OPUS

Introduction

1003198, Version 8

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www.bruker.com

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The description given in this manual is based on the technical specifications and the technical design valid at the time of publication. Technical specifications and technical design may be subject to change.

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

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1 Introduction

1.1 About this manual

This manual is a quick reference guide about the OPUS spectroscopy software. For important information the manual uses the following format:

i The *i* provides important information given to the user to facilitate system operation, and make the best possible use of the software.

1.2 Terms

This manual uses the term *OPUS* when the software is described.

1.3 Gender-neutral form

The manual uses the male form in a neutral sense and does not differentiate between male and female users. We would kindly ask all female users to have understanding for this simplified form.

1.4 Questions and concerns

If you have questions or concerns about operating the software, contact Bruker at the numbers listed below:

- Service hotline: +49 (0) 7243 504-2020
- Fax: +49 (0) 72 43 504-2100
- E-mail: service.bopt.de@bruker.com
  service.bopt.us@bruker.com
- Internet: www.bruker.com/optic
- International service: www.bruker.com/about-us/offices/offices/bruker-optics

2 Installation Instructions

2.1 System requirements for software

PC data system:	• parallel and serial interface[a] • Ethernet, RJ45, 10Base T (10 or 10/100MHz) • USB[b] • Mouse, keyboard • PCI and PCIe-x1 interface[c]
Processor:	**Minimum:** Intel Pentium III, 800MHz **Recommended:** Intel I5 or Dual Core
RAM:	2 GB
Hard disk:	250 GB, IDE
Graphics card:	XVGA, >128MB RAM, 32 color-bit depth, open GL and support of Direct-X, version 9 or higher (for OPUS/VIDEO, OPUS/3D)
External drive:	**Minimum:** CD ROM burner **Recommended:** DVD ROM burner

Table 2.1: System requirements for software

Monitor:	**Minimum resolution:** 1024 x 768 **Recommended resolution:** 1600 x 1200
Operating system:	**Minimum (OPUS 8 and higher):** • Windows 7 Home Premium or better (recommended: Professional or better), 32 or 64 bit[d] • Windows 10
Ethernet:	**Windows 7 or 10 and OPUS 8 or higher:** • Internet explorer 10 **General (for any OPUS version):** • TCP/IP must be configured • Address range of PC network card must include spectrometer IP • Port 80 to spectrometer via network card must be available • No proxy is allowed to interfere with the communication to the optics • USB port must be available

Table 2.1: System requirements for software

a. Only required when connecting external devices, e.g. temperature controller, and Sadtler libraries (parallel interface).

b. USB 2.0 is required for loading OPUS and operating the digital cameras built-in the Hyperion, Ramanscope III, SENTERRA (2x) and LUMOS (requires 2 ports; optionally 3 ports, if a network adapter is to be used) microscope.

c. Some types of accessories (e.g. A673-X, A750/x, S522-20, S522-200, Frame-Grabber etc.) require a data system which accommodate one or more cards in their entirety.

d. The 64 bit variant is only allowed in case of special types of spectrometers.

2.2 Access rights

- Windows Administrator rights required to install or register OPUS
- Complete write access required to the target path
- Complete access required to USB ports, no restrictions on access rights by services such as *DeviceLook Service*

2.3 Miscellaneous

Configure Windows so that it is possible to see the file extensions of registered file types.

1. Open the Windows Explorer.
2. On the *Tools* menu, click the *Folder Options* command.
3. Click the *View* tab.
4. Delete the checkmark in front of the *Hide extensions for known file types* option.
5. Click *OK* to confirm the settings.

2.4 Installing OPUS using Windows 7 or 10

When using Windows 7 or 10 it is not sufficient to be logged into the operating system as a user with Administrator rights. You need to perform the installation explicitly as administrator, and start the installation manually as follows:

1. If the installation starts automatically after inserting the OPUS stick, interrupt the installation procedure.
2. In the *C:\Program Files\Bruker\OPUS_<version>* directory, right click the *SETUP.EXE* file.
3. From the pop-up menu that opens, select the *Run as Administrator* option.
4. Confirm the message that pops up to be able to continue.

2.5 Modifying, repairing or removing single OPUS features

i For technical reasons not all features are deleted when de-installing the OPUS program. If you want to remove OPUS completely, you have to delete the OPUS directory manually after de-installation. Before you do this, store all important data (e.g. workspaces, printing templates, macros etc.) in a different directory.

1. Click the Windows Start menu.
2. Select the *Control Panel* command.
3. On the view that opens, select the *Programs and Features* command.
4. Right click the current OPUS version installed.
5. From the pop-up menu displayed, select the *Change* command.
6. On the view that opens, check the particular option button depending whether you want to modify, repair or remove OPUS features.
7. Click the *Next* button.
8. Use the InstallShield Wizard to make the settings.
9. Click the *Finish* button.

3 Installing OPUS

i By default, the OPUS spectroscopy software is supplied on a USB stick.

3.1 Installation procedure

1. Insert the OPUS stick supplied into the USB port of your PC.
   ➢ *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 the stick.*
2. Follow the on-screen installation instructions.
3. Enter the OPUS registration date.[1]
   ➢ *The registration data are provided on the OPUS stick. The registration has to be performed only once and is valid for all users.*
4. Define whether OPUS is to run in the 21 CFR Part 11 validation mode or not.[2]
5. Select the language to be used for OPUS.
6. Restart the PC at the end of the installation procedure.
   ➢ *If you are prompted to restart your computer when you install different program components, do NOT restart before the OPUS setup has been completed.*

1. If you want to install an OPUS test version (valid for 30 days), you do not need to enter any registration data. In this case, set a checkmark for the test option.
2. This one-off setting (to be activated in the program options) cannot be undone and has comprehensive effects on the work with OPUS. 21 CRT part 11 is a quality regulation legally approved by the United States Food and Drug Administration (FDA), which also regulates the requirements on data integrity. If OPUS 8 or higher has to run in validation mode with a user-specific database connected, you have to define the user-specific database during installation.

