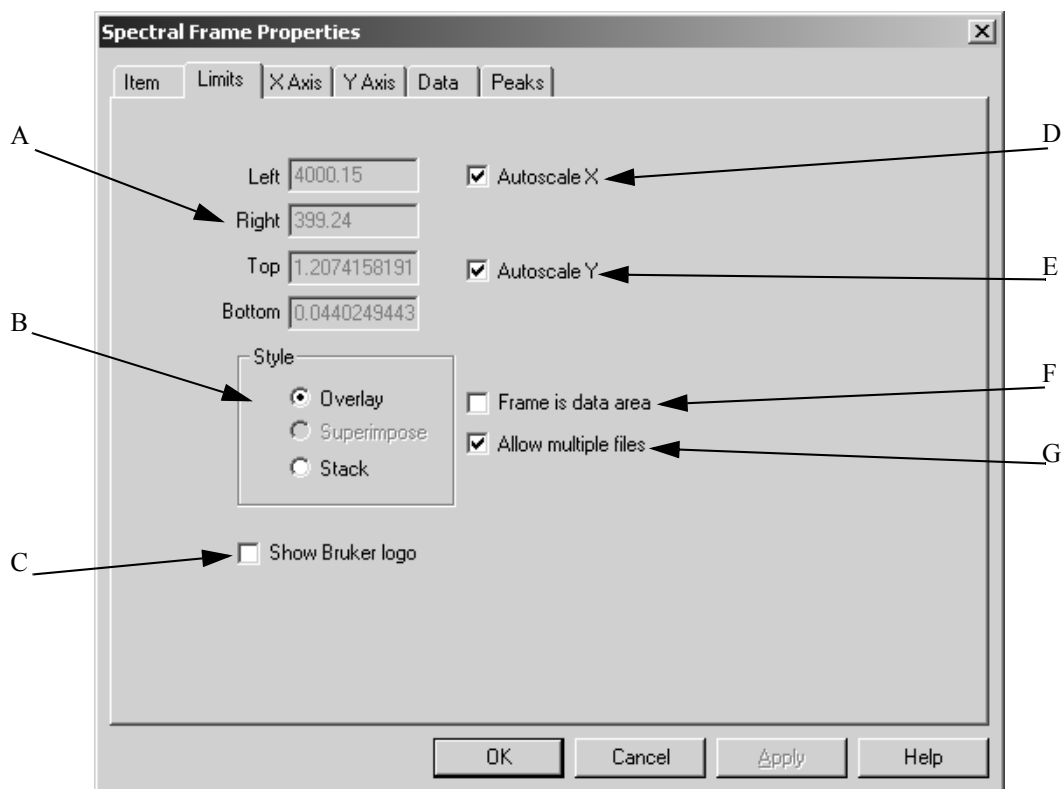


Figure 288: Spectral Frame Properties – Limits tab

- A) The entry fields allow to define the frame limits. The unit of the values entered has been specified in the *PLE Page* dialog on the *Page* tab.
- B) The style type selected determines the presentation of the data within the frame. You can have the spectra displayed in overlaid or stacked mode.
- C) Activate the *Show Bruker Logo* check box if you want to have the logo displayed within the spectrum frame.
- D) If you activate the *Autoscale X* check box, the x axis of the spectra will be autoscaled within the particular frame.
- E) If you activate the *Autoscale Y* check box, the y axis of the spectra will be autoscaled within the particular frame.
- F) The frame displayed on the drawing area can either include the entire spectrum (with axes and annotations), or can be used as boundary for the spectrum itself. If you activate the *Frame is Data Area* check box, the axes and annotations will be drawn outside the frame.
- G) If you do not activate the *Allow multiple files* check box, only one spectrum can be displayed within the frame.

11.5.8.3 Axes

The *X Axis* and *Y Axis* tabs are identical except for the *Rotate Numbers* check box on the *Y Axis* tab. This function allows to turn the y axis annotations by 90°. The *Show axis for stacked spectra* and the *Compressed Wavenumbers* check boxes are only available for the x axis.

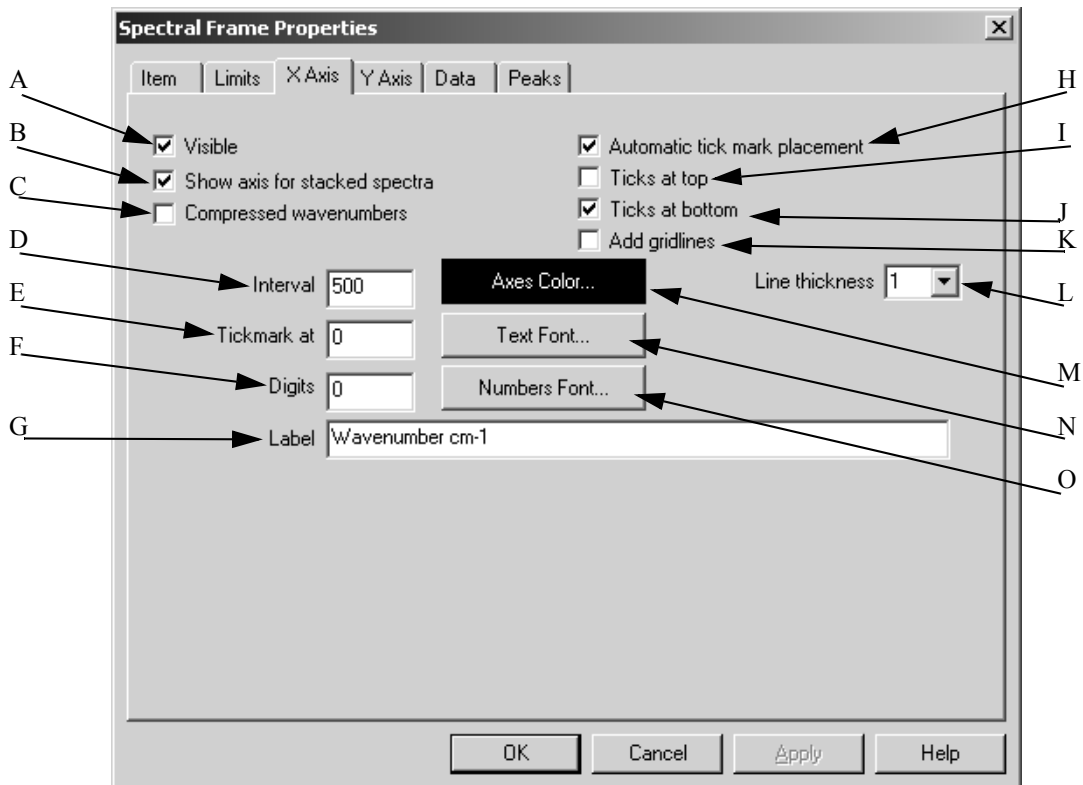


Figure 289: Spectral Frame Properties – X Axis tab

- A) Activate the *Visible* check box if the axes, tick marks and labels have to be displayed.
- B) Activate the *Show axis for stacked spectra* check box if each spectrum has to be displayed with a separate x axis. Otherwise, one common x axis will be used for all spectra.
- C) If you activate the *Compressed Wavenumbers* check box, wavenumbers above 2000cm^{-1} will be displayed using a smaller linear scale.
- D) If you have not activated the *Automatic Tick Mark Placement* check box (H), you can specify the interval between two tick marks.
- E) In the *Tickmark at* entry field you determine the position of a tick mark, provided you have not activated the *Automatic tick mark placement* check box.
- F) Specify the number of digits used to for the numeric tick mark labels, provided you have not activated the *Automatic tick mark placement* check box.
- G) The axes are labelled according to the spectrum file loaded by PLE. The axis label can later be changed.
- H) PLE can automatically sub-divide axes. Activate the *Automatic tick mark placement* check box.
- I) If you activate the *Ticks at top* check box, the tick marks will be displayed on top of the frame. In case of the y axis activate the *Ticks at right* check box on the *Y Axis* tab.
- J) If you activate the *Ticks at Bottom* check box, the tick marks will be displayed at the bottom of the frame. In case of the y axis activate the *Ticks at left* check box on the *Y Axis* tab.

- K) Activate this check box if you want to have the grid lines displayed on the frame.
- L) Determine the thickness of the axis lines.
- M) Click on the *Axes Color* button to select a color used for the axes from the color palette displayed.
- N) If you click on the *Text Font* button, a drop-down list will be displayed. Use this list to determine the font and size of the axis label.
- O) If you click on the *Numbers Font* button, a drop-down list will be displayed. Use this list to determine the font and size of the tick mark (numeric) labels.

11.5.8.4 Data

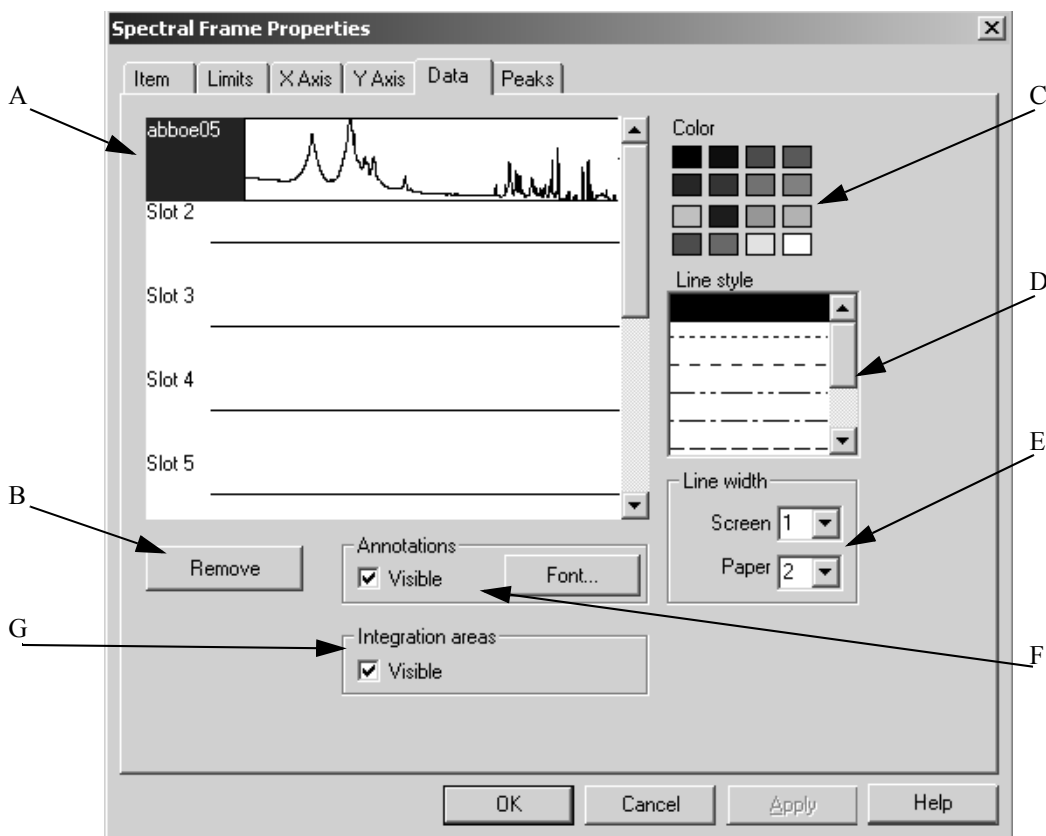


Figure 290: Spectral Frame Properties – Data tab

- A) Spectra added to a frame, are put into a *slot*. This slot just determines the position of spectra. To change the spectra view, you first have to select the corresponding slot of this spectrum. Then, you have to define the properties for that slot using the control elements for color, line style and line width.
- B) If you click on the *Remove* button, the spectra data selected in (A) will be deleted from the slot.
- C) The color palette allows to determine the color of the spectrum displayed.
- D) Use the drop-down list to determine the line style of the spectrum displayed.
- E) Define the line width of the spectrum displayed. Separate line widths can be specified for the screen view and printout.
- F) If the spectrum file contains an ANNO data block, this block can be displayed in the PLE plot by activating the *Visible* check box. Use the *Font* button to determine the font for the annotations.
- G) If the spectrum file contains an INTEG data block, this block can be displayed in the PLE plot by activating the *Visible* check box.

11.5.8.5 Peaks

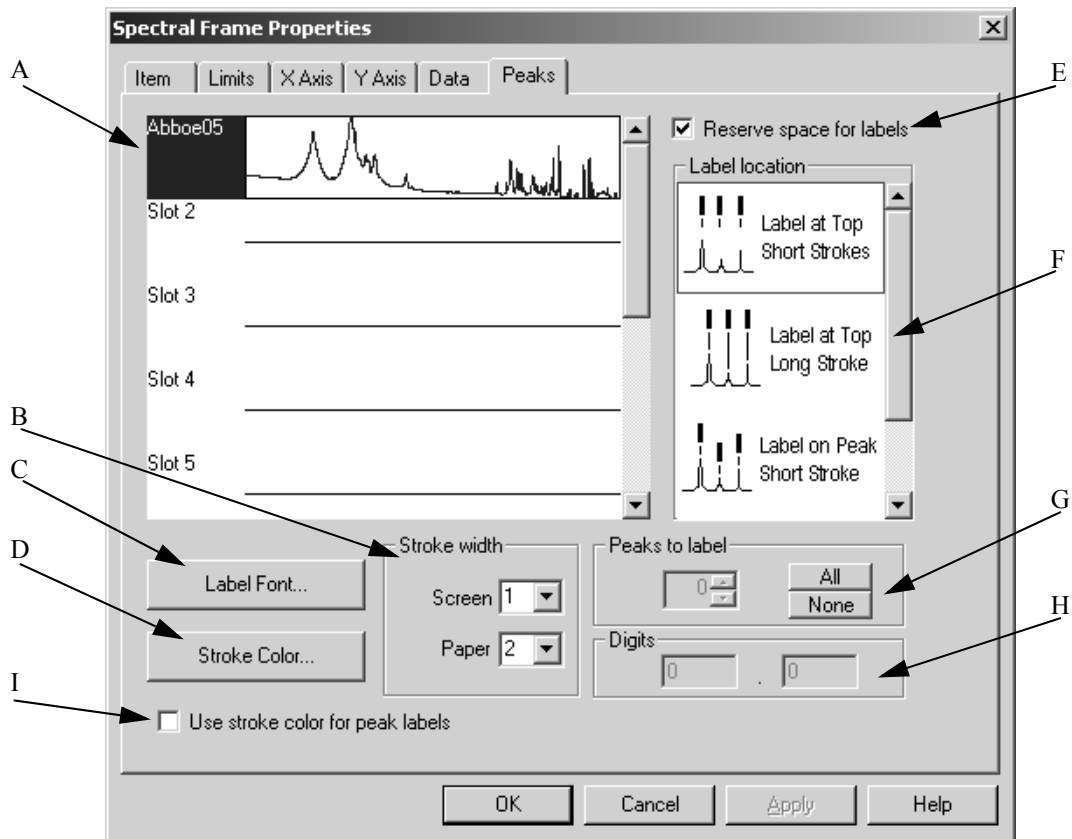



Figure 291: Spectral Frame Properties – Peaks tab

- A) Similar to the *Data* tab you first have to select the corresponding slot for the spectrum.
- B) Define the stroke width of the spectrum displayed. Separate line widths can be specified for the screen view and printout.
- C) Click on the *Label Font* button to determine the font type used for the labels.
- D) Click on the *Stroke Color* button to determine the color for the label strokes.
- E) If you activate the *Reserve Space for Labels* check box, extra space between the highest peak and the spectrum frame for the peak labels is available.
- F) Use the drop-down list to select the type and position of the labels you want to assign to the peaks.
- G) Starting with the highest peak you specify the number of peaks to be labelled, using the *All* and *None* buttons.
- H) Enter the number of digits and decimals for the peak labels.
- I) Activate this check box if the stroke color has to be the same as the one for the spectrum labels. This helps to get a clear display, which is especially useful if the PLE contains more than one spectrum. By means of the *Stroke Color* button (see D) you can define an individual stroke color for each spectrum, which will be the same for the spectrum label if you activate the check box (I).

11.5.9 PLE Table Properties

A table can be created by using the  icon from the PLE toolbar. Tables consist of 2 columns and 2 rows by default. The number of columns and rows can be changed using the *Table Properties* dialog.

It is also possible to edit the table cells separately. Right click into the particular table cell and select the *Edit* command from the pop-up menu. When editing table cells you can change between the different cells by using the tab key.

The *Table Properties* dialog consists of several tabs which will be described in the following. The *Item* tab has already been described in chapter 11.5.8.1.

11.5.9.1 Parameters

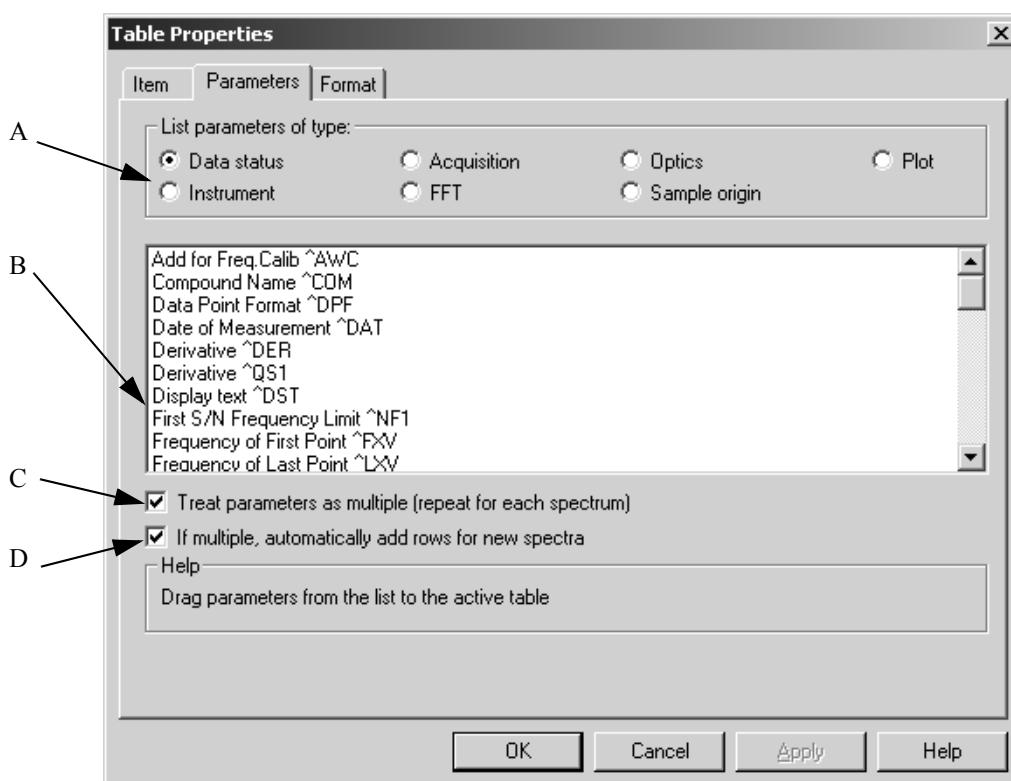


Figure 292: Table Properties – Parameters tab

- A) Different types of parameters are available. Select one of them.
 B) The entries of the drop-down list depend on the type of parameter selected (A). To add information to a table, select an item from this drop-down list and drag & drop it to the particular table cell.

The entries in the drop-down list are meta strings, i.e. three-letter codes preceded by a ^ character. When PLE encounters such a code, it interprets it as an instruction to extract information from the data slot of the linked spectral frame, and to substitute the information by the code. If you edit the table by means of the *Edit* command from the pop-up menu, you will see the actual codes which the meta string consists of. If you want to customize the default format, edit the cell and change the format.

- C) Normally, the information extracted by PLE to expand the meta strings is taken from the corresponding spectral frame in *Slot 1*. If you activate the *Treat Parameters as Multiple* check box, the parameters will be repeated for each spectrum within a particular frame until the maximum number of rows defined on the *Format* tab has been reached.
- D) The more spectra you add to a frame, the more additional table cells can be created to be able to display the parameters for each spectrum. If you activate the *If Multiple, automatically add rows for new spectra* check box, the number of rows set on the *Format* tab will become meaningless.

11.5.9.2 Format

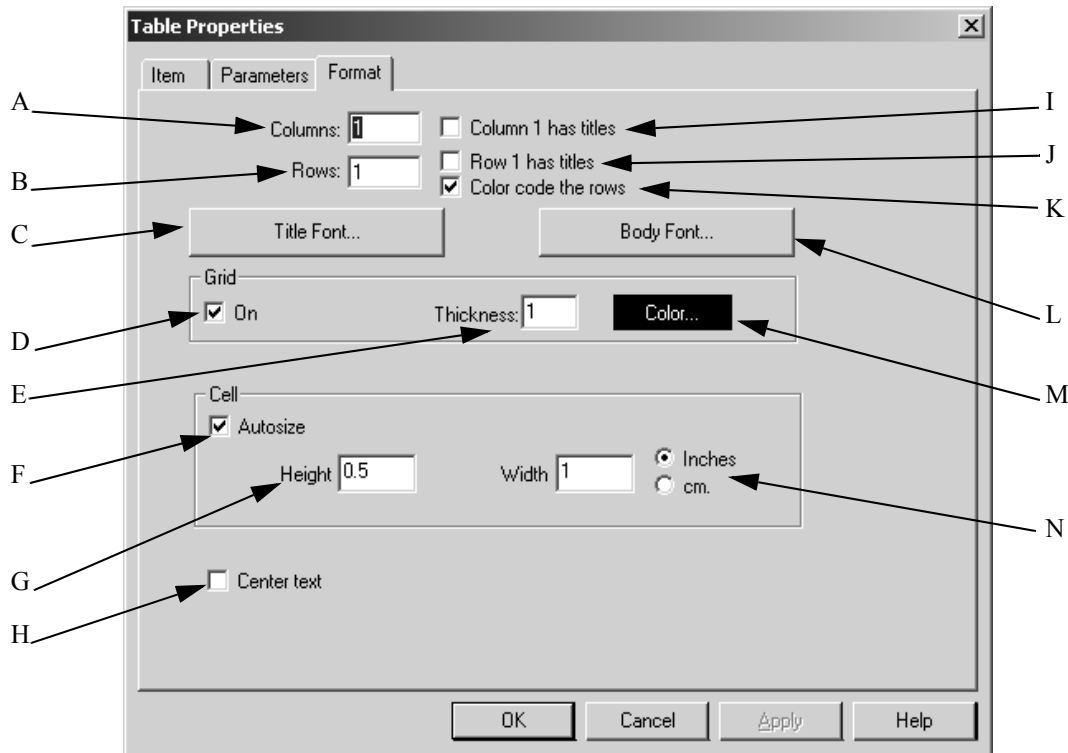


Figure 293: Table Properties – Format tab

- A) Define the number of columns included in the table.
- B) Define the number of rows included in the table.
- C) Use the *Title Font* button to determine the font for the title. Make sure that you first activate the *Row 1 has titles* check box.
- D) If you activate the *On* check box, a grid is displayed around each table cell for better distinction.
- E) The value entered into the *Thickness* entry field determines the thickness of the grid in pixels.
- F) If you activate the *Autosize* check box, cells will automatically be adjusted to the size of the table frame.
- G) If you do not activate the *Autosize* check box, define the height and width of the cells by means of the two entry fields according to the unit specified (M).
- H) Activate the *Center text* check box if you want to center text within the table.
- I) If you activate this check box, the text in column 1 is used as column header, and displayed in the font specified by the *Title Font* button (C).
- J) If you activate this check box, the text in row 1 is used as row header, and displayed in the font specified by the *Title Font* button (C).

- K) To better distinguish the rows you can activate the *Color code the rows* check box. The parameters will then be displayed by the corresponding spectral color.
- L) The *Body Font* allows to specify the body font for the table text. This font applies to all table cells, provided you have not activated the *Column 1 has titles* and *Row 1 has titles* check boxes.
- M) The *Color* button allows to specify the color of the grid to be displayed. As soon as you have selected a color from the color palette the *Color* button will be displayed in this color.
- N) Define the unit for the height and width of table cells if you have not activated the *Autosize* check box.

11.5.10 Text Properties

If a frame includes text, you can format this text by means of the *Text Properties* dialog. The text can consist of meta strings (see chapter 11.5.9.1) or manually typed characters. The meta strings used for table parameters can also be directly typed into a text frame, and 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 described in the previous chapters (11.5.8.1 and 11.5.9.1).

11.5.10.1 Text

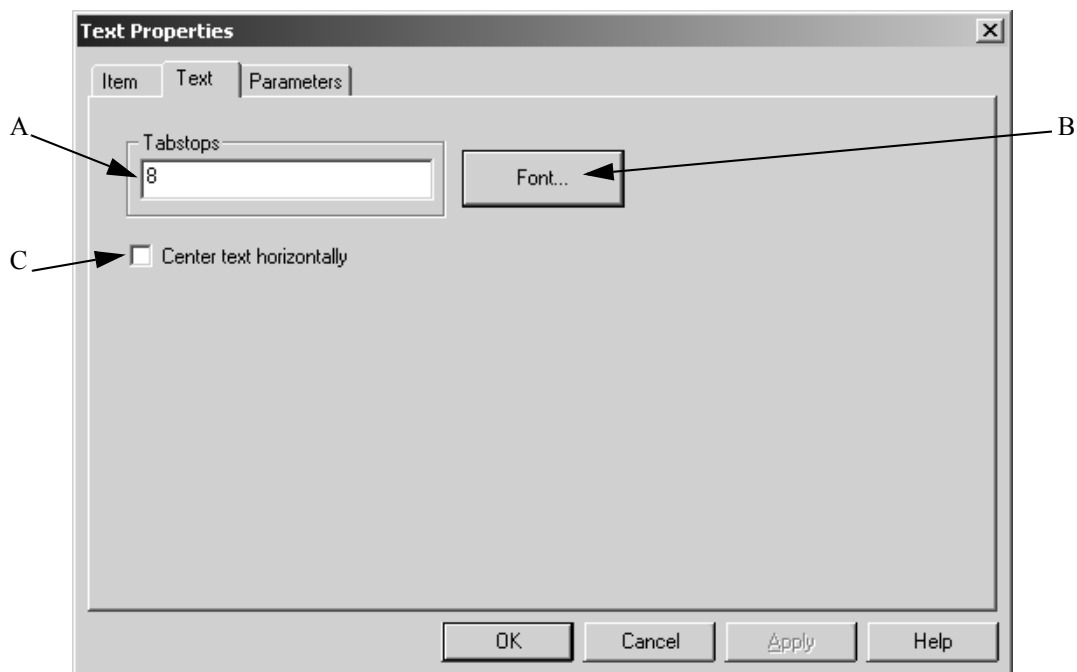


Figure 294: Text Properties – Text tab

- A) Defines the position of tab stops for the text in the frame. The value entered represents the distance to the next tab. Multiple positions can be used, separated by spaces, e.g. *8 12 20 40*. The last tab spacing is used for subsequent tab stops, if more tabs are required.
- B) By means of the *Font* button you determine the font and font size of the text.
- C) To better align text within a frame activate the *Center Text Horizontally* check box, as the text lines will be horizontally centered.

11.6 Open Layout

The *Open Layout* command shows a list of existing templates. When using this command for the first time after the OPUS installation you have to navigate to the particular directory. Templates have the file extension **.ple*.

11.7 Print / Print Preview

You can view the result of a printout using the *Print Preview* command. The *Print* command starts printing immediately.

12 Macro

Macros can be created for regularly used OPUS functions. An OPUS macro is a sequence of OPUS commands that can be executed all in one. In addition to the standard OPUS commands there is a set of macro functions which allow to control the macro execution, interaction with the user and the evaluation of results.

Basically, an OPUS macro is a text file using the extension *.MTX*, which can be edited by any kind of text editor. For a detailed description of all macro functions and their syntax, see the OPUS Programming manual.

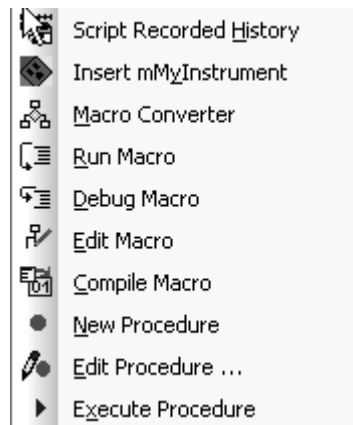



Figure 295: Macro menu

12.1 Script Recorded History

The data stored in the HISTORY data block () can also be stored in a script. Select the file which you want to extract the performed manipulations from. Drag & drop the file into the *File to extract manipulations from* entry field.

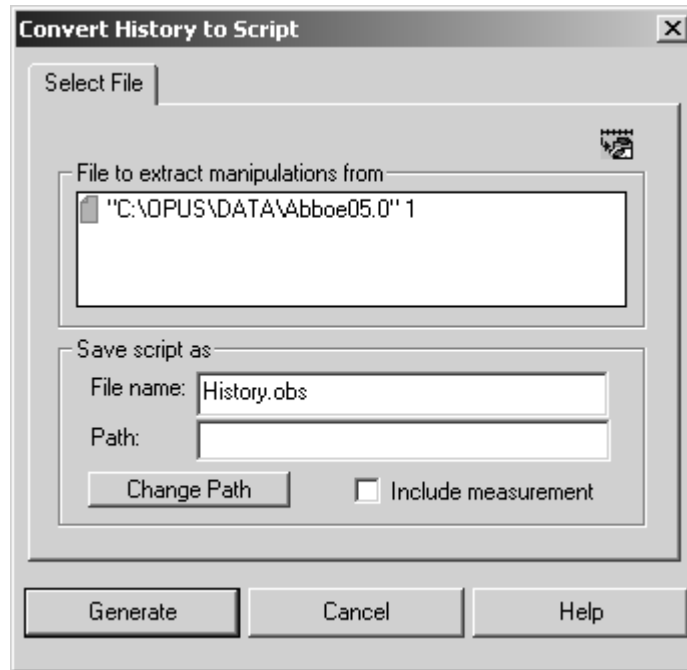


Figure 296: Convert History to Script - Select File tab

Define a file name for the script and specify the directory path, where the file is to be saved to. If you activate the *Include Measurement* check box, you add the corresponding measurement parameters as well.

Once the script has been saved, it can also be applied to other files using the *VisualBasic Script* command from the *File* menu.

12.2 Insert MyInstrument

MyInstrument 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 VisualBasic Script.

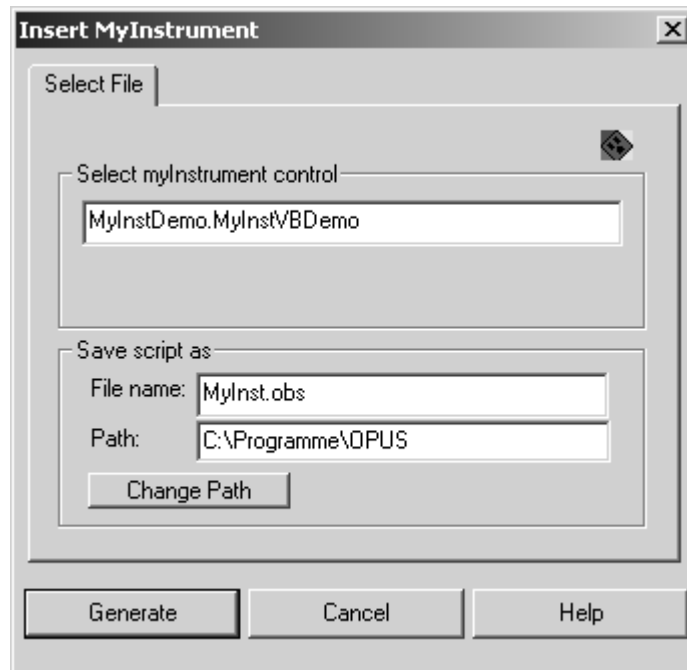


Figure 297: Insert MyInstrument - Select File tab

Enter the name of the registered *MyInstrument* control element into the *Select MyInstrument control* entry field, and define the file name and path for the resulting VisualBasic Script.

12.3 Macro Converter

Use the Macro Converter to translate macros written by OPUS-OS/2 into the OPUS format. The conversion may require some changes as a result of the different macro syntax. For any further details, refer to the OPUS Programming manual.

If you have selected the *Macro Converter* command, a wizard starts and helps you with the conversion steps. Follow the on-screen instructions.

12.4 Run Macro

To run a macro click on the *Run Macro* command and select the appropriate macro from the dialog box that opens. Any further actions depend on the macro selected.

12.5 Debug Macro

The *Debugging* term means executing macros step-by step or selectively executing single macro lines. The program is executed until a specified break point has been reached. Debugging simplifies the localizing and analyzing of macro errors.

Click on the *Debug Macro* command and select the correct macro from the dialog that opens. For any further details on this subject, refer to the OPUS Programming manual.

12.6 Macro Editor

OPUS includes an editor to generate and edit macros. Click on the *Macro Editor* command and create a new macro or load an already existing one using the *Open Macro* button. For any further details on this subject, refer to the OPUS Programming manual.

12.7 Compile Macro

Macros are written and stored as text files. The *Compile Macro* command allows to convert these text files to executable binary codes. Compiled macros are started faster than macros in text format. For any further details on this subject, refer to the OPUS Programming manual.

12.8 Adding Macros

Macros which you use regularly can be added to the toolbar or any menu. To do this you have to add an entry to the *USERMAC.LST* file in the *OPUS* directory. If this file is not available in the directory, create the file using the text editor.

For each macro you want to add to the toolbar you have to enter the following information to the *USERMAC.LST* file using the text editor:

- 1) Name and path of the macro file
- 2) Number of the menu (see table below)
- 3) Text to be included in the menu
- 4) Text for tooltips in the tool bar
- 5) Text for the status bar

Entries in one line have to be separated by the “@” sign, e. g.:

```
E:\OPUS\MACRO\IT.MTX@8@Instrument test@IT-Test@Start IT
```


If you want to have an icon displayed in the toolbar, the macro directory also has to include a bitmap file with the icon. Make sure that the bitmap is of 16*15 pixels.

To add a macro to a particular menu, use the menu 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

12.9 New Procedure

The *New Procedure* editor allows to create a specific structure used to automate ordinary procedures. When creating such a structure you can either follow the on-screen instructions provided by the Macro Wizard, or click on single OPUS icons in the toolbars to define the course of actions manually.

If you select the *New Procedure* command, the following dialog opens:

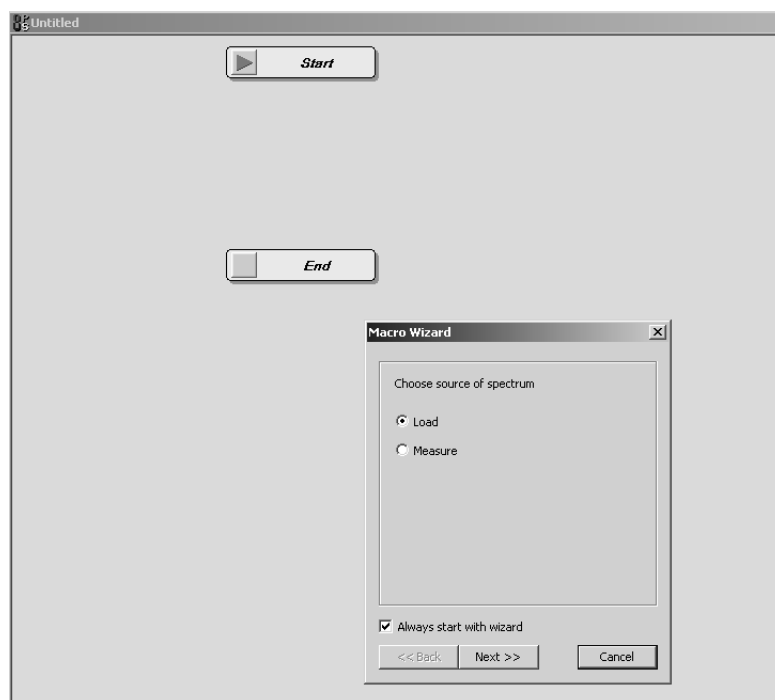



Figure 298: New Procedure workspace with Macro Wizard

By default, the Macro Wizard is displayed. If you want to change this default setting, deactivate the *Always start with wizard* check box. In this case you have to define the course of actions manually.

If you do not use the wizard and you want to define a *Load File* structure block, e.g., click on the  icon, select the file from the dialog displayed and click on the *Open* button. A *Load File* block will be created and automatically added to the procedure. This also applies to evaluation, manipulation, save or printing blocks. To adjust the parameters of these blocks double click on the structure block, and the respective OPUS command dialog opens.

To delete a certain structure block, left click on the block and press the *Del* key on the keyboard.

12.9.1 Macro Wizard

The different dialogs of the Macro Wizard will be explained in the following. As figure 298 exemplifies, on the first macro wizard dialog you have to select the source of spectrum, i.e. you can either activate the *Load* or *Measure* option button. In the latter case a file has to be actually loaded and displayed in the OPUS browser window, as the procedure will only have an effect on a loaded file. Click on the *Next* button.



Figure 299: Macro Wizard - manipulation functions

Select one of the manipulation functions and activate the appropriate option button. The *Other* drop-down list includes all manipulation functions provided by OPUS except those already displayed in the dialog. This dialog will be closed not until you activate the *No manipulation* option button.

Click on the *Next* button to continue.

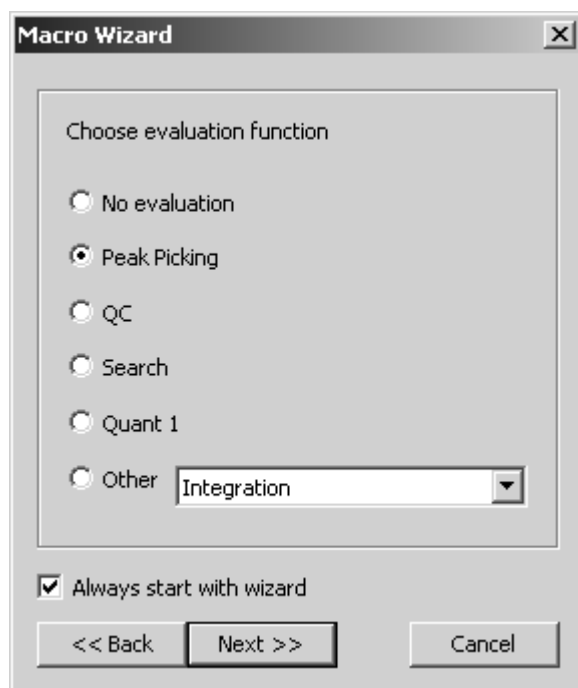


Figure 300: Macro Wizard - evaluation functions

Select one of the evaluation functions and activate the appropriate option button. The *Other* drop-down list includes all evaluation functions provided by OPUS except those already displayed in the dialog. This dialog will be closed not until you activate the *No evaluation* option button.

Click on the *Next* button to continue.



Figure 301: Macro Wizard - final dialog

Activate the *Save* check box if you want to save the file at the end of the procedure. The same applies to the *Print* options if you want to have the file automatically printed. Activate the *Loop* check box to repeat the course of actions previously defined *n* times. As soon as you click on the *Finish* button the macro structure created will be displayed.

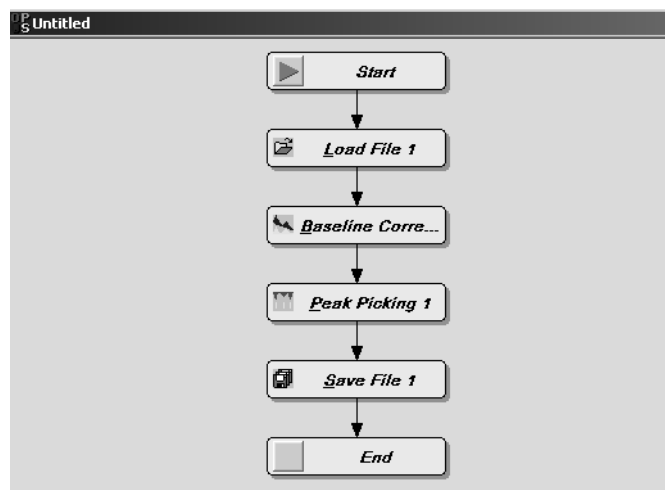


Figure 302: Procedure created

12.9.2 Pop-up menu

Right clicking somewhere on the procedure workspace opens a pop-up menu which consists of the following commands:

- Macro
- Tools
- Blocks
- Edit

These commands can be used to edit, validate or save the procedure created. In the following each of the commands will be described in more detail.

