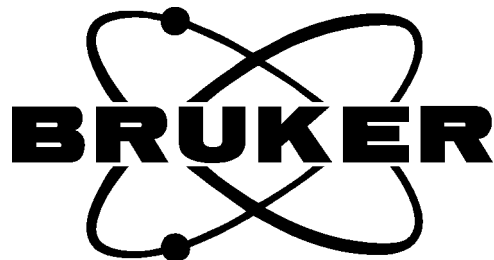


Spektroskopiesoftware

OPUS



OPUS-ROUTINE
for OPUS/IR

(Version 3)

08/2000

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Dieses Buch ist die Originaldokumentation zur Spektroskopiesoftware **OPUS**.

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1. General

ROUTINE provides an easy to use interface for OPUS-NT designated for routine work in laboratories. It offers a set of functions which can be executed with single mouse clicks. The interface is based on a combination of VB-Scripts and macros.

OPUS – ROUTINE has been designed to be as flexible as possible, i.e. the button captions and all functions on the second page of the interface can be changed. The configuration of the interface is stored in a parameter file. A separate setup program is used to easily modify this parameter file. A few predefined parameter files are available and can be used to easily switch between different versions and to demonstrate the possibilities of this interface.

If required a choice of different sample techniques can be used with ROUTINE. For each sample technique the measurement parameters, manipulation and evaluation functions can be specified individually.

The current version of ROUTINE has the following limitations:

- The forms and control elements are not adapted to screen resolution. The current version is optimized for 800x600 pixel.
- ROUTINE does not interact with the automatic accessory recognition software (AAR).

1.1 System requirements

- OPUS 3.02 Beta or a newer version
- Screen resolution 800x600 Pixel

1.2 Installation

ROUTINE is automatically installed during OPUS installation. If the default ROUTINE interface shall be used the measurement experiments have to be set up to run with your instrument first. During installation the following paths are set up as sub-directories of OPUS:

| | | |
|-------------------|--------------|--|
| [OPUS Path] ----- | ROUTINE | (VB-Scripts and Parameter Files) |
| | | |
| | -----MACRO | (macros used by Routine) |
| | | |
| | -----MEAS | (measured spectra are stored here) |
| | | |
| | -----METHODS | (Methods used by Routine e.g. for Quant) |
| | | |
| | -----XPM | (Measurement experiments) |

After installation go through the following steps:

- Open the measurement dialog
- Load the experiment files from the \ROUTINE\XPM directory one after the other
- Correct inconsistencies (if any) and save each modified experiment
- Do not change the spectral ranges. Otherwise the QUANT 2 evaluation might cause an error.

The name of the parameter file which is used for the ROUTINE configuration is "ROUTINE.PAR". You will find a few other parameter files in the routine subdirectory demonstrating examples of alternative user interfaces. To use one of those parameter files instead just copy the parameter file into routine.par

e.g. *COPY THREEEXPM.PAR ROUTINE.PAR