3.2 OPUS Login

1. When the installation has been finished, click the OPUS icon on the Windows Start menu.
2. On the dialog that opens, select the user ID[1] from the drop-down list.
3. Enter *OPUS* as password.
   ➢ *The password is case sensitive. Once you have assigned yourself a user account in OPUS, it is possible to determine your own user ID and password. In 21 CFR Part 11 validation mode, you will be requested to change the password immediately after the first login. Details are described in chapter 3.2.1.*
4. Select a workspace.
   ➢ *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 very first time, we recommend to accept the standard 'default.ows' workspace.*
5. Click the *Login* button.
6. On the dialog that opens, click the *OK* button.
   ➢ *The OPUS user interface opens.*

3.2.1 Changing password in 21 CFR Part 11 validation mode

1. After the very first OPUS login you are requested to change the password. Click OK to confirm the request.
2. In the dialog that opens, enter the new password and verify it.
   ➢ *According to the 21 CFR Part 11 validation mode the password has to comply with special complexity requirements. In the activated validation mode, the password has to fulfill the following minimum conditions:*

1. By default, OPUS provides the following user IDs: Admin, LabManager and Operator. Detailed information on the user ID are described in the OPUS Reference Manual.

- ➢ *Total length: 8*
- ➢ *Number of numerals: 1*
- ➢ *Number of letters: 1*
- ➢ *Number of lower case letters: 1*
- ➢ *Number of upper case letters: 1*
- ➢ *Number of special characters: 1*

3. Click the *Change Password* button.
4. In the *Login* dialog, enter the new password and click the *Login* button.

3.3 OPUS user interface

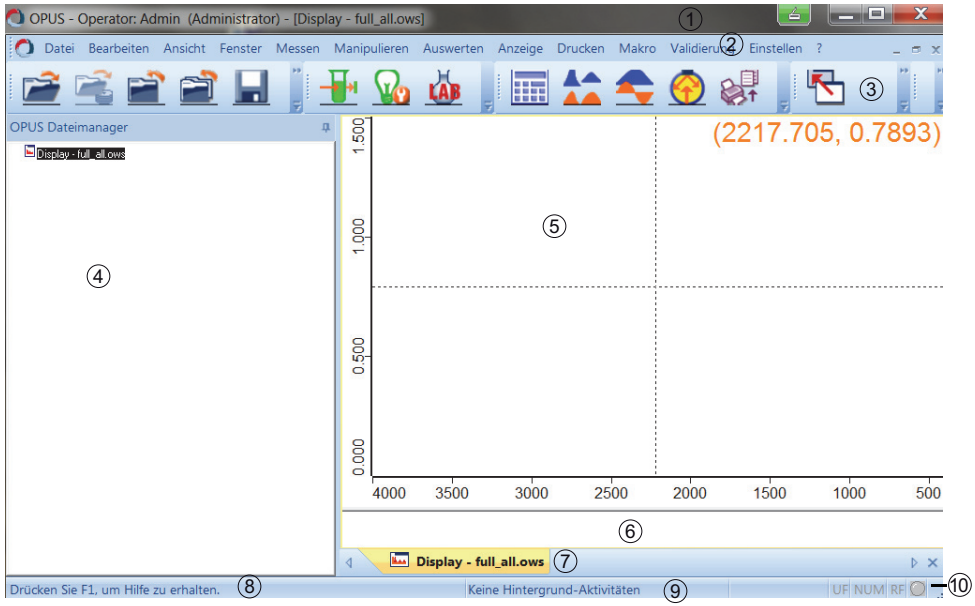


Figure 3.1: OPUS user interface

	Element	Definition
1	Title bar	The title bar shows the user ID and the work-space assigned to the user.
2	Menu bar	The menu bar shows all menus available in OPUS. The individual menus allow access to all OPUS commands.
3	Toolbar	The toolbar contains frequently-used OPUS commands, individually configured by means of icons.
4	Browser	The browser shows the spectrum files loaded, with the particular data blocks.
5	Spectrum window	The spectrum window shows the spectrum file loaded. By default, a crosshair is displayed. The current position of the crosshair (e.g. wavenumber and intensity) are displayed on the upper right edge. This allows to read out the x/y positions directly from the spectrum. Right clicking the spectrum window hides the crosshair.
6	Overview window	The overview window shows the complete frequency range of the spectrum file loaded.

Table 3.2: Elements of OPUS user interface

	Element	Definition
7	OPUS view	The OPUS view you work with is indicated by a tab. Each tab has a different color to be able to distinguish between the OPUS views. If several OPUS views are open simultaneously, click the respective tab or use the buttons on the left and right to change between the different OPUS views.
8	Online help	The OPUS online help provides detailed information on all OPUS commands and can be opened by clicking the F1 key.
9	Status bar	The status bar informs about active tasks currently running in OPUS Introduction, and shows their status.
10	Instrument status	The instrument status is indicated by the OPUS status light ( ) as follows: • Gray: no spectrometer connected • Green: spectrometer connected • Yellow: warning • Red: error

Table 3.2: Elements of OPUS user interface

3.4 Access control

OPUS has an access control system which is shown in figure 3.2.

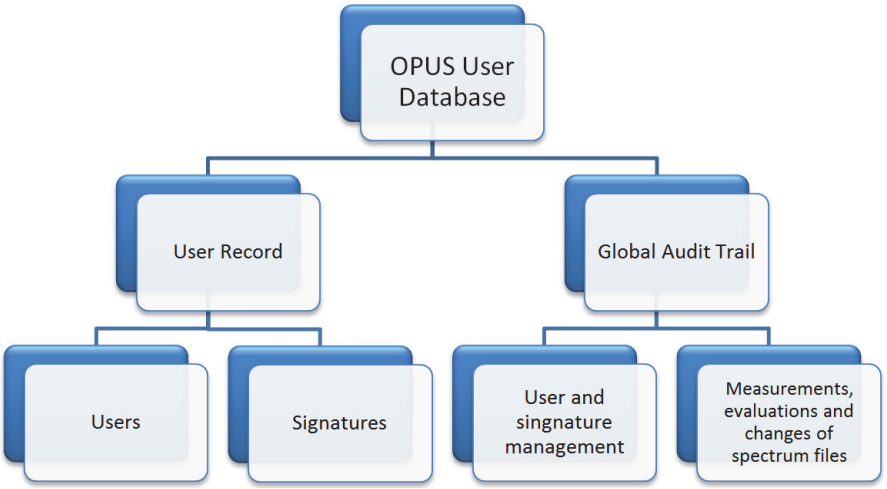


Figure 3.2: Access control in OPUS

3.4.1 User record

The user records in the OPUS user database comprise:

- User ID
- Password
- Operator name
- User group (Administrator, Operator)
- Signature categories
- Accessible workspaces

3.4.2 OPUS workspace

The workspaces comprise:

- Menu contents
- Toolbar contents
- Access rights within OPUS
- Other settings (e.g. file increment mode, display limits)

Detailed information on the user management e.g. to add, modify or remove users from the user database are described in the OPUS Reference Manual.