Macro

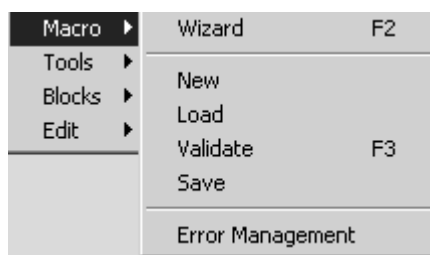
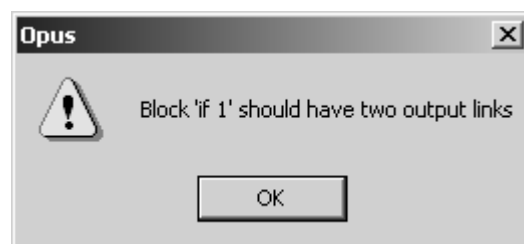
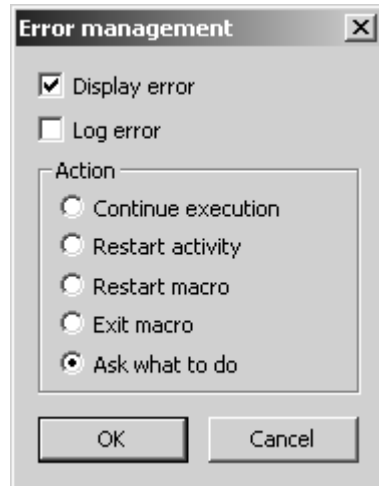


Figure 303: Pop-up menu - Macro

- **Wizard:** starts the wizard.
- **New:** provides new procedure workspace.
- **Load:** loads existing procedure structure.
- **Validate:** allows to validate the procedure created, i.e. it will be checked whether the course of actions within the structure is valid. If not, a message box pops up indicating how the existing structure has to be modified, as the following example shows:



- **Save:** saves the procedure. Define the file name and directory path in the dialog displayed. As the macro structure is stored as OPUS basic script, it has the file extension **.obs* and can also be started by the *Visual Basic Script* command from the *OPUS File* menu.
- **Error Management:** global setting which specifies how the script should react in case of an error. If you click on *Error Management*, the following dialog opens:



Activate the appropriate check box and option button to further define the error management.

Tools



Figure 304: Pop-up menu - Tools

- **Select:** allows to select a certain procedure block. This option is checked by default. To select a procedure block, left click on it, and it will be marked by a broken line:



. Now, you can move any structure block to a different place if you press and hold down the left mouse button.

When positioning a structure block on a black connecting arrow between two different structure blocks, this arrow becomes red, visualizing that you are now changing the original structure. As soon as you release the mouse button the structure block moved will exactly be positioned between these two different structure blocks.

- **Create Link:** to explicitly create an arrow link, e.g. in case of *IF* structure blocks. To delete a link, click on the arrow which turns red and press the *Del* key on the keyboard.

Blocks

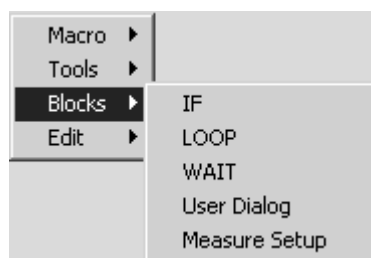
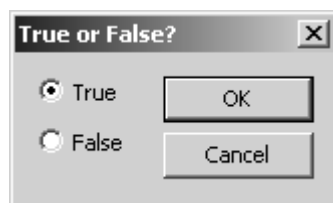


Figure 305: Pop-up menu - Blocks

- **IF**: creates an *IF* structure block which always requires two output links. If you integrate the *IF* block into an existing procedure, the following dialog opens:



Specify which *condition*, i.e. *True* or *False* has to be used to continue. Double clicking on an *IF* structure block displays the following window:

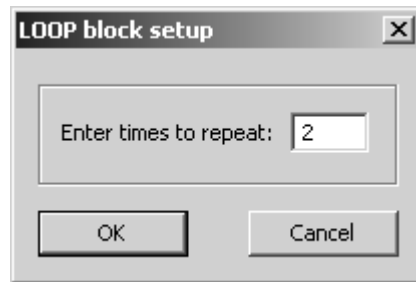


If you activate the *Dialog answer* option button, you have to enter an appropriate question into the entry field. You can also define whether the *IF* block shall be based on a previous evaluation report. Depending on the report selected from the drop-down list further details with regard to the condition can be defined. If you have, e.g., selected *Peak Picking*, you can further determine whether the

number of peaks should be  than the number specified in the

entry field. In case of a *Search* or *IDENT* report the value to compare with will be the hit quality.

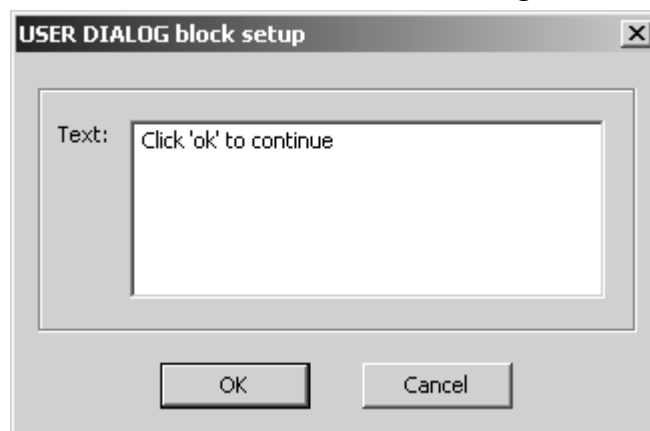
- **LOOP:** creates a *LOOP* structure block. This kind of structure block is used to repeat certain functions. Define the loop count in the dialog that pops up when double clicking on the *LOOP* structure block.



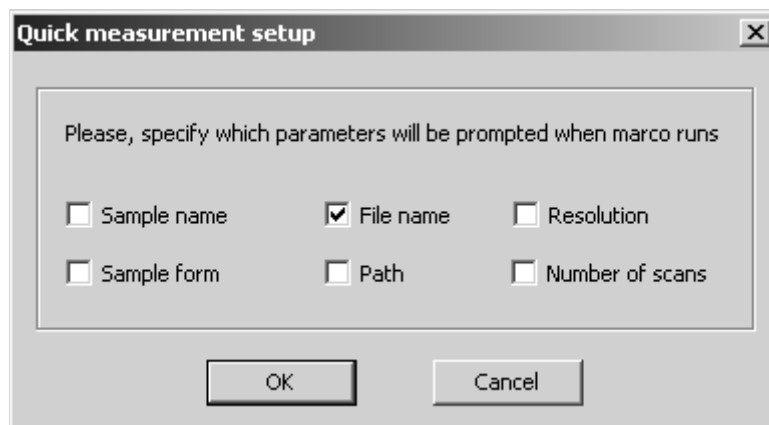
- **WAIT:** creates a *WAIT* structure block. This kind of structure block is used to interrupt the current course of action. The period of time can be exactly defined in the dialog that pops up when double clicking on the *WAIT* structure block.



- **User dialog:** creates a *Message Box* structure block. To manually enter the text double click on the *Message Box* structure block.



- **Measure setup:** creates a *QUICK MEASURE* structure block. If you integrate such a block into the procedure, specific parameters will be prompted when running the macro. To explicitly define these parameters double click on the *QUICK MEASURE* structure block.



Edit



Figure 306: Pop-up menu - Edit

- **Move to back:** in case of two structure blocks on the same position moves the one selected behind the other.
- **Invert selection:** inverts the structure selected.
- **Arrange:** arranges the procedure as exemplified in figure 302.
- **Select All:** selects all structure blocks.

12.10 Edit Procedure

The *Edit Procedure* command can be used to edit a procedure created. Select the respective procedure from the dialog that opens.

12.11 Run Procedure

To run a procedure click on the *Run Procedure* command and select the appropriate macro from the dialog box that opens. Any further actions depend on the macro selected.

13 Validation

The *OPUS Validation Program* (OVP) is part of the OPUS software and allows a validation of the spectrometer with the PQ test (Performance Qualification¹) and OQ test (Operational Qualification²).

The *Validation* menu contains the following commands:

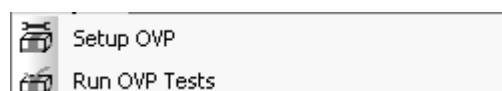



Figure 307: Validation menu

OVP is based on a modular concept and works as follows:

- Test channels can be defined and assigned to OVP by specifying a measurement configuration for each channel. 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.
- If the tests have 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 status light  changes its color to green. The operator can continue using the spectrometer as the instrument has been properly tested.
- 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. This, however, assumes that the tests themselves do not require any interaction.

Measurement and test parameters are stored in a set of databases which have also been installed when installing OPUS. If you have received a separate database CD, you also have to install this CD. For details on the installation instructions refer to the database CD.

1. Qualification of spectrometer performance in daily routine work

2. Qualification of spectrometer performance after installation and maintenance

13.1 General Settings

OVP modules, databases, test spectra measured and reports are stored in the OVP standard directory *C:\OPUS\VALIDATION*. If you want to change this directory, select the *User Settings* command from the *Setup* menu (see figure 308) and change the validation path. Make sure that you also move the data files of the previous standard directory to this new path, and restart OPUS.

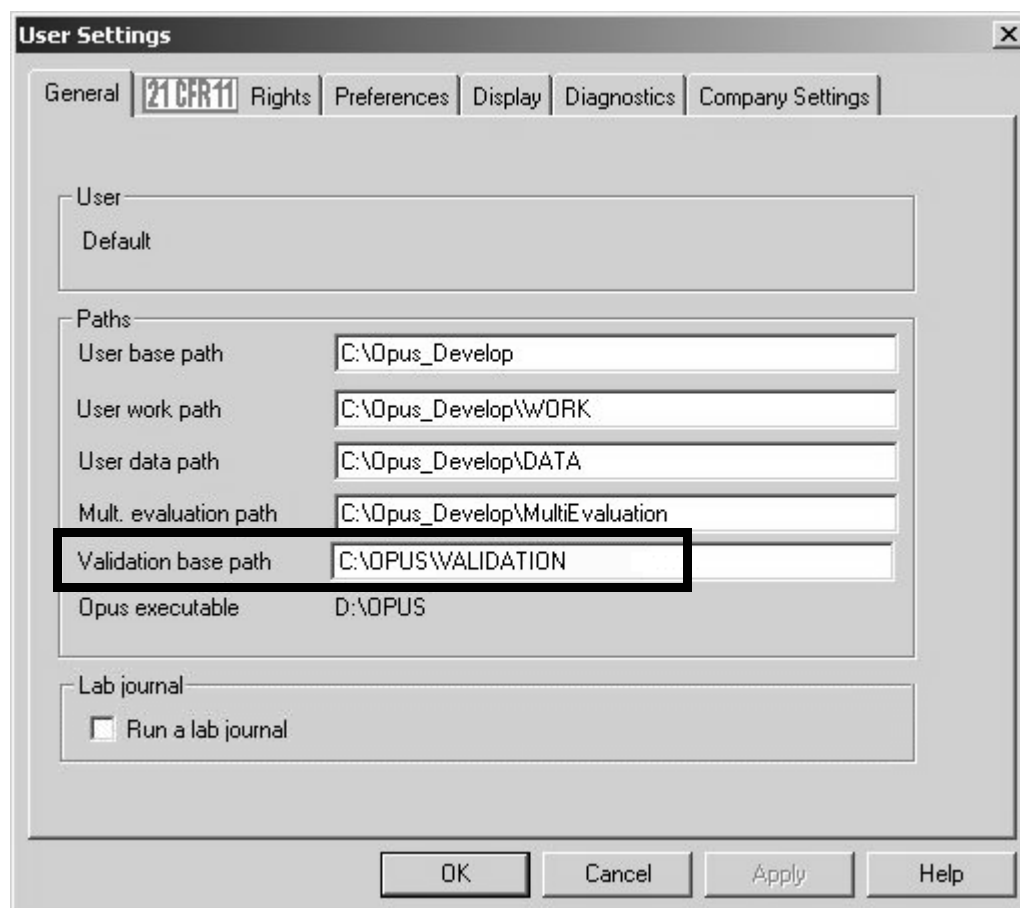


Figure 308: User Settings - Validation base path

13.2 OVP Setup

Before you can work with OVP you have to set the corresponding parameters in the OVP dialog *Setup OVP*. Select the *OVP Setup* command from the *Validation* menu to open the following dialog:

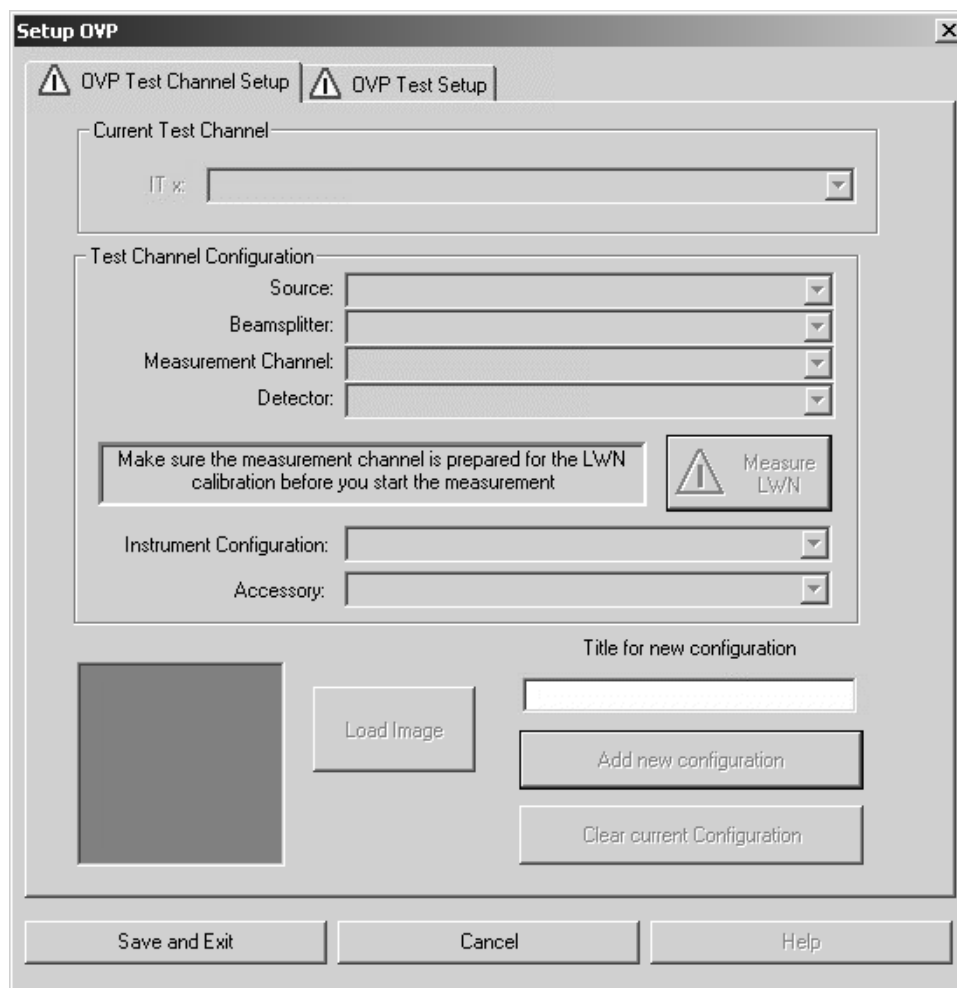


Figure 309: Setup OVP

Enter a title for the current configuration into the *Title for new configuration* entry field, to specify the current setup by a descriptive text.

Click on the *Add new configuration* button. Now, all the other selection fields will no longer be hidden and can be filled in.

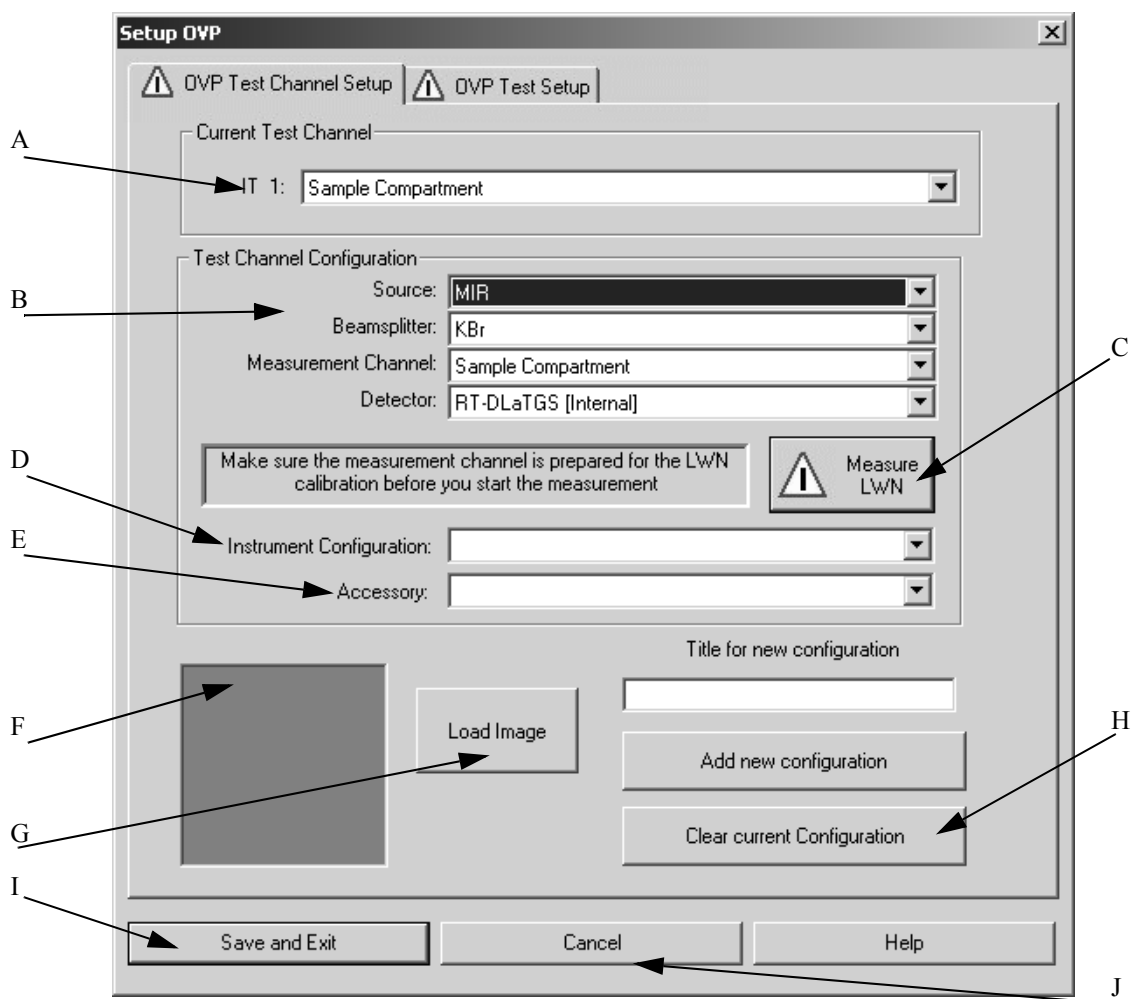


Figure 310: Setup OVP - Activated drop-down lists

- A) The drop-down list shows the test channel used by OVP.
- B) For each spectrometer test channel you have to assign a measurement configuration to be used during actual validation measurement. This is a valid combination of source, beam splitter, measurement channel and detector. As soon as you have selected all components the appropriate instrument configuration (D) and the bitmap (F) specified for the measurement channel will automatically be displayed.
- C) Click on this button to set up the laser wavenumber. See also chapter 13.2.2.
- D) In general, the instrument configuration is automatically displayed as soon as you have selected all components. Always check whether the correct instrument configuration has been suggested. If required, select a different instrument configuration.
- E) Depending on the test channel, the drop-down list contains appropriate accessories. The following example shows an accessory selection of fiber-optics probes:

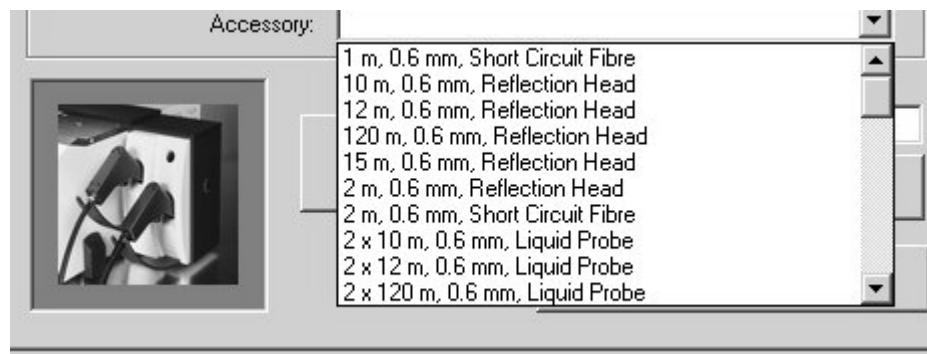



Figure 311: Accessory selection

- F) Depending on the measurement channel or accessory selected a configuration-specific bitmap will be displayed.
- G) Use the *Load Image* button to load further instrument images available in OPUS (see chapter 13.2.1). The bitmaps are stored in the *OPUS\VALIDATION\Bitmaps* directory.

Select the *Thumbnail* option from the pop-up menu when clicking on the  button to be able to see at once which bitmap belongs to which file name.

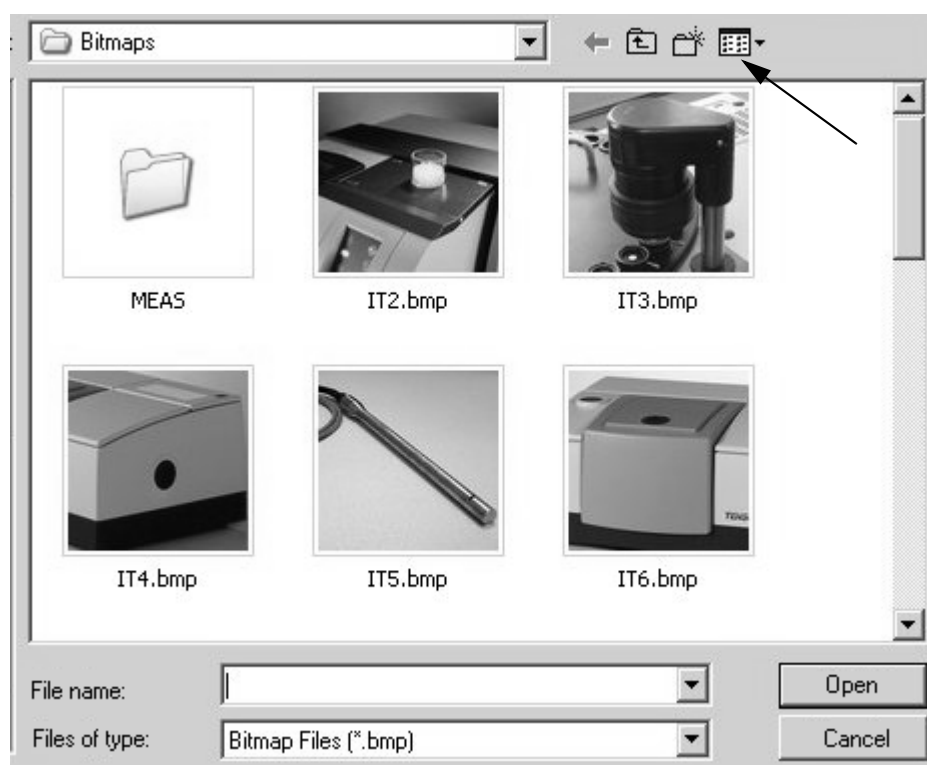


Figure 312: Bitmaps in Browse view

You can also make your own photo with a size of 90 x 90 and store it into the bitmap directory using the *ITnn.bmp* file name (*nn* is a consecutive number).

- H) To delete the current configuration click on this button. Once deleted the settings cannot be reloaded. If you have accidentally deleted a channel, you have to repeat the complete setup again. OVP configurations are stored in the *OPUS\VALIDATION\Database\<Instrument>* (<Instrument> e.g. MPA) directory.
- I) To save the configuration click on the *Save and Exit* button.
- J) Click on this button to cancel the OVP setup without saving.

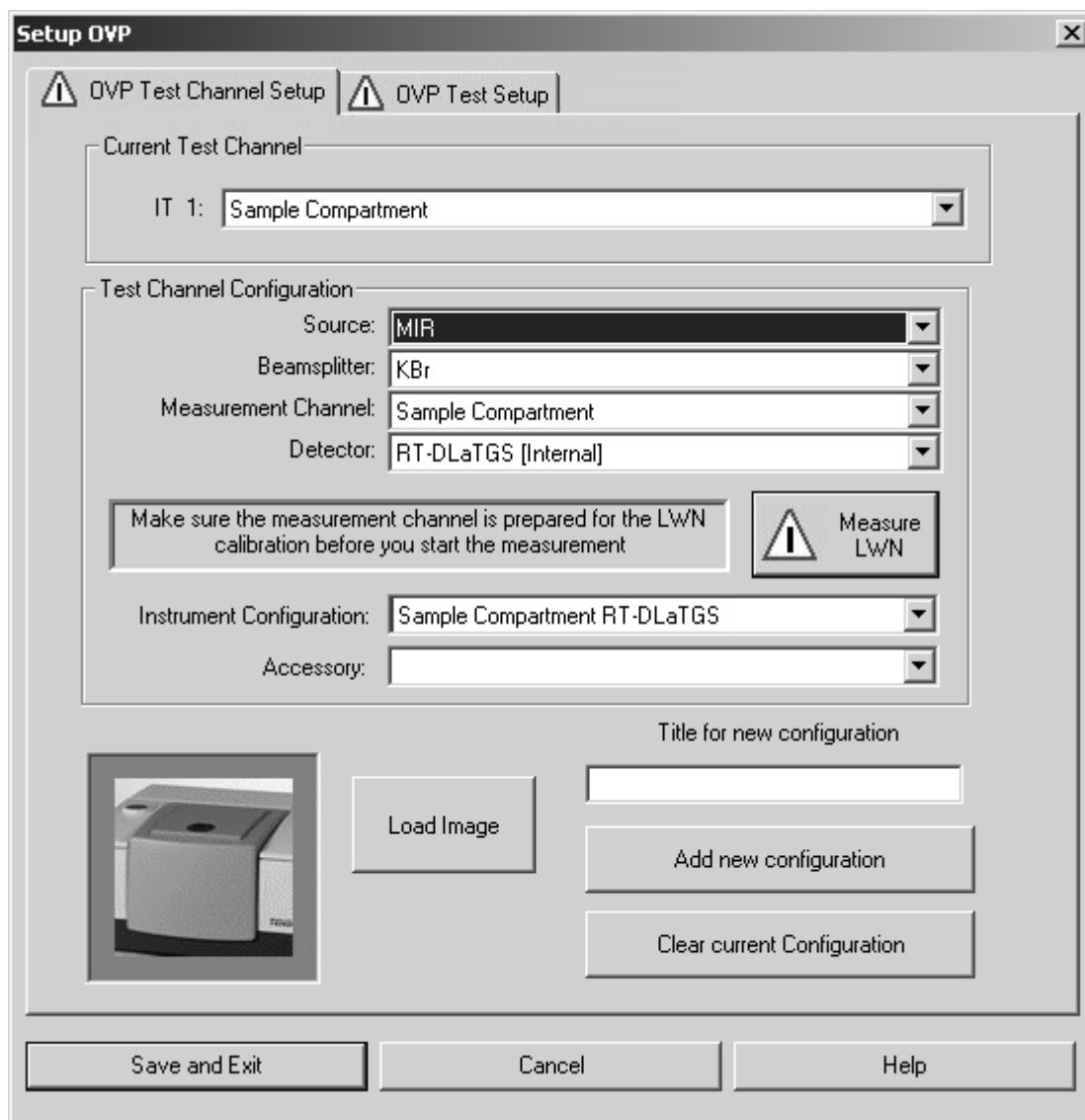


Figure 313: Setup OVP - Bitmap of instrument type

13.2.1 Bitmaps for OVP

The following bitmaps of different instrument configurations are available for the OVP setup:



IT2.bmp: MPA integration sphere



IT3.bmp: VECTOR 22/N, external transmission



IT4.bmp: TENSOR 27, external port



IT5.bmp: Liquid probe



IT6.bmp: TENSOR, sample compartment



it7.bmp: MPA, sample compartment



it8.bmp: MPA, fiber-optic probes



it9.bmp: MPA, external transmission



IT10.bmp: Fiber-optic probe



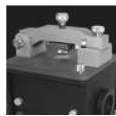
IT11.bmp: Solid probe



IT12.bmp: Emission head



it13.bmp: DuraSampler



It14.bmp: Golden Gate



IT15.bmp: Pike MIRacle, reflection unit



IT16.bmp: Liquid probe



IT17.bmp: HTS-XT



IT18.bmp: HTS-XT, transmission



IT19.bmp: HTS-XT, reflection



IT20.bmp: Equinox 55, sample compartment



IT21.bmp: MATRIX-E



IT22.bmp: MATRIX-F



IT23.bmp: MATRIX-I



IT24.bmp: VECTOR 22/N



IT25.bmp: VERTEX 70, sample compartment



IT26.bmp: VERTEX 70, external port



IT27.bmp: VERTEX 80V



IT28.bmp: TGA



IT29.bmp: TANDEM



IT30.bmp: RAM II



IT31.bmp: RFS 100



IT32.bmp: RAMSYS



IT33.bmp: SENTERRA



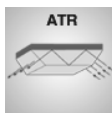
IT34.bmp: SENTINEL



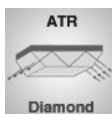
IT35.bmp: FRA 106



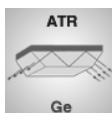
IT36.bmp: IRcube



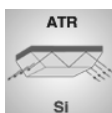
IT37.bmp: ATR (Attenuated Total Reflection)



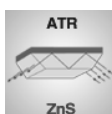
IT38.bmp: ATR Diamond



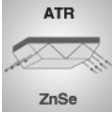
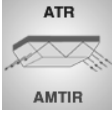

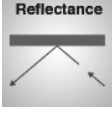

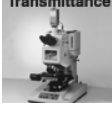
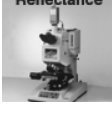

IT39.bmp: ATR Ge (Germanium)




IT40.bmp: ATR Si (Silicon)



IT41.bmp: ATR ZnS (Zinc sulphide)

	IT42.bmp: ATR ZnSe (Zinc selenide)
	IT43.bmp: ATR AMTIR (IR transmission substance)
	IT44.bmp: DRIFT (Diffuse reflection)
	IT45.bmp: Reflectance
	IT46.bmp: Transmittance
	IT47.bmp: Hyperion, Transmittance
	IT48.bmp: Hyperion, Reflectance
	IT49.bmp: ATR objective, Hyperion

13.2.2 Measure Laser Wavenumber

The  warning symbol indicates that the settings for the current configuration have not yet been completed. To be able to define the settings for the single tests you first have to measure the laser wavenumber (LWN). Therefore, click on the



button to perform a test using the optics configuration for the currently selected IT channel.

Proper assignment of test-channel-specific laser wavenumbers may require an update of the instrument firmware as well. In case of doubt contact Bruker service.

The laser wavenumber is affected by changes in the optical path length. This can cause considerable deviations when using optical fibers of different lengths. Measuring and assigning the laser wavenumber for each test channel ensures the wavenumber accuracy of spectral data.

The test first measures a spectrum of water vapor and uses a specific water band to determine the optimum laser wavenumber. To verify the validity of the water

band adjacent water bands are checked as well. In a second step the appropriate wavenumber 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.

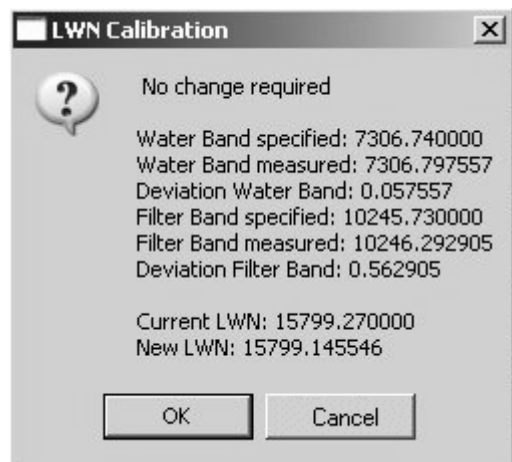


Figure 314: OVP - Test result of LWN calibration

The LWN test result shows the water bands specified and measured. You can also see the water band deviation as well as the laser wavenumber, i.e. both the specified and newly calculated one.

If the current LWN for this channel is within a certain tolerance, the test has passed and no further changes are required. If the deviation is beyond a certain tolerance, the LWN value for the current measurement channel is set to the currently computed optimal value when clicking on the *OK* button. Now, a

green check mark is added to the  button in the *Setup OVP* dialog.

If the water band could not be detected properly as the water vapor concentration of your instrument may be too low or too high, first a warning pops up.

In this case examine the water vapor spectrum *LWN_Water.x* (with *x* being any number) which is located in the *OPUSVALIDATIONTEMP* 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. If the water vapor contents are too high, you have to replace the desiccant cartridge or purge by using dry air. Repeat the measurement until the result is OK.

Important: Since OPUS 5 the laser wavenumber has been stored and used based on the test channel specified in OVP. In case of measurements in the empty sample compartment, and measurements in the sample compartment equipped with an accessory, both configurations have to be setup as two different test channels in OVP. The laser wavenumber can be different for both test channels, even if both configurations use the sample compartment as

measurement channel. Therefore, it is important to register the empty sample compartment and the sample compartment equipped with accessory in different test channels.

In case of spectrometers equipped with a Quick Lock™ baseplate (TENSOR and VERTEX only) the accessory is both identified when calibrating the laser wavenumber, and the settings are displayed in the measuring configuration. This is to ensure a unique allocation of the test channel.

It is not necessary to measure the laser wavenumber separately in case of transmission accessories. This means that neither an entry is required in the *Accessory* drop-down list nor an additional OVP channel has to be set up.

13.2.3 Setting up OVP tests

If you click on the *OVP Test Setup* tab, the following dialog opens:

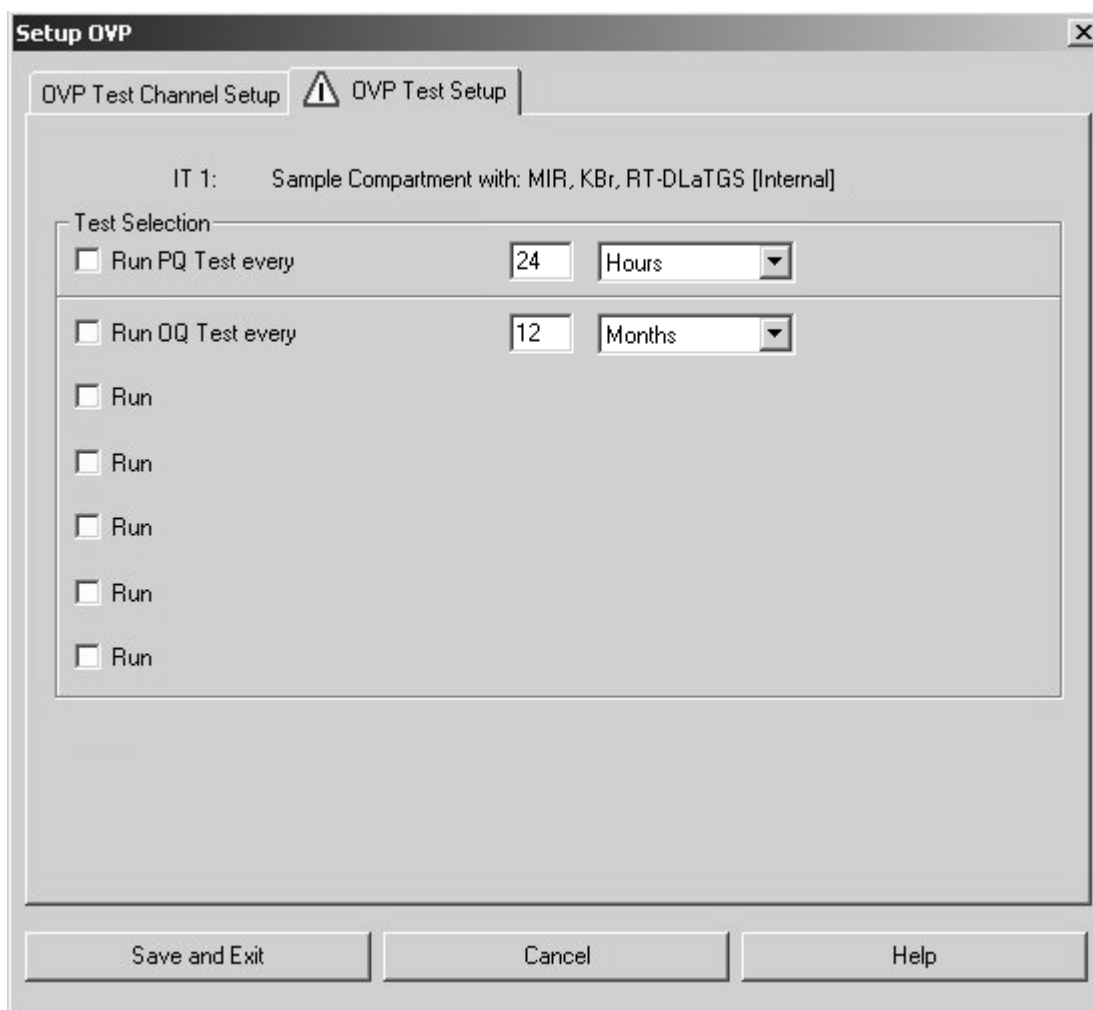


Figure 315: OVP Test Setup tab

The line on the very top shows the test channel selected on the *OVP Test Channel Setup* tab.

You have two basic categories for testing:

- PQ test
- OQ test

Define a specific test interval for both test categories to determine when the tests have to be performed.

Note: It is 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.

If you activate the *Run PQ Test every* check box, the following line will be displayed:

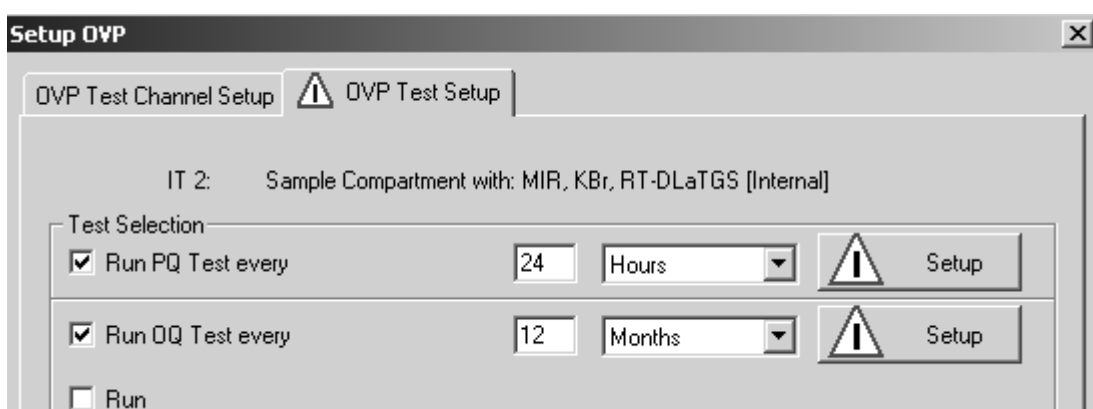


Figure 316: Configuring PQ test

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 PQ test protocol is a short-term test which verifies that the instrument performance is suited for daily operation.

