



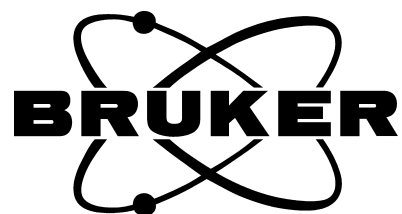
OPUS

Spectroscopy Software

Version 6

User Manual

SUPPLEMENT



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This manual is the supplement documentation for OPUS 6.

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Introduction

This supplement comprises new features designed for the OPUS version 6, which have not yet been described in the corresponding manuals, as well as updated information on existing OPUS commands.

New Features:

- Easy Measurement Mode: for quality control using MPA and TENSOR 27 only
- Accessories in measurement and OVP

Up-dated Information:

- Correlation Modes
- AAR Test Result
- Rapid Scan Measurement
- Interleaved Time Resolved Measurement
- Step Scan Measurement
- ATR Correction
- Spectrum Search

1 Easy Measurement Mode

The *Easy Measurement* mode has been designed for quality control when using TENSOR 27 and MPA spectrometers. To switch off this mode you need to have Administrator rights in OPUS.

If you work in this mode, specific parameters are pre-defined and interferograms will automatically be stored. The Bruker standard experiments have been adapted to this mode.

1.1 Installation

When installing OPUS follow the on-screen instructions. Make sure that you select the correct instrument for quality control. Depending on the instrument used either select:

- TENSOR 27 for quality control or
- MPA

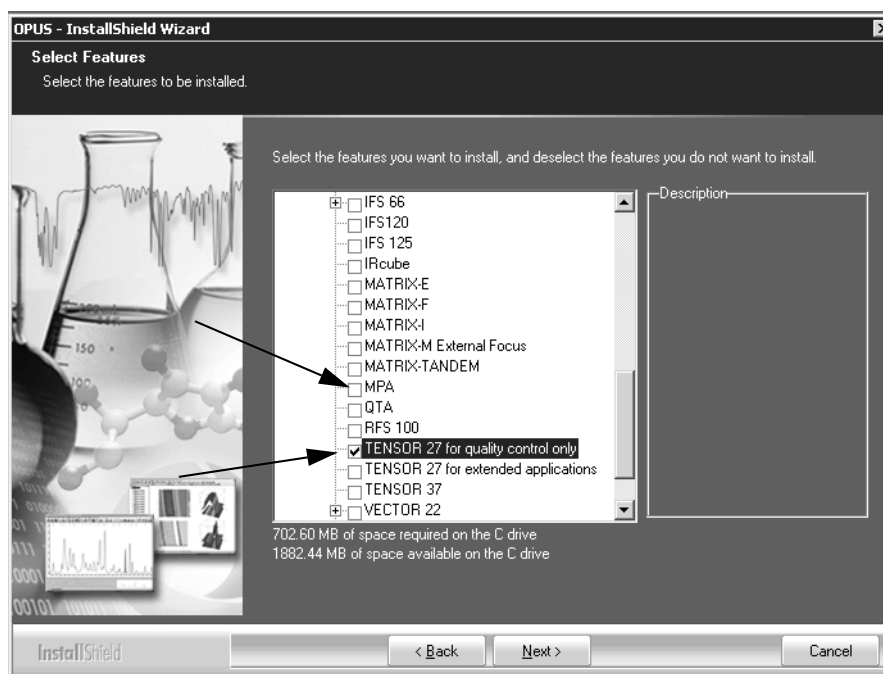


Figure 1: Selecting instrument type during OPUS installation

For further details on the installation procedure refer to the OPUS Installation Instructions. If the installation has been finished, start OPUS.

1.2 Routine Workspace

When working in the *Easy Measurement* mode the respective routine measurement workspace opens by default. The workspace is defined as:

- *MIR_Routine_Quali.ows* (in case of TENSOR)
- *NIR_Routine_ows* (in case of MPA)

The *Measure* menu as well as all the other OPUS menus, e.g. *Manipulate* or *Evaluate* include only those commands which are required for routine measurement. Figure 2 exemplifies the *Measure* menu.

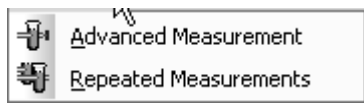


Figure 2: Measure menu in *Easy Measurement* mode

To perform a measurement select the *Advanced Measurement* command from the *Measure* menu. The following dialog opens:

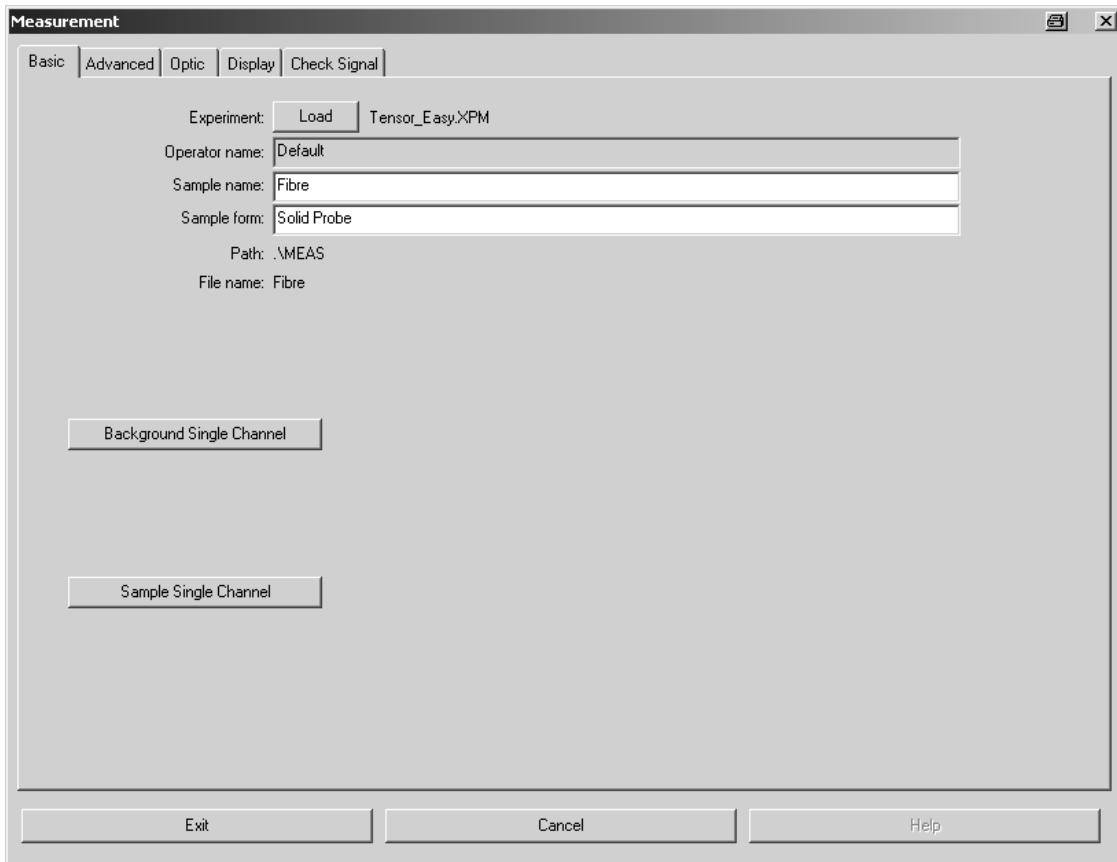


Figure 3: Measurement - Basic tab

The DEFAULT measurement experiment with parameters specified by Bruker is automatically loaded. Click on the *Load* button if you want to load a different experiment.

If the parameters defined for a user-specific experiment differ from the parameters specified by Bruker, the following error message pops up:

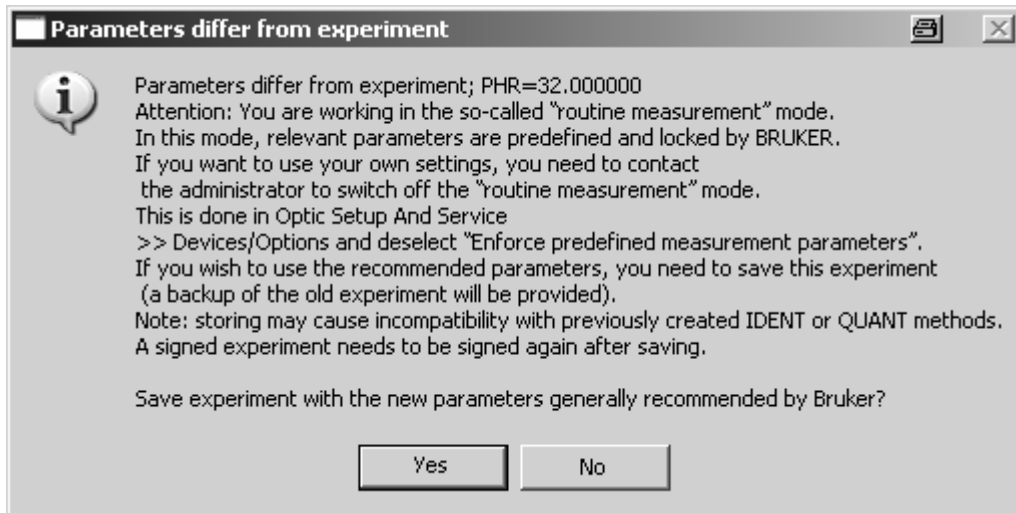


Figure 4: Error message

This may occur in case of loading existing experiments in the *Easy Measurement* mode. Measurements using non-conforming parameters are not possible, by default.

Note: Before storing the experiment file with the new parameters a backup is made of the original file (*.xpm.bak). If you work in validated mode, you have to sign the experiment once again after the experiment file has been stored.

On the *Optics* tab all registered accessories are displayed (only in case of TENSOR). Select the appropriate accessory from the drop-down list (A in figure 5).

If the accessory currently inserted has already been registered, the name of the this accessory is also displayed (B in figure 5) in the measurement dialog.