3.4.3 Audit trail

The global audit trail logs all actions which have been performed in OPUS in connection with the user and signature management, as well as with the single spectrum file, within a defined period of time (chapter 4.4).

Next to the type of action the audit trail also shows the user ID of the user who is responsible for this action. Details on the single manipulations and/or evaluations on spectra files are listed in the HISTORY data block (chapter 4.3).

5. Click *OK* to confirm the entries.

Detailed information on the OPUS registration are described in the OPUS Reference Manual.

Installing OPUS 3

4 Working with OPUS

4.1 Measuring a spectrum

Chapter 4.1 et seq. describes the individual steps to be performed or observed BEFORE, DURING or AFTER measuring spectra. Observe the order of the steps described.

The dialogs depend on the spectrometer configuration currently used. Therefore, the following dialogs may be slightly different from the ones displayed on your screen.

4.1.1 Connecting to spectrometer

1. On the *Measure* menu, select the *Optic Setup and Service* command, or click the icon from the toolbar.
2. In the dialog that opens on the *Optical Bench* tab, check whether the spectrometer settings are OK. If yes, close the dialog. If no, continue with step 3.
3. From the *Configuration* drop-down list, select the particular spectrometer type.
4. Enter the spectrometer's IP address into the *Optical Bench URL* entry field.
5. Click the *Connect* button.
6. Wait until the connection to the spectrometer has been established.
   ➢ *The spectrometer is connected as soon as the spectrometer name and firmware version are displayed (figure 4.3). If the connection has been successful, the OPUS status light is green.*

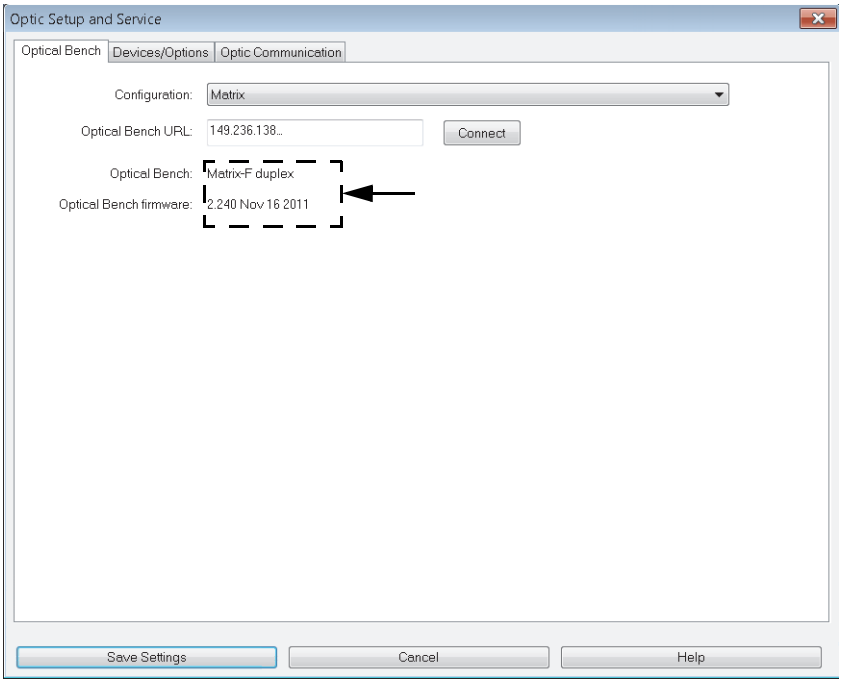


Figure 4.3: Spectrometer connecting data

7. Click the *Save Settings* button.

4.1.2 Setting up measurement parameters

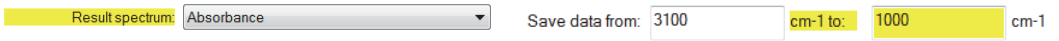
1. On the *Measure* menu, select the *Measurement* command, or click the icon from the toolbar.
2. On the dialog that opens, define the measurement parameters on the different tabs.
   ➢ *To learn more about error diagnostics when setting measurement parameters refer to chapter 4.1.2.1. Details on the individual measurement parameters are described in the OPUS Reference Manual.*
3. Click the *Accept & Exit* button.

4.1.2.1 Error diagnostics when setting measurement parameters

Display in OPUS	Meaning
	The yellow exclamation mark indicates that the particular tab contains a warning for one or more measurement parameters. **i** Measurement still possible.

Example:

➢ Yellow marking in front of the drop-down list or in the entry field of a measurement parameter.



☞ If you position the cursor on the drop-down list or entry field, a tooltip explains why a warning is available for the particular measurement parameter.

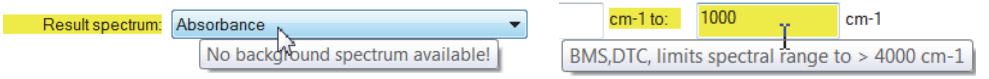


Table 4.3: Error diagnostics when setting measurement parameters

Display in OPUS	Meaning
	The warning symbols indicate that the particular tab contains one or more measurement parameters[a], which are missing or have not been correctly defined as they do not match the optic configuration. **i** Measurement not possible.
Example: ➢ Red marking in front of the drop-down list or in the entry field of a measurement parameter. ☞ If you position the cursor on the drop-down list or entry field, a tooltip explains the missing or wrong measurement parameter. 	

Table 4.3: Error diagnostics when setting measurement parameters

a. Some types of measurement parameters interact with other ones, i.e. if one measurement parameter is corrected, the warning indicated for other measurement parameters affected by the correction may no longer apply.