Click on the *Setup* button to open the following dialog:

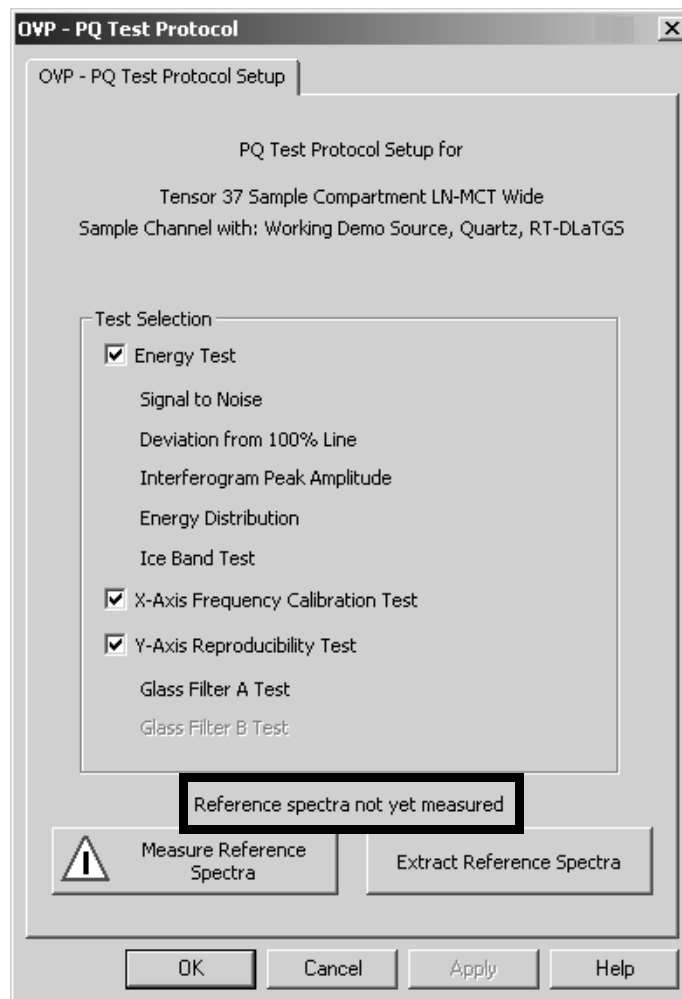


Figure 317: OVP - Selecting PQ tests

All tests available for a particular type of spectrometer have already been selected. In exceptional cases (not recommended) you can deactivate certain tests by deleting the check mark.

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.

13.2.3.1 PQ Tests

The PQ test protocol consists of the following single tests (for further details on each test see also chapter 13.2.3.2:

Energy Test

The energy test includes the following single tests:

- **Signal to Noise**
Verifies that the signal-to-noise ratio is better than a specified limit.
- **Deviation from 100% Line**
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 Distribution**
The energy tests verifies, by means of different methods, the total energy of the spectrometer and its different components.
- **Ice Band Test**
This test verifies the leak tightness of MCT detectors.


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. The test is performed by using one or two filter(s) with different absorbing properties.

- Glass Filter A Test
- Glass Filter B Test (not available in each spectrometer)

Tests which are not available for the given spectrometer type cannot be selected. For some PQ tests reference measurements are required which are generally performed after the OQ test has been passed. No PQ test can be performed without these reference data. This is indicated by a warning written in the lower part of the dialog (see marking in figure 317), and the  symbol displayed.

Click on the *Measure Reference Spectra* button. If the reference measurement has been successfully finished, the date of measurement will be displayed and a green check mark is added to the *Measure Reference Spectra* button.

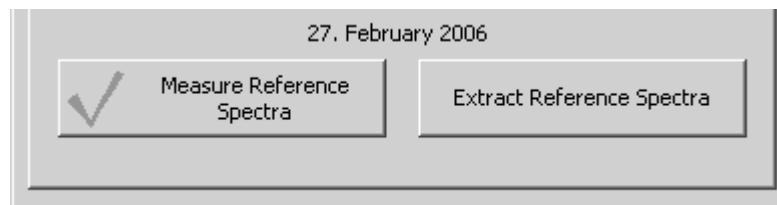


Figure 318: Reference measurement passed with PQ test

Reference spectra are stored in the user database. Whenever used the reference data are temporarily extracted and afterwards removed again. This avoids accidental deleting or overwriting.

If you click on the *OK* button, the current setup status is indicated by a green check mark on the *Setup* button of the *OVP Test Setup* tab.



Figure 319: PQ test setup status

If you close the dialog without measuring any reference spectra, or without any existing reference spectra from previous measurements, a warning pops up and the warning symbol remains on the *Setup* button.

13.2.3.2 PQ Test Description

Signal to Noise (S/N) Ratio:

The signal-to-noise ratio test determines the sensitivity of the spectrometer by calculating the average signal-to-noise ratio of ten 100% spectra.

The S/N ratio is determined by collecting and analyzing a 100% spectrum. A 100% spectrum is the ratio of two successively acquired single-channel spectra with no sample in the sample compartment. The ratio of these two single-channel spectra is used to generate a transmission spectrum.

The S/N ratio is 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 is calculated differently for systems used in the MIR and NIR region.

Figure 320 shows a peak-to-peak noise of 0.1%, referring to 100% transmittance in MIR region. To calculate the S/N ratio the reciprocal value is multiplied by 100 ($1 / 0.1 * 100$). Figure 321 shows a 100% line in NIR region.

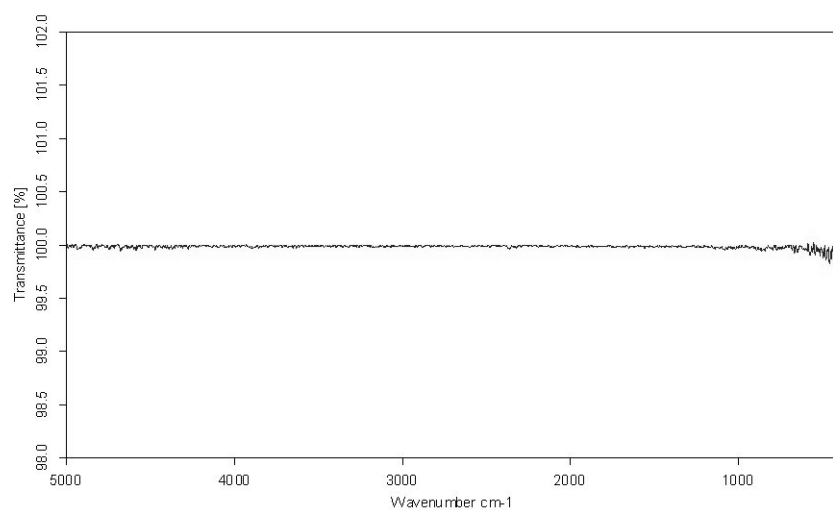


Figure 320: MIR 100% line

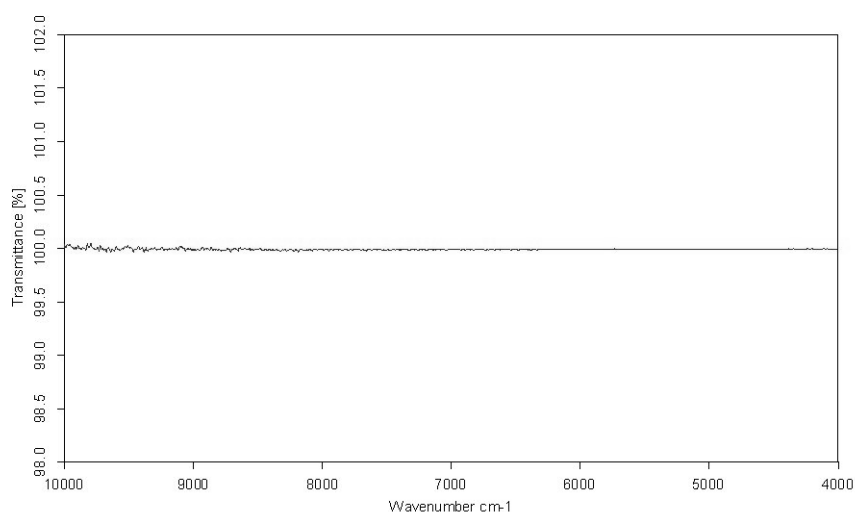


Figure 321: NIR 100% line

Deviation from 100% Line:

This test measures the maximum deviation of a 100% line within a larger frequency range.

The average determined by 10 measurements must not exceed the predefined limit.

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 the reference interferogram stored.

The amplitude of the reference interferogram corresponds to 100%. In the PQ 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 PQ test report relative to the reference value and must not fall below a specified limit. Figure 322 shows an interferogram, which has been measured by the *Double Sided, Forward-Backward* acquisition mode.

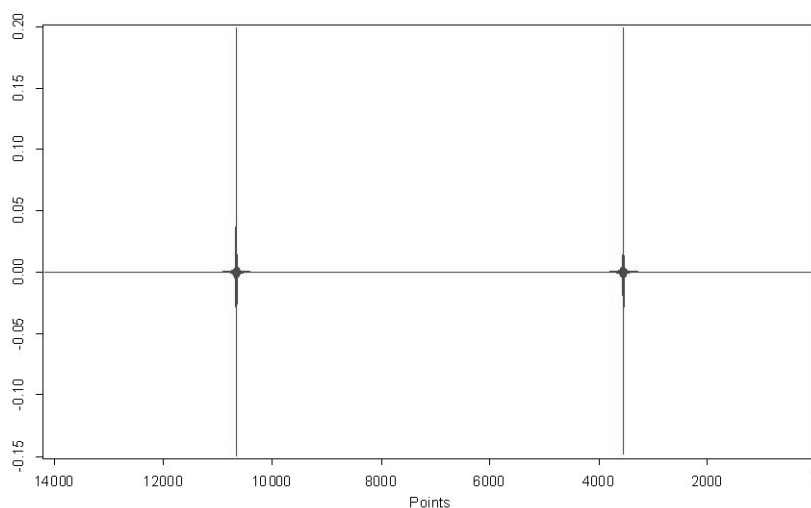


Figure 322: Double-sided interferogram

Energy Distribution (Single-Channel Spectrum):

The energy distribution test is a long-term stability test which compares the amplitude of a measured single-channel spectrum to that of a stored reference single-channel spectrum.

Figure 323 and 324 show the single-channel spectra of the reference file 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. In case of this long-term stability test, test spectra are compared to the reference spectrum stored.

A new reference spectrum has to be measured as soon as the instrument has been realigned, or the source changed.

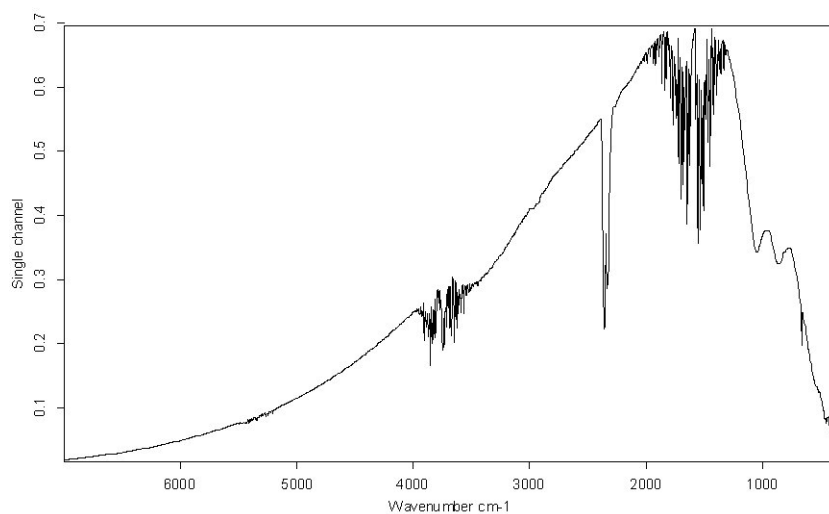


Figure 323: MIR reference spectrum

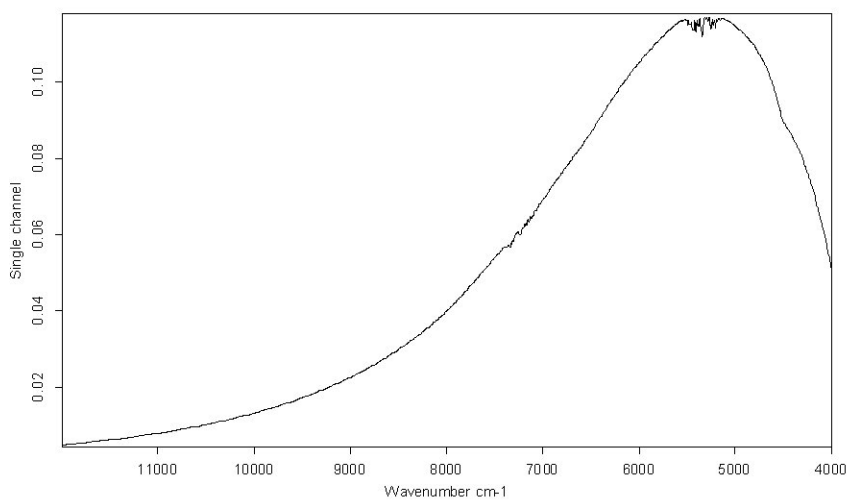


Figure 324: NIR reference spectrum

Ice Band Test:

If the vacuum of an MCT detector decreases you can observe the ice band caused by condensed water vapor in the single-channel spectrum.

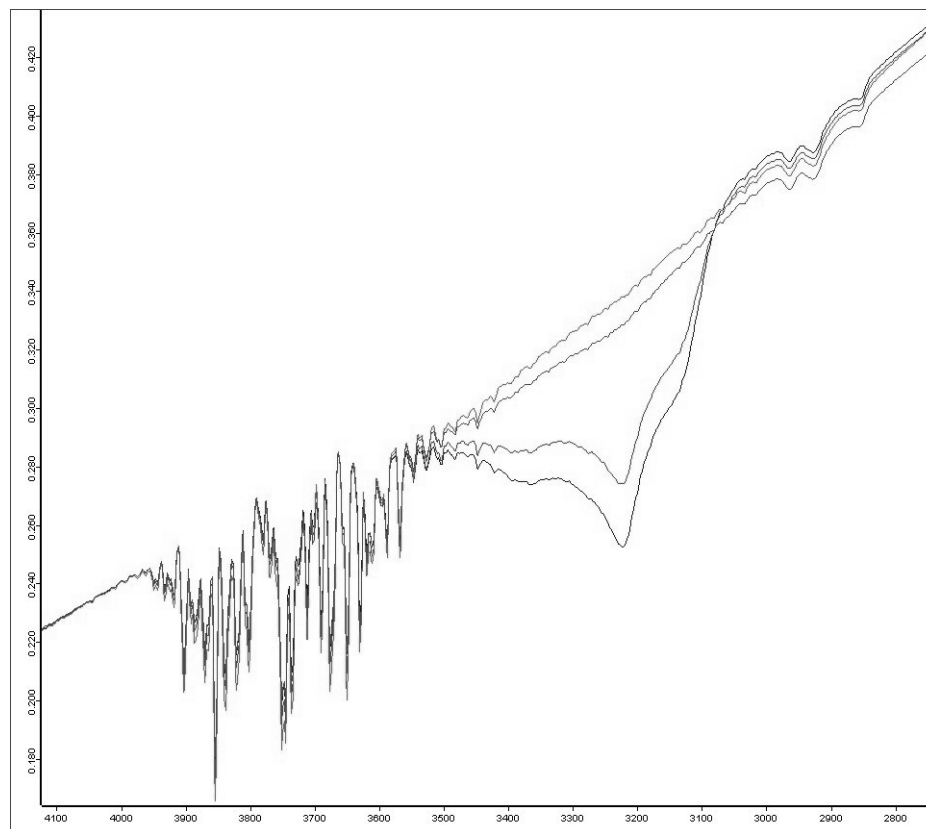


Figure 325: Spectra showing ice bands of different intensities

The ice band test is part of the energy test and compares the integral in the ice band region ($3485 - 3050\text{cm}^{-1}$) with the integral of the reference spectrum measured for the PQ test. The integral should not exceed a preset limit.

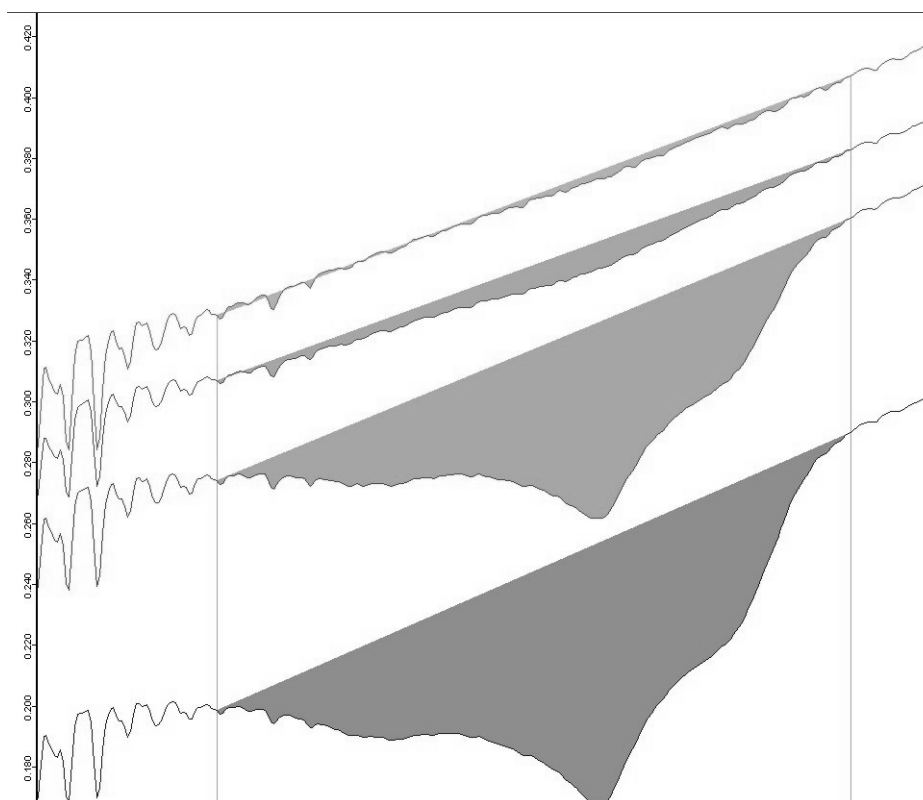


Figure 326: Integrals of ice bands (of different thickness)

X-Axis Frequency Calibration Test (Wavenumber accuracy):

The x-axis frequency calibration test ensures that the frequency calibration of the instrument is within the specified limits. If possible, water vapor is used to determine the wavenumber accuracy. Water vapor has the advantage of having an extremely narrow band(s) and therefore 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 327 and 328 show typical water vapor spectra in the MIR and NIR region.

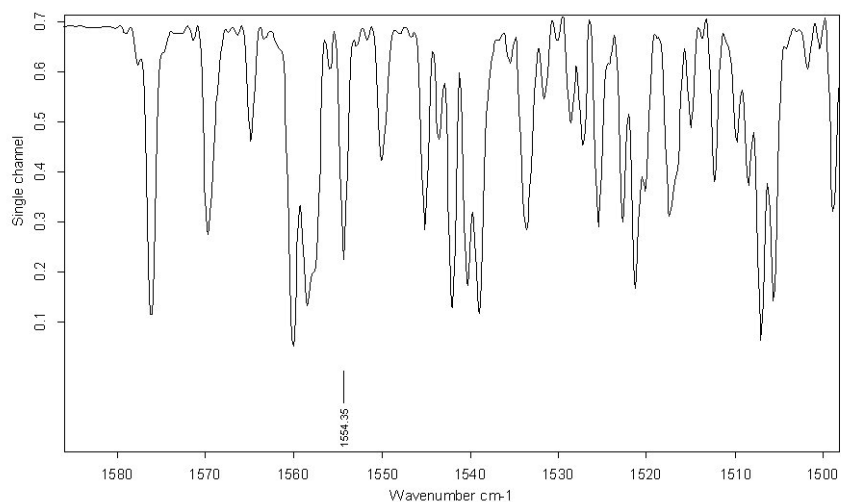


Figure 327: MIR water vapor spectrum

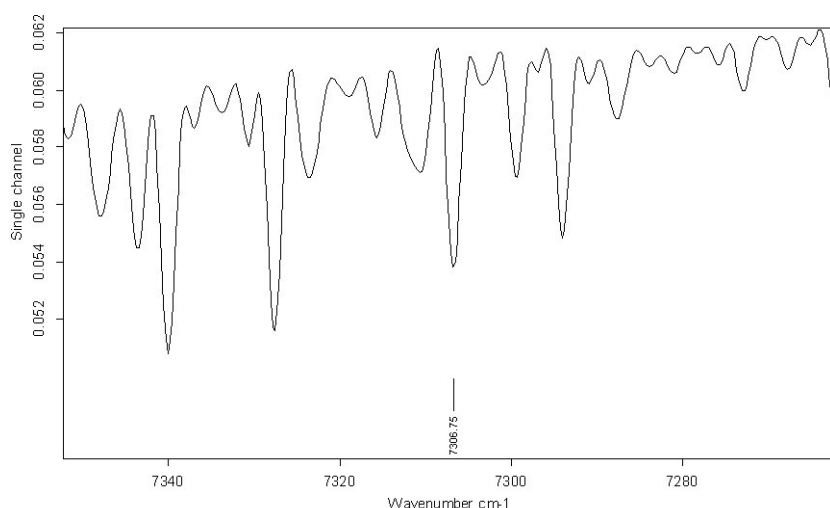


Figure 328: NIR water vapor spectrum

A second measurement verifies the frequency calibration. It is used either a polystyrene standard sample (MIR and NIR) or a glass filter with a mixture of rare earth oxides (BRM 2065, only NIR) which composition is identical to the NIST standard *SRM 2065*. The standard (either polystyrene or BRM 2065) is on the internal validation unit. Thus, no further actions are 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 the water vapor band 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 Test (Photometric Accuracy):

The y-axis reproducibility test is a long-term stability test which compares the total intensity values of glass filter spectra to those of the reference spectra.

A glass filter transmission spectrum is used to test the precision of the y-axis. The test spectra of glass filters are compared to the reference spectra by calculating the mean difference over a large spectral range (MIR: 4000 - 2000 cm^{-1} , NIR: 1000 - 45000 cm^{-1}). Figure 329 and 330 show the spectra of two different glass filters in NIR and MIR.

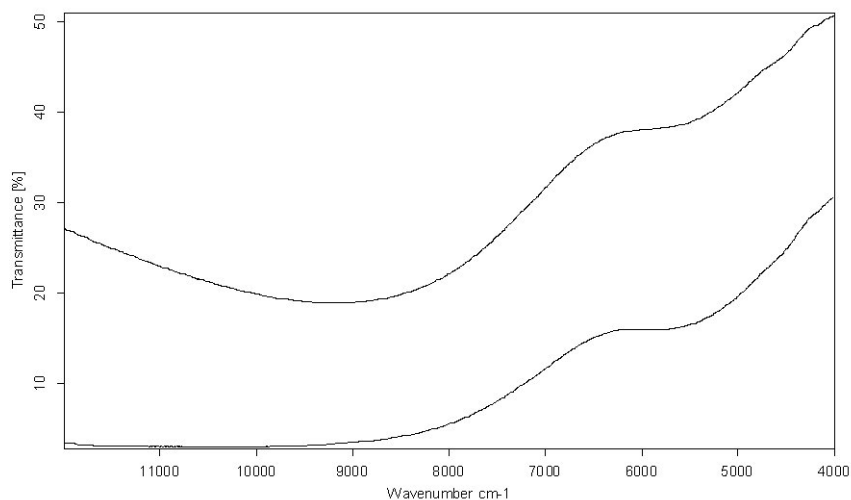


Figure 329: Glass filter NIR reference spectra

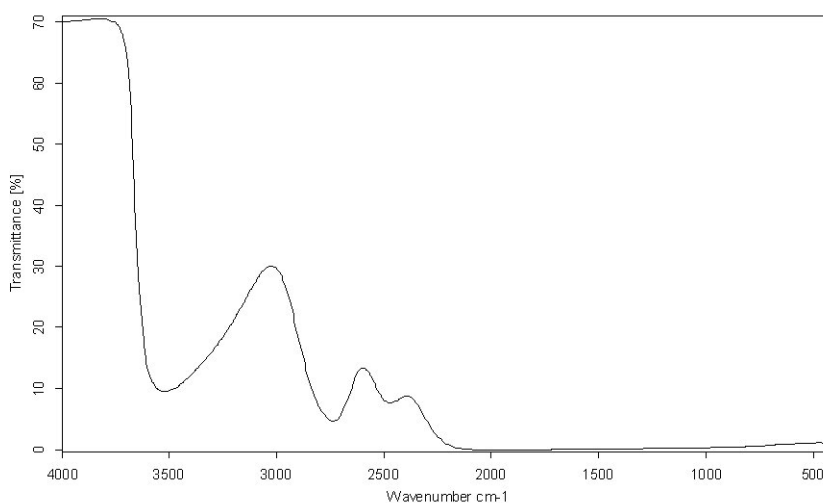


Figure 330: Glass filter MIR reference spectrum

13.2.3.3 OQ Tests

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 performed during final testing before an instrument is delivered to the customer. The OQ test should be performed after each major repair, exchange of optical components which may influence the instrument performance, and on a regular yearly basis, e.g. after maintenance.

If you activate the *Run OQ Test every* check box, the following drop-down list will be displayed:

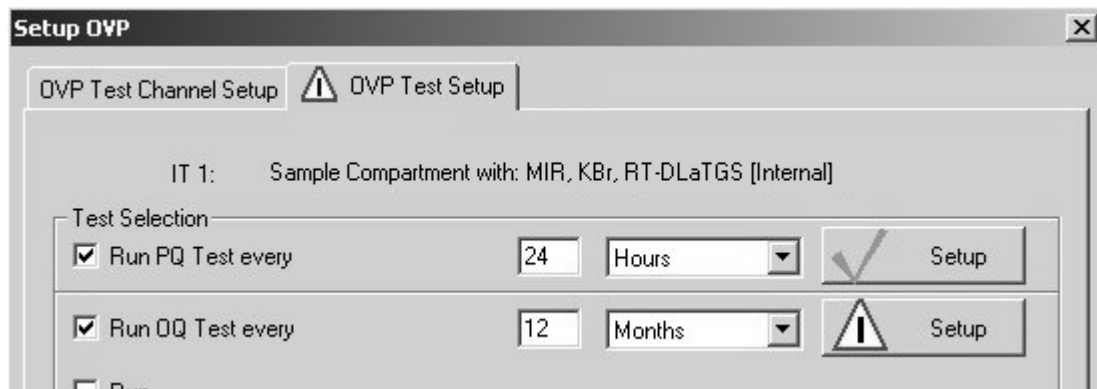


Figure 331: Configuring OQ test

Type the interval period into the entry field and select the units from the drop-down list. Available units are hours, days, or months. Click on the *Setup* button to open the following dialog:

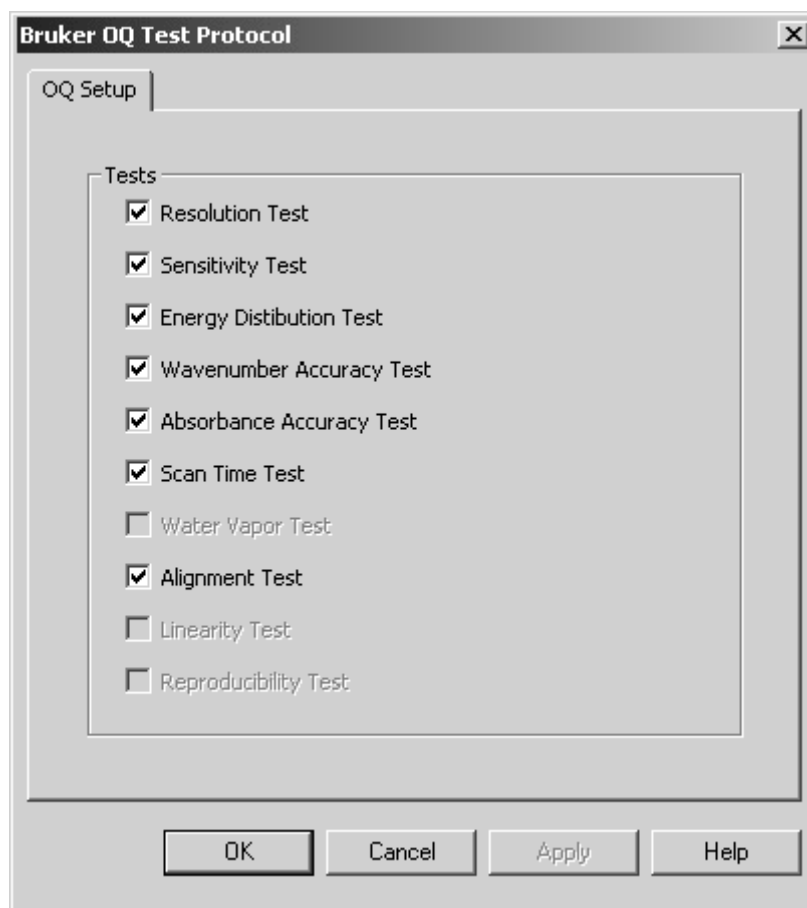


Figure 332: Bruker OQ Test Protocol - OQ Setup

The OQ test protocol consists of the following single tests (for further details on each test see also chapter 13.2.3.4):

- **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 energy distribution of an empty channel over the spectral range completely achievable.
- **Wavenumber Accuracy Test**
Verifies the absolute x-axis accuracy of the instrument.
- **Photometric Accuracy Test**
Verifies the photometric accuracy of the spectrometer.
- **Scan Time Test**
Verifies the mechanical properties of the interferometer and the control electronics functioning.

- **Water Vapor Test**
Verifies that the water vapor concentration does not exceed a specified value.
- **Alignment Test**
Verifies that the interferogram peak is within the specified range.
- **Linearity Test**
Verifies the detector linearity below the detector cutoff frequency.
- **Reproducibility Test**
In case of instruments with several measurement channels verifies the proper mode of functioning of all mechanical parts which change the instrument beam path (e.g. mirrors).

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.

Tests which are not available for the selected instrument type are disabled, all the other tests are activated. If you do not want to perform a specific test, deactivate the respective check box.

As soon as you have set up all tests click on the *OK* button. The current setup status is indicated by a green check mark on the *Setup* button of the *OVP Test Setup* tab.

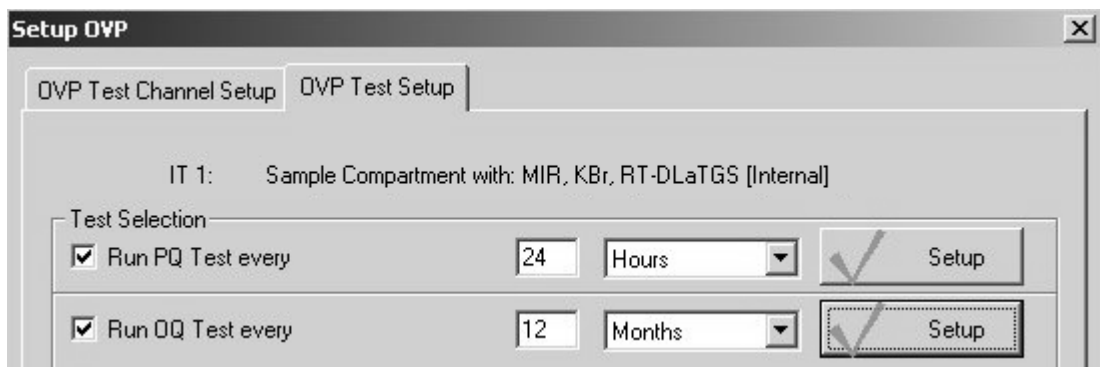


Figure 333: OQ test setup status

13.2.3.4 OQ Test Description

Resolution Test:

The resolution test verifies the achievable spectrometer resolution by measuring a single-channel (single-beam) spectrum of the water vapor available inside the spectrometer. The spectrum will be measured using the maximum spectrometer-specific resolution. This means for most spectrometer types: 1cm^{-1} for MIR and 2cm^{-1} for NIR, see figure 334. The spectrum is first logarithmized. Then, the full width at half maximum (FWHM) of a water band ($7306,74\text{cm}^{-1}$ for NIR and $1554,353\text{cm}^{-1}$ for MIR) is determined. The result is compared to the specified resolution of the spectrometer.

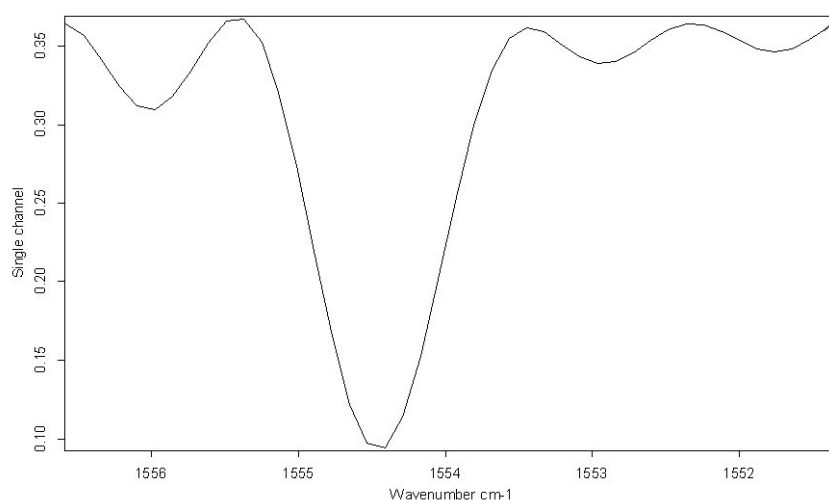


Figure 334: Water vapor band at 1553.353cm^{-1} (MIR)

Sensitivity Test:

The sensitivity test determines the sensitivity of the spectrometer by calculating the average S/N ratio of ten 100% spectra. A 100% spectrum is the ratio of two successively measured single-channel spectra with no sample in the sample compartment. The ratio of these two single-channel spectra is used to calculate 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, and the test result will be the mean value of all 10 results. The region to measure the S/N ratio is different for systems used in the MIR and NIR region, and is displayed in the corresponding report.

The spectrum shown in figure 335 has a peak-to-peak noise of 0.1% from 100% transmittance in the MIR region. To calculate the S/N ratio the reciprocal value is multiplied by 100 ($1 / 0.1 * 100$). Figure 336 shows a 100% spectrum in the NIR region.

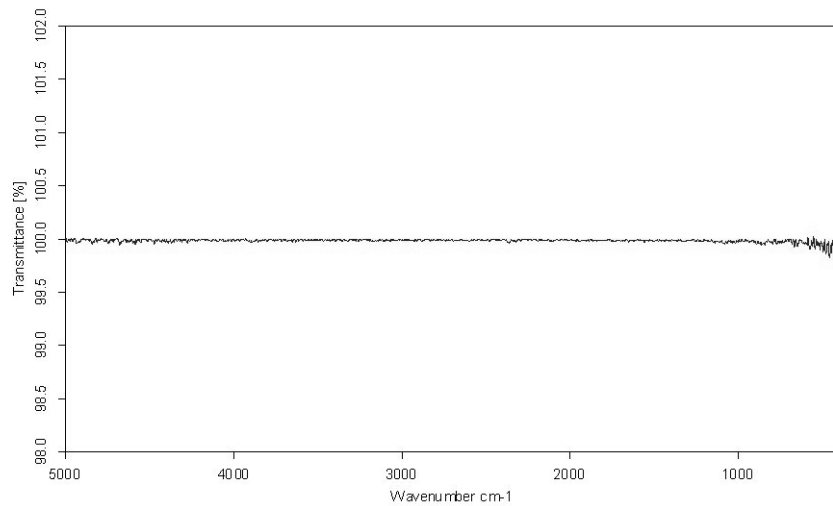


Figure 335: MIR 100% spectrum

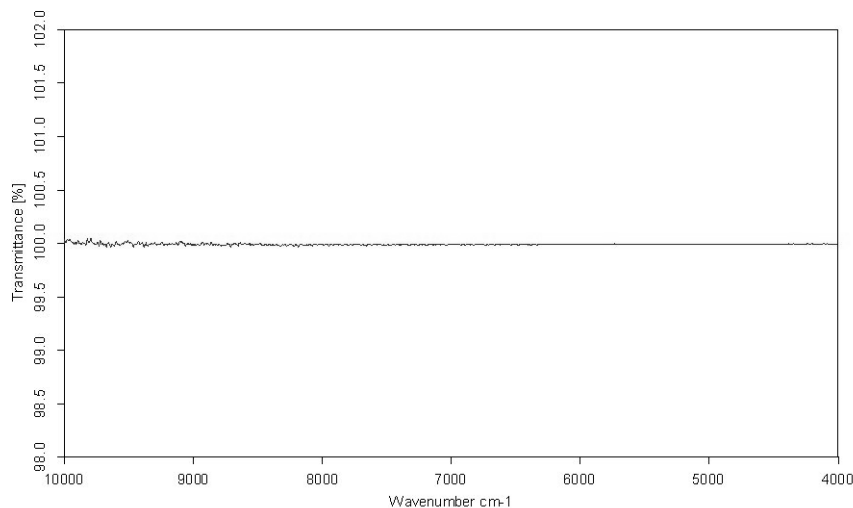


Figure 336: NIR 100% spectrum

Energy Distribution Test:

The energy distribution test verifies the achievable frequency range and the energy at the maximum position of the single-channel spectrum.

A single-channel spectrum is measured for this test. The absolute values of energy measured are measured at different wavenumber positions, see

figure 337. These values are divided by the value achieved, compared to acceptance values and indicated in per cent.

Optical components (e.g. detector, source and beam splitter) as well as the sampling accessory have an effect on the limits of the frequency range.

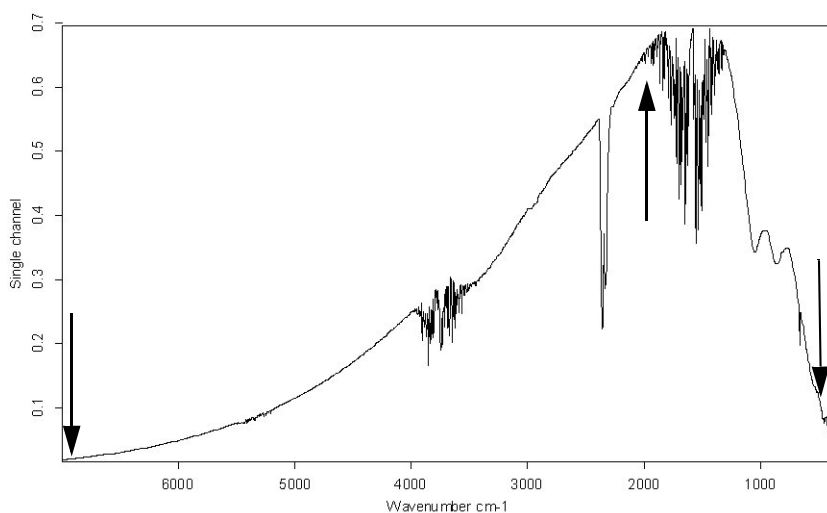


Figure 337: Single-channel spectrum

Wavenumber Accuracy Test (X-axis):

The wavenumber accuracy test verifies that the frequency calibration of the spectrometer is within the limits defined. To test the wavenumber accuracy water vapor is used. Water vapor has the advantage of having extremely narrow bands, and the position of these bands 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 7306.74cm^{-1} for calibration, and the MIR region at 1554.353cm^{-1} .