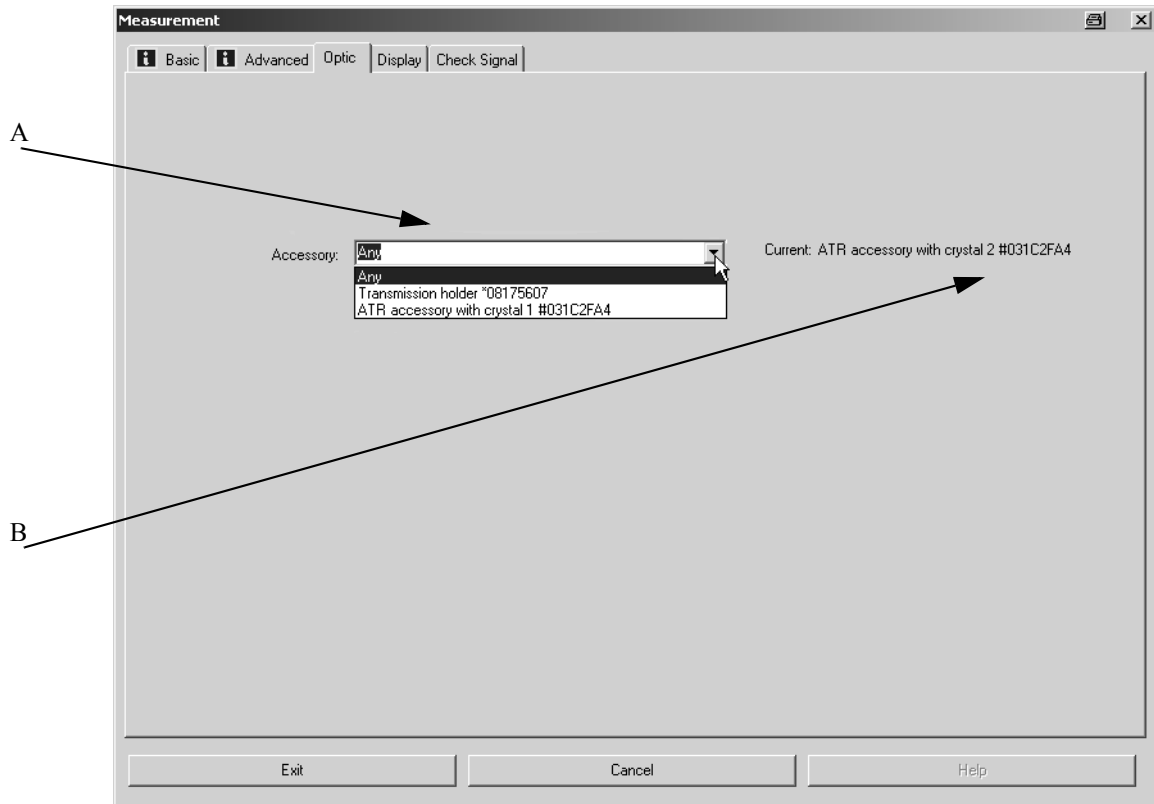


Figure 5: Measurement - Optic tab

1.3 Switching off Mode

The *Easy Measurement* mode can only be switched off by the Administrator. Select the *Optic Setup and Service* command from the *Measure* menu and click on the *Devices/Options* tab.