4.1.3 Calibrating interferogram peak

The exact interferogram peak position must be determined and stored BEFORE the very first measurement. Once determined, the interferogram peak position must be determined only if hardware changes have arisen.

1. On the *Measure* menu, Select the *Advanced Measurement* command.
2. Click the *Check Signal* tab.
3. On the dialog that opens, activate the *Interferogram* option button.
4. Use the arrow buttons (figure 4.4) to move the scan region to the left or right if no interferogram peak is displayed.

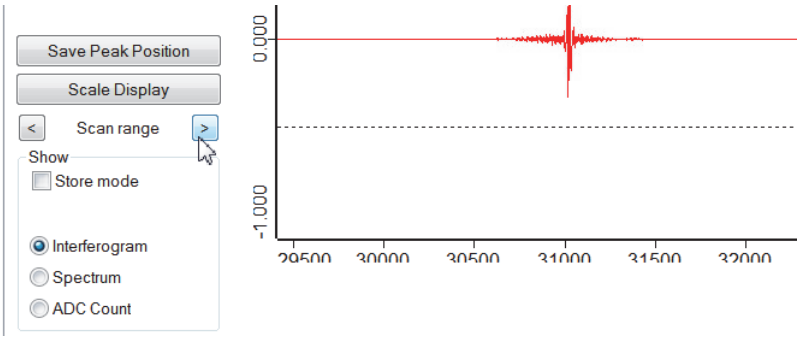


Figure 4.4: Moving scan region

5. Click the *Save Peak Position* button to store the interferogram peak.
   ➢ *The exact peak position is required to be able to perform Fourier Transformation.*
6. Click the *Accept & Exit* button.

4.1.4 Storing experiment file

1. On the *Measure* menu, select the *Advanced Measurement* command.
2. Click the *Advanced* tab.
3. On the dialog that opens, define the number of scans in the *Sample/Background Scan Time* entry fields (figure 4.5).

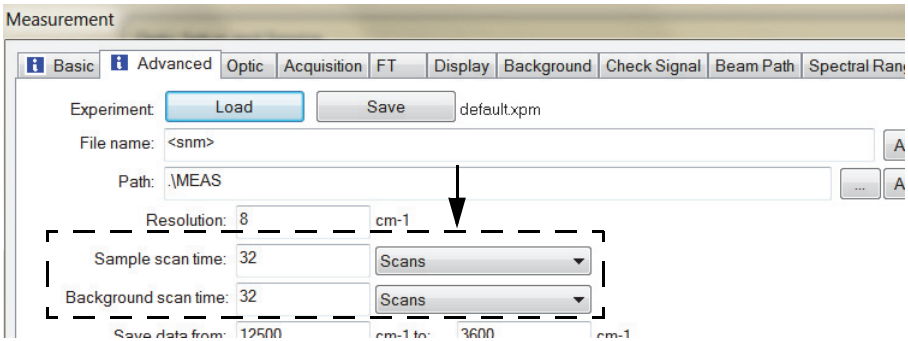


Figure 4.5: Defining number of scans

4. Define the path to automatically store the measuring data, e.g. *\MEAS.

   ➢ *Use the* ... *button to exactly select the storage path. If OPUS is used in the 21 CFR Part 11 validation mode, special requirements on the storage path must be fulfilled. Details are described in chapter 4.1.4.1.*

5. Determine the data type for the result spectrum.

   ➢ *It is recommended to select 'Absorbance' as result spectrum data type. Figure 4.6 shows possible result spectrum data types.*

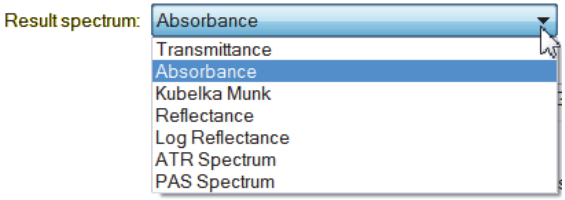


Figure 4.6: Result spectrum data types

➢ *The data type of the result spectrum can be changed at any time.*

6. Click the *Save* button.
7. On the dialog that opens, define a name for the experiment file and save this name.

   ➢ *It is recommended to repeatedly use the experiment file. When working with macros, experiment files are essential.*

4.1.4.1 Storing path in 21 CFR Part 11 validation mode

When working in validation mode 21 CFR Part 11 the storage path refers to the *Protected Pool* area[1] in the *Public Documents* directory. Paths which do not refer to the *Protected Pool* area are not accepted by OPUS, and the spectrum files cannot be stored into these paths.

4.1.5 Measuring background spectrum

In case of a background spectrum you measure an open-beam spectrum without any sample in the optical path. Therefore, a background spectrum is also called single-channel reference spectrum. Before starting sample measurement you have to measure a background spectrum, if not yet available.

1. In the *Protected pool* area, files can be edited but not deleted nor overwritten. Programs other than OPUS have no access to the files stored in the *Protected Pool* area.

The background spectrum reflects the effects that the spectrometer itself has on measured spectra. For example, the performance of the light source varies at some frequencies, or the optics absorbs light stronger at a certain wavelength.

1. Make sure that the OPUS status light is green.
2. Make sure that there is no sample available in the sample compartment.
3. On the *Measure* menu, select the *Advanced Measurement* command.
4. Click the *Optic* tab.
5. On the dialog that opens, click the *Aperture* setting drop-down list and select the same value used to acquire a sample spectrum.
6. Click the *Basic* tab.
7. On the dialog that opens, click the *Background Single Channel* button.
   ➢ *The status bar below the spectrum window indicates the progress of the background measurement, e.g. the number of scans already measured. Background measurement has finished if the status bar reads 'No Active Task'.*
8. Wait until the background measurement has finished, then measure the sample spectrum (chapter 4.1.6).

4.1.6 Measuring sample spectrum

1. If the background measurement (chapter 4.1.5) has finished, place the sample into the optical path of the spectrometer.
   ➢ *How to do this depends on the spectrometer configuration.*
2. On the *Measure* menu, select the *Advanced Measurement* command.
3. Click the *Basic* tab.
4. On the dialog that opens, define the sample description and sample form in the particular entry field.
   ➢ *This information is stored together with the spectrum.*
5. Click the *Sample Single Channel* button to start measurement.
   ➢ *The 'Measurement' dialog closes and the spectrum window opens. The status bar below the spectrum window indicates the progress of the sample*

measurement. The sample measurement has finished if the measured spectrum is displayed in the spectrum window (figure 4.7).