Figure 338 and 339 show a typical water vapor spectrum in the MIR and NIR region. Depending on the source the BRM 2065 is alternatively used in NIR for testing if the water vapor band specified is beyond the limits defined.

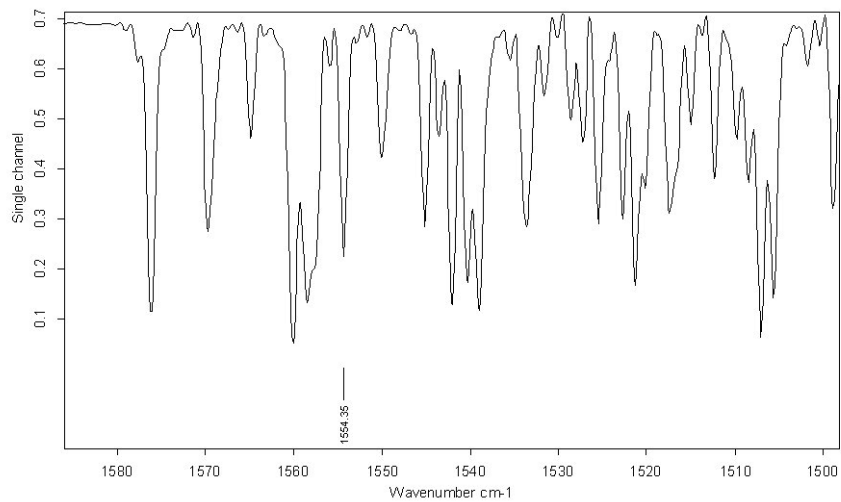


Figure 338: MIR water vapor spectrum

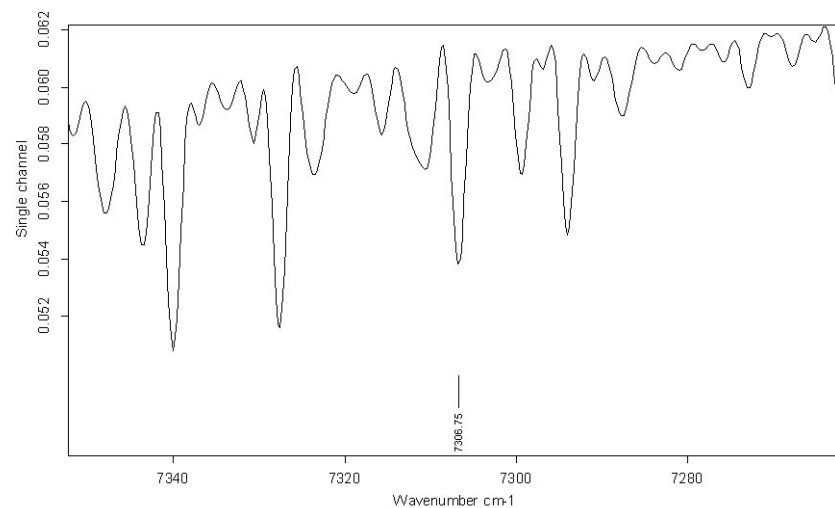


Figure 339: NIR water vapor spectrum

Photometric Accuracy Test (Y-axis):

The absorbance accuracy test verifies, amongst others, whether the y-axis of a measured spectrum is accurate.

The test uses a polystyrene transmission spectrum in MIR and a water spectrum in NIR which shows total absorption in several regions (see figure 340 and 341). At these positions the theoretical transmission of the spectrum should be 0. It is tested whether the deviation of the transmission value of 0 is within the limits specified in these regions.

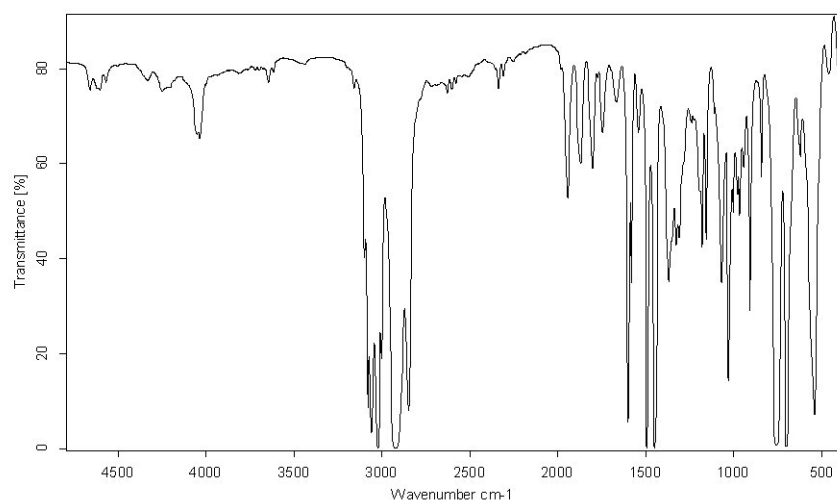


Figure 340: Polystyrene spectrum for MIR

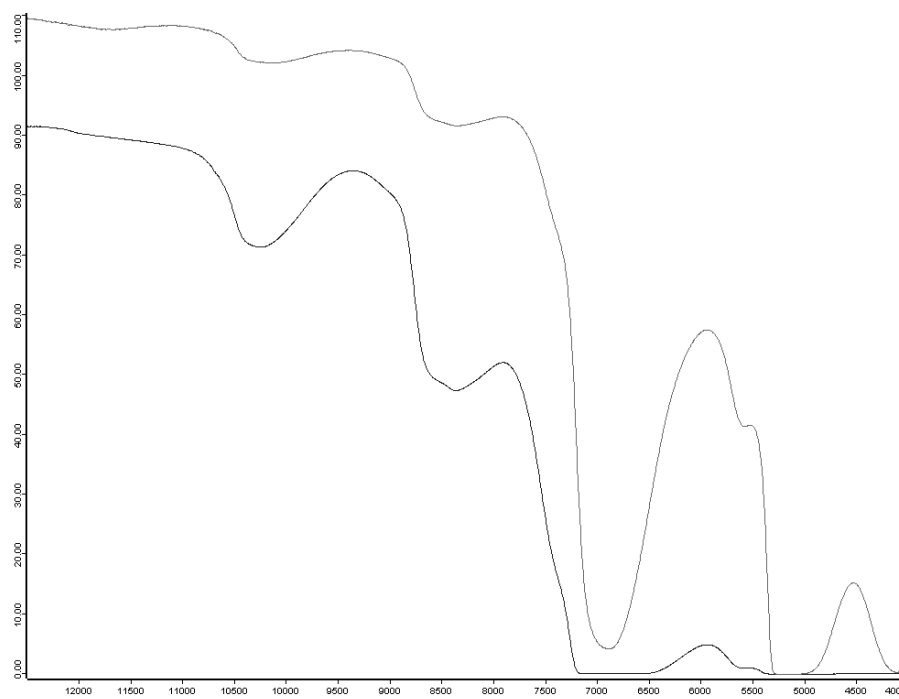


Figure 341: Water spectra for NIR with different layer thickness

Scan Time Test:

The scan time test is used to test the interferometer functioning. A single-channel spectrum is measured with a defined number of scans, at the highest scan 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 inside the instrument.

A single-channel spectrum is measured to determine the peak height of a water band within a small frequency region, i.e. $1660 - 1643\text{cm}^{-1}$ for MIR (figure 342) and $7315 - 7297\text{cm}^{-1}$ for NIR (figure 343).

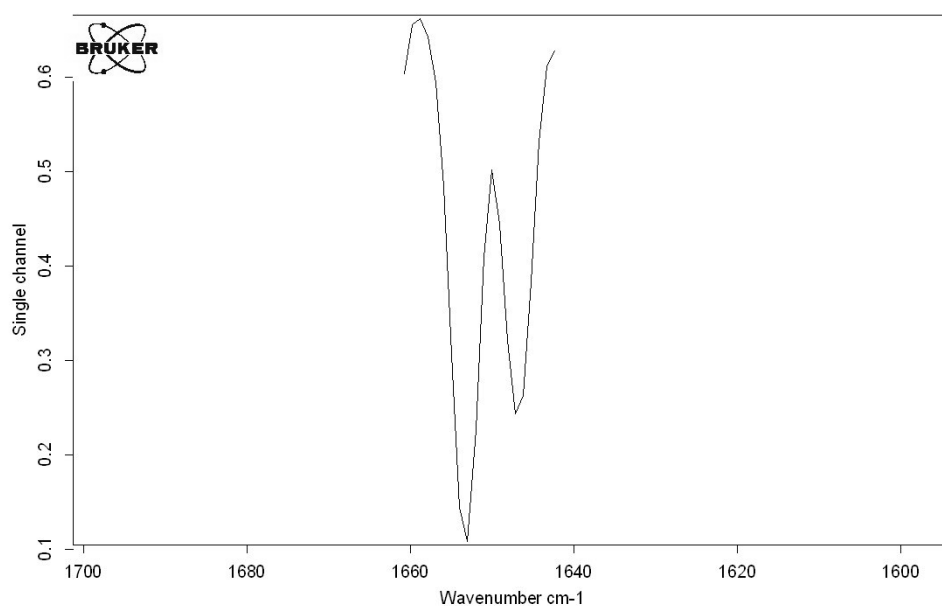


Figure 342: MIR water vapor band, $1660 - 1643\text{cm}^{-1}$

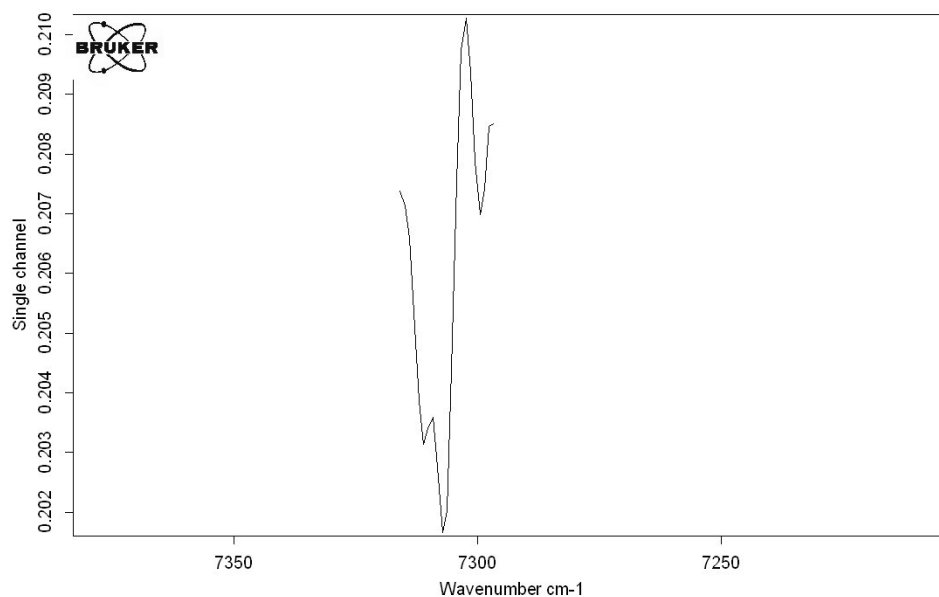


Figure 343: NIR water vapor band, 7315 - 7297cm⁻¹

The water vapor concentration is calculated from the measured data as follows:

$$\text{Water vapor concentration} = 100 - ((Y_{\text{Min}} * 100) / Y_{\text{Max}})$$

The value calculated is compared to the maximum value allowed.

Alignment Test:

The alignment test verifies that the absolute peak position of the interferogram is within the range specified.

A single-channel spectrum is measured and the absolute peak position is determined 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 up to 0cm⁻¹ (figure 344). The energy contribution in the region below the detector cutoff frequency is determined and compared to the energy value of the single-channel spectrum at the maximum.

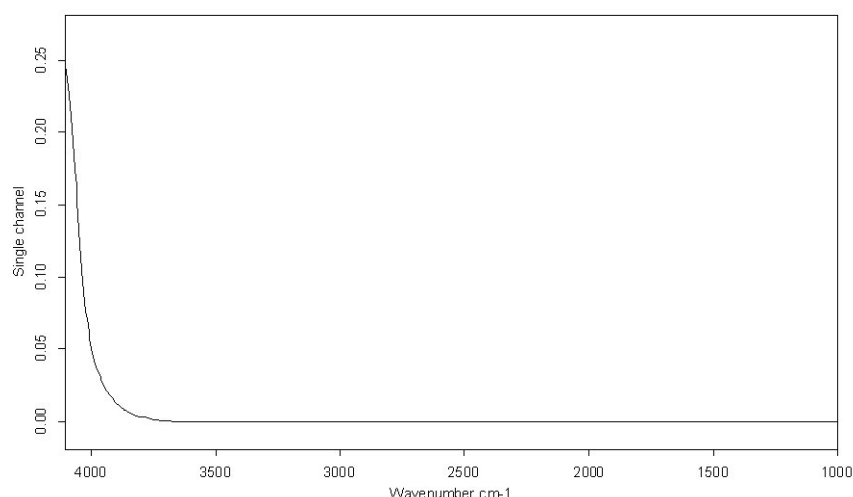


Figure 344: Single-channel spectrum around detector cutoff frequency

The following formula is used to calculate the linearity value:

$$\text{Linearity Value} = ((\text{Abs}(Y_{\text{MaxCutoff}} + Y_{\text{MinCutoff}}) / 2) / Y_{\text{MaxSpectrum}}) * 100$$

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 positioned correctly and in a reproducible way.

A single-channel 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 single-channel transmittance spectrum is recorded in the channel position. This procedure is repeated 10 times. The deviation of each of the ten single-channel spectra from the reference spectrum is computed. The greatest deviation must not exceed a maximum value.

13.2.3.5 Further Tests (optional)

Further tests are available as plug-ins:

- PhEur 2.2.40 (European Pharmacopoeia for NIR)
- PhEur 2.2.24 (European Pharmacopoeia for MIR)
- Raman
- USP 1119 (US Pharmacopoeia for NIR)

Note: For detailed information on these tests separate documentation is available.

To select the optional tests activate the *Run* check box on the *OVP Test Setup* tab.

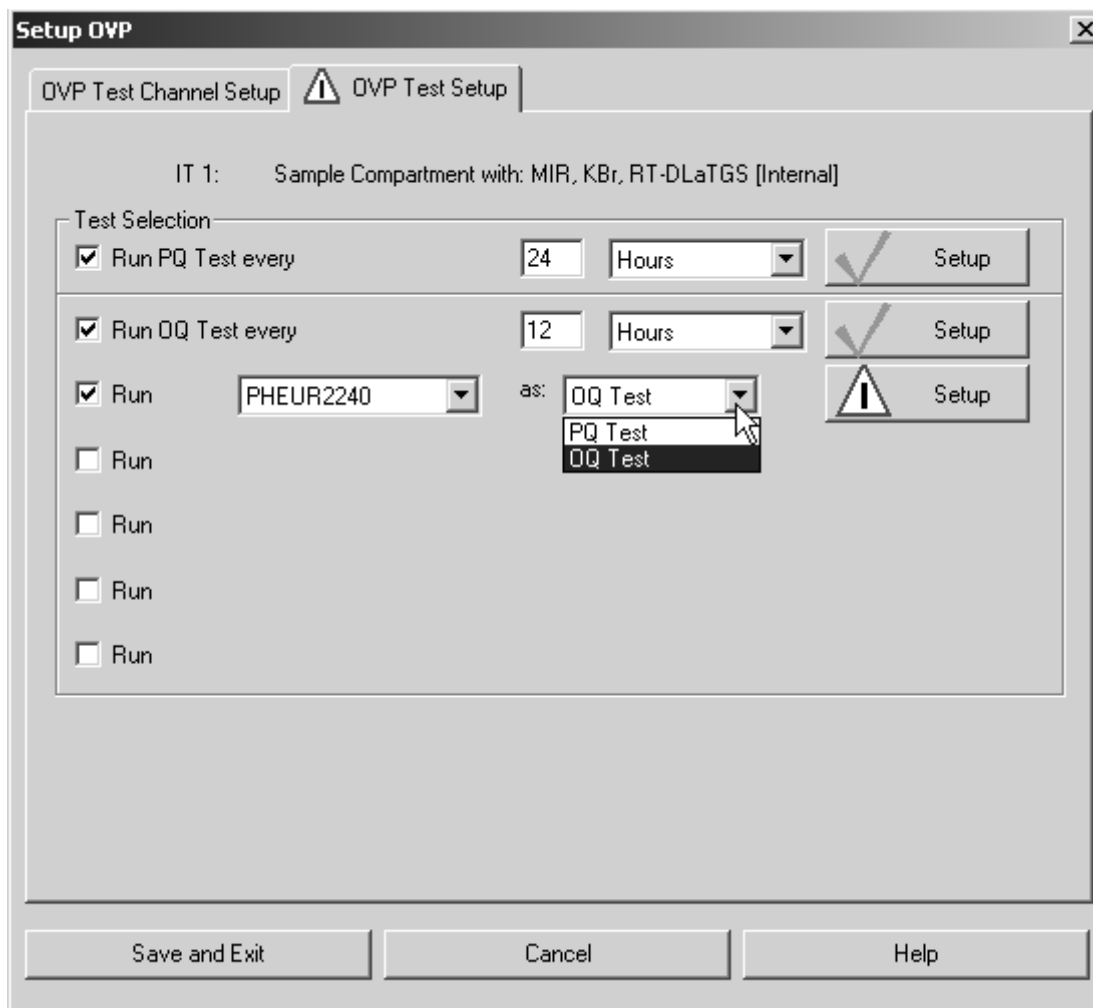


Figure 345: OVP - Further tests (optional)

Select the correct test from the first drop-down list, and the test interval (OQ in general) or the kind of test, i.e. PQ or OQ if they are different (e.g. in case of Raman), from the second drop-down list. Click on the *Setup* button. For a separate description of these optional tests refer to the corresponding OVP manual.

If you have selected a test which is not available for a certain kind of instrument configuration, a warning will be displayed when clicking on the *Setup* button. Note that you have to acquire a separate licence for most of these tests. Make sure that you have a correct registration, otherwise you will not be able to run these tests.

If you do not want to perform a specific test, deactivate the respective check box. The current setup status of the respective test is indicated by a green check mark on the *Setup* button of the *OVP Test Setup* tab. As soon as you have set up all tests click on the *Save and Exit* button.

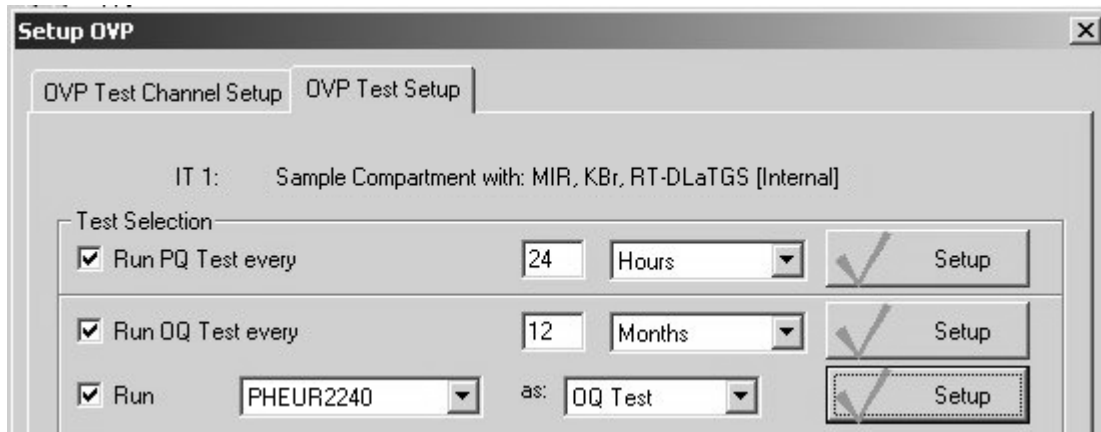


Figure 346: OVP - Raman test setup status

13.3 Run OVP Tests

13.3.1 Measuring by Instrument Status dialog

The *Instrument Status* dialog can be opened by clicking on the status light in the bottom right corner of the OPUS interface. The status light always indicates both the hardware status as well as the current test status of the active test channel. The test status is displayed in different colors and can be as follows:

- **Green:** all tests have passed and have not been expired
- **Yellow:** at least one of the tests has expired
- **Red:** the last test has failed or has not yet been performed

Click on the status light to display the *Instrument Status* dialog.



Figure 347: Instrument Status

The first row of icons represents the instrument hardware test status (see also chapter 7.7). The second and third row of icons are reserved for OVP tests. In figure 347 two test channels have been set up in OVP, therefore the corresponding icons are displayed for both channels in the second row.

The test status is indicated as follows:

- **PASSED** (green): test successfully performed and still valid
- **FAILED** (red): test failed or has not yet been performed
- **EXPIRED** (light-blue): test expired

The activated measurement channel is indicated by a blue text below the bitmap. In case of non-activated test channels the text is gray.



Figure 348: Current measurement channel

If you click on one of the measurement channels, the following dialog is displayed:

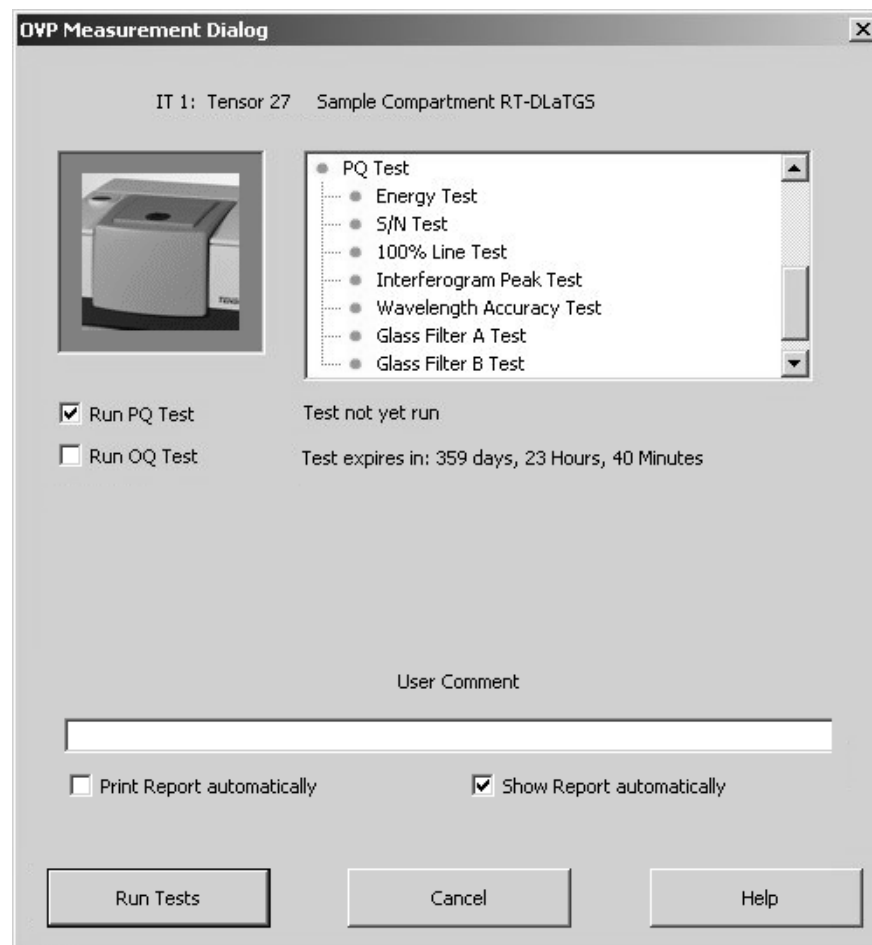


Figure 349: OVP Measurement Dialog

The browser-like window next to the bitmap contains all tests selected in the setup, and which will actually be performed. Activate the *Run...Test* check boxes for the respective test measurement. If you want to have a comment displayed in the report, write a comment into the *User Comment* entry field.

Activate the *Print Report automatically* check box if a test report has to be automatically printed after each test.

Clicking on the *Run Tests* button closes the dialog. The tests will run in the background, not visible for the operator.

If the tests have been finished, click again on the status light. The test status is displayed in the *Instrument Status* dialog. Click on the respective test channel to see the test status also on the *OVP Measurement Dialog*.

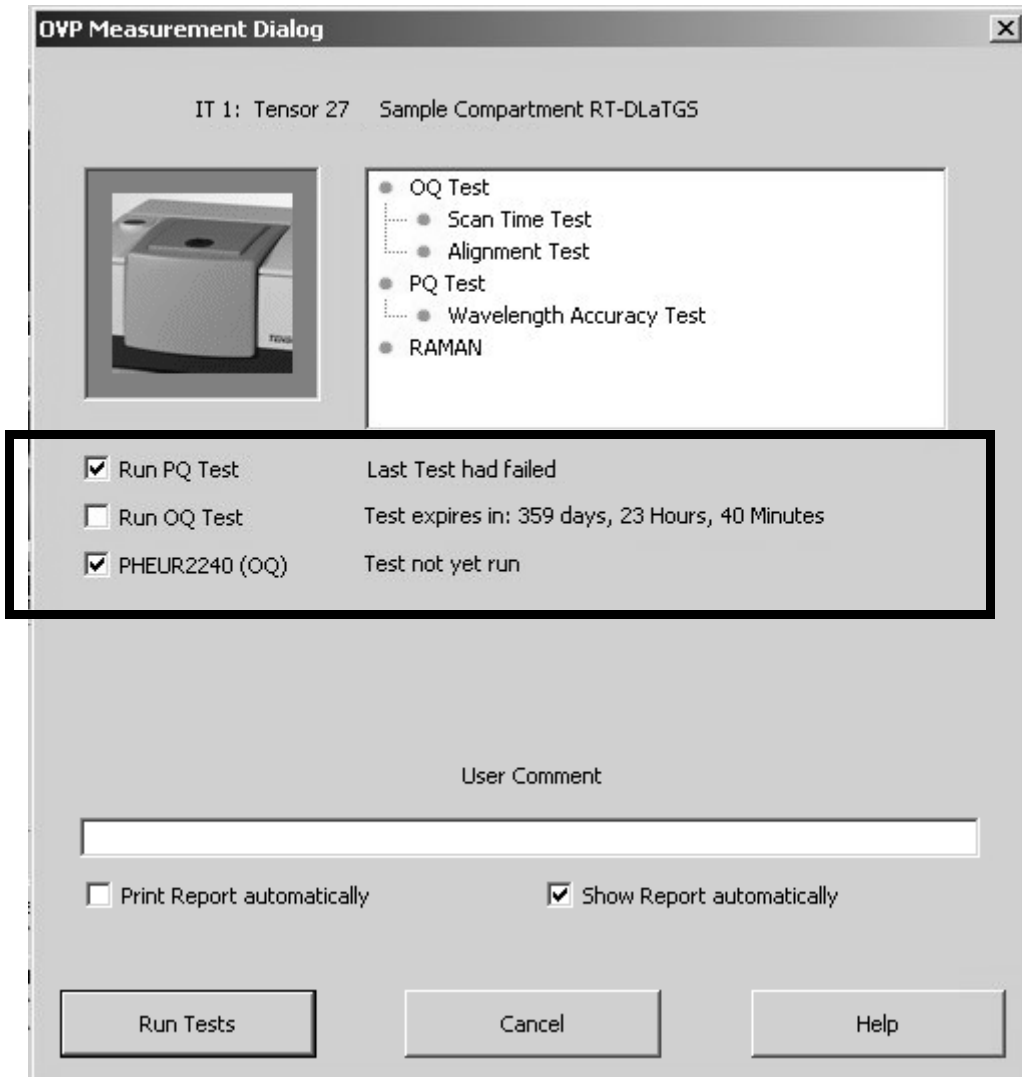


Figure 350: OVP - Test results

13.3.2 Measuring by means of the menu

To start running the tests click on the *Run OVP Tests* command in the *Validation* menu. The following dialog opens:

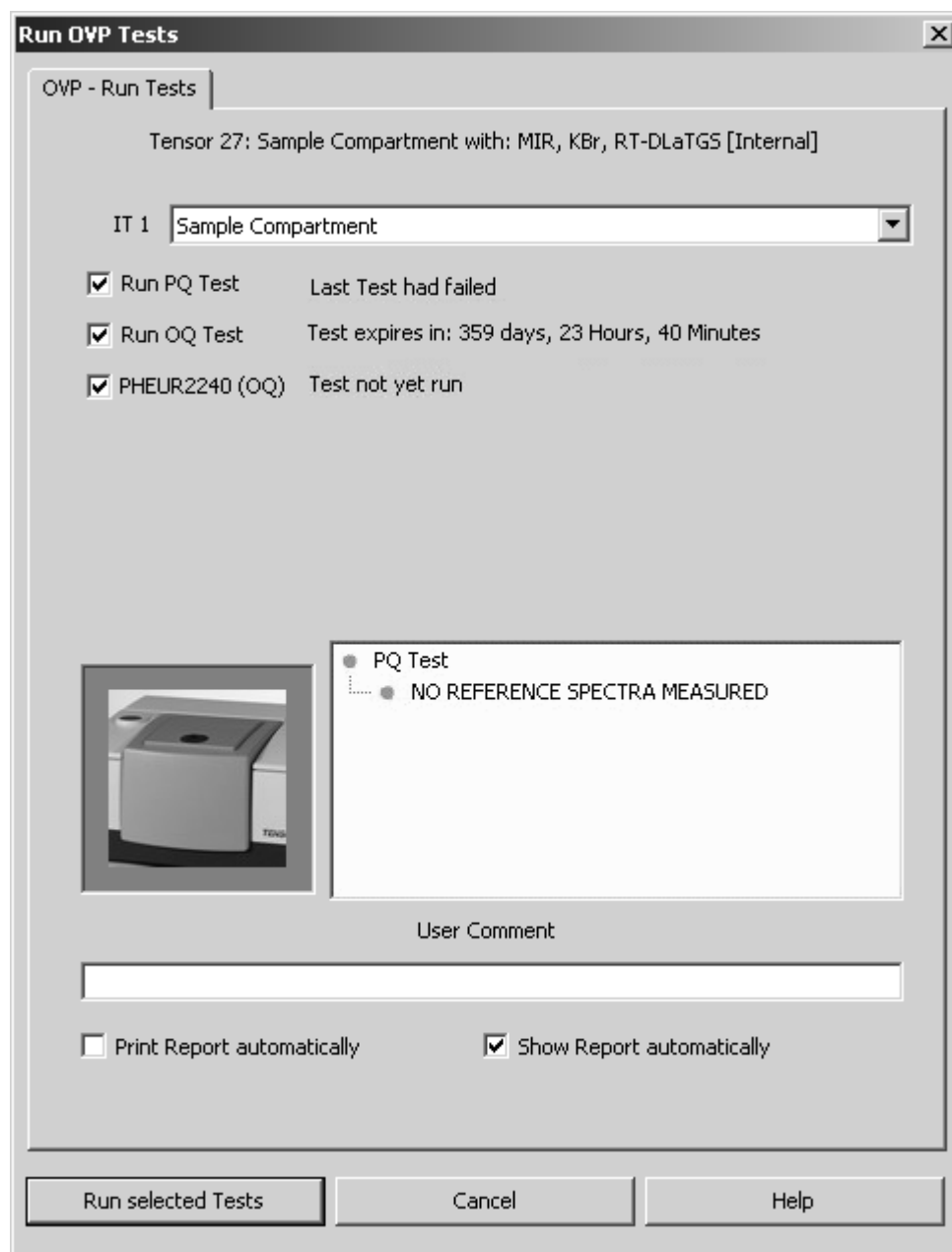


Figure 351: Run OVP Tests

The $IT\ n$ drop-down list allows to select the appropriate IT test channel. The lines below show the tests set up for the IT test channel selected, as well as the test status. Tests which have expired, or which have not yet been performed are automatically activated for measurement. Tests which have not yet expired are not activated, and their remaining time is indicated as a reminder.

If a test has not expired, but the interval has only e.g. 2 hours left you can activate the check box for that test and run the test earlier.

If a test has expired, but you are not prepared to perform that test (external standards required), you can deactivate the check box for the corresponding test.

Note: If you decide not to perform a test which has already been expired, you will not be able to use this channel in routine environment.

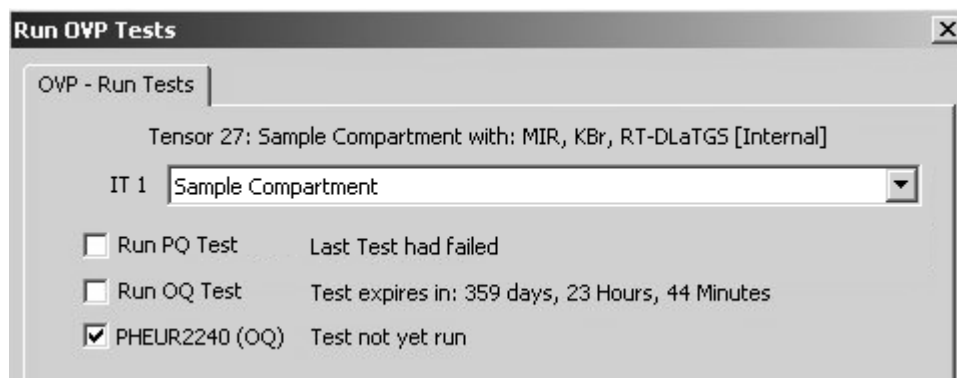


Figure 352: Different types of OVP test status

As soon as you have activated the check box for the respective test protocol you can see which test(s) will be performed by the browser-like display next to the bitmap. The example in figure 351 shows that reference spectra have not yet been measured. Before you can start this PQ test you first have to perform the reference measurement.

All measurement results are stored in a report (PDF file) and in the *UserData* database. To append a comment to the current test protocol entry write a comment into the *User Comment* entry field.

To have the reports displayed make sure that the Adobe Acrobat Reader is installed on your computer. The Adobe Acrobat Reader is available on the OPUS installation CD.

Click on the *Run selected Tests* button to start the respective tests. If you do not want to perform any test, click on the *Cancel* button.

13.4 Test Spectra

The spectra produced when running the tests are stored in a directory structure which will be automatically generated. In the *\Validation\Data* directory a sub-directory is created for the current date, supporting the following format: *YYYYMMDD*¹ (e.g. 20060212). A further sub-directory for the time is created in the directory for the current date, supporting the following format: *HHMMSS*² (e.g. 113423).

The spectrum file name always starts with either PQ or OQ and a test name (e.g. *PQ_MPA_Sample_Compartment_Energy.0*). The date and time is also used for

1.Y= year, M= month, D= day

2.H= hour, M= minute, S= second

the report name to allow a clear correlation between spectra and reports. The spectra contain the test result together with other important data in the INFO data block.

13.5 Measurement with test channel-specific laser wavenumber

Generally, you have to measure the laser wavenumber for each measurement channel or setup separately. This mainly affects multi-channel spectrometers or measurements which optionally use special accessories (e.g. ATR unit). The laser wavenumber may slightly change due to the different optical paths. A change of the laser wavenumber directly influences the frequency calibration of the spectrometer.

Select the *Advanced Measurement* command from the *Measure* menu and click on the *Optic* tab.

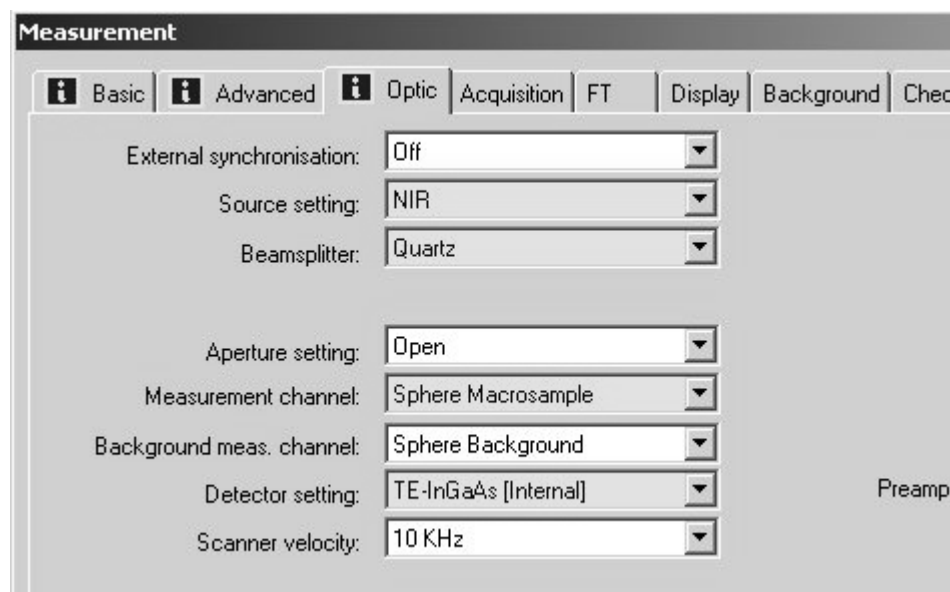



Figure 353: Measurement - Yellow drop-down lists

In case of spectrometers supported by OVP it is ensured that the correct laser wavenumber is automatically used for each measurement. This requires, however, that the measuring configuration (combination of source, beamsplitter, measurement channel and detector) has first been defined in OVP.

OVP automatically checks during each measurement whether the respective measuring configuration has already been defined in OVP. If not, the  symbol will be displayed on the *Optics* tab, and the drop-down lists for the source, beamsplitter, measurement channel and detector settings will be yellow.

If you position the cursor above a yellow drop down list, a tool tip is displayed containing the following text: *OVP Configuration not found, measurement will use wrong LWN. Add configuration in OVP Setup.*

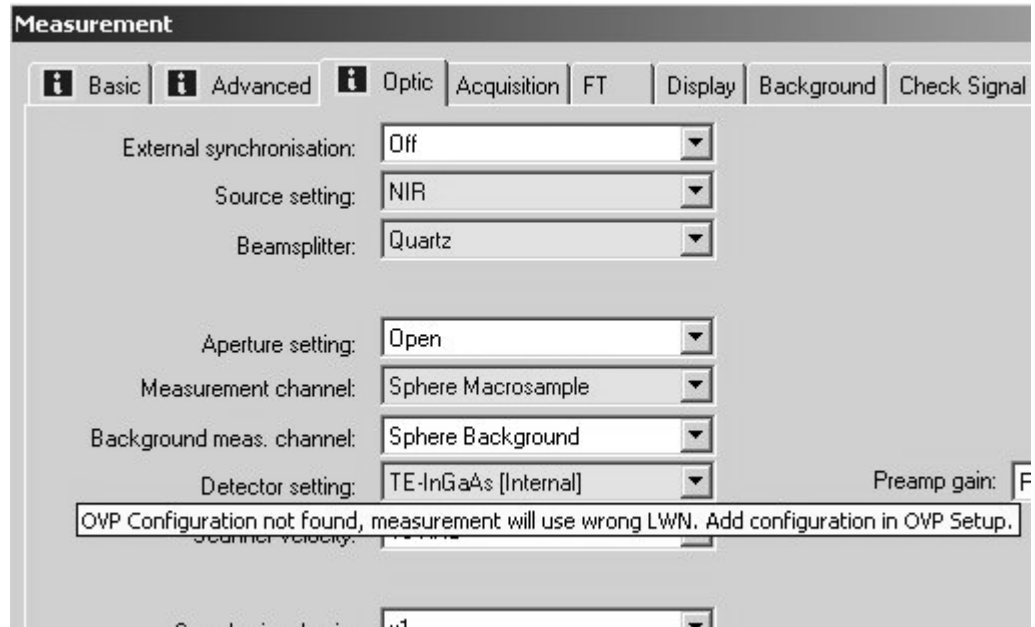


Figure 354: Measurement - Tool tip displayed

The tool tip indicates what kind of problem has occurred and how it can be solved. If you use OPUS in validated mode, make sure that the measurement configurations are set up in OVP. Otherwise, an error message pops up.