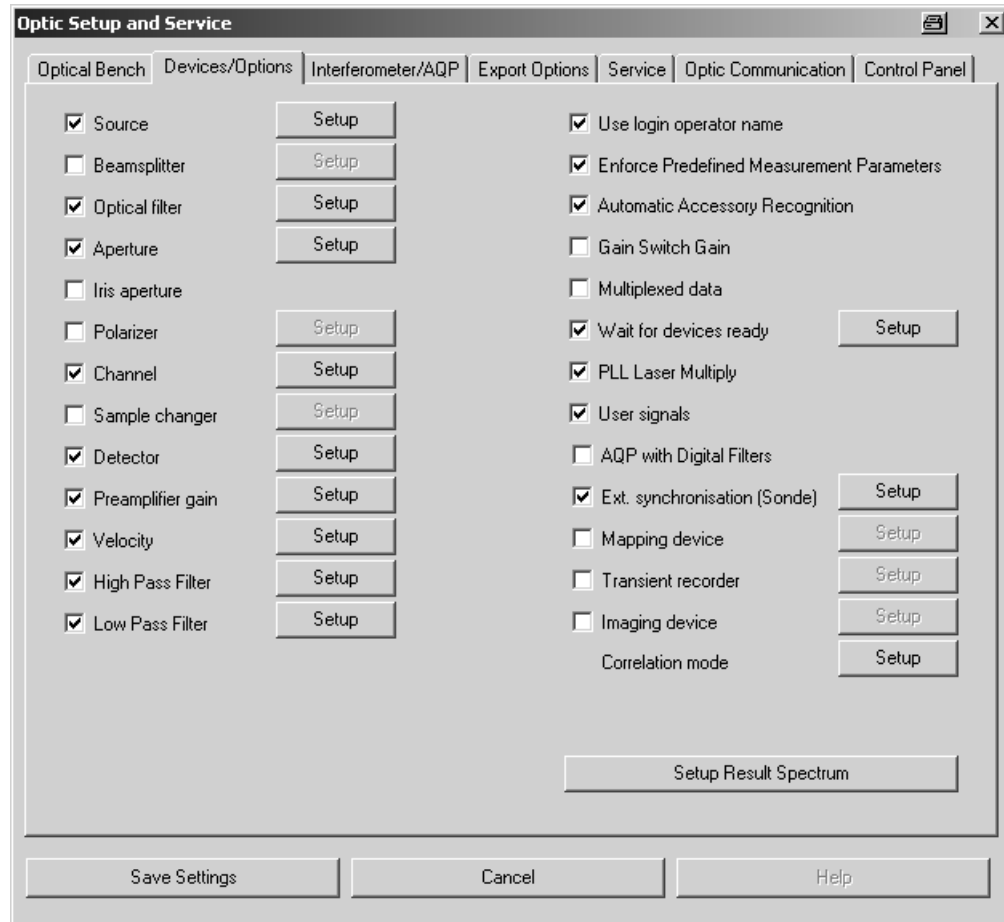


Figure 6: Optic Setup and Service - Devices/Options tab

The *Enforced Pre-defined Measurement Parameter* check box is automatically activated if OPUS is installed for the first time to perform measurements by using MPA or TENSOR. To deactivate the mode remove the check mark.

2 Accessories in Measurement Dialog and OVP

Note: Refers to chapter 13 in the OPUS Reference Manual

The following describes the QuickLock accessory recognition in OVP. This kind of feature is available for TENSOR and VERTEX spectrometer series only.

2.1 Accessories in Measurement Dialog

If you select the *Advanced Measurement* command to open the measurement dialog, a drop-down list is displayed on the *Optics* tab, which includes all accessories registered for the respective spectrometer.

Note: For information on how to register accessories by Automatic Accessory Recognition (AAR) refer to the OPUS AAR manual.

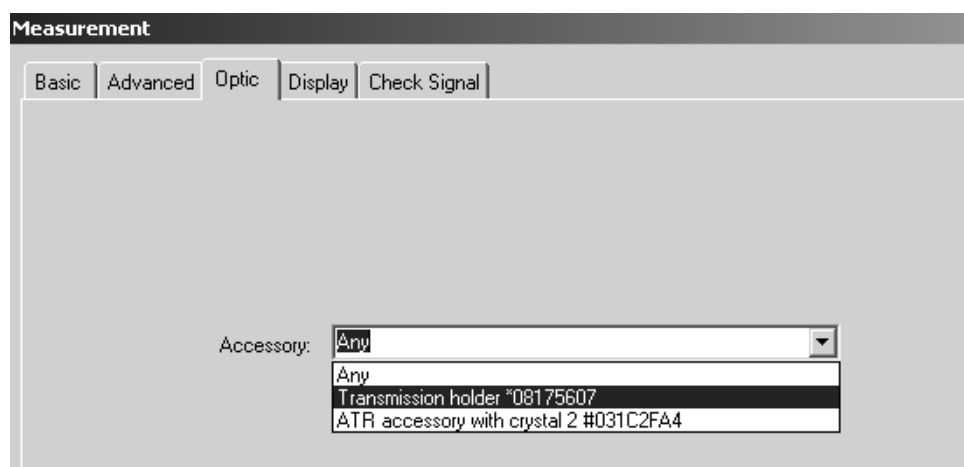


Figure 7: Measurement - Accessory list

The accessory currently inserted into the spectrometer is also shown to the right of the drop-down list (see figure 5).

If you store a measurement experiment, the accessory selected from the drop-down list will be stored as a parameter. This means that the measurement using this experiment can only be performed by inserting the correct accessory.

If you load an experiment which uses an accessory not currently inserted into the sample compartment, the drop-down list field in the measurement dialog is marked red. In this case no measurement can be performed.

2.2 Accessories in OVP

If you have selected any accessory in OVP (A in figure 8) the measurement configuration, i.e. the combination of source, beamsplitter, measurement channel and detector, will be extended by this accessory (B).