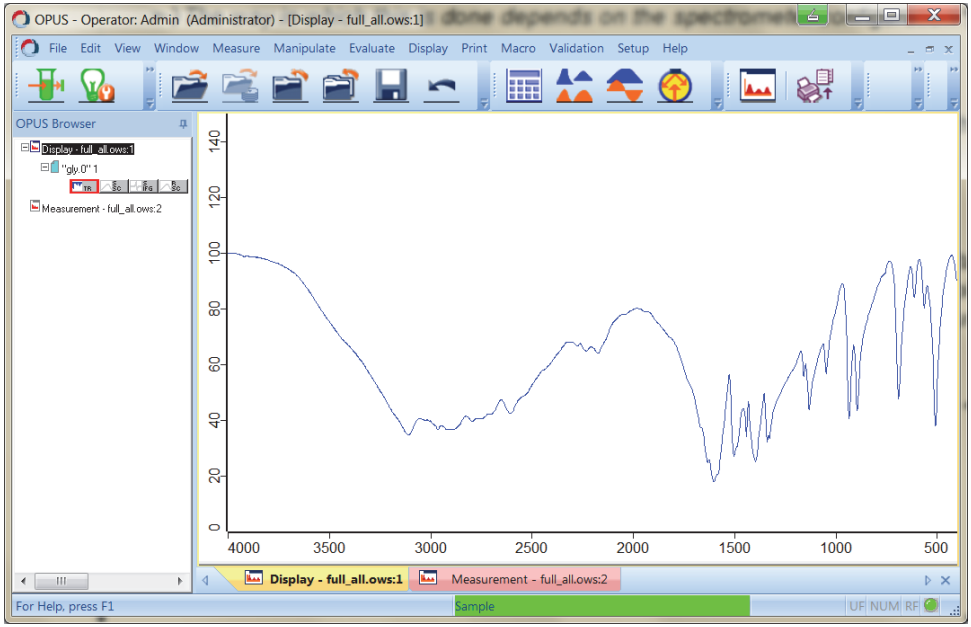


Figure 4.7: Measured sample spectrum displayed in the spectrum window

Strictly speaking, the spectrometer measures an interferogram rather than a spectrum. Using Fourier Transformation this interferogram is transferred into a single-channel spectrum. On the basis of this single-channel spectrum and the background spectrum measured, a result transmission spectrum is calculated.

To better understand the different types of spectra, figure 4.8 shows the single-channel spectrum, background spectrum and the calculated transmission spectrum. The particular data blocks are displayed in the browser.

Details on the data blocks are described in the OPUS Reference Manual.

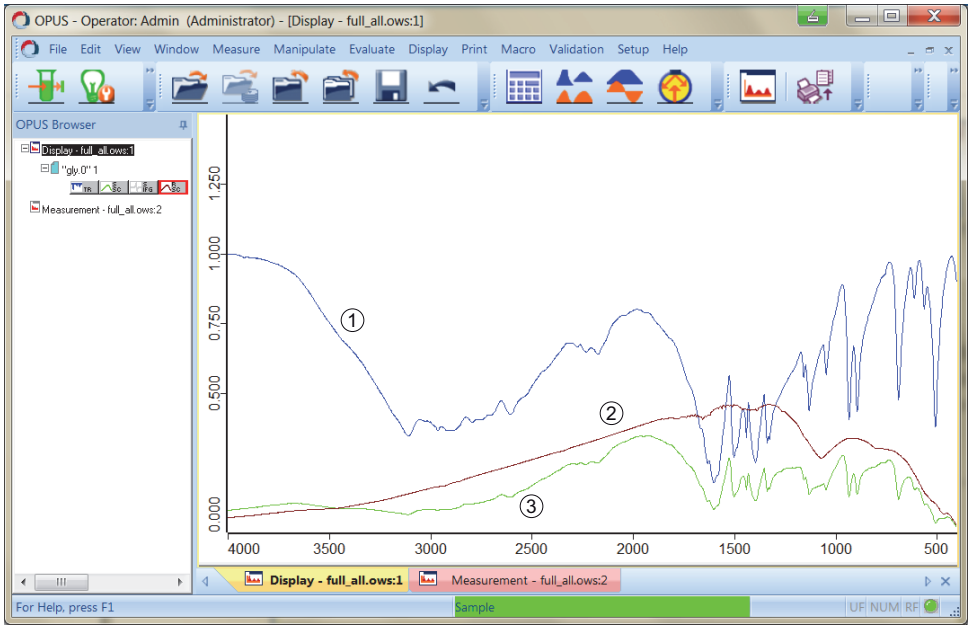


Figure 4.8: All spectrum types of a measured sample spectrum

	Definition	Data block in the browser
1	Transmission spectrum	TR
2	Background spectrum (single-channel)	RSC
3	Sample spectrum (single-channel)	SSC

Table 4.4: Definition of spectrum types

4.2 Baseline correction

Directly after sample measurement has finished, the baseline correction is useful to manipulate spectra which could not have been measured very well due to the sample material available.

If the baseline of the spectrum is sloped, curved or significantly below 100% transmission, the sample preparation might have been insufficient. Instead of measuring the sample again, perform a baseline correction. In many cases, this will solve the problem.

However, you should always try to prepare the samples properly to get good spectra, instead of correcting them after measurement.

Figure 4.9 shows an example for baseline correction. The upper spectrum is the original spectrum, the lower one is baseline corrected.