When working in validation mode make sure that the measuring configuration has actually been setup before. Otherwise, you will not be able to perform any measurement at all and an error message pops up:

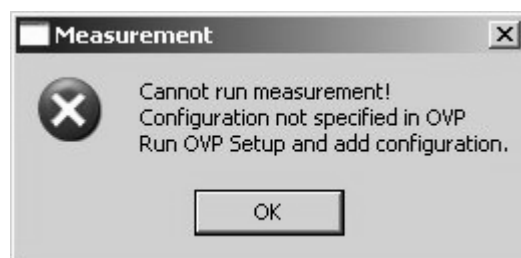


Figure 355: Error message when measuring in validation mode

13.6 Printing Reports

The results of test measurements are stored in a report (PDF format). The test report contains a summarized test result page and subsequent pages for each test with all the test spectra and measuring parameters displayed. Reports are stored in the separate *VALIDATIONREPORTS* directory and can automatically be printed. To have the report displayed and printed you require the Adobe Acrobat Reader which is available on the OPUS installation CD.

Bruker PQ Test Protocol

Company:	Bruker Optik GmbH		
Operator:	Default		
Instrument Type:	Tensor 27 Sample Compartment RT-DLaTGS		
Optics Configuration:	Sample Compartment with: MIR, KBr, RT-DLaTGS [Internal]		
Accessory:	None		
Instrument Serial Number:	MID0028		
Instrument Firmware Version:	1.440 Jul 14 2005		
OPUS/DB Version:	20060215/DATABASE VERSION		
Overall Test Result:	PASS		
Test expires:	2006/02/27 15:25:09		
Test Date/Time:	2006/02/27 15:25:09		
Test Spectra Path:	C:\Programme\OPUS6_0\validation\Data\20060227\152509		
Comment::			
Signal to Noise Test			
Signal to Noise Limit:	3000	Measured S/N:	8043
100% Line Deviation Test			
Maximum 100% Line Deviat	0.5	Measured 100% Line Deviat	2.979
Interferogram Peak Amplitude Test			

Figure 356: OVP - PQ test protocol

As the example in figure 357 shows, the overall test result is displayed by a green check mark, i.e. the OQ test has passed.

Bruker OQ Test Protocol			
Company:	Bruker Optik GmbH		
Operator:	Default		
Instrument Type:	Tensor 27 Sample Compartment RT-DLaTGS		
Optics Configuration:	Sample Compartment with: MIR, KBr, RT-DLaTGS [Internal]		
Accessory:	None		
Instrument Serial Number:	MID0028		
Instrument Firmware Version:	1.440 Jul 14 2005		
OPUS/DB Version:	20060215/DATABASE VERSION		
Overall Test Result:	PASS		
Test expires:	2006/02/29 13:46:11		
Test Date/Time:	2006/02/28 13:46:11		
Test Spectra Path:	C:\Programme\OPUS6_0\Validation\Data\20060228\134611		
Comment:			
Resolution Test ✓			
Water Vapor Band:	1554.35	Measured Resolution:	0.66
Maximum Resolution:	1.00		
Overall Test Result = PASSED ✓			

Date and Signature			

Date and Signature			

Figure 357: OVP - OQ test protocol

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.

The *Open Planner* command from the *Setup* menu allows to automatically run the OVP PQ test. For detailed information on the *Open Planner* command refer to chapter 14.10.

You can also define single OVP tests as recurring items at a daily, weekly or monthly interval. Click on the *Open Planner* command from the *Setup* menu. To create a calendar item right click on the respective day and select the *New Appointment* command from the pop-up menu.

The screenshot shows a dialog box titled "Edit Appointment". At the top, there are three buttons: "Save and Close", "Recurrence...", and "Delete". Below these are several input fields: "Subject" (a drop-down menu), "Location" (a text field), and "Label" (a drop-down menu with "None" selected). Below these are time fields: "Start time" (13. Mrz. 2006, 09:00) and "End time" (13. Mrz. 2006, 10:00), with an "All day event" checkbox. At the bottom, there is a "Show time as" field (set to "Busy") and three checkboxes: "Private", "Meeting", and "Phone call". A large empty text area is at the bottom of the dialog.

Figure 358: Edit OVP appointment

Select the respective OVP test configuration from the *Subject* drop-down list. Make sure that the particular test configuration has been defined in the OVP setup, before. Determine the time interval for the test configuration. For detailed information on this subject refer to chapter 14.10.2.

To perform single test on a daily basis click on the *Recurrence* button.

Figure 359: Appointment Recurrence

Define the start time of the test, either manually or by means of the arrow keys. The recurrence pattern helps to exactly set up at what intervals the test has to take place. Activate the respective option button.

The range of recurrence refers to the duration of a complete test recurrence. Define the start and end of the test recurrence and confirm your settings by clicking on the *OK* button.

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, e.g. 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 you can also use the OVP Accessory Manager.

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 user 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 Bruker database update will not have any impact on the contents of the user accessory data. 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
- 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 started from the Windows explorer.

Note: Do not move the accessory manager to a different sub-directory as the program automatically expects the user databases to be located in the *DATABASES* folder of the *VALIDATION* sub-directory.

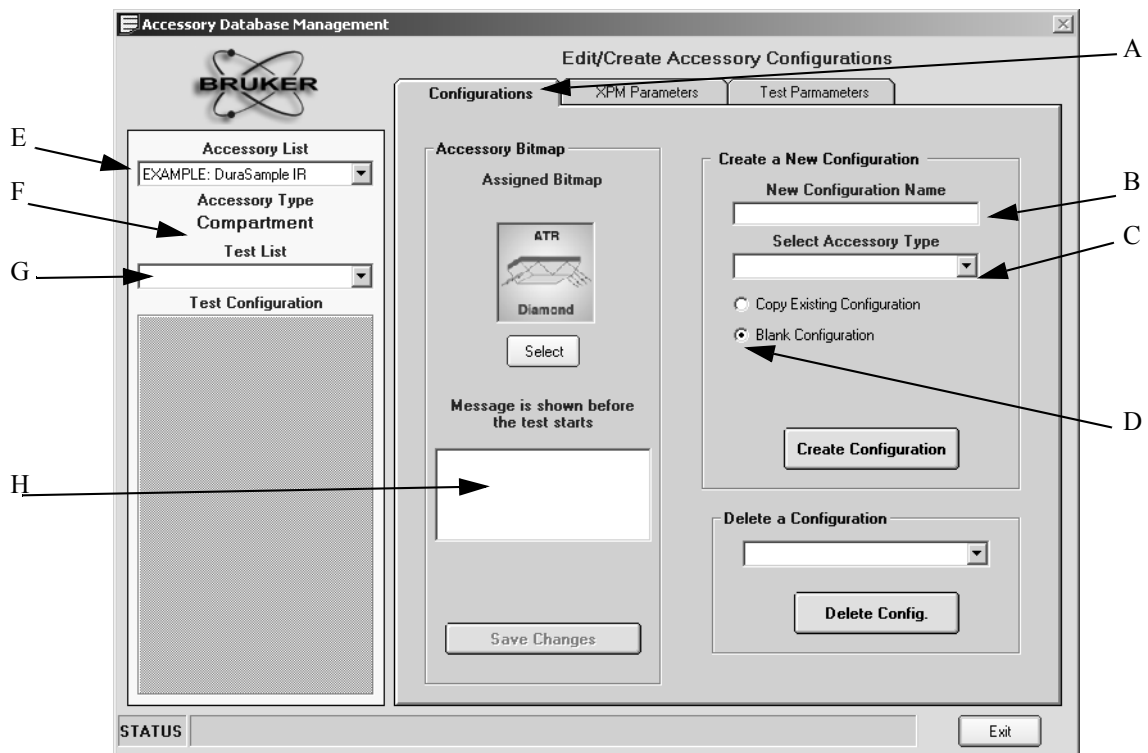


Figure 360: OVP Accessory Manager - Accessory Database Management dialog

After starting the accessory manager make sure that the *Configurations* tab (A) is selected.

The accessory database contains two example configurations which you can use as basis for the new accessory used. In this case copy one of the configurations (see chapter 13.8.3) and adapt the parameters, accordingly.

The following step-by-step instruction describes how to add a new accessory configuration to the database.

- 1) Enter the accessory name into the *New Configuration Name* entry field (B).
- 2) Select the type of accessory from the *Select Accessory Type* drop-down list (C).

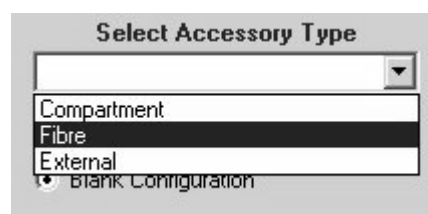


Figure 361: OVP Accessory Manager - Accessory type

It is distinguished between different types of accessories which can either be mounted into the sample compartment, connected to a fiber port or mounted at an external port of the instrument.

- 3) Make sure that the *Blank Configuration* option button (D) is selected and click on the *Create Configuration* button. The new accessory 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).

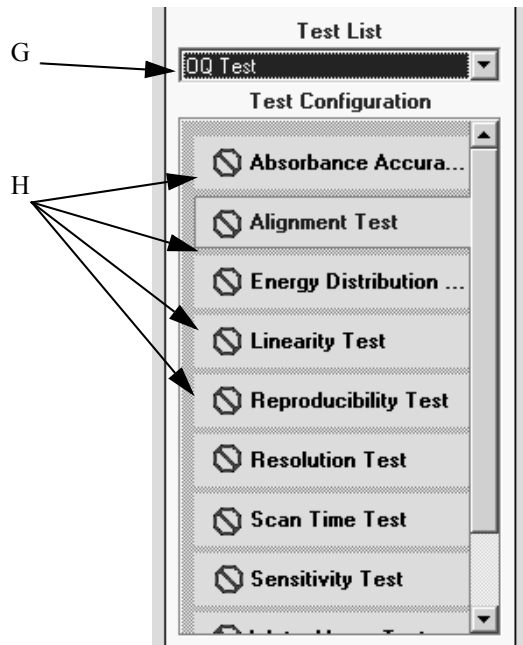


Figure 362: OVP Accessory Manager - Test configuration

- 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. **Make sure that you only select tests which are also available for the basic configuration.**

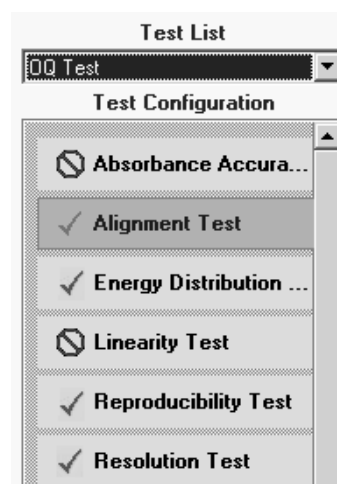


Figure 363: OVP Accessory Manager - Tests activated

- 6) The *Accessory Bitmap* group field allows to select one of the existing bitmaps for the accessory used. The bitmaps assigned will later be shown when selecting the accessory. Click on the *Select* button.

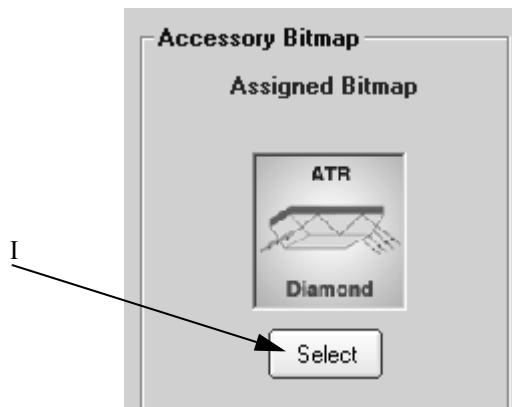


Figure 364: OVP Accessory Manager - Assigned bitmap

- 7) If you want to add a user-specific bitmap for the particular accessory, create a bitmap with the size of 90 x 90. Copy the bitmap, using the *ITnn.bmp* file name (nn = consecutive number) into the *\Validation\Bitmap* directory. After this you can select the bitmap by means of the *Select* button.

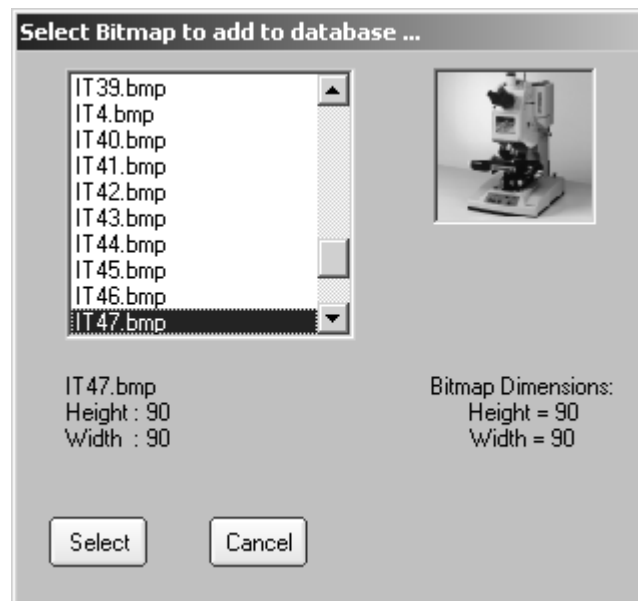


Figure 365: OVP - Add bitmap to database

- 8) In the message entry field (H in figure 360) you can enter an accessory-specific text which will be displayed at the beginning of the tests. This kind of text should reflect the steps required for preparing a test measurement.
- 9) Select the *XPM Parameters* tab to change the measurement parameters for the particular accessory, if required.

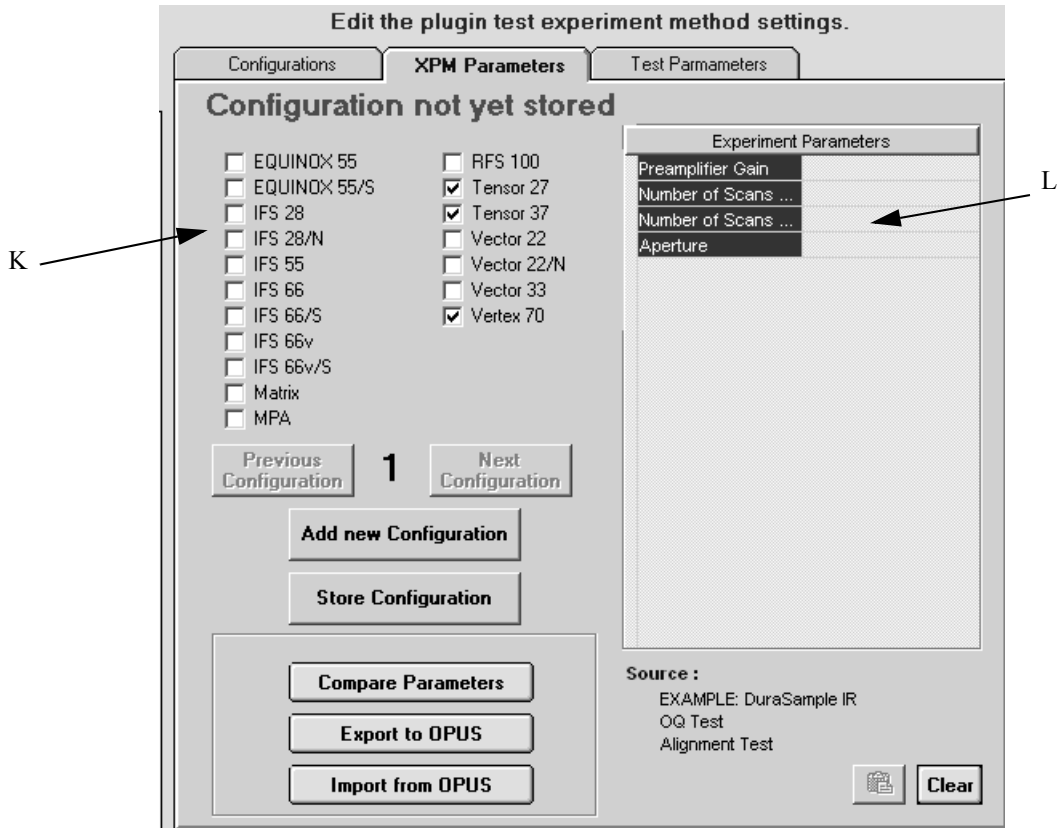


Figure 366: OVP Accessory Manager - XPM Parameters tab

- 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.

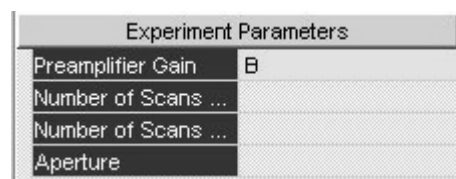


Figure 367: OVP Accessory Manager - Experiment parameters selected

- 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 in figure 368) 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 368: OVP Accessory Manager - Measurement parameters options

12) Click on the *Store Configuration* button (P).

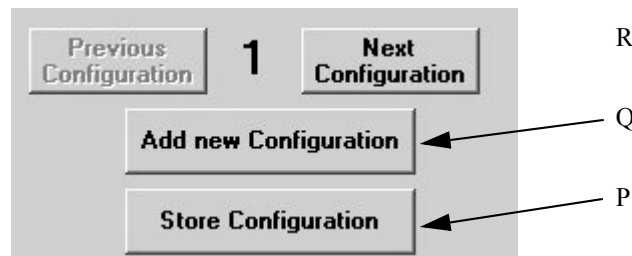


Figure 369: OVP Accessory Manager - Parameter configuration buttons

- 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 Params* button (S in figure 370).

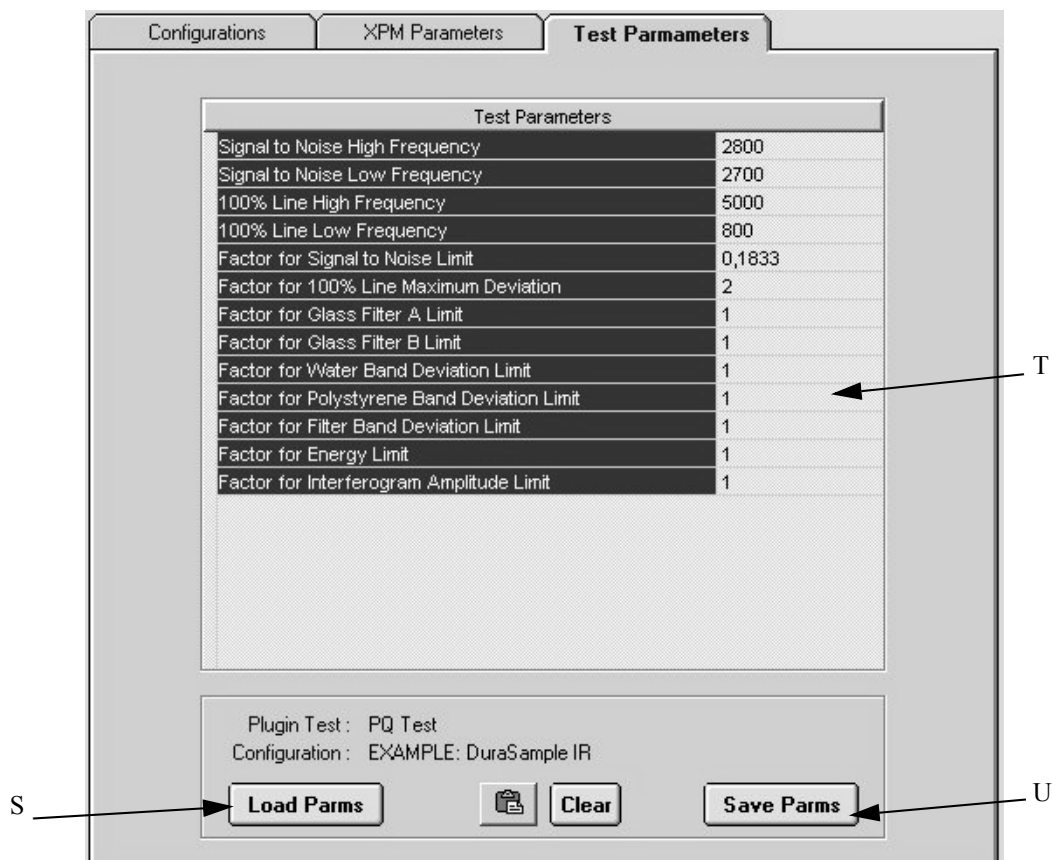


Figure 370: OVP Accessory Manager - Test Parameters tab

16) Enter appropriate frequency limits and factors into the parameter section (T). Offsets are entered in wavenumber units and used instead of the value specified for the basic setup. If an instrument increases, e.g., the lower frequency limit for the signal-to-noise test by 4500cm^{-1} , enter *4500* into the appropriate field.

By means of factors you can define test limits which have been changed. 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. Frequency limits which do not have to be changed have to be set to 0, while parameter limit factors which do not change need to be set to 1.

Test Parameters	
Offset for Signal to Noise High Frequency	0
Offset for Signal to Noise Low Frequency	100
Factor for Signal to Noise Limit	0.5
Offset for 100% Line High Frequency	0

Figure 371: OVP Accessory Manager - Test parameter settings

- 17) Store the settings by clicking on the *Save Params* 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 362). 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. **Make sure that you only select tests which are also available for the basic configuration.**

13.8.3 Copying Accessory Configurations

You can also set up another configuration by copying the existing example configurations.

Figure 372: 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 new accessories listed in the *Accessory* drop-down list (see figure 311 on page 325).

13.9 OVP Program Modules and Databases

The main directories and databases required for OVP, and their meaning are outlined in the following:

\\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 Results
VALIDATION\\DATA	Basic Directory for Measurement Data
\\VALIDATION\\DATA	Test Spectra Directory:
\\<YYMMDD>\\<HHMMSS>	Sub-Directory named with test date and time
VALIDATION\\REPORTS	Reports Sub-Directory
\\VALIDATION\\TEMP	Directory for Temporary Data
VALIDATION\\BITMAPS	Directory for instrument bitmaps
<i>ITnn.bmp</i>	Bitmap files (nn = consecutive number)
Definition of spectra and reports:	
<i>PQ_configuration_Testtype.0</i>	PQ Test spectra named by instrument configuration and test (e.g. PQ_MPA_SAMPLE_
COMPARTMENT_	FREQTEST.0)
<i>OQ_configuration_Testtype.0</i>	OQ Test spectra named by instrument configuration and test (e.g. OQ_MPA_SPHERE_LINEARITY.0)
<i>PQ_configuration_date_time.pdf</i>	PQ Test Report (e.g. PQ_MPA_FIBRE_040217_124909.pdf)
<i>OQ_configuration_date_time.pdf</i>	OQ Test Report (e.g. OQ_MPA_FIBRE_040216_103545.pdf)

14 Setup

The *Setup* menu includes all functions to be required to configure menus and toolbars as well as the workspace.

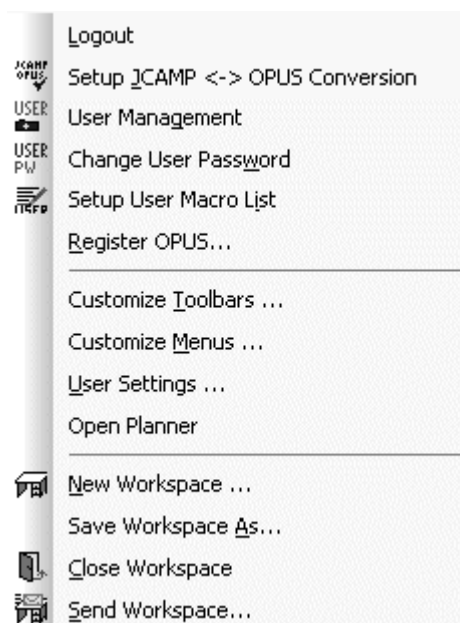


Figure 373: Setup menu

14.1 Logout

To log in a new user or log out and terminate OPUS click on the *Logout* command.

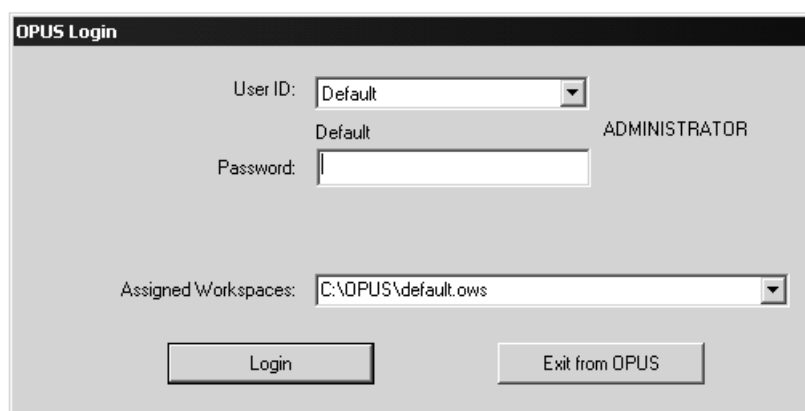


Figure 374: OPUS Login dialog

To log in select the corresponding *User ID* from the drop-down list. The user to be the last to log in will be displayed by default. Enter the correct user

password. The password will be displayed by a number of “*”. Always the user type (*Operator* or *Administrator*) for the currently selected user is displayed.

Select one of the workspaces using the drop-down list. The workspaces included in the drop-down list substantially depend on the user selected. In case of *Operator* only the assigned workspaces are shown, whereas in case of *Administrator* all workspaces stored in the OPUS directory are shown.

Click on the *Login* button to log in the new user. Click on the *Exit from OPUS* button to close the login procedure and terminate 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 both to the *Convert3dJCAMP* command in the *Edit* menu and to the *Load File* command in the *File* menu.

To avoid the loss of information when converting JCAMP files define how the JCAMP labels correlate with OPUS parameters and information lines. This has to be done by using a conversion table. A conversion table is a text file with the extension **.PCT*, and can be generated by any kind of text editor. Additionally, you have to specify the file containing the info text definition.

The general syntax of the file with the **.PCT* extension 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 is a three-character OPUS parameter.
LABEL is the name of the JCAMP label.

It is mandatory to determine the consecutively numbered info line. Each line needs 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.

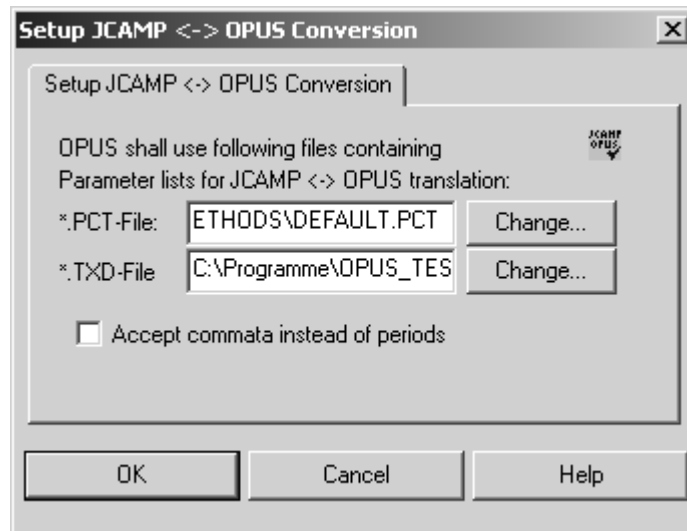


Figure 375: Setup JCAMP - OPUS Conversion

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 more than 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 Workspaces	Unlimited access to all user workspaces		

We recommend not to delete these user records or to change the password to be able to have access to 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.

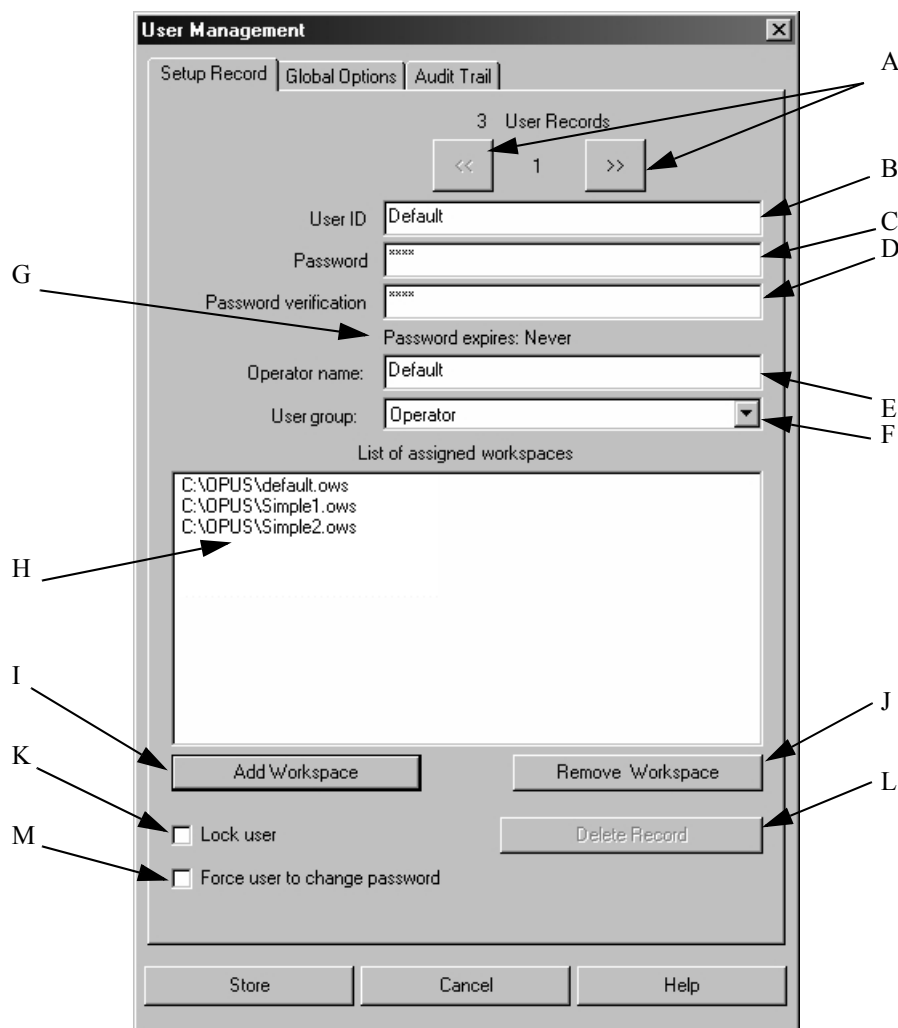


Figure 376: User Management - Setup Record tab

- 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 by a number of “*”.
- D) Re-enter the password for verification. The entry in the *Password Verification* entry field is indicated by a number 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 administrator (NT, XP...)	All	Yes
OPUS Administrator and user/power user of operating 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, whereas users with *Administrator* or *Labmanager* rights both have unlimited access to all workspaces.
- D) 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 users with *Operator* rights 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 377: 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.

H) If you activate the *Lock OPUS if not worked at for* check box, OPUS will be locked after a certain period of time has passed in which you have not performed any steps in OPUS. As soon as you have activated the check box, an entry field is enabled. Use this entry field to define the period of time in minutes.

OPUS will be locked if the defined period of time has passed. Any program access will be impossible. The *OPUS Login dialog* is displayed. Note that only the previous user or the administrator can log in again.

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
- Changing password

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

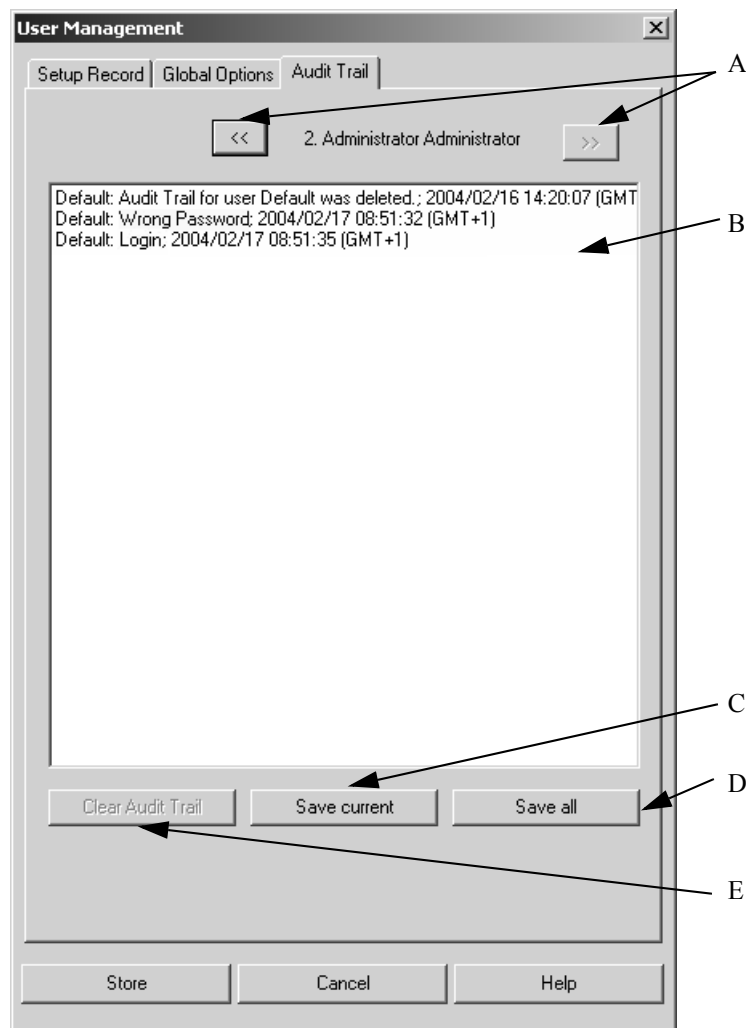


Figure 378: User Management - Audit Trail tab

- 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 according to 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:

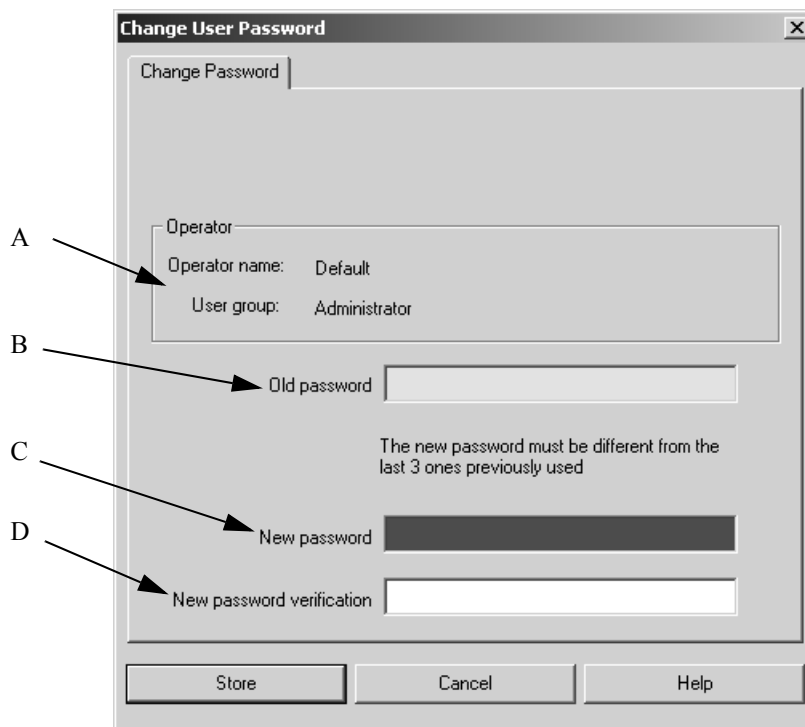


Figure 379: Change User Password

- 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 try to start OPUS, a warning pops up.



Figure 380: Warning - password expired

If you click on the *OK* button, the *OPUS Login* dialog opens. Enter the new password and verify it.

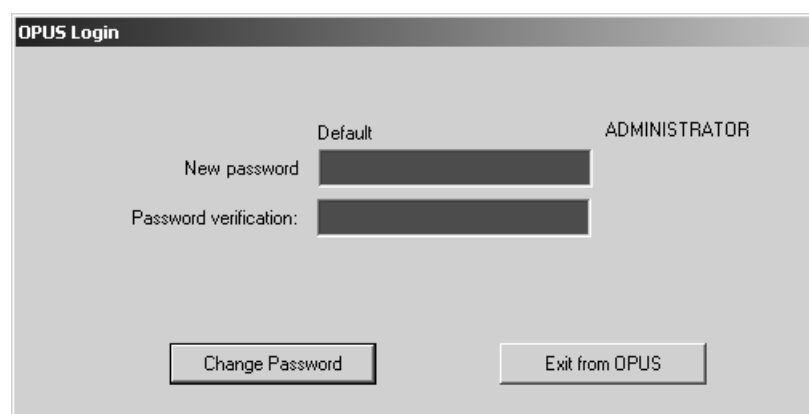


Figure 381: Change expired password

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 or scripts are integrated into the menu and can be added to the toolbars. It is possible to add macros and scripts in different languages.

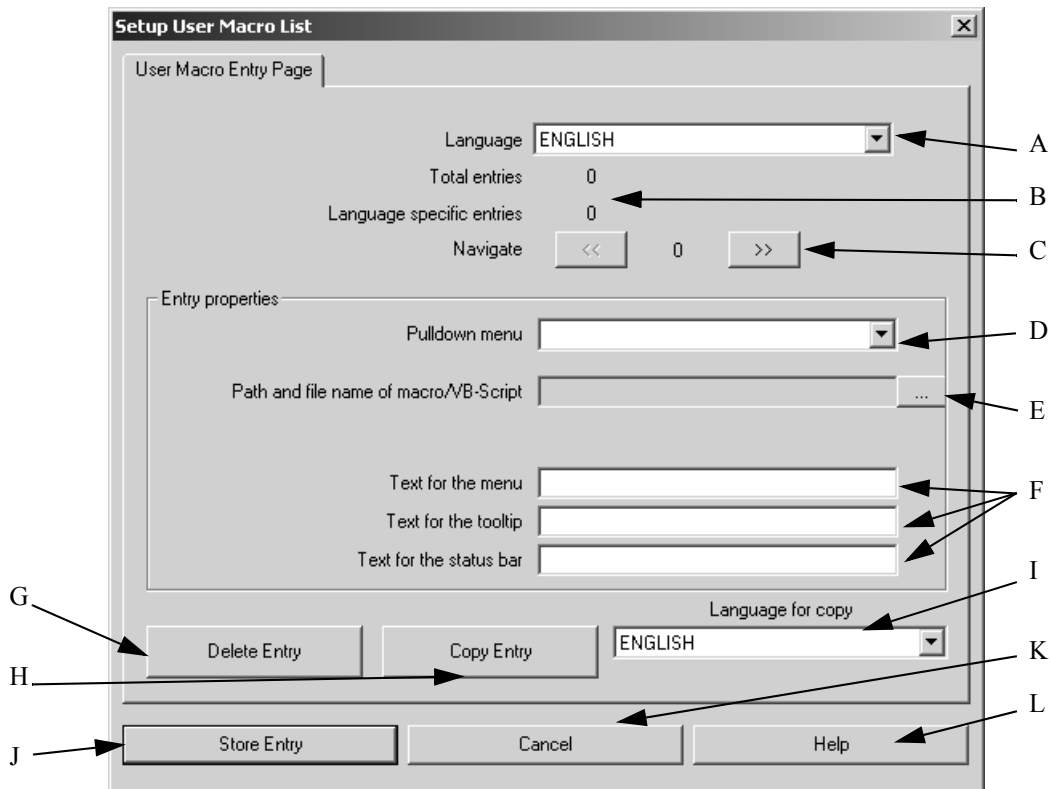


Figure 382: Setup User Macro List - User Macro Entry Page tab

- A) Select the correct language for the entry from the drop-down list. The following languages are available: ENGLISH, GERMAN, FRENCH. The default language is the language in which OPUS has been started. You can only edit the entries for the selected language. If the language has been changed, the entries for the newly selected language can be accessed.
- B) Shows the total number of entries and the number of entries for the current language.
- C) Use these buttons to go to the previous or next user record to scroll between the different entries for the current language.
- D) Select the menu which the macro/script is to be added to from the drop-down list.
- E) Use the browse button to select the macro/script for the entry. To prevent errors the path and file name of the macro/script cannot be entered manually.
- F) Fill in the entry fields by the correct text for the menu, tooltip and status bar.
- G) If you want to remove the current entry from the list, click on the *Delete Entry* button.
- H) You can also copy an entry for a different language into the list by clicking on the *Copy Entry* button. Before, you have to select a language from the drop-down list (I). Make sure that the language is not the same as specified in (A). Otherwise, an error message pops up indicating that you cannot copy an entry using the same language. Translate or modify the entry accordingly.
- I) Use this drop-down list to select the target language for copying. See also (H).
- J) Use this button to store all entries for all languages in the *USERMAC.LST* file.
- K) Exit by using the *Cancel* button. The modifications will not be stored.
- L) To have the online help displayed click on the *Help* button.