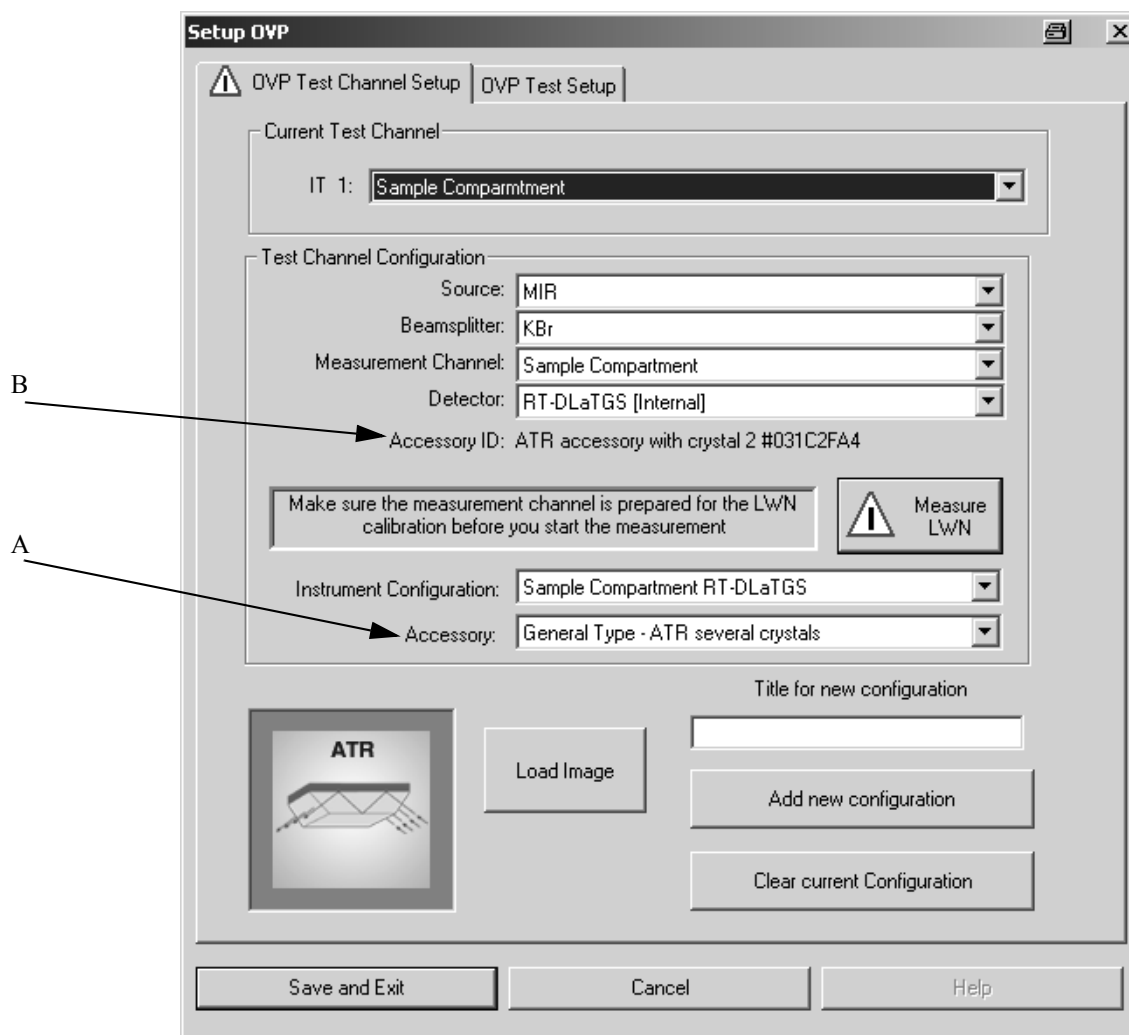


Figure 8: Setup OVP

In this case make sure that you measure the laser wavenumber with the accessory being inserted. The measurement will then recognize the correct test channel and thus the correct laser wavenumber, depending on the accessory being inserted.

2.3 Inserting accessory with activated AAR

Inserting a QuickLock accessory for the first time enables the firmware to recognize that any accessory exists in the sample compartment. The firmware, however, cannot recognize the type of accessory and writes a question mark as type of accessory.

If the Automatic Accessory Recognition (AAR) is activated by means of the *Optic Setup and Service* command from the *Measure* menu, OPUS recognizes that an unknown type of accessory is in the sample compartment. Use AAR to exactly define the name and type of the accessory.

Note: AAR only runs if you first have defined a test channel in OVP for the sample compartment. Otherwise, an error message pops up in AAR. Afterwards AAR sets up a second test channel for the respective accessory type.

When inserting the accessory AAR starts and tries to recognize the type of accessory by means of a measurement. In case of a non-registered accessory AAR provides a drop-down list which you use to select a general accessory type or an accessory which has already been registered in the OVP database.

If you have activated the *Accessory has to be tested* check box (figure 9), an OVP test channel is automatically set up for this kind of accessory and a shortened S/N test (one measurement) performed.

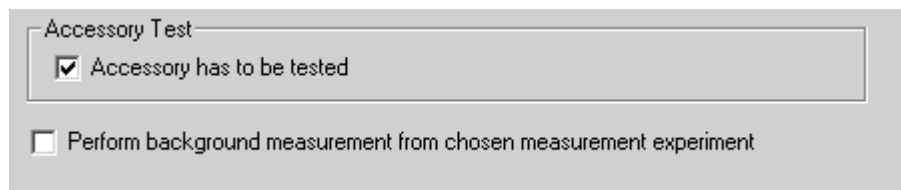


Figure 9: AAR - Accessory to be tested

If you deactivate the check box, no OVP test channel will be set up. Select the new test channel in OVP for the respective type of accessory.