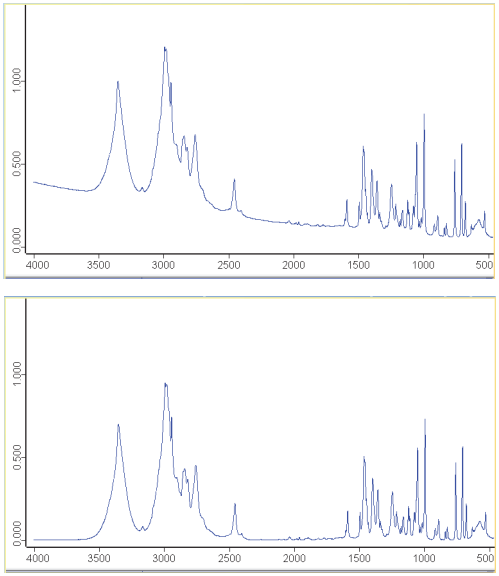


Figure 4.9: Spectrum before (top) and after (bottom) baseline correction

4.2.1 Performing baseline correction

1. On the *Manipulate* menu, select the *Baseline correction* command, or click the icon from the toolbar.
2. On the browser, double click the spectrum block (AB or TR) of the sample spectrum measured.
   ➢ *The spectrum file is displayed in the 'File(s) to correct' selection field.*
3. Click the *Select Method* tab.
4. On the dialog that opens, select a baseline correction method (figure 4.10).
   ➢ *Details on the single method types are described in the OPUS Reference Manual.*

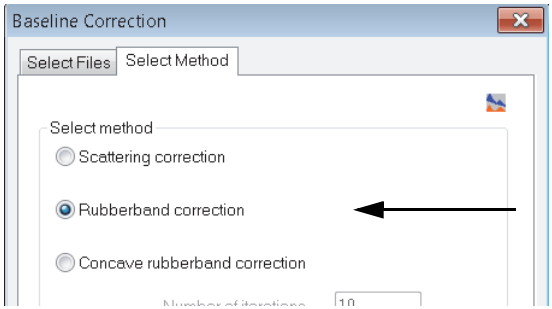


Figure 4.10: Baseline correction - Select method

5. Enter the number of baseline points manually.
   ➢ *It is recommended to accept the default value of 64.*
6. Activate the *Exclude CO2 bands* checkbox to exclude the CO_2 range during baseline correction.
7. Click the *Correct* button.
   ➢ *Baseline correction will be executed immediately.*

The browser window shows a red document symbol (figure 4.11) on top of the blue document symbol (original data). The red document symbol indicates that the spectrum file has been manipulated.

Figure 4.11: Spectrum file displayed in browser after baseline correction

4.2.1.1 Baseline correction completed

After baseline correction has been completed the spectrum has not yet been saved to hard disk and exists only as a temporary file. Save the file on hard disk, use a different file name to prevent the original file from being overwritten (chapter 4.5.2).

4.2.1.2 Undo baseline correction

1. On the browser, right click the red document symbol.
2. From the pop-up menu that opens select the *Undo all Manipulations* command.
3. On the dialog that opens, click the *Undo* button (figure 4.12).

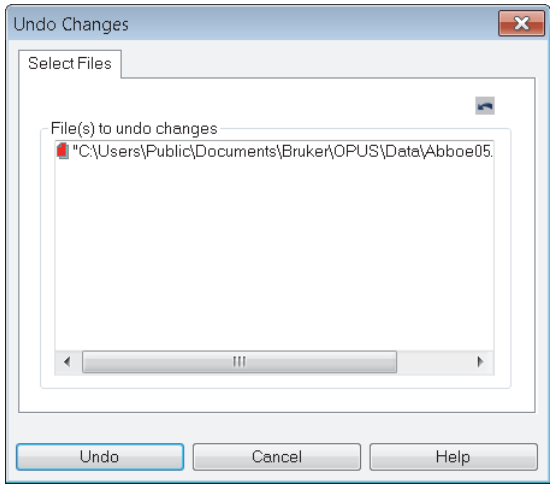


Figure 4.12: Undo baseline correction

➢ *The red document symbol is no longer displayed in the browser, and the original data are available again.*

4.3 History of spectrum files

In OPUS, measurements or manipulations and evaluations of spectrum files are reported and logged by the audit trail[1] (chapter 4.4).

If a spectrum file loaded has been edited or changed or if global measuring settings have been changed, all these actions can be recorded in a non-editable, non-deletable history data block (HISTORY).

Figure 4.13 shows parameters from a HISTOTRY data block of a spectrum file with several types of manipulations performed.

☞ To have the parameters displayed right click on the red document symbol and select the *Show Report* command.

1. The audit trail reports and logs all actions performed in OPUS within a defined period of time.

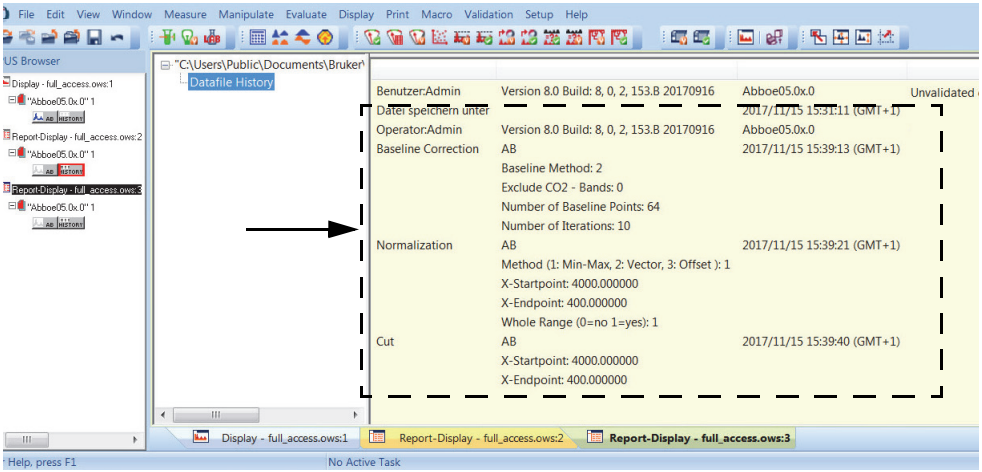


Figure 4.13: Parameters of HISTORY data block

The HISTORY data block contains the following parameters:

- user ID
- OPUS version
- spectrum file name
- all previous manipulations (in the order of performance)

The parameters are stored in one single spectrum file, together with the spectrum edited. This ensures that all data manipulations are recorded, e.g. type of manipulation method, time etc.

4.4 Viewing audit trail

The global audit trail records all actions which have ever been taken in OPUS, in chronological order. Details on the audit trail are described in the OPUS Reference Manual.