14.5.1 Contents of the USERMAC.LST File

The *USERMAC.LST* file in the OPUS directory is stored as 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 these sections each line represents a macro or script. The different parts of the lines are separated by the "@" character and have the following meaning:

```
.\macro\it.mtx@8@Instrument Test@Instrument Test@Run the Instrument Test
(1)      (2)      (3)      (4)      (5)
```

- 1) Path and file name of macro or script
- 2) Number of menu
- 3) Text for menu
- 4) Text for tool tip
- 5) Text for status bar

14.6 Register OPUS

After installing OPUS you can use the program for 30 days without registering.

You have to register OPUS if

- you buy additional OPUS packages.
- you want to use Bruker libraries.
- the 30-days'-trial period has expired.

The data required (key, serial number etc.) to register OPUS can be obtained from Bruker. The registration has to be performed only once and is valid for all users. To be able to register OPUS you need to have Administrator rights in Windows.

Start the OPUS registration by selecting the *Register OPUS* command in the *Setup* menu.

Figure 383: Registration Dialog

Fill in the entry fields by using the data which are written on the OPUS CD for the OPUS registration.

Note: You only have to fill in those fields which you received registration data for.

The OPUS serial, package and library number consist of figures only, whereas the key consists of both figures and capital letters. When entering the key for the first time it is displayed in plain text, later it is hidden by "*".

Activate the correct option button for your registration data in the *Dialog mode* group field. If you have registration data for OPUS 5.5 (or previous versions), activate the corresponding option button. In this case a message pops up requiring to define the respective additional software packages from the drop-down list. These additional packages are defined as *Extended packages* in your registration data.

To check whether the registration data are correct click on the *Check Registration Data* button. If they are correct, the selection field lists all available OPUS packages and libraries.

The *Select packages....* option button allows to deactivate single software packages and libraries. If you activate this option button, you can remove the check mark in front of the respective package or library. If you close the dialog, these packages or libraries will not be registered until you restart OPUS.

Click on the *OK* button to have the data permanently registered.

14.7 Customize Toolbars

Customizing toolbars in OPUS is similar to any other software package based on Windows. OPUS provides the following options:

- Adding or deleting toolbars
- Moving toolbars or copying toolbar icons
- Customizing or generating toolbars
- Grouping icons on toolbar
- Creating user-defined icons

14.7.1 Adding or deleting toolbars

To call OPUS icons either select the *Customize Toolbars* command or click on the arrow head (A in figure 384) at the end of each toolbar. In the latter case an edit field (B in figure 384) pops up. If you position the cursor on the edit field arrow head, the main OPUS menus with the specific icons are displayed.

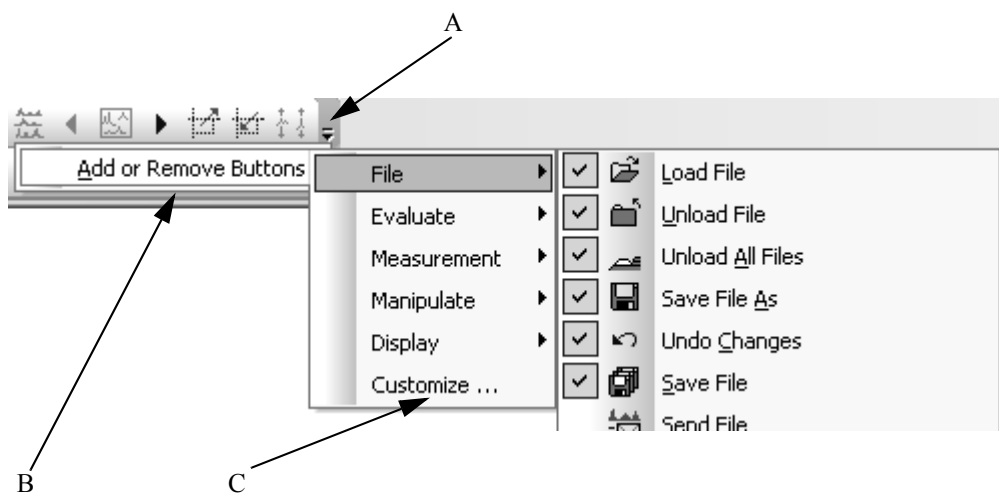




Figure 384: Customizing toolbars

To add a new icon to the toolbar click on the particular icon from the menu shown in figure 384. A check mark is set next to the icon. All icons with a check mark are activated and displayed in the toolbar.

To delete an icon from the toolbar click on the check mark. The check mark is then deleted and the icon is no longer displayed in the toolbar. If you click on the *Customize* command (C in figure 384) the dialog shown in figure 385 opens. To learn how to add or delete icons by means of this dialog refer to chapter 14.7.3.

14.7.2 Moving toolbars or copying toolbar icons

Toolbars can be freely moved. Position the cursor over the  button at the beginning of the toolbar. The cursor changes into . Now, press the mouse button and move the toolbar to any position you like.

Toolbar icons can also be copied. First, select the *Customize Toolbars* command from the *Setup* menu to open the *Customize* dialog. Then, right click on the respective icon in the toolbar and select the *Copy Button Image* command from the pop-up menu. Click on the icon and drag it to the position desired. When copying icons by means of the pop-up menu have the *CTRL+ALT* keys pressed while dropping the icon to the new position. Otherwise, the icon will only be moved.

14.7.3 Customizing or generating toolbars

If you click on the *Customize Toolbars* button, the following dialog opens:

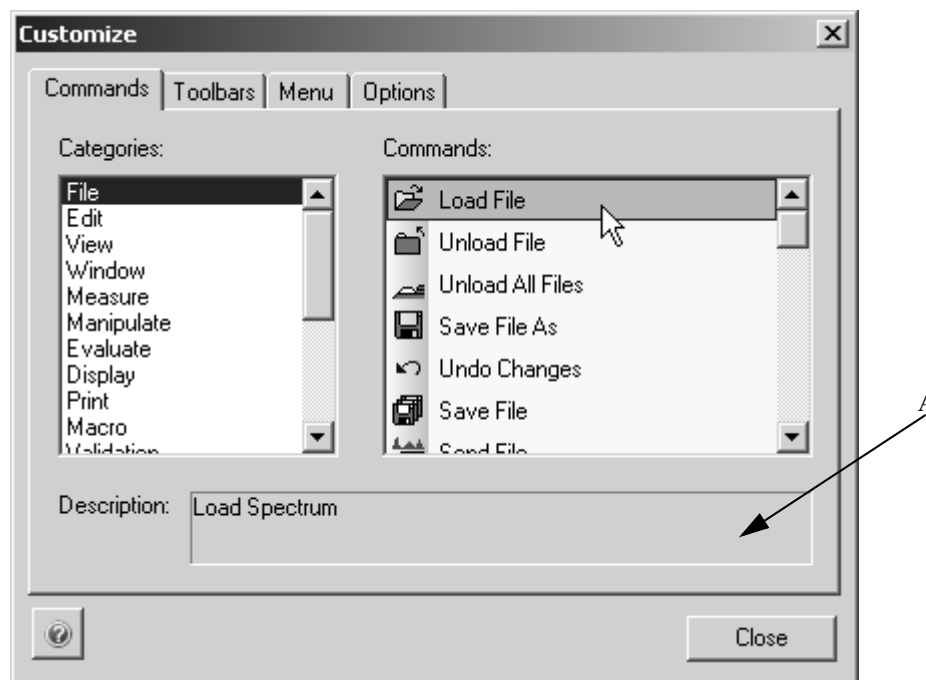



Figure 385: Customize Toolbars – Commands tab

The *Commands* tab contains both the different menu categories and menu commands with the respective icons. If you, e.g., select the *File* category, all commands available for the *File* menu are displayed in the *Commands* list box. If you click on any command in this list box, a short text (A in figure 385) comes up describing this command.

To add an icon to a specific toolbar proceed as follows:

- Click on the respective icon in the *Command* list box.



- The cursor changes into .
- Drag and drop the icon to the desired position in the toolbar.
- You have two possibilities to delete the icon from the toolbar. Either click on the icon and remove it from the toolbar while pressing the mouse button. If you release the mouse button, the icon is deleted from the toolbar. You can also right click on the icon and select the *Delete* command from the pop-up menu. **Note:** Make sure that the *Customize* dialog is open, otherwise no pop-up menu will be displayed.

You can also add single menus or sub-menus to a toolbar by means of the *New Menu* category in the *Categories* list box. Drag and drop the *New Menu* entry displayed in the *Commands* list box to the desired position in the toolbar. If you want to change the name of the entry, right click onto it and select the *Button*

Appearance command from the pop-up menu. Enter the new name into the *Button text* entry field (also see chapter 14.8.4). The new menu has an arrowhead on the right side. Clicking on this arrowhead opens a small field in which you can drag and drop single menu commands.

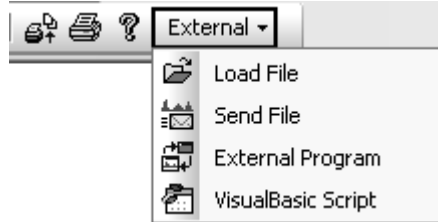



Figure 386: Example of a menu entry in the toolbar

By means of the  button you can open the online help for each tab. Click on the *Toolbars* tab to open the following dialog:

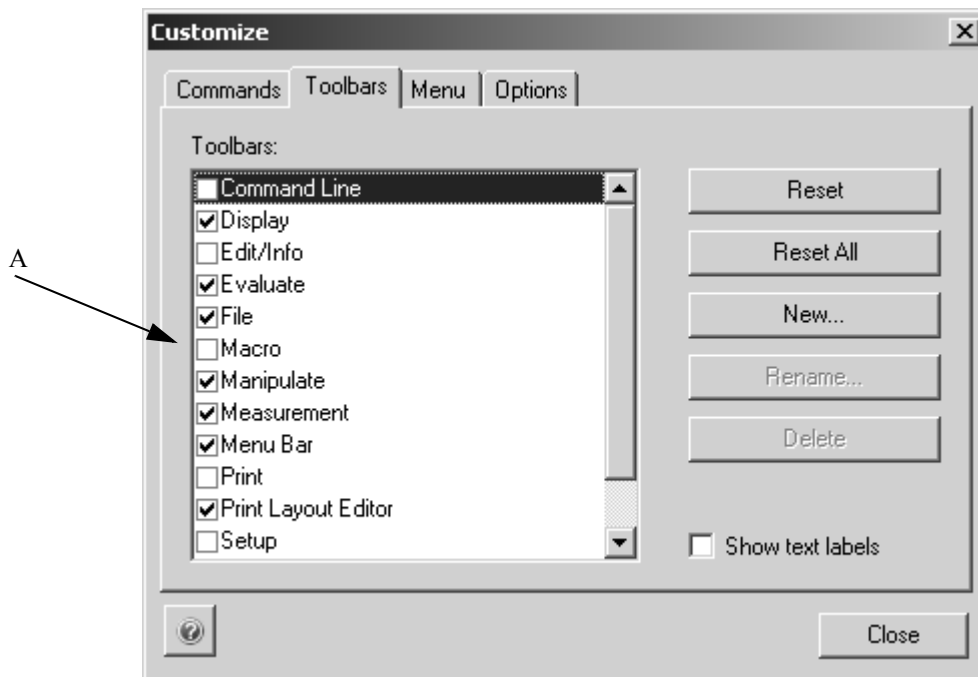


Figure 387: Customize - Toolbars tab

The *Toolbars* list box (A in figure 387) helps to define which OPUS toolbar is to be displayed. Therefore, set a check mark in front of the toolbar name. If you remove the check mark, the toolbar will not be displayed.

To generate additional toolbars proceed as follows:

- Click on the *New* button.
- Enter the name of the new toolbar into the *Toolbar Name* entry field.
- Confirm the name by *OK*. The new entry will then be displayed on the lower end of the *Toolbars* list box.
- If you want to rename or delete this new entry, select it and click on either the *Rename* or *Delete* button.

Note: Toolbars which have not been created by the user **cannot** be deleted. If you select such a toolbar the *Reset* button will be enabled. This button allows to reset the standard icons of the toolbar.

To reset the standard OPUS toolbars, i.e. have them displayed by their default symbols, names and commands, select the toolbar name and click on the *Reset* button. Similar to this, all toolbars can be set to their default contents by clicking on the *Reset All* button.

Toolbars can also be displayed with their text labels. Select the name of the toolbar and activate the *Show text labels* check box. The toolbar will be displayed as follows:



Figure 388: Toolbars with text label

14.7.4 Depicting Icons

In general, OPUS icons can be depicted as follows in the toolbar:

- Image:
- Text:
- Image and text:

Right click on any icon in the toolbar and select the appropriate depiction from the pop-up menu. For further information on this pop-up menu refer to chapter 14.7.5 and 14.7.6.

Note: Make sure that the *Customize* dialog is open. Otherwise, the pop-up menu will not be displayed

The *Menu* tab contains options to customize single menus and is described in detail in chapter 14.8.

Further settings on the appearance of toolbars can be made on the *Options* tab. Activate or deactivate the respective check box.

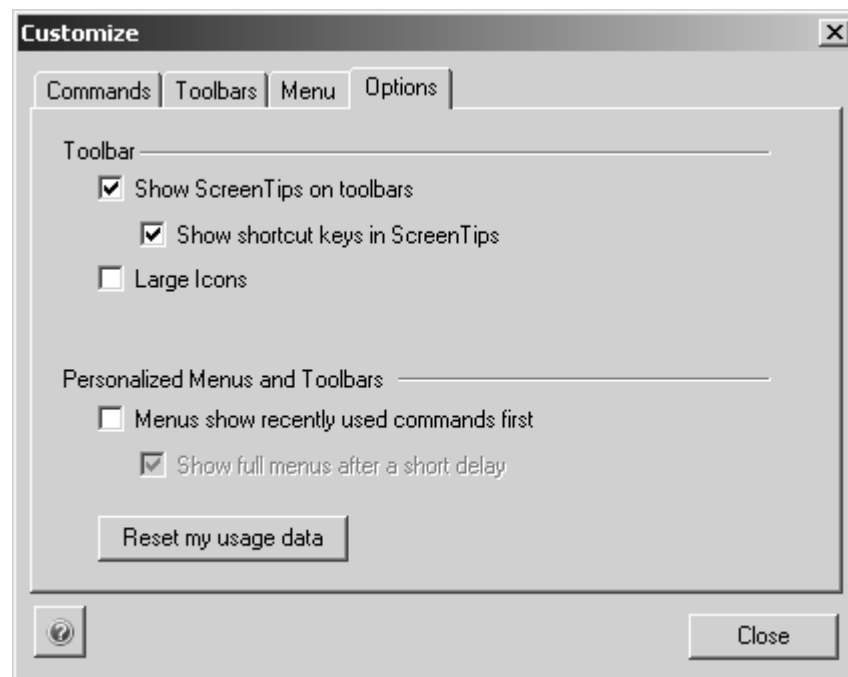



Figure 389: Customize - Options

- **Show screen tips on toolbar:** screen tips (tooltips) will be shown as soon as you move the cursor over a toolbar button.
 - **Show short cut keys in screen tips:** screen tips will also include the short cuts for the icon
- **Large icons:** the toolbar icons will be double the normal size

For details on the menu settings in this dialog refer to chapter 14.8.

14.7.5 Grouping icons on the toolbar

Icons which belong together regarding subject matter can be grouped on the toolbar. In this case you can set a dividing line in front of the first and after the last group element to differentiate between this group and the other icons and menus on the toolbar.

To add a dividing line right click on the desired icon while the *Customize* dialog is open. Select the *Start Group* command from the pop-up menu, and a check mark is set in front of the command. On a horizontally positioned toolbar the dividing line is added to the left side of the icon (). In contrast, on a vertically positioned toolbar the dividing line is added above the icon.

To delete a dividing line between two icons you can choose between two possibilities. Either move one icon into the direction of the other or right click

on one of the icon and remove the check mark at the *Start Group* command in the pop-up menu.

14.7.6 Creating user-defined icons

Right clicking on a toolbar pops-up a menu. To create user-specific icons select the *Button Appearance* command from this pop-up menu.

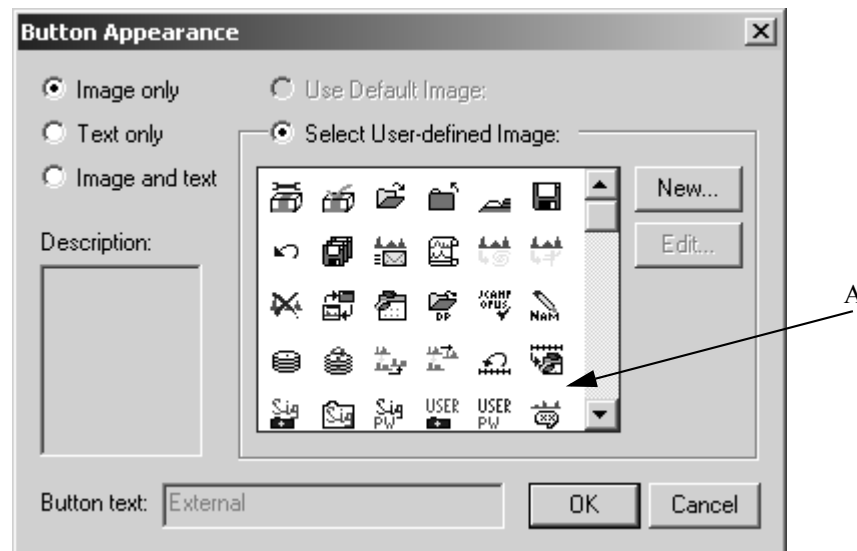


Figure 390: Pop-up menu - Button appearance

Activate the *Select User-defined Image* option button and click on the *New* button. Another dialog opens:

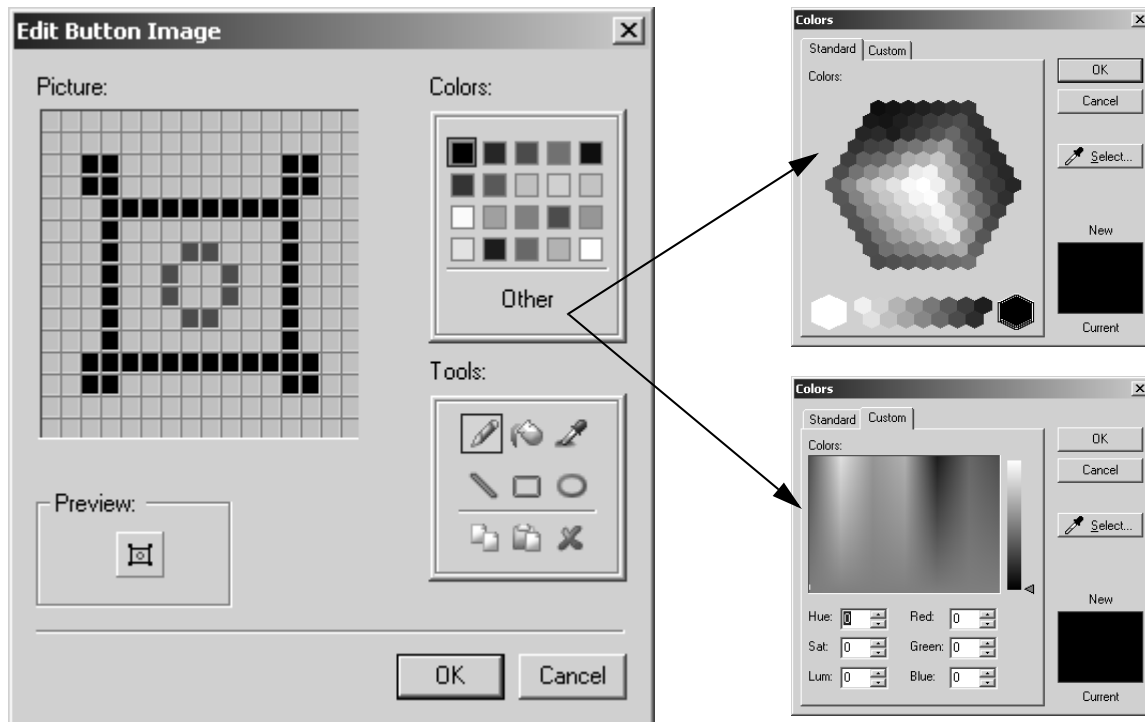


Figure 391: Pop-up menu - Edit button image

Similar to any other drawing program a color palette and different tools are available to create your own icons. The icon drawn is displayed in the preview. You can further customize the colors or create your own color shades. Click on *Other* in the color palette and select the respective options from the dialogs displayed.

To store the newly created icon click on the *OK* button. The icon will be included in the icon drop-down list (A in figure 390).

If you want to create a name for the icon, activate the *Image and text* option button. The *Button text* entry field will be enabled. Now, enter an appropriate name for the icon.

14.8 Customize Menus

Similar to the toolbars you can also customize the OPUS menus. OPUS provides the following options:

- Adding or deleting menu commands
- Moving or copying menu commands
- Moving or copying menus and menu commands on toolbar
- Creating sub-menus
- Grouping menu commands

Click on the *Customize Menus* command. In the following the *Menu* and *Options* tab is described. The *Commands* and *Toolbars* tabs are mainly about on how to customize toolbars and are described in chapter 14.7.

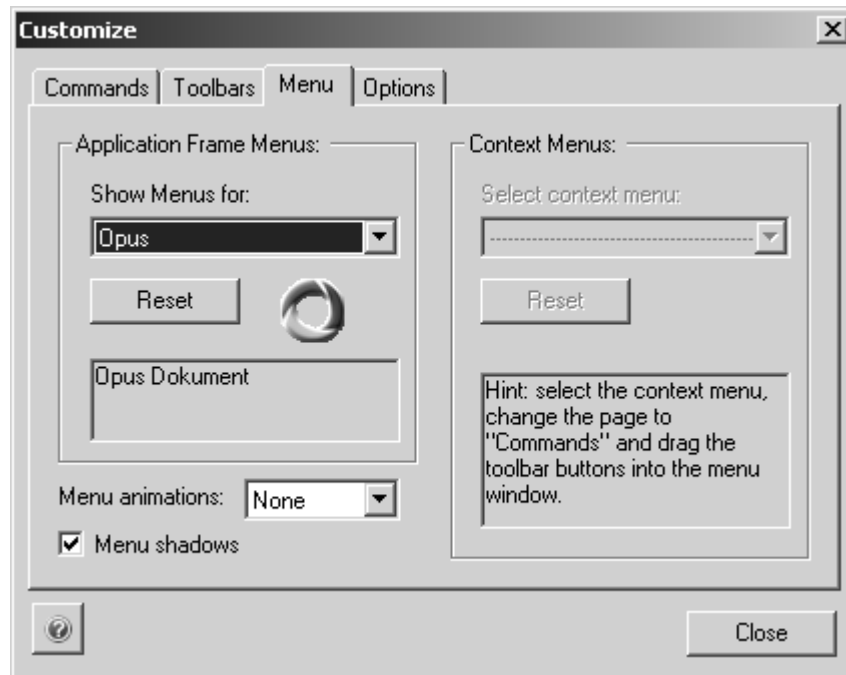


Figure 392: Customize - Menu tab

Select the workspace for the menu to be customized from the *Show Menus for* drop-down list. You can edit the menus for the following OPUS workspaces:

- OPUS
- PLE (Plot Layout Editor)
- VBScript
- GMacro
- Default Menu

To undo the changes made click on the *Reset* button, and the menus of the workspace in question are displayed again with their standard icons and commands.

Menus can also be animated. Select one type of animation from the *Menu animations* drop-down list. The following types of animations are available:

- Unfold
- Slide
- Fade

The *Menu shadows* check box is activated by default and displays the menus with a light grey shadow on the right side.

Two additional general settings can be made on the *Options* tab. These settings influence the appearance of the user-defined menus and toolbars.

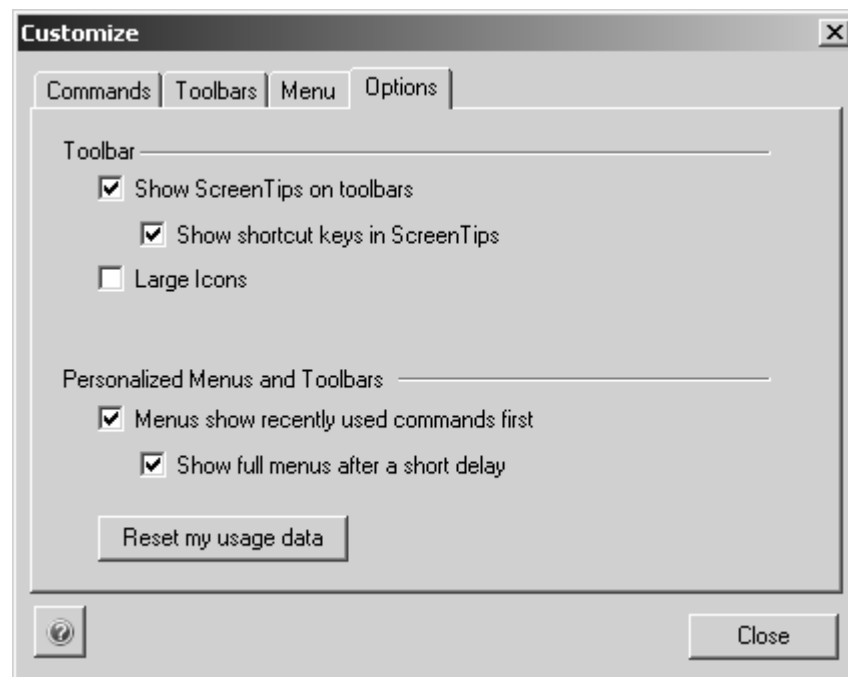



Figure 393: Customize - General settings for menus

If you activate the *Menus show recently...* check box, only those commands are displayed in the menu which have been used recently. To open the complete menu view click on the double arrow () below the last command shown.

You can have the complete menu view automatically be displayed after a short period of time. Activate the *Show full menus....* check box.

The settings of the customized menus are stored in the particular workspace. If you are not entitled to customize a particular workspace, the menus and commands will continue to be deactivated (also see chapter 14.9). To have all menus and commands displayed you may have to load a different workspace.

14.8.1 Adding or deleting menu commands

In both cases first select the *Customize Menus* commands from the *Setup* menu.

Note: Menus can only be configured, if the *Customize* dialog is open.

- Open the menu which has to be edited.
- Click on the *Commands* tab in the *Customize* dialog. For further information on this tab refer to chapter 14.7.3.
- Use the *Categories* list box and select the menu which you want to add the command from.

- Click on the respective command icon in the *Commands* list box. The

cursor changes into .

- Drag and drop the icon to the desired position in the menu you want to edit.
- To delete a command from a menu, click on this command and remove it from the menu.

14.8.2 Moving or copying menu commands

To move menu commands click on the respective command while the *Customize* dialog and the menu are both open. Move the command to the desired position while pressing the mouse button.

To copy menu commands right click on the respective command while the *Customize* dialog and the menu are both open. When copying have the *CTRL+ALT* buttons pressed and drag and drop the command to the new position. Otherwise, the command is only moved.

14.8.3 Moving or copying menus and menu commands on toolbar

Both single menu commands and complete menus can be moved within or copied to any toolbar. Click on the respective command or menu while the *Customize* dialog is open and drag and drop it to the desired position in the toolbar.

When copying press the *CTRL* button and drag and drop the menu command or menu to the desired position in the toolbar.

14.8.4 Creating sub-menus

Menu commands which belong together regarding subject matter can be sorted in sub-menus and subsumed under a main menu. First, create the main menu. Click on the *Commands* tab in the *Customize* dialog and select the *New Menu* command from the *Categories* list box. The *New Menu* entry is displayed in the *Commands* drop-down list.

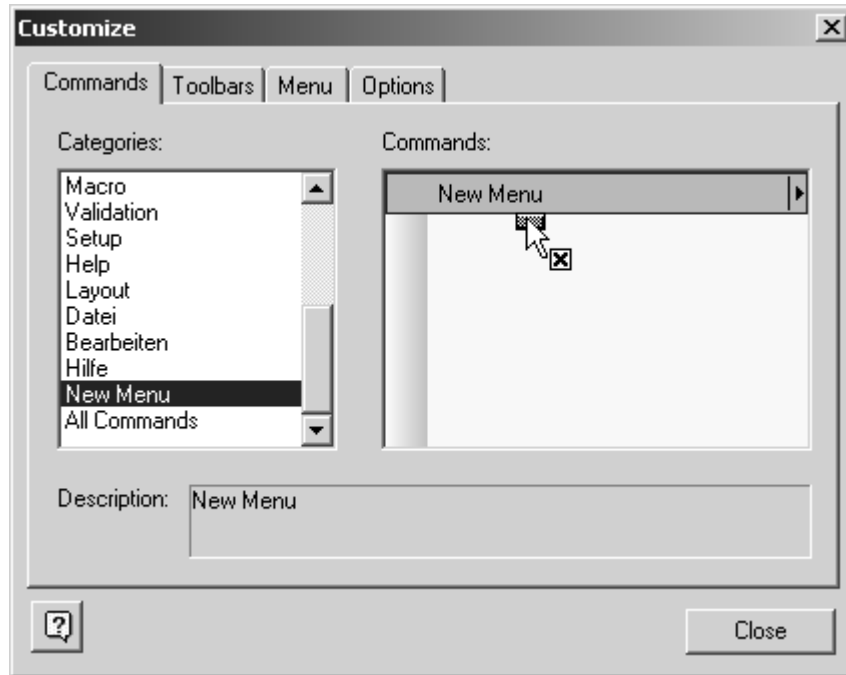
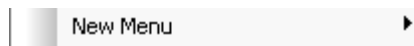


Figure 394: Customize - Creating sub-menu

Open the menu which you want to edit and drag and drop the *New Menu* entry into this menu. The new entry is now displayed in the menu:



The name of the menu entry can be changed. Right click on the entry and select the *Button Appearance* command from the pop-up menu. The following dialog opens:

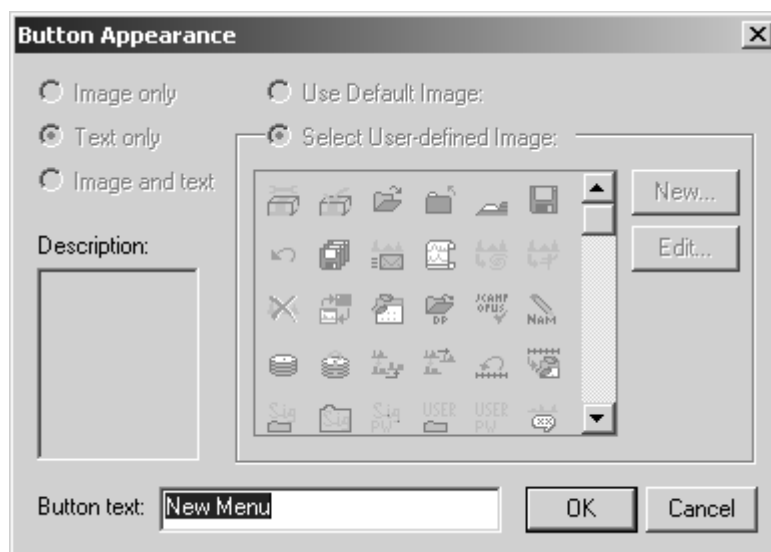


Figure 395: Changing button text

Define an appropriate name for the new menu entry in the *Button text* entry field.

The new menu entry has a small arrow head on the right side. If you click on this arrow head, a small field opens in which you can drag and drop the sub-menus. Select the respective command with the appropriate icon either from the *Commands* list box in the *Customized* dialog or from the menu itself. Drag and drop this command into the small entry field next to the arrow head.



Figure 396: Example of a main menu command with sub-menus

14.8.5 Grouping menu commands

Menu commands which belong together can be grouped within a particular menu, i.e. in front of the first and after the last element of a group you can add a dividing line. This allows to distinguish the group from other commands within a specific menu.

To add a dividing line right click on the menu command while the *Customize* dialog is open. Select the *Start Group* command from the pop-up menu, which is activated by a check mark. The dividing line is displayed above the menu command selected.

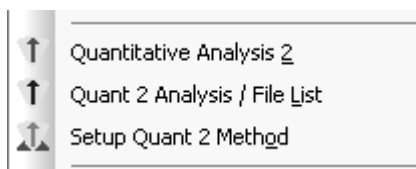


Figure 397: Example of grouping menu commands

To delete a dividing line between different menu commands right click on one of the command and click on the *Sort Group* command from the pop-up menu. The check mark will be deleted and the command deactivated.

14.9 User Settings

OPUS user accounts can be created and managed by means of the *User Settings* command. Make sure that you have the necessary user rights to do so.

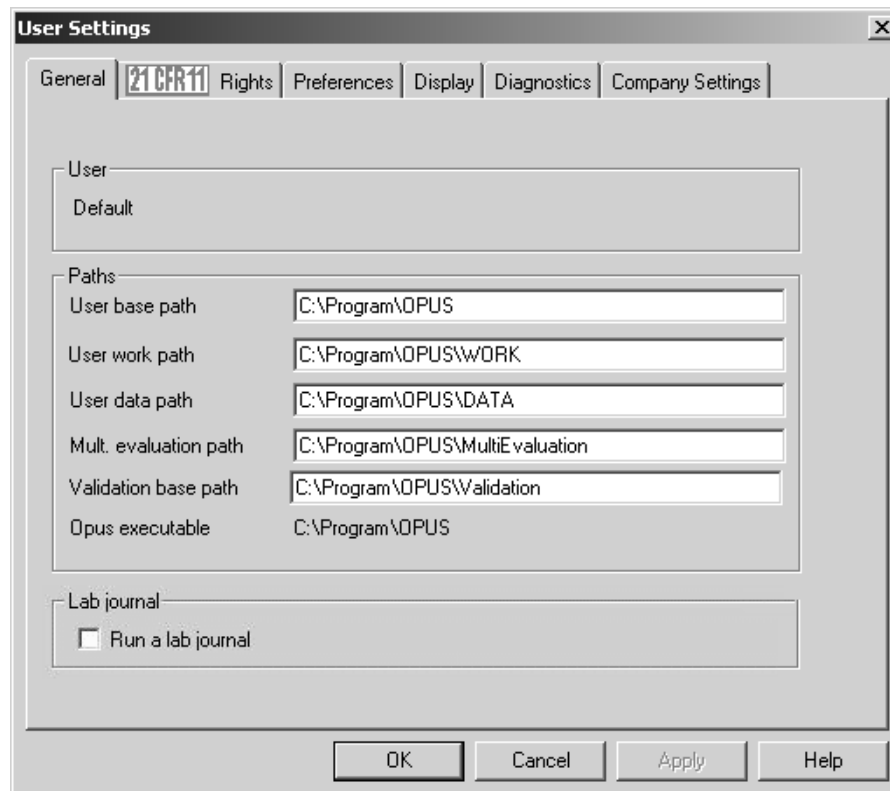


Figure 398: User Settings – General tab

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. For details on the lab journal refer to chapter 3.20.

Click on the *21CFR11 Rights* tab to assign the particular rights for the account.

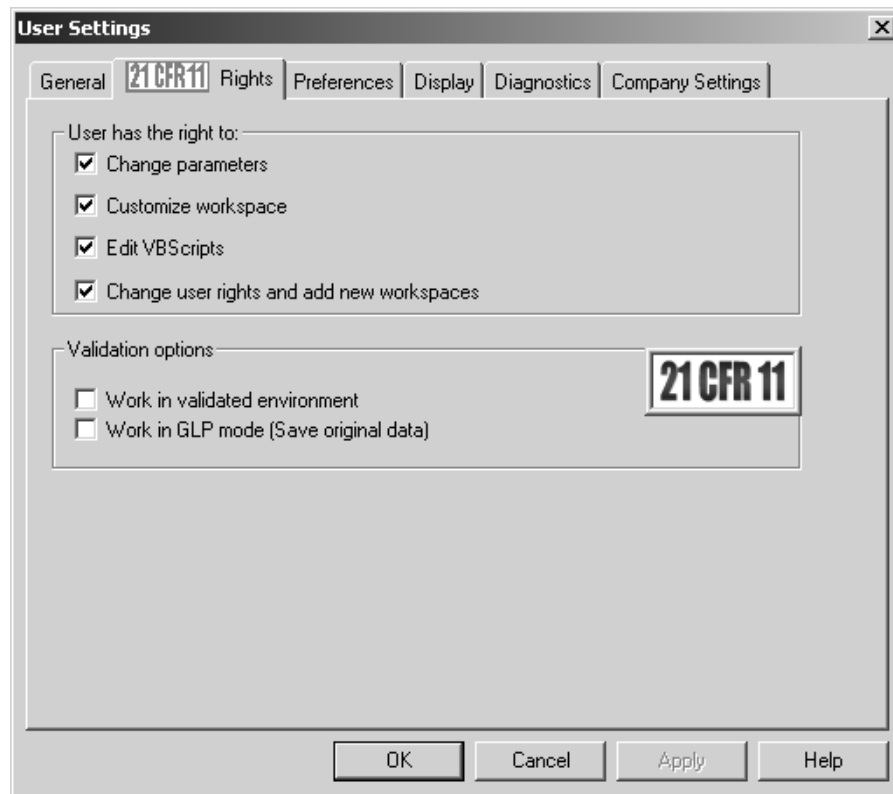


Figure 399: User Settings – 21CFR11 Rights tab

Select the user rights by activating 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.

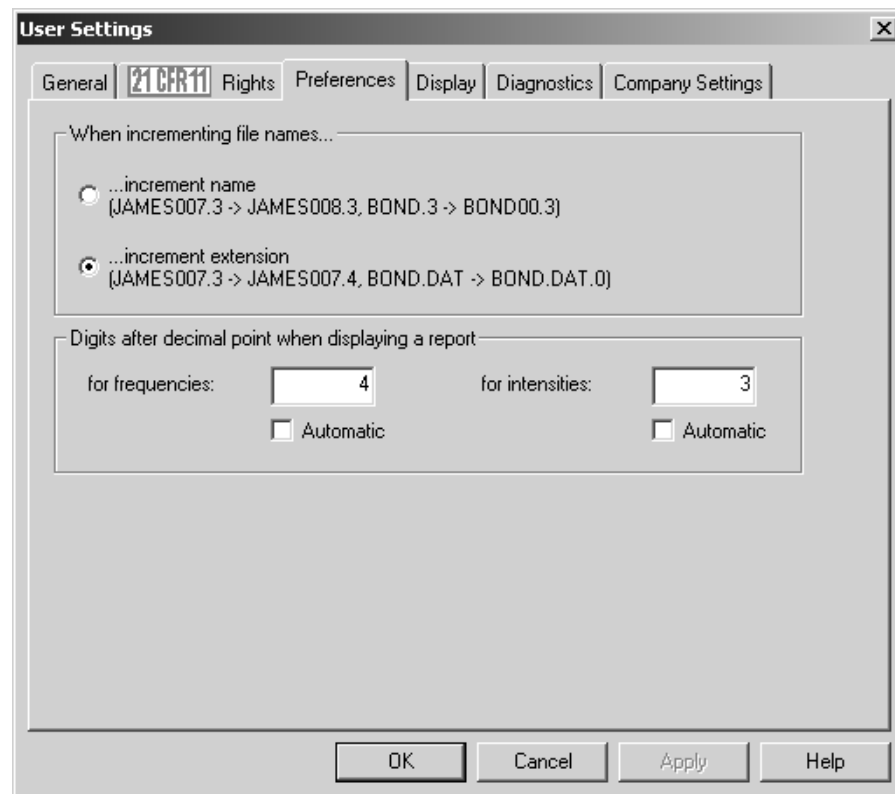


Figure 400: User Settings – Preferences tab

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.