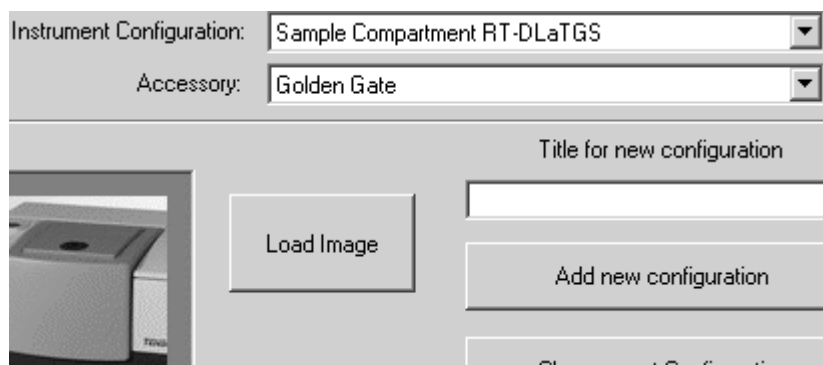


Figure 10: Setup OVP - Accessory selected

Afterwards, click on the *Measure LWN* button to measure the laser wavenumber. OVP will then enter the accessory recognition into the test channel configuration (as defined in AAR). If you perform measurements by using this type of accessory, the test channel will automatically be recognized and the correct laser wavenumber used. When inserting a different registered type of accessory, only the S/N test will be performed OVP.

2.4 Inserting accessory without activated AAR

In this case the firmware defines all accessories inserted by a question mark in the optics. Therefore, these types of accessories will neither be recognized by OVP nor displayed in the measurement dialog (see figure 7).

You have to manually set up a separate OVP channel for this type of accessory. As soon as you measure the laser wavenumber the name of the accessory selected in OVP will be used and replaced by this name in the optics. Thus, the accessory is also displayed in the measurement dialog even if AAR is not activated.

If you perform a measurement by using this type of accessory, the test channel will also be automatically recognized and the correct laser wavenumber used.

Note: This feature is only activated for *Sample Compartment* measurement channels. In case of an external channel (e.g. *External Port*) the sample compartment accessory currently inserted for this measurement channel will not be taken into account.

2.5 Special case: ATR Several Crystals

In case of ATR accessories with changeable crystals neither the optics nor OVP recognizes what type of crystal is currently used. This requires a separate OVP test channel to be set up for every possible kind of crystal.

Select *General Type - ATR Several Crystals* from the *Accessory* drop-down list in OVP for each one of these test channels.

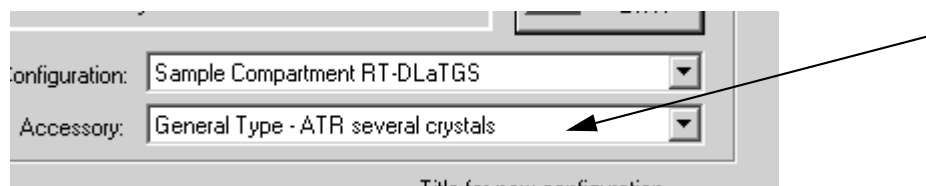


Figure 11: Setup OVP - General Type ATR several crystals

Consequently, the same configuration exists several times in OVP. In case of several identical configurations OVP always uses the laser wavenumber of the first configuration found. Tests have shown that the crystal type has an insignificant influence, if at all, on the laser wavenumber.

Due to the different optical characteristics of crystals you have to measure reference spectra for each crystal separately to run PQ tests.

2.6 Special case: HYPERION

As Hyperion is no QuickLock accessory it cannot be recognized by the spectrometer optics. To ensure an OVP accessory assignment OVP writes accessory information into the optics as soon as the laser wavenumber has been measured for a Hyperion configuration.

The following kind of information is written into the optics:

- Type of accessory: *HYPERION*
- Accessory ID: *HYPERI01_xx* with being xx = IT Channel No (01, 02, 03...)
- Name of accessory: as indicated in the OVP accessory list (e.g. *Hyperion 1000/2000 ATR Objective*)
- Accessory location: *0x0*

Hyperion configurations are also displayed in the *Accessory* drop-down list of the measurement dialog. They are recognized by OVP and assigned to the correct test channel. This ensures that the correct laser wavenumber is used when a measurement is performed.

3 Up-dated Information

This chapter includes up-dated information on existing OPUS commands.

3.1 Correlation Modes

Note: Refers to chapter 7.2.5 in the OPUS Reference Manual

The correlation mode determines whether a data integrity check is performed during data acquisition. Depending on the spectrometer type OPUS provides different correlation modes.

Spectrometer Type	Mode	Definition
AQP instruments	No	No data check
	Around Peak, Low	This mode 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 rejected. Otherwise, the interferogram will be used for averaging.
	Around Peak, High	Same as <i>Around Peak Low</i> , but the limit is more sensitive to minor changes (e.g. caused by thermal drift in case of long-term measurements).
AQP instruments with Raman	Full Igram Length	All interferogram data points are compared to each other. An interferogram is rejected 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.
TENSOR, MATRIX, MPA, VERTEX, IFS 125HR	OFF	No data check
	ADC FS (Full Scale)	The complete scan is rejected if the inteferogram amplitude is greater than 80%. If this mode is activated, acquisition and co-addition of overloaded signals is avoided.
	Vel (Velocity)	Rejects all scans which velocity deviation is greater than the specified limit during data acquisition. The default deviation limit is set to >2% and can be customized.
	IFG_Length_Difference	The number of interferogram data points is not identical to the nominal number. This mode should be activated in case of non-frequent and intense mechanical disturbances to have the scan automatically rejected.