1. On the *Validation* menu, select the *View global audit trails* command.
2. In the view that opens, define a start and end date for the search period.
3. Click the *Request* button.
   ➢ *The query result is displayed in chronological order in a table (figure 4.14).*

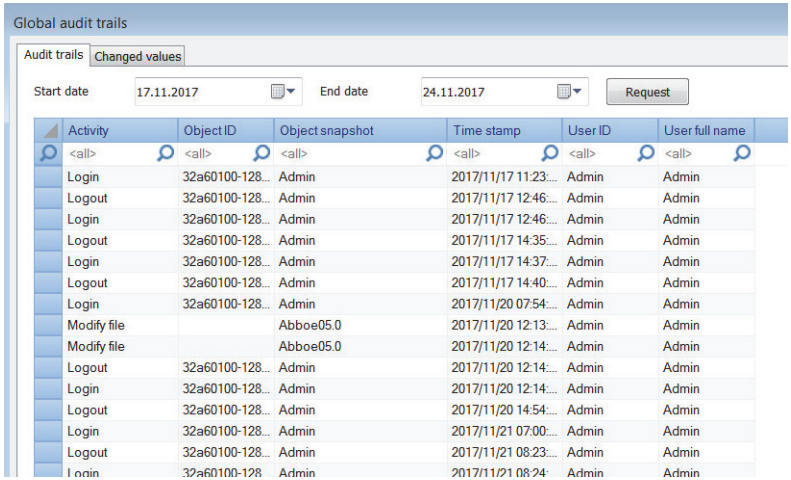


Figure 4.14: Example of an audit trail result view

4.4.1 Loading HISTORY data block from audit trail

Modifications performed on a spectrum file are saved in the HISTROY data block, which is added to the spectrum file. The HISTORY data block can be directly loaded from the audit trail for a particular spectrum file.

1. In the result view of a query, search the spectrum file which has been modified.
2. Double click the name of the modified spectrum file in the *Object Snapshot* column.
   ➢ *The parameters of the HISTORY data block are displayed in a separate report view.*

4.5 Saving spectrum

By default, the sample spectrum measured (original file) is saved in the path defined in chapter 4.1.4. If the original file has been manipulated, it is recommended to save the original file by using a different file name (chapter 4.5.2), to prevent the original file from being overwritten. Once overwritten, restoring the original file is not possible anymore.

4.5.1 Saving and overwriting the original file

1. On the *File* menu, select the *Save File* command, or click the icon from the toolbar.
2. On the dialog that opens, drag & drop the spectrum file from the browser to the *File(s) to save* list box.

3. Click the *Save* button.
   ➢ *The original file is overwritten. Restoring the original data is not possible anymore.*

4.5.2 Saving without overwriting the original file

1. On the *File* menu, select the *Save File As* command, or click the icon from the toolbar.
2. On the dialog that opens, drag & drop the spectrum file from the browser to the *File to save (OPUS format)* list box (figure 4.15).

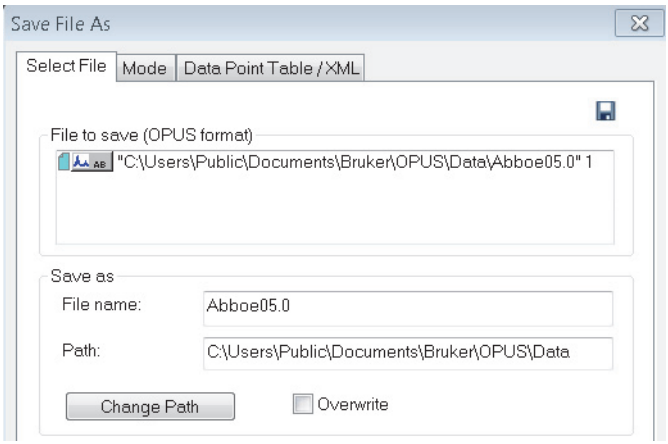


Figure 4.15: Save File As

3. Define the file name.
   ➢ *By default, OPUS provides a file name which can always be changed.*
4. Define the path.
   ➢ *The 'Change Path' button allows to exactly select the storage location.*

5. Activate the 'Overwrite' checkbox if a previous file is to be overwritten.
   ➢ *If the checkbox is deactivated, the file name is incremented. The 'Overwrite' checkbox is disabled when the spectra have been measured in validation mode.*
6. Make the settings on the *Mode* and *Data Point Table/XML* tab.
   ➢ *The spectrum file is normally saved in OPUS format. However, the 'Mode' and 'Data Point Table/XML' tabs allow to save the file in different formats, e.g. JCAMP-DX or XML format, as a plain XY data table, in Pirouette (DAT) or in GALACTIC format (SPC). Details on the tabs are described in the OPUS Reference Manual.*
7. Click the *Save* button.

4.6 Load spectrum file

1. On the *File* menu, click the *Load File* command, or click the icon from the toolbar.
2. On the dialog that opens, select the particular spectrum file.
   ➢ *The dialog is described in chapter 4.6.1.*
3. Click the *Open* button.
   ➢ *The spectrum is displayed in the spectrum window.*

4.6.1 Description of *Load Spectrum* dialog

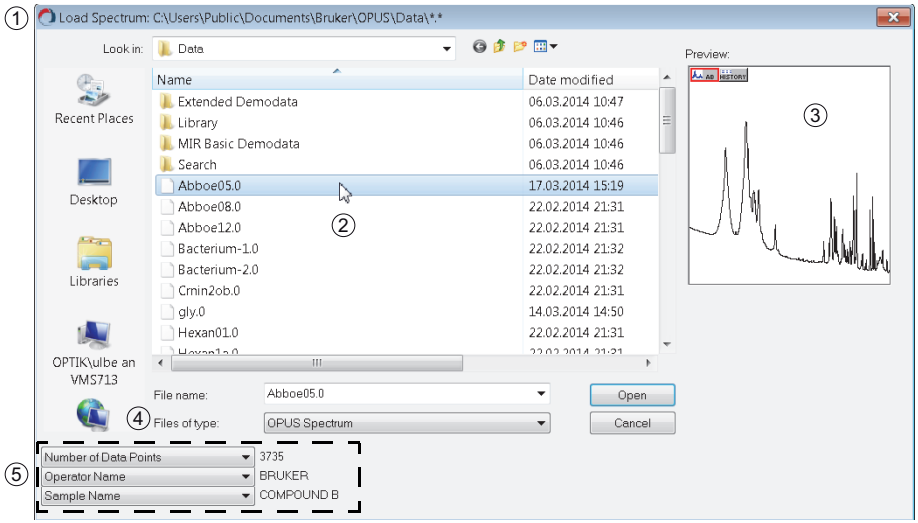


Figure 4.16: *Load Spectrum* dialog

	Element	Definition
1	Title bar	The title bar shows the directory in which the spectrum files are saved.
2	Spectrum files	Depending on the data type (4) selected all spectra files are displayed, which are available in the particular directory.
3	Preview	The preview shows the spectrum without axes, and the data blocks of the spectrum file.