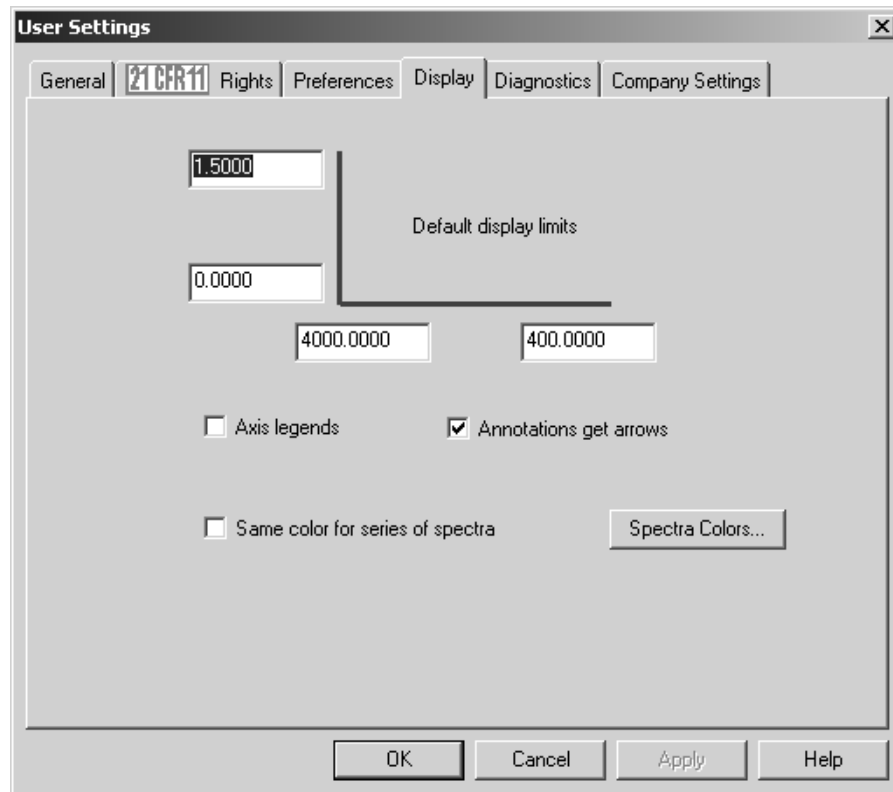


Figure 401: User Settings –Display tab

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.

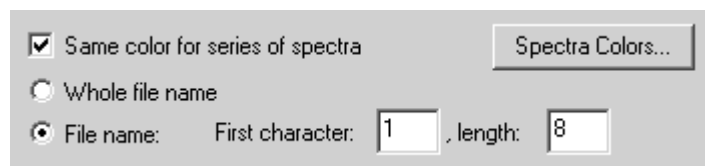


Figure 402: User Settings - Display tab with additional features

The *Whole file name* option button indicates that the file name (without extension) of the spectra series has to be identical to be able 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 conform with the file name series.

Click on the *Spectra Colors...* button to assign a color sequence to the spectra. The following dialog opens:

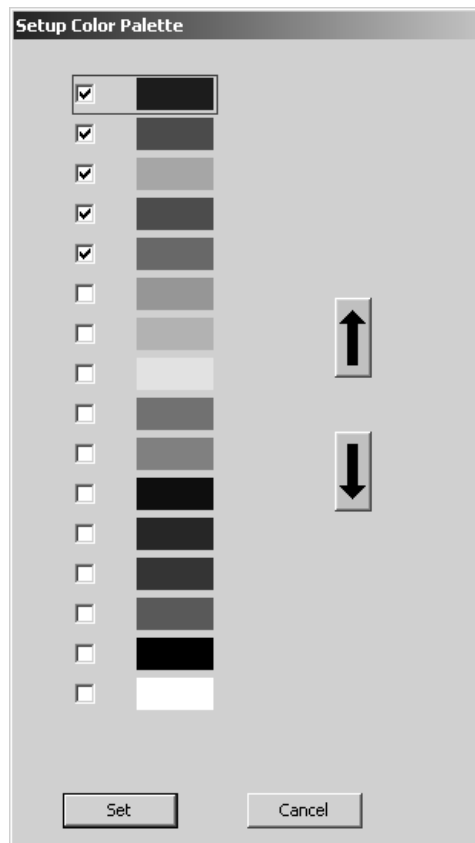


Figure 403: User Settings - Setup Color Palette

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:

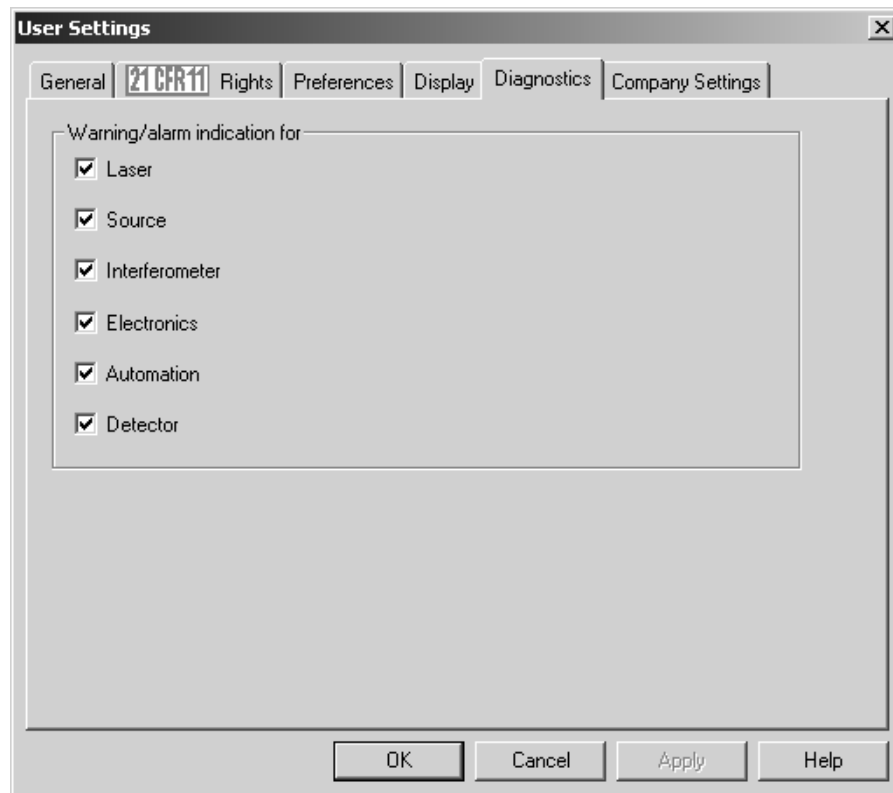


Figure 404: User Settings – Diagnostics tab

On the *Company Settings* tab you can optionally define standard data for different company features. Once these entries have been defined they will be written in each OPUS file when a measurement is performed.

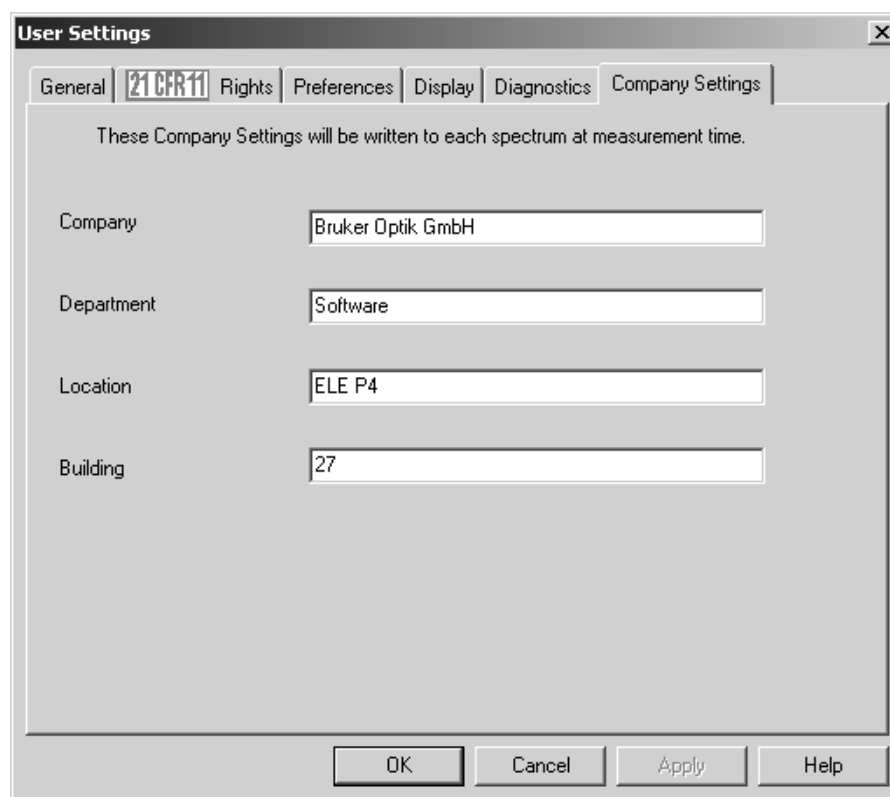


Figure 405: User Settings – Company Settings tab

14.9.1 Instrument Test (only in case of non-OVP supported instruments)

For spectrometers which are not supported by OVP, e.g. EQUINOX or 120/125 HR there are two additional tabs for the instrument test. Each of the *Instrument Test 1* and *Instrument Test 2* tab includes 6 test channels. Each of these test channels can assign one program to be used from within OPUS for validation purposes, and correlates with an icon position on the second or third row of the *Instrument Status* dialog, see chapter 7.7.

Note: 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: Configuring 12 test channels is only possible in OPUS 5 and higher versions. In previous OPUS versions you can only assign a maximum number of 6 channels. Thus, these versions only have one *Instrument Test* tab in the *User Settings* dialog.

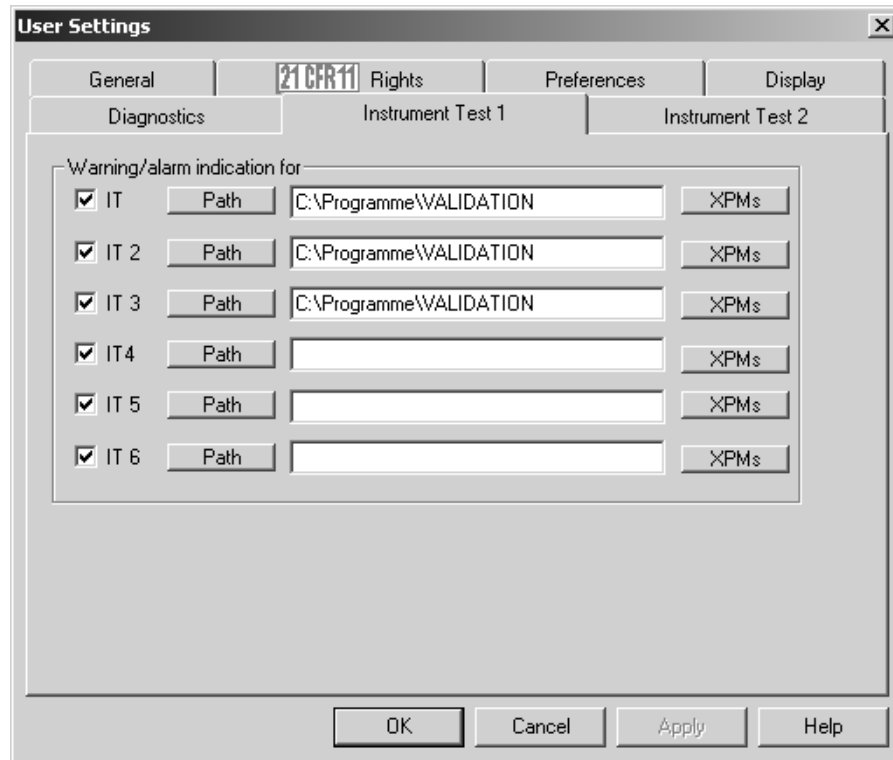


Figure 406: User Settings – Instrument Test 1 tab

First, activate the *IT* check box which represents the active test channel, and either enter the path manually or click on the *Path* button.

Notes when selecting the path:

If you have selected 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.

Example:

Assuming the instrument uses both a sample chamber and an external port as measurement channel, to validate both configurations you would assign OVP to 2 IT channels on the *Instrument Test* tab.

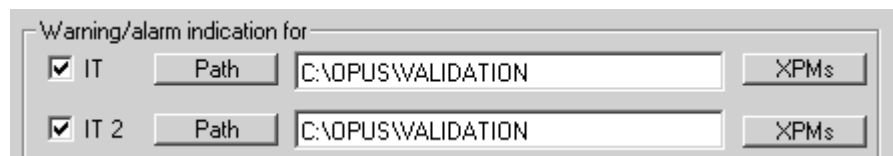


Figure 407: Two configurations assigned for the instrument test

In this example we would arbitrarily designate the first position (IT) to be used for all experiment files that use the sample compartment. All experiment files that use the external port channel will be designated for the second position (IT2).

If you have entered a path into the appropriate *IT* entry field on the *Instrument Test* tab, an icon is assigned for that particular channel on the *Instrument Status* dialog (see chapter 7.7).

Measurement experiments:

Use the *XPMs* button to register one or more measurement experiment files to the validation channel. These are the experiment files which you will use for normal daily measurement.

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.).

If you click on the *XPMs* button the following dialog opens:

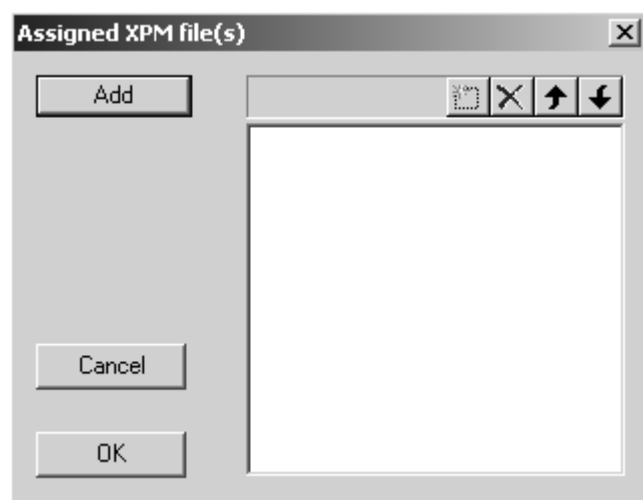


Figure 408: Assign XPM file(s)

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 selection field. Confirm the selection by clicking on the *OK* button. Undo the selection by clicking on the *Cancel* button.

If you load an experiment file, OPUS checks all the experiment files registered. If the experiment selected has been registered for a channel, this channel 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:

If you deactivate one of the *IT* check boxes, this particular channel becomes inactive. OPUS does not update the status light if that particular channel is selected as the active channel.

The following summarized sequence of actions ensues:

- 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.
- The status light reflects the current status.

14.10 Open Planner

The *Open Planner* command allows to exactly schedule appointments or events in a calendar. Appointments are planned activities in your calendar which you can also define as recurring items at a daily, weekly or monthly interval.

In this context an event is an activity that lasts at least 24 hours and normally takes place once (e.g. yearly) during one day or several days.

OPUS allows to schedule the following activities:

- Switching on and off the internal IR source of the spectrometer
- Starting OVP PQ tests
- Activating user-specific messages

Basically, the general calendar setup in OPUS is similar to any other comparable calendar feature based on Windows.

Note: The *Open Planner* command can only be accessed if you are entitled to change user rights and add new workspaces (see also chapter 14.9).

If you double click anywhere on the calendar, you can start defining the entry. It is also possible to colorize the entry to see at once what kind of appointment or event it is about.

When a timer item starts a message pops up and reminds you of the OPUS activity running soon. Postponing a timer item may be possible by using a respective macro. For details on how to generate macros refer to the OPUS Programming manual.

OPUS has to run before being able to start the scheduled item at the pre-defined time. If you click on the *Open Planner* command, the following dialog opens:

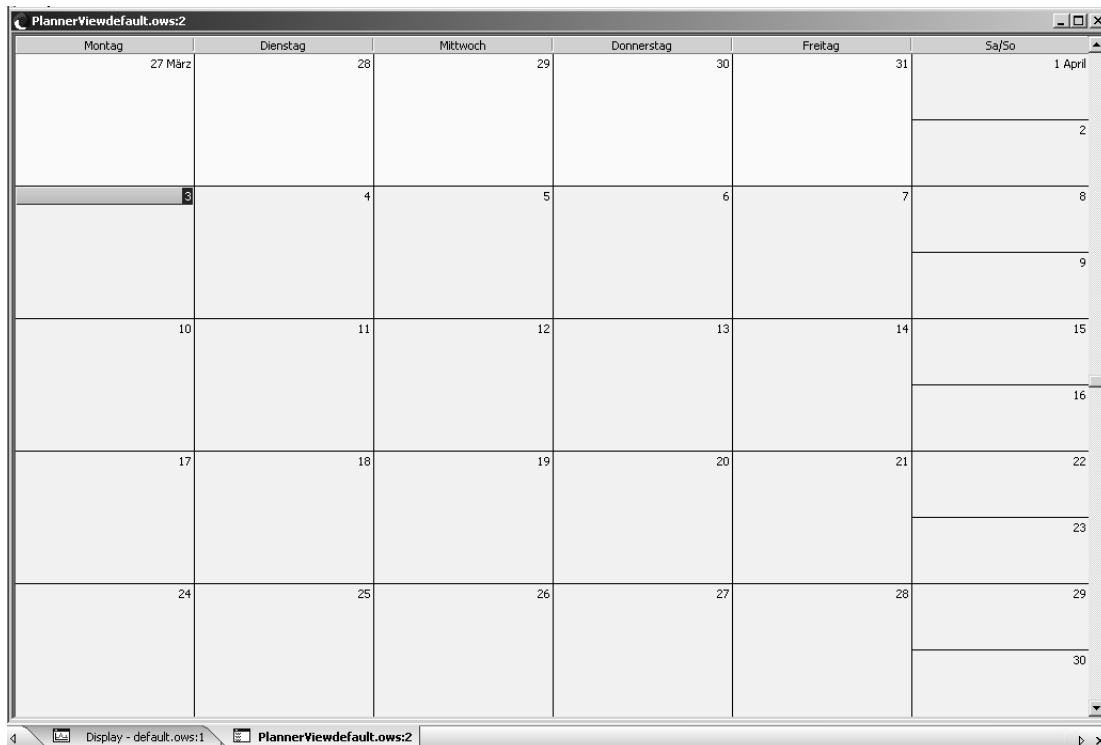


Figure 409: OPUS Planner view

14.10.2 View Options

OPUS provides different calendar view options. By default, the month panel is displayed which you can change at any time. Right click on the panel and select the *Go to Date* command from the pop-up menu.

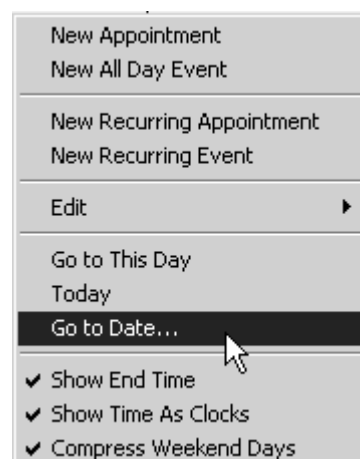


Figure 410: Planner - Pop-up menu

Select the desired calendar panel from the *Show in* drop-down list. To undo the setting made select the *Go to Date* command again and change the panel, accordingly.

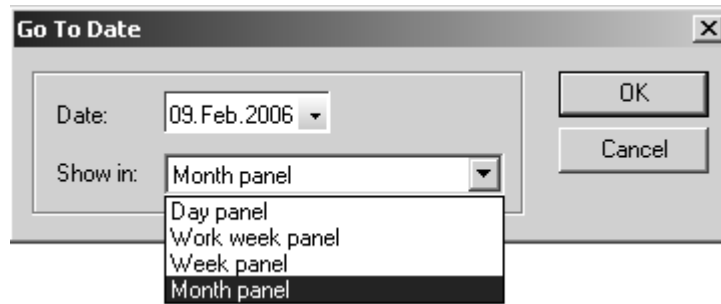




Figure 411: Calendar panel selection

The following calendar view options are set by default:

- Show end time: 08:00 10:00
- Show time as clock:  
- Compress weekend days: i.e. Saturday and Sunday are displayed in one column, one below the other

To change these default settings remove the check mark in front of the respective command in the pop-up menu (see figure 410).

The day panel of a particular day can also be opened by the pop-up menu. Right click on the respective day and select the *Go to This Day* command from the pop-up menu. The day panel opens. To undo this panel setting right click again on the calendar and select the *Go to Date* command. Use the *Show in* drop-down list (figure 411) to select the panel desired.

14.10.3 Creating Calendar Items

There are two possibilities to create a calendar item. Either double click on the particular day to open the *Edit Appointment* dialog. Or right click on the respective day and select the *New Appointment* command from the pop-up menu.

The screenshot shows the 'Edit Appointment' dialog box. At the top, there are three buttons: 'Save and Close', 'Recurrence...', and 'Delete'. Below these are three main sections. The first section has a 'Subject' drop-down menu. The second section has a 'Location' text field and a 'Label' drop-down menu with 'None' selected. The third section has 'Start time' and 'End time' fields, each with a date and time selector. The 'Start time' is set to '13. Mrz. 2006' and '09:00', and the 'End time' is set to '13. Mrz. 2006' and '10:00'. There are also checkboxes for 'All day event', 'Private', 'Meeting', and 'Phone call'. A 'Show time as' field is set to 'Busy' with a color swatch. At the bottom is a large empty text area with a vertical scrollbar.

Figure 412: Edit Appointment

Select the OPUS activity desired from the *Subject* drop-down list. The following options are available:

- SOURCE ON/OFF
- RUN OVP PQ TEST
- COMMAND LINE


Single OPUS commands can be defined by command line parameters. In this case make sure that you use the right OPUS command line syntax. A macro editor in OPUS allows to write command lines. For further details on the macro editor refer to the OPUS Programming manual.

Single entries can be colorized to see at once what kind of appointment it is about. Select the color desired from the *Label* drop-down list. The entry will then be displayed by an additional color bar.

There are two possibilities to define the start and end time of an entry. Either enter the date manually into the entry fields, or use the small arrows. In the latter case a small month panel pops up from which you can select the desired day for the respective entry.



Figure 413: Define date - Month panel

Starting from today's date you can also use the arrow keys  to define the date desired. The time can be set either manually or by using the arrow keys.

If you activate the *All day event* check box, the entry becomes an event that lasts at least one day. An all day event does not occupy blocks of time in your calendar. Instead, it is displayed at the top of the date which you have specified in the calendar. This kind of event can also be created by using the *New All Day Event* from the pop-up menu (see figure 410).

The *Show time as* drop-down list allows to define the time status of the entry. This is recommended if others have access to your calendar.

Note: Each single appointment or event can be changed into a recurring item, i.e. have it occurred repeatedly. In this case click on the *Recurrence* button (for details see the following chapter).

To save your settings click on the *Save and Close* button.


14.10.4 Creating Recurring Items

If single appointments or events are to be repeated, define these appointments or events as recurring items. A typical example of a recurring daily event is to start particular OVP tests at a fixed period of time, or shut down the IR source inside the spectrometer.

To create recurring events right click on the calendar view and select the *New Recurring Appointment* or *New Recurring Event* command. The dialog that opens is the same for both commands.

Figure 414: Appointment Recurrence

Define the start and end time of the actual appointment or event, either manually or by means of the arrow keys. The recurrence pattern helps to exactly set up at what intervals the appointment or event recurrence has to take place.

The range of recurrence refers to the duration of a complete appointment or event recurrence. Define the start and end of the recurrence. Recurring items are always indicated in the calendar by the  symbol.

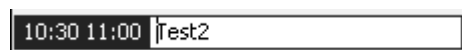
As soon as you confirm your settings by clicking on the *OK* button the *Edit Appointment* dialog (figure 412) is displayed. Enter the name of the recurrence into the *Subject* entry field, or select the corresponding activity from the *Subject* drop-down list.

14.10.5 Editing Calendar Items

To edit appointments or events double click on the respective entry. The *Edit Appointment* dialog (see figure 412) is displayed. Now, you can make all the changes desired.

You can also right click on the appointment or event and select the *Open* command from the pop-up menu to have the *Edit Appointment* dialog displayed.

To rename single appointments or events in the calendar click on the name (not on the time) of the respective entry. A small white entry field will open in which you can change the current name:



To copy or delete particular entries right click on the appointment or event and select the *Copy* or *Delete* command from the pop-up menu.

14.10.6 Editing Recurring Calendar Items

Editing recurring appointments or events is similar to editing single appointments or events. However, a warning pops up indicating that this kind of entry selected is a recurring item. You can either change any aspect of a recurring appointment for the entire series, or edit one instance of an appointment without affecting the entire series of items. Activate the corresponding option button and confirm the setting by clicking on the *OK* button.

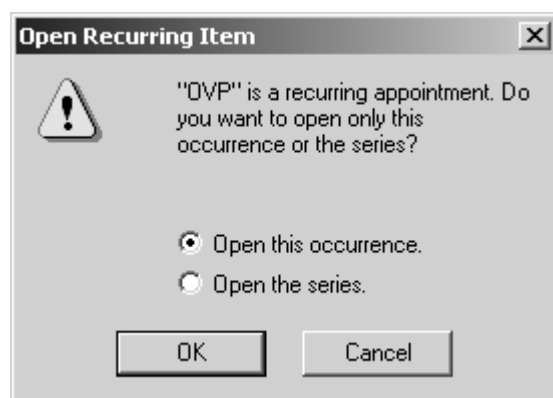


Figure 415: Warning in case of recurring items

The *Edit Appointment* dialog (figure 412) is displayed. If you want to change the complete recurrence pattern, click on the *Recurrence* button.

Recurring items can also be copied or deleted. In the latter case a warning pops up indicating that the entry in question is a recurring item.

14.11 New Workspace

The OPUS workspace stores the following settings:

- All user rights
- Configuration of toolbar and windows
- Parameters (settings) of all commands
- Configuration of menus and pop-up menu
- User name and password

For details on how to customize a new workspace also see chapters 1, 14.7 and 14.8.

14.12 Save Workspace as

If you have changed a workspace, e.g. by re-positioning toolbars, this modified workspace will automatically be stored when you exit OPUS. If you have created a new workspace, a dialog pops up requesting the name of this new workspace when you exit OPUS.

14.13 Close Workspace

Using the *Close Workspace* command would close the current OPUS workspace.

14.14 Send Workspace

It is possible to send the OPUS configuration by e-mail. In this case the e-mail addressee accepts all OPUS settings valid on your computer. The addressee has to store the OPUS workspace file on his computer, and open the file by OPUS.

Make sure that each path correlate to the OPUS settings. Therefore, sending workspaces does only make sense if the computer configuration with regard to the installation paths is identical. The workspace addressee has to know the configuration password to be able to use the workspace.

15 Help

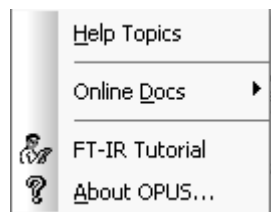


Figure 416: OPUS Help Menu

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, 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:

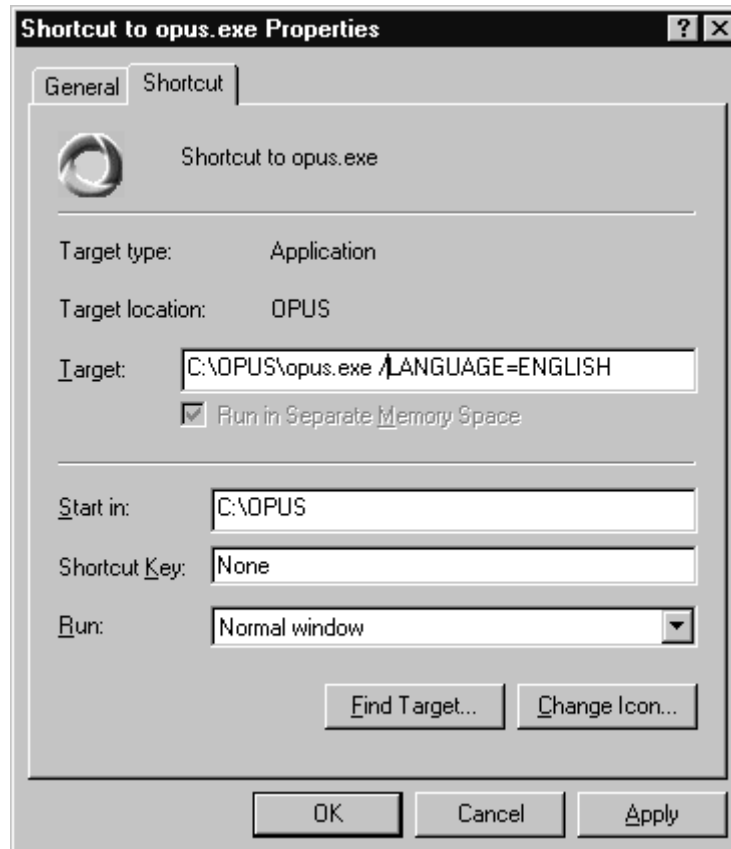


Figure 417: Properties Dialog - Shortcut tab

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=CHINESE starts OPUS in Chinese
- OPUS/LANGUAGE=ENGLISH starts OPUS in English
- OPUS/LANGUAGE=FRENCH starts OPUS in French
- OPUS/LANGUAGE=GERMAN starts OPUS in German
- OPUS/LANGUAGE=JAPANESE starts OPUS in Japanese
- OPUS/LANGUAGE=SPANISH starts OPUS in Spanish

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.

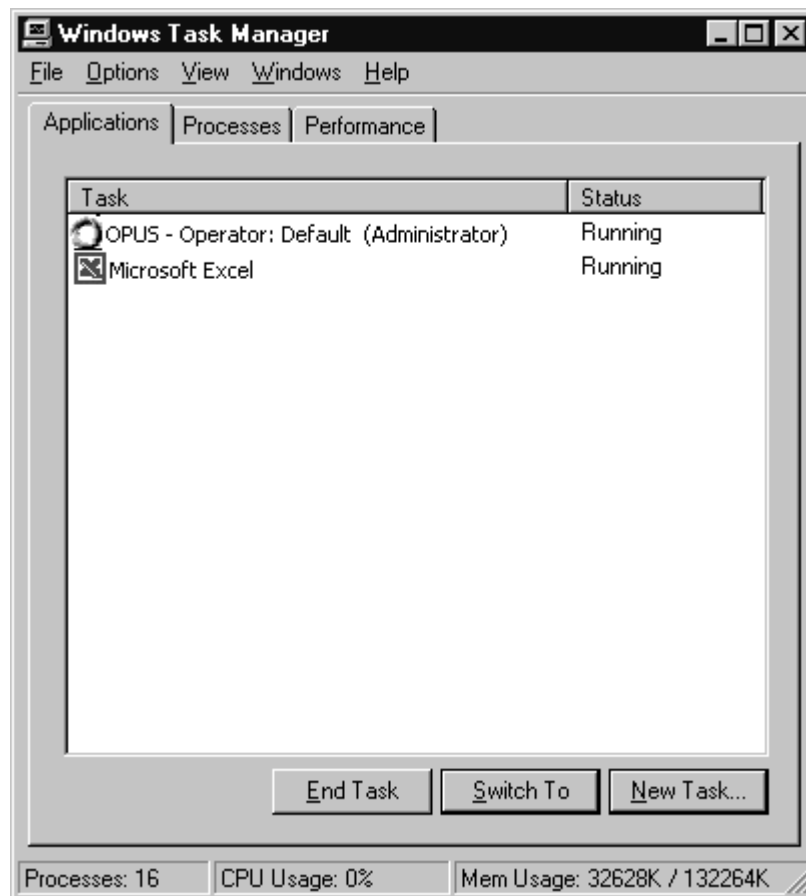


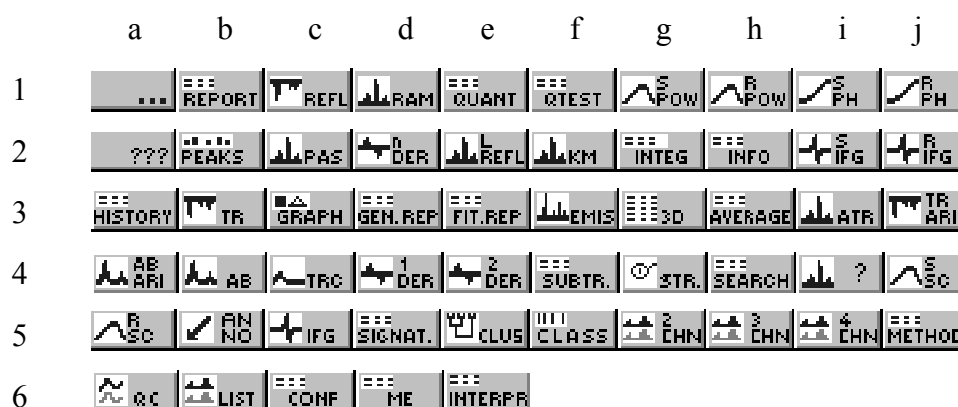
Figure 418: Windows Task Manager

Select OPUS from the *Applications* tab and click on the *End Task* button. **OPUS will terminate without saving any data.**

Appendix A

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	Unknown block	...
1b	Report	REPORT
1c	Reflectance spectrum	REFL
1d	Raman spectrum	RAM
1e	QUANT report	QUANT
1f	Quality test	QTEST
1g	Sample, power spectrum	SPOW
1h	Reference power spectrum	RPOW
1i	Sample, phase spectrum	SPH
1j	Reference, phase spectrum	RPH

2a	Unknown block	???
2b	Peak table	PEAKS
2c	Photoacoustic spectrum	PAS
2d	n th derivative	nDER
2e	Logarithm of reflectance	LREFL
2f	Kubelka-Munk spectrum	KM
2g	Integration report	INTEG
2h	Information block	INFO
2i	Sample, interferogram	SIFG
2j	Reference, interferogram	RIFG

3a	Protocol	HISTORY
3b	Transmittance spectrum	TR
3c	Video image(s)	GRAPH
3d	General report	GEN.REP
3e	Fit report	FIT.REP
3f	Emission spectrum	EMIS
3g	3D spectrum	3D
3h	Average report	AVERAGE
3i	ATR spectrum	ATR
3j	Arithmetical result, transmittance	TRARI

4a	Arithmetical result, absorbance	ABARI
4b	Absorption spectrum	AB
4c	Trace	TRC
4d	First derivative	1DER
4e	Second derivative	2DER
4f	Subtraction report	SUBTR
4g	Molecular structure	STR
4h	Search result	SEARCH
4i	Unknown spectra type	?
4j	Single channel spectrum, sample	SSC
















5a	Single-channel spectrum, reference	RSC
5b	Annotation	ANNO
5c	Interferogram	IFG
5d	Signature	SIGNAT
5e	Cluster analysis	CLUS
5f	Classification	CLASS
5g	2nd data channel	2CHN
5h	3rd data channel	3CHN
5i	4th data channel	4CHN
5j	Method	METHOD




















6a	Quick Compare	QC
6b	Spectra file list	LIST
6c	Conformity test	CONF
6d	Multi Evaluation	ME
6e	Interpretation	INTERPR

























































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
-  Open
-  Close workspace
-  Send workspace
-  Cut
-  Copy
-  Paste
-  New spectrum window
-  New report window
-  New 3D window
-  Tile
-  Cascade
-  Quick print
-  Print
-  About OPUS

-  Draw ellipse
-  Draw line
-  Draw rectangle
-  Insert table
-  Move
-  New page
-  Delete page
-  Delete
-  Clear frame
-  Page properties
-  Object properties
-  Lock
-  Back (frequency range)
-  Forward (frequency range)
-  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
	Make compatible		Spektum search
	Convert spectra		Peak search
	Smooth		Information search
	Derivative		Structure search
	Frequency calibration		Initialize library
	Raman correction		Store spectrum in library
	Black body		Library editor
	Interferogram to spectrum conversion		Library browser
	Inverse FT		Quantitative analysis 2
	Post zerofilling		Quant 2 analysis / file list
	Fourier self-deconvolution		Set up Quant 2 method
	Symmetric FT		Identity test
	Kramers-Kronig Transformation		Set up Identity test method
	Extrapolation		Cluster analysis
	1/cm <-> μm		Carbon Oxygen Analysis
	Averaging		2D Correlation
	Merging spectra ranges		Quick Compare Setup
	Atmospheric compensation		Quick Compare
	Straylight correction		Multi Evaluation Setup
	Noise generation		Multi Evaluation Test
	Moving mean		
	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		Load file
	Motorised stage control		Unload file
	Video assisted measurements		Unload all files
	Time resolved step scan		Save file as
	Chromatography		Undo changes
	Step scan modulation		Save file
	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
	Macro converter		VisualBasic Script
	Run macro		Load data point table
	Debug macro		Scan OPUS files
	Macro editor		Find OPUS files
	Compile macro		Clone entry
			Clone original

Parameters

The main parameters which may be included in the parameter data blocks are listed

Data Status Block

General

AOZ = "Map Origin Z"
 DDZ = "Map Delta Z"
 DPF = "Data Point Format"
 NPT = "Number of Data Points"
 NPZ = "Map Points in Z"
 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 Multiplier"
SSP = "Sample Spacing Divisor"
SGP = "Switch Gain Position"
SGW = "Gain Switch Window"
INS = "Instrument Type"
P2A = "Peak Amplitude 2nd Channel"
P2L = "Peak Location 2nd Channel"
P2R = "Backward Peak Amplitude 2nd Channel"
P2K = "Backward Peak Location 2nd Channel"
P3A = "Peak Amplitude 3rd Channel"
P3L = "Peak Location 3rd Channel"
P3R = "Backward Peak Amplitude 3rd Channel"
P3K = "Backward Peak Location 3rd Channel"
P4A = "Peak Amplitude 4th Channel"
P4L = "Peak Location 4th Channel"
P4R = "Backward Peak Amplitude 4th Channel"
P4K = "Backward Peak Location 4th Channel"
DAQ = "Data Acquisition Status"
SSM = "Sample Spacing Multiplier"
SSP = "Sample Spacing Divisor"
SGP = "Switch Gain Position"
SGW = "Gain Switch Window"
TPX = "Total Points X"
NSN = "Scan Number"
MVD = "Max. Velocity Deviation"
HUM = "Humidity Interferometer"
TSC = "Scanner Temperature"
TSM = "Sample Temperature"
PIM = "Pressure Interferometer"

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. μ sec"
IDL = "Interleave Trigger Delay μ sec"
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-DEM
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"
PTH = "Measurement Path"
EXP = "Experiment"
PAT = "Path of File"
NAM = "Filename"
NA2 = "Ch. 2 Filename"
ATX = "Annotation Text"
XPP = "Experiment Path"
RAT = "TRS Method name"
CPR = "Copyright message"

Additional Information

Run OPUS from CD

It is possible to copy OPUS directories (even write-protected ones) on CD and run OPUS from CD. This will not install OPUS on your system! Note that possible changes made, e.g. in the workspace, when running OPUS on CD are only stored temporarily. Therefore, they will not be available when restarting OPUS from CD.