Spectrometer Type	Mode	Definition
	Signal Amplitude Limits	Scans of a particular interferogram amplitude range are used only. The range can be customized.
	Start on Signal Amplitude Limits	The measurement starts only if one scan is within the defined amplitude limit. Thus, the measurement is triggered by intensity. Example: sample inserted, measurement starts
	Stop on Signal Amplitude Limits	The measurement stops if a scan is beyond the defined amplitude limit. Example: sample removed, measurement stops
	Raman	Detects Raman spikes in the interferogram and substitutes them by other scans of the same measurement. If more than 10% of the interferogram data points have to be substituted, the scan will be rejected.

3.2 AAR Test Result

The result of the AAR reference tests is also displayed in the AAR dialog.

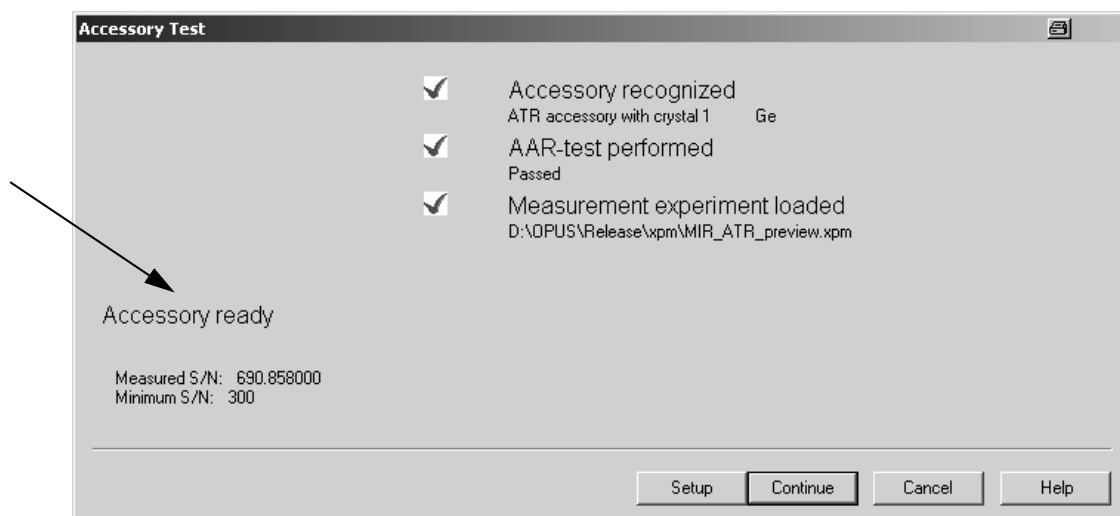


Figure 12: AAR test result OK

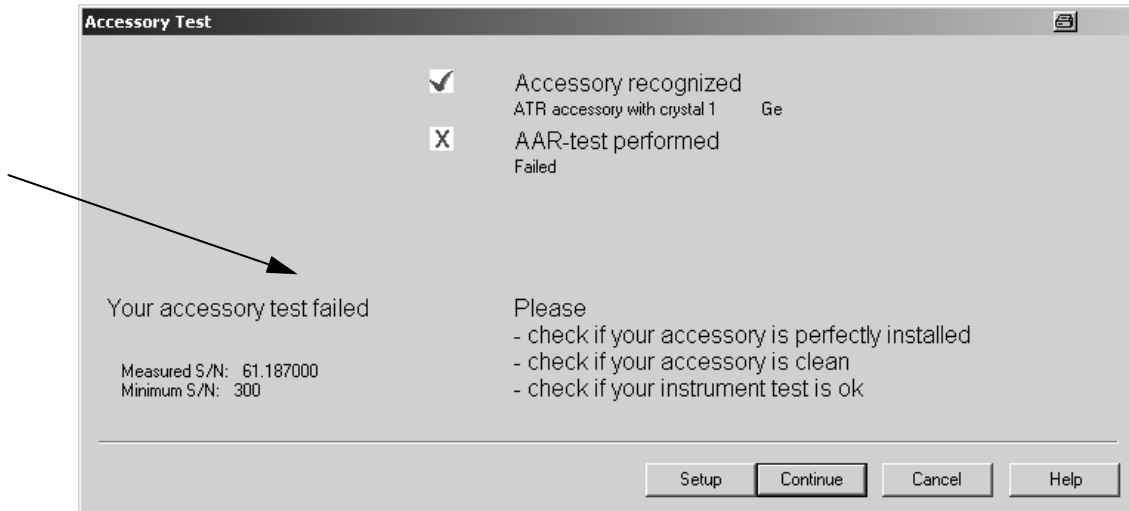


Figure 13: AAR test result not OK

3.3 Rapid Scan Measurement

Note: Refers to chapter 7.4 in the OPUS Reference Manual

The Rapid Scan measurement parameters described in chapter 7.4 do not apply to MATRIX and MPA spectrometers. The description in the OPUS Reference Manual refers to AQP instruments. In case of TENSOR and VERTEX spectrometer series the parameters have to be adapted individually. For further information on typically-used measurement parameters in case of TENSOR and VERTEX series refer to the separate documentation which can be provided on request.

3.4 Interleaved Time Resolved Measurement

Note: Refers to chapter 7.5 in the OPUS Reference Manual

The Interleaved Time Resolved measurement parameters described in chapter 7.5 apply to the IFS 66(v)/S and IFS 120HR spectrometers only.

3.5 Step Scan Measurement

The Step Scan measurement parameters available in OPUS do not apply to TENSOR, MATRIX, MPA and IFS 125HR spectrometers. The description in the OPUS Step Scan manual refers to EQUINOX 55 and IFS 66(v)/S. In case of VERTEX spectrometer series the parameters have to be adapted individually. For further information on typically-used measurement parameters in case of VERTEX refer to the separate documentation which can be provided on request.

3.6 ATR Correction

Note: Refers to chapter 8.24.2 in the OPUS Reference Manual

Load the spectra measured by an ATR unit into the OPUS browser. Make sure that the spectrum contains no ranges with strong noise. Otherwise, use the *Cut* or the *Straight Line Generation* command from the *Manipulate* menu to modify these ranges. As the extended ATR correction is sensitive to noise wrong results may be produced.

3.7 Spectrum Search

Note: Refers to chapter 9.11 in the OPUS Reference Manual and 2.3.1 in the OPUS SEARCH manual.

The following search algorithms which can be selected from the drop-down list on the *Search Parameters* tab are available in OPUS.

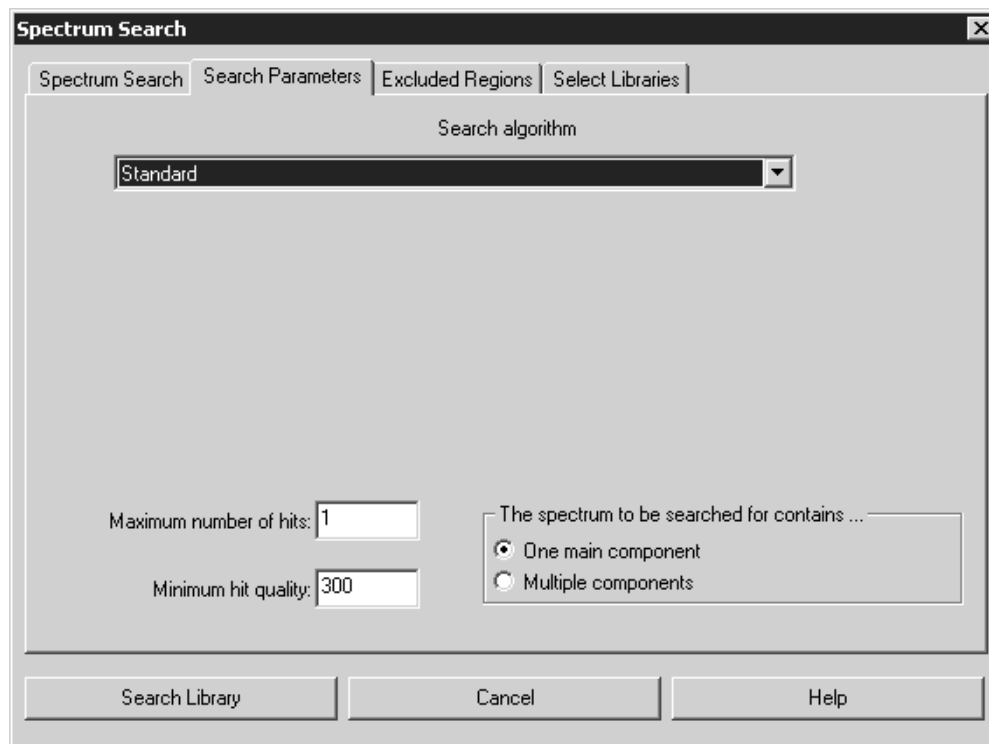


Figure 14: Spectrum Search - Search Parameters tab

- **Standard**

All pieces of band information, which are available from the query and library spectrum, are reflected in the hit quality. The information contains the position, relative intensity and half-width of each band. A library spectrum band is considered to be identified in the query spectrum if this spectrum contains a band

- which position does deviate from the position in the library spectrum by less than the half-width,
- which difference between the half-widths and relative intensities is less than factor 2, respectively.

This algorithm also allows to further specify the search result. Select the appropriate option button to define whether the query spectrum consists of one main component or multiple components.

- **Use Existing Peak Table**

This algorithm uses an already existing peak table, which enables you to suppress the influence of peaks originating from the substrate. Depending on the measurement you can additionally define whether the spectrum to be searched for contains one component (in case of a single substance) or multiple components (in case of compounds).

- **Spectrum Correlation**

This algorithm calculates the sum of the squared deviations between the query spectrum and the result spectrum for the data points of the range defined. The summation can be limited to a spectral range selected by the user. If you use this algorithm, two additional drop-down lists, *Normalization Method* and *Derivative*, are displayed.