Table 4.5: Elements of the *Load File* dialog

	Element	Definition
4	Data type	The drop-down list contains different data types. Spectra measured in OPUS have the *OPUS Spectrum* data type.
5	Parameter	By default, 3 parameters are displayed per each spectrum file. The drop-down lists contain different types of parameters. If a spectrum file has been selected, the values are displayed next to the parameters on the right (figure 4.16). As not all parameters must be specified for each spectrum, some of the parameter values may be missing even if the spectrum file has been selected.

Table 4.5: Elements of the *Load File* dialog

4.7 Printing spectrum file

4.7.1 Using the *Quick Print* command

☞ On the *Print* menu, select the *Quick Print* command, or click the icon from the toolbar.

➢ *Depending on the window type currently used, OPUS selects an appropriate plot layout. For example, if you work in the spectrum window, the spectrum will be printed within a frame. If you search a spectrum library, the results as well as a hit list, spectral information and the structure of the product will be printed. More details on pre-defined layout plots are described in the OPUS Reference Manual.*

4.7.2 Using the *Print Spectra* command

1. On the *Print* menu, select the *Print Spectra* command, or click the icon from the toolbar.
2. On the dialog that opens (figure 4.17), you can individually define the basic settings for the print-out.

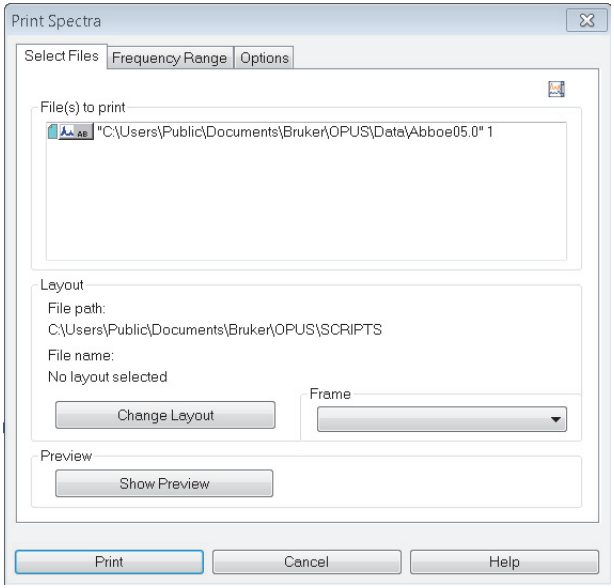


Figure 4.17: *Print Spectra* dialog

3. Select a layout.
4. If required, make further settings on the *Frequency Range* or *Options* tabs.
   ➢ *More details on the single tabs are described in the OPUS Reference Manual.*
5. Click the *Print* button.

5 Analysis Report

OPUS allows to depict sample parameters and evaluation results for one or several spectrum files in an analysis report. The spectra files need to contain the data block of the respective evaluation. Evaluation data blocks are e.g. PEAK, INTEG, QUANT, IDENT, SEARCH, CT.

Figure 5.18: Spectrum file with data blocks of different evaluation types

5.1 Generating report

1. On the *Print* menu, select the *Generate Analysis Report* command, or click the icon from the toolbar.
2. On the dialog that opens, click the *Load* button.
3. Select the particular spectrum file and click the *Open* button.
   ➢ *The spectrum file is displayed in the 'File(s) for report generation' list box (figure 5.19).*

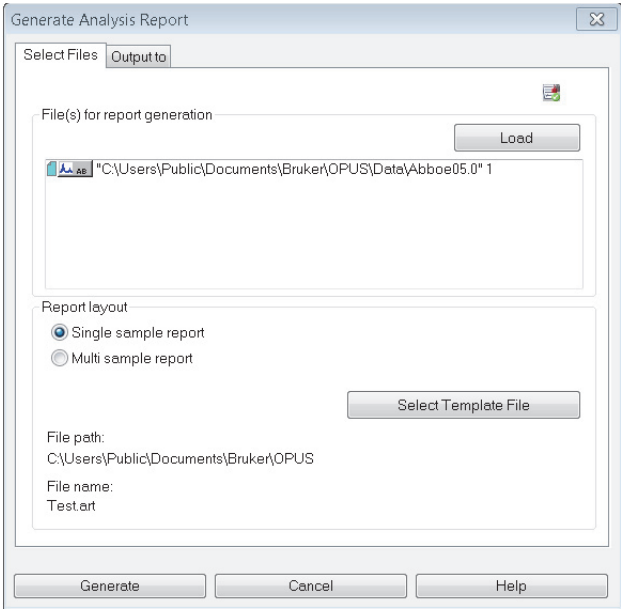


Figure 5.19: Generating analysis report

4. Define the report layout.
   - ➢ *Single sample report[1]: one report for each spectrum file*
   - ➢ *Multi sample report[2]: one report for all spectrum files*
5. Select the template file.
   - ➢ *By default, OPUS provides several types of template files. Template files have the extension *.art and are stored in the C:\Users\Public\Public Documents\Bruker\OPUS_<version> directory.*
6. Click the *Output to* tab and define how the report is to be printed.
   - ➢ *If you want to print the report as PDF or csv file, you have to define the file name of the report and the path to store the report.*
7. Click the *Generate* button.

1. To generate a single sample report you can use several spectra files at once. In this case, a separate report will be generated for each spectrum file separately.
2. A multi sample report lists all spectrum files with the respective data in one report.

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