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 evaluation 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	X	Macro file
.MTB	N	Macro file
.MTD	X	Library method
.MTX	N	Macro file
.NTI	N	Optical bench configuration file
.OWS	N	OPUS workspace
.PCT	X	Parameter correlation table used for JCAMP-DX
.PLE	N	Printing template
.PLT	X	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...

Extension	Used By^a	Description
.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. N: used by OPUS

X: used by both programs



Appendix B

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

$$n = n + ik \quad (\text{B-1})$$

complex dielectric constant

$$\varepsilon = \varepsilon' + i\varepsilon'' \quad (\text{B-2})$$

and the logarithm of the amplitude-reflectivity

$$\ln(re^{i\Phi}) = \ln(r) + i\Phi \quad (\text{B-3})$$

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 KKT to first calculate the phase rotation angle $\Phi(\nu)$ as function of the wavenumber ν from the measured reflectance spectrum $R(\nu) = r^2(\nu)$ of an optically thick sample. Then, the reflectivity of the air/sample edge (vertical incidence) is calculated from $r(\nu)$ and $\Phi(\nu)$ using the Fresnel equation:

$$\Gamma(\nu)e^{i\Phi(\nu)} = [n(\nu) - 1]/[n(\nu) + 1] \quad (\text{B-4})$$

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

$$n(\nu) = [1 - R(\nu)]/[1 + R(\nu) - 2R^{1/2}(\nu)\cos(\Phi(\nu))] \quad (\text{B-5})$$

$$\kappa(\nu) = 2R^{1/2}(\nu)\sin(\Phi(\nu))/[1 + R(\nu) - 2R^{1/2}(\nu)\cos(\Phi(\nu))] \quad (\text{B-6})$$

If desired, the dielectric function is calculated:

$$\varepsilon' = n^2 - \kappa^2 \quad (\text{B-7})$$

$$\varepsilon'' = 2n\kappa \quad (\text{B-8})$$

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

$$A(\nu) = \log(e)2\pi\nu d\kappa(\nu) \quad (\text{B-9})$$





In principle, KKT enables to determine all important optical sample properties on the basis of one single measurement (reflectance spectrum $R(\nu)$). At least two measurements are required to determine the real and imaginary part of the complex quantities (B-1) to (B-3).

Equation (B-9) is implemented such that OPUS does not calculate $A(\nu)$ from a given thickness d but selects d , with the maximum of $A(\nu)$ being 1.0. This results in comparable intensities similar to absorption spectra measured in transmission. Therefore, the intensities of $A(\nu)$ are only defined up to a freely selectable scaling factor.

$A(\nu)$ according to equation B-9 is not directly comparable with the measured $A_g(\nu)$ absorption spectrum of a layer of thickness d as the absorptivity only describes the absorption of the pure medium without any reflection losses. In contrast, the measured $A_g(\nu)$ absorption spectrum is always a combination of absorption and reflection at the two boundaries of the sample. In case of simple reflection this can be considered by the additional factor $(1 - R)^2$, with multiple reflections and interference being neglected.

$$A_g(\nu) = -lgT = -lg[(1 - R)^2 10^{-A(\nu)}] \quad (\text{B-10})$$

Performing KKT

The *Kramers-Kronig-Transformation* dialog is called from the *Manipulate* menu. The desired result function can be selected in the *Compute* group field. The *Refractive index (complex)* and *Dielectric function (complex)* both produce two data blocks, with the real part being stored in the ABR reference data block () and the imaginary part in the ABI sample data block (). One data block only is created in case of *Absorbance* () and *Phase* ().

To define the frequency limits used to perform KKT click on the *Frequency Range* tab.

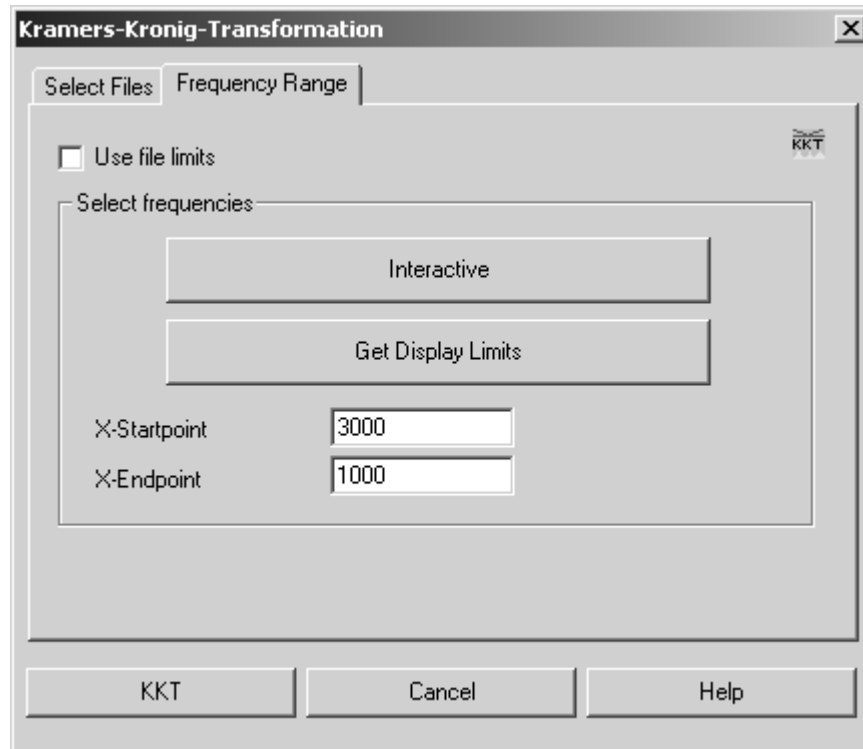


Figure 419: Kramers-Kronig-Transformation - Frequency Range tab

If you activate the *Use file limits* check box, you specify the entire frequency range. In this case the other options in the *Select frequencies* group field will be disabled.

To select a particular part of the frequency range either click on the *Interactive* or *Get Display Limits* button. You can also determine the frequency range manually by means of the *X-Startpoint* and *X-Endpoint* entry fields.

Note: When selecting the frequency range make sure that the spectrum is as flat as possible at the edges, and does not abruptly break off at high intensity changes.

Preconditions and Restrictions

KKT can only be used reasonably if the following preconditions are met as best as possible. Thus, a large number of errors can be avoided.

Limited Frequency Range

Strictly speaking, KKT is only valid on condition that the function to be transformed is known for the entire spectral range from $\nu = 0$ to $\nu = \infty$. This can, however, never be achieved in practice. Therefore, KKT of the logarithmized reflectance spectrum is only an approximation of the $\Phi(\nu)$ phase. When selecting the frequency range make sure that the reflectance spectrum is flat at the edges. Avoid any significant structures at the edges of the spectrum.

The KKT software in OPUS extrapolates the $\ln(R)$ spectrum in horizontal direction at the edges, which is a suitable approximation for insulators. In case of semiconductors, however, this kind of approximation cannot be used as their reflectivity with $\nu \geq 0$ tends to 1. You can only extrapolate to $\nu \geq 0$ correctly in case of semiconductors if you have appropriate information on the effective mass and concentration of free charge carriers. Furthermore, you have to be able to measure far enough in the FIR range such that $R(\nu)$ monotonously tends to 1 again and can be fitted by a model function. At present, an automatic $\nu \geq 0$ extrapolation in case of semiconductor reflectance spectra is not yet possible with OPUS.

Measuring Accuracy

In general, calculating optical constants by KKT on the basis of reflectance data requires a very reliable measuring accuracy. Therefore, noise, insufficient water vapor and CO₂ compensation, non-linearities or baseline drifts have an adverse effect on the measuring accuracy.

The reflectance spectrum should not contain any zero lines as otherwise the $(\ln R)$ KKT integrand becomes singular. In case of highly absorbing material, e.g. NaCl, SiO₂, the reflection decreases in some positions from 10^{-3} to 10^{-4} which may lead to the fact that the measuring errors are greater than the wanted signal.

The result of KKT substantially depends on the correct spectrum intensity within these critical ranges. Wrong intensities in the reflectance spectrum can frequently be detected by a sometimes negative absorption coefficient $k(\nu)$. In this case spectral noise effects can be minimized by smoothing. Furthermore, at least the reflectance value can be set to the correct order of magnitude by adding/subtracting a linear offset.

Incorrect Model

The sample used has to correspond to the model of an optically thick sample (half-space reflection), i.e. no radiation, which has been reflected on a rear boundary, may emit from inside the sample. If, e.g., the reflectance spectrum contains interference patterns, the sample has certainly be too thin.

If the sample you use is not thick enough, roughen the sample to avoid back reflection. Strictly speaking, the calculation of optical constants outlined before on the basis of the reflectance spectrum is only valid in case of vertical incidence. Therefore, this kind of calculation should only be used in case of measurements which have been performed by using *almost vertical* incidence (10° reflection unit).

Examples

KKT can be verified quite well by theoretical reflectance spectra which have been acquired from the following oscillator model for dielectric function:

$$\varepsilon(\nu) = \varepsilon_{\infty} + \sum((\Omega_{pj}^2)/[\Omega_{tj}^2 - \nu^2 - i\nu\Omega_{rj}]) \quad (\text{B-11})$$

With Ω_{pj} , Ω_{tj} and Ω_{rj} being the intensity, resonance frequency and line width of the j^{th} oscillator. ε_{∞} is a linear contribution to the dielectric function. Based on the real and imaginary part of the above model with the dielectric function ε' and ε'' the real and imaginary part of the refractive index

$$n = [0,5\varepsilon' + 0,5(\varepsilon'^2 + \varepsilon''^2)^{0,5}]^{0,5} \quad (\text{B-12})$$

$$k = [-0,5\varepsilon' + 0,5(\varepsilon'^2 + \varepsilon''^2)^{0,5}]^{0,5} \quad (\text{B-13})$$

can be calculated. This yields to the reflectivity R (for vertical incidence, optically thick sample) with

$$R = [(n - 1)^2 + k^2]/[(n + 1)^2 + k^2] \quad (\text{B-14})$$

and the phase shift Φ with

$$\Phi = \arctan[2k/(n^2 - 1 + k)] \quad (\text{B-15})$$

Figure 1 shows a reflectance spectrum (R) of NaCl, which has been calculated by the following model parameters (3 oscillators, with all Ω values being cm^{-1}):

$\varepsilon_{\infty}(2.3)$

	j = 1	j = 2	j = 3
Ω_{tj}	164	233	254
Ω_{pj}	284	60	40
Ω_{rj}	5,5	28	16

The corresponding phase spectrum (Φ), real and imaginary part of the refractive index (N, K) and dielectric function $\varepsilon', \varepsilon''$ have been calculated both on the basis of the model parameters (equations B-10 to B-14) and per KKT, as well as compared with each other. In both cases the data points have been quite conform.

Figure 2 shows a measured reflectance spectrum of NaCl as well as the refractive index and dielectric function both derived by KKT. Compared to figure 1 considerable errors can be detected (strong negative parts in the K and ε'' spectra).

This erroneous result is mainly due to the inaccuracy of the measured spectrum in the range of the lower limit at about 340cm^{-1} .

Figure 3 is the same as figure 2, however, the experiment spectrum has been smoothed first, to get a more even band in the range of the lower limit. Afterwards, a linear offset has been deducted to reduce the intensity in the range of the lower limit from 0.008 to the value of the theoretical spectrum R in figure 1 (0.002). Thus, the erroneous parts of the K and ε'' spectra could be substantially decreased as shown in figure 3.

Figure 4 shows the influence of extrapolation at the low-frequent end of the spectrum. The theoretical spectrum of figure 1 has been cut at 50cm^{-1} and transformed by KKT. Compared to figure 1 there are insignificant amounts of negative parts and higher intensities in the K and ε'' spectrum, however, these effects are less distinctive than in figure 2.

Figure 5 and **figure 6** are further examples to verify KKT on the basis of the theoretically calculated reflectance spectra of SiO_2 and polystyrene (PS), analog to figure 1. The results received by KKT are again quite conform. The following model parameters have been used:

$$\varepsilon_{\infty}(2.4)$$

	j = 1	j = 2	j = 3	j = 4
Ω_{tj}	1445	800	1075	1190
Ω_{pj}	422	240	867	266
Ω_{rj}	30	70	20	70

Polystyrene (5 oscillators):

$\varepsilon_{\infty}(2.4)$

	j = 1	j = 2	j = 3	j = 4	j = 5
Ω_{tj}	542	699	763	1452.5	1493.5
Ω_{pj}	57	100	65	40	50
Ω_{rj}	60	7	12.5	5	10

Figure 7 shows both a measured reflectance spectrum (R_{xp}) of polystyrene (PS) and the absorption coefficient (K_{xp}) as well as the absorptivity (A_{xp}) calculated therefrom by KKT. To enable a direct comparison both the theoretical reflectance spectrum (R_{th}) and the spectra (K_{th}) and (A_{th}) calculated therefrom by KKT are also displayed. This comparison makes it possible to assess the error to be expected in practice.

When calculating the absorptivity A from the absorption coefficient k according to equation B-9 the intensities are scaled proportionally to the wavenumber. This means that noise and interferences in the reflectance spectrum in case of high wavenumbers additionally increase by transformation.

The example spectra of the different figures are available as OPUS files.

Figure 1: NaCl, theoretical

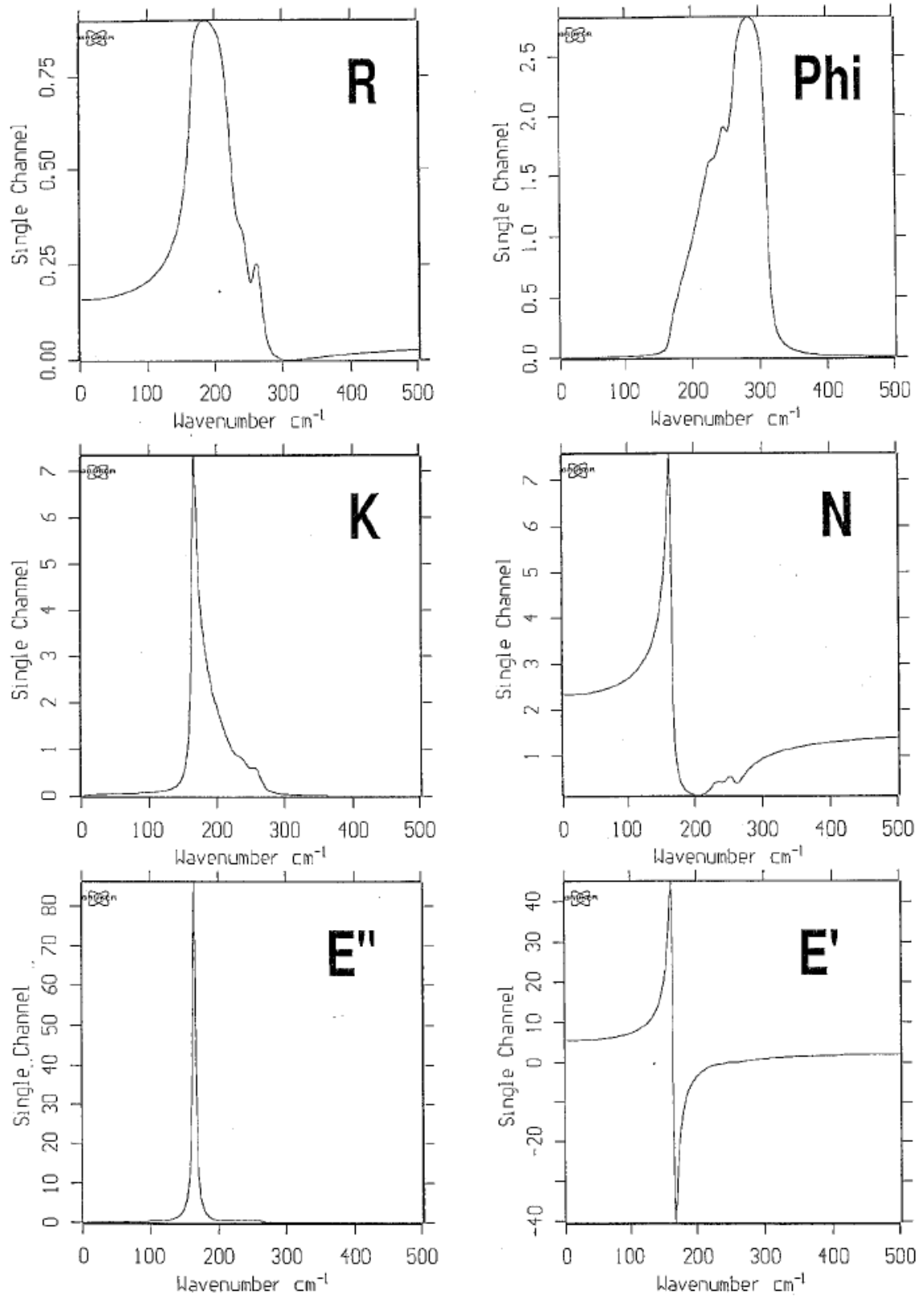


Figure 2: NaCl, measured

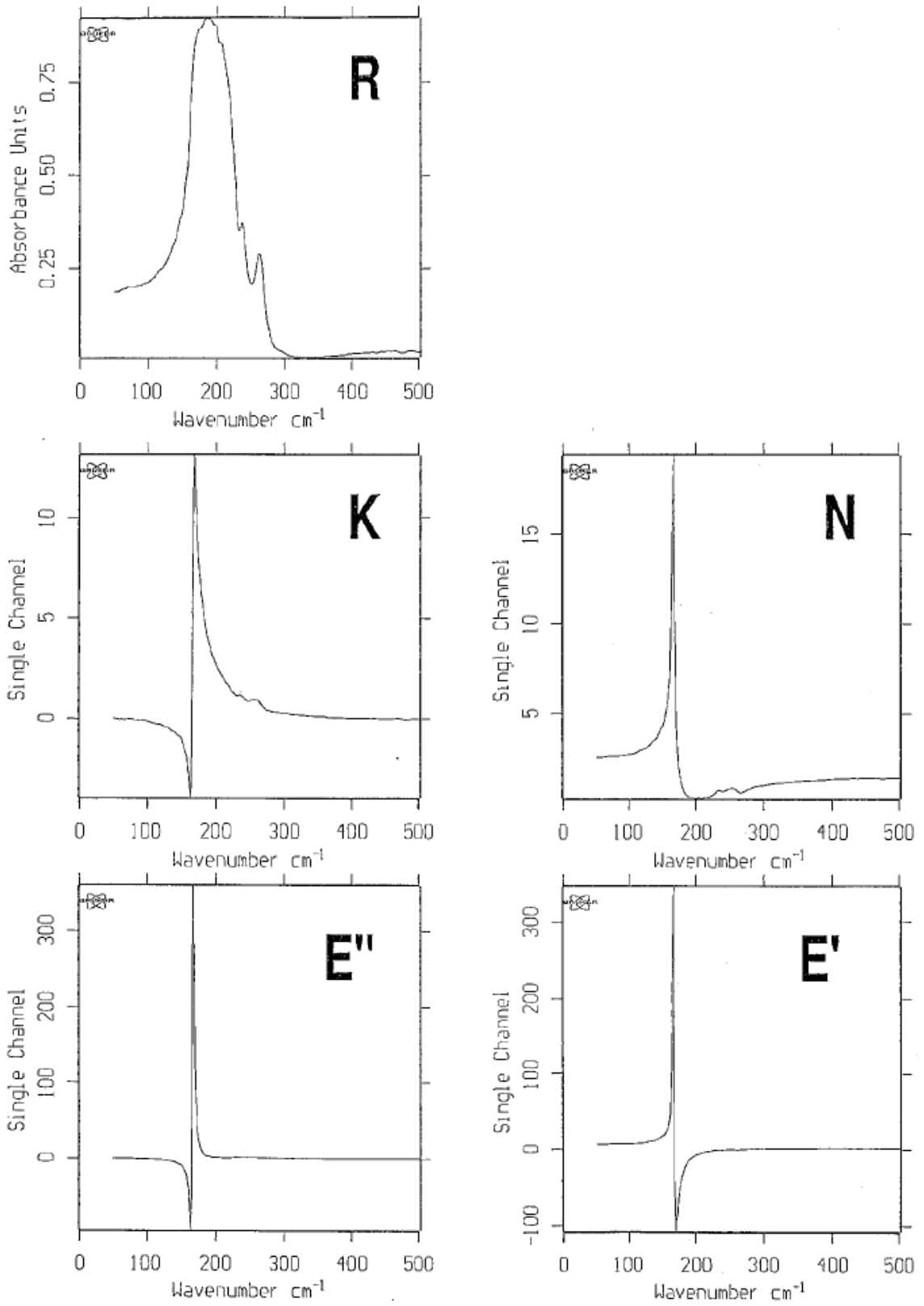


Figure 3: NaCl, measured, transformed

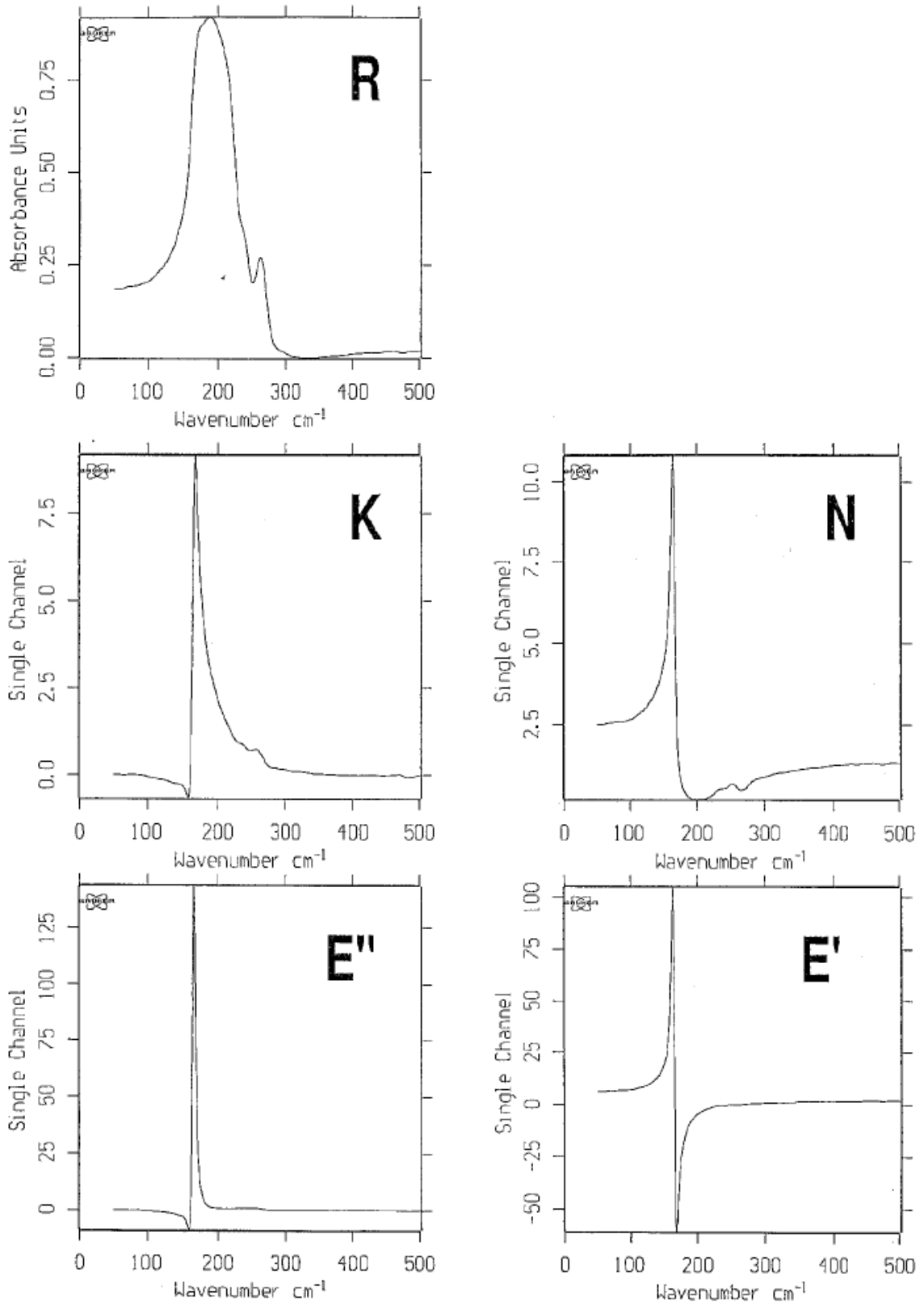


Figure 4: NaCl, theoretical up to 50cm⁻¹

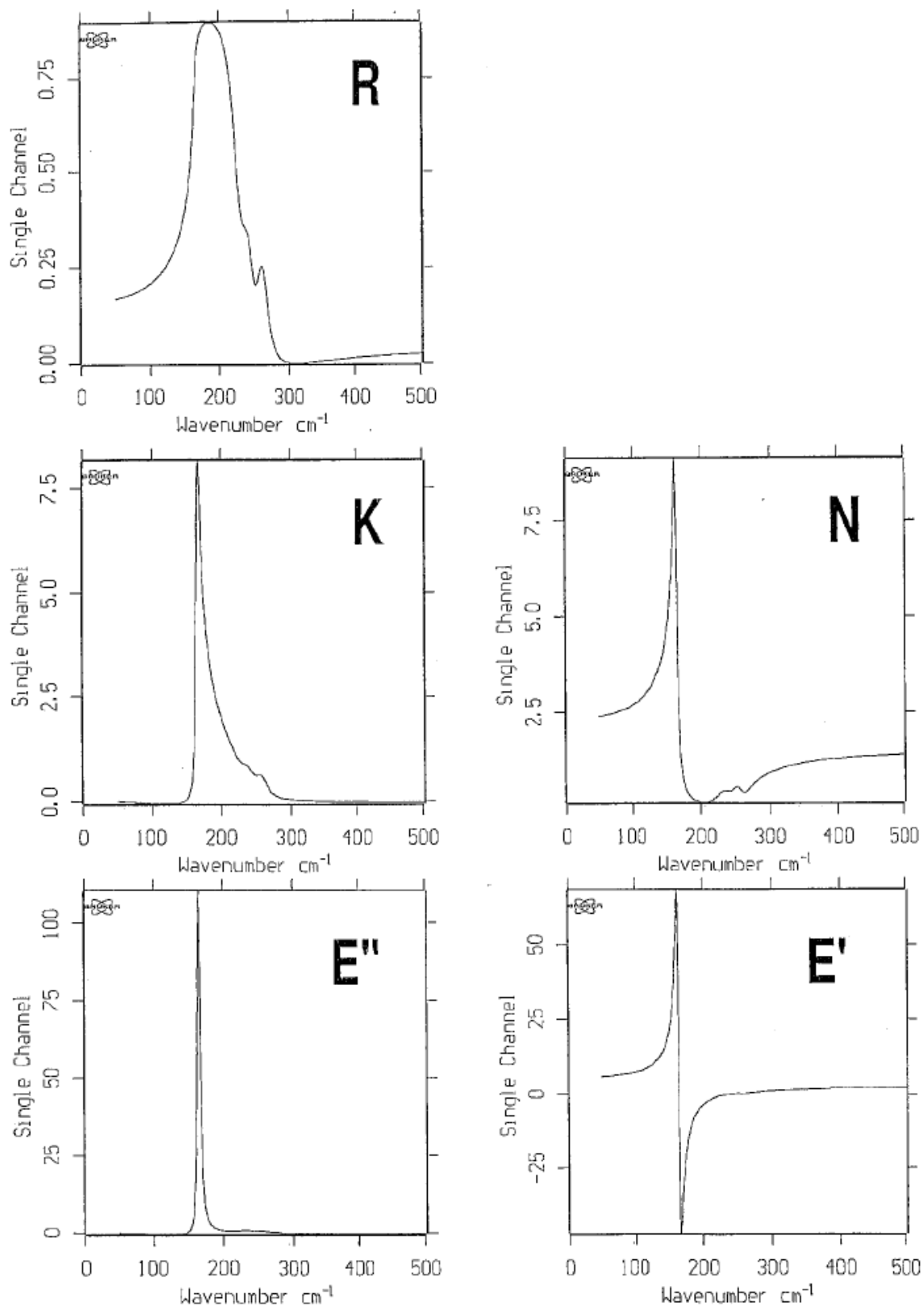


Figure 5: SiO₂, theoretical

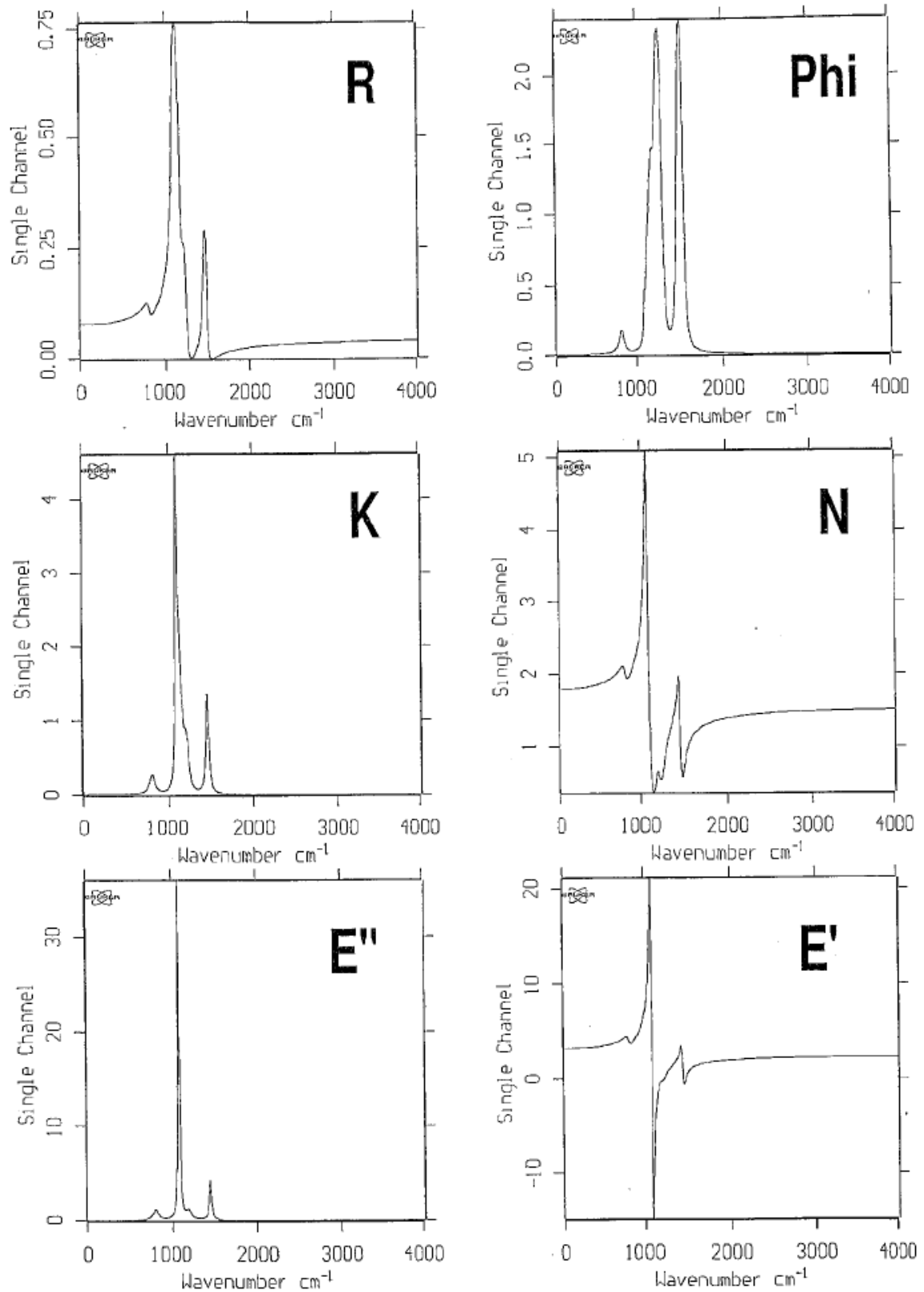


Figure 6: PS, theoretical

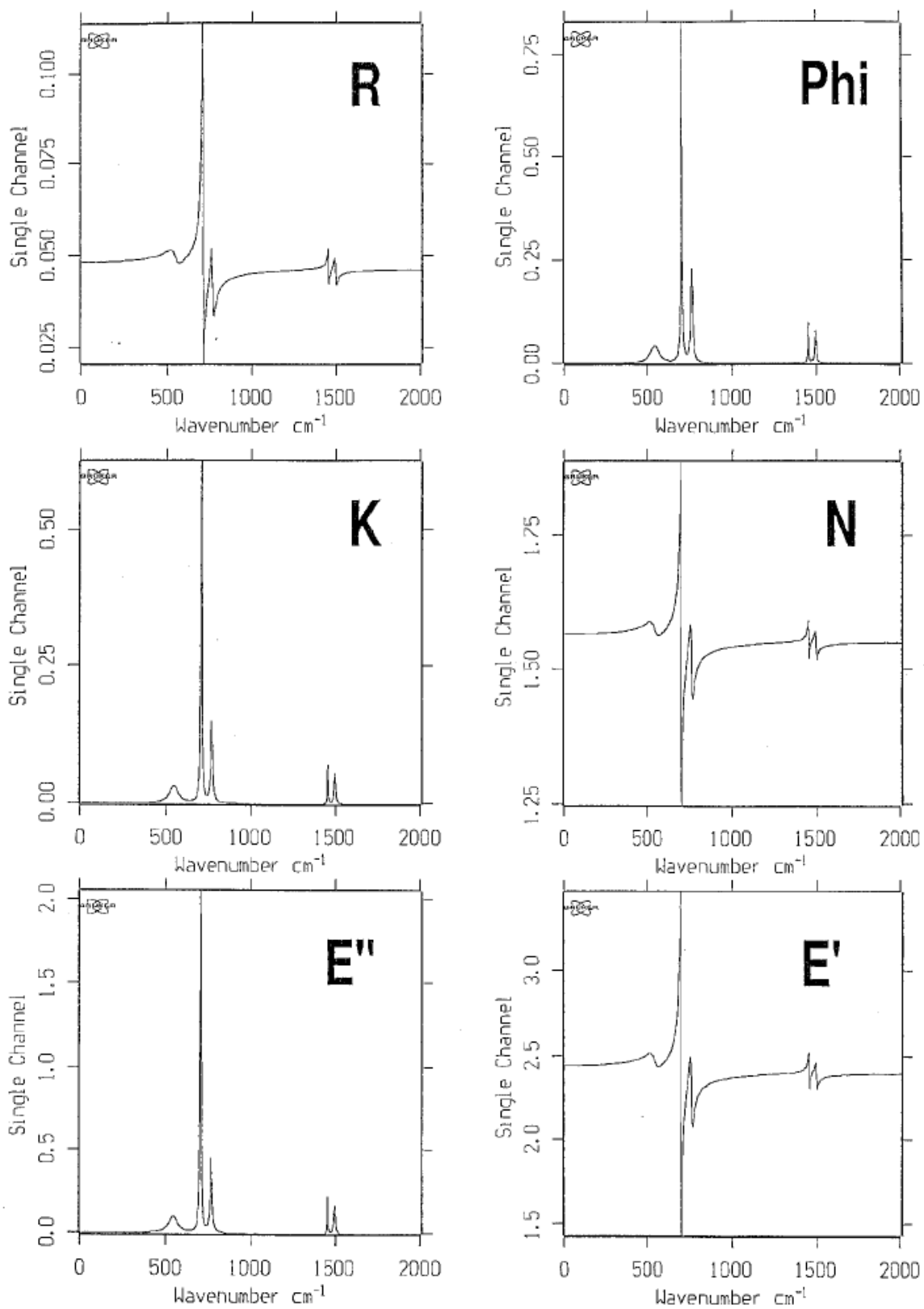
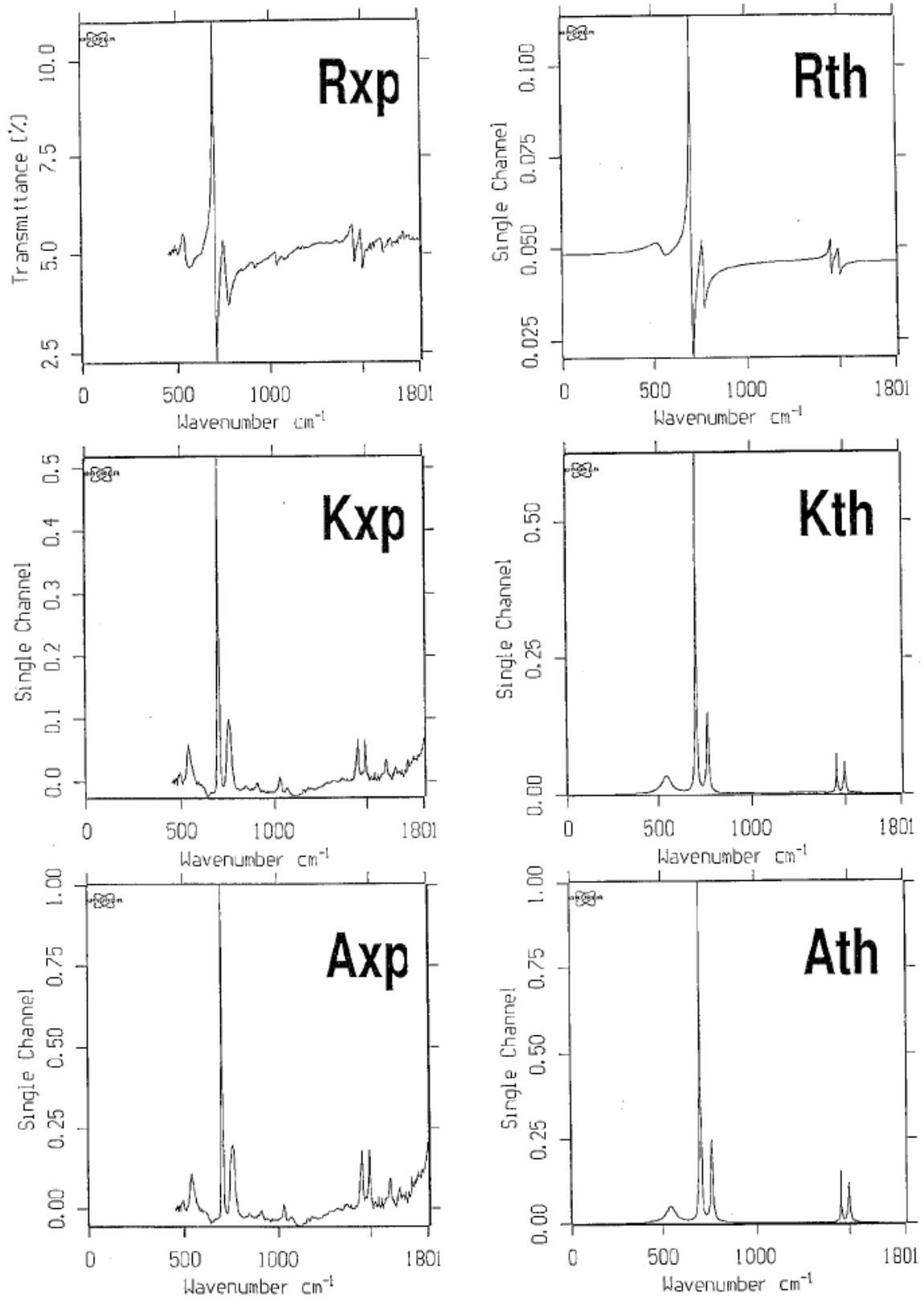


Figure 7: PS, absorbance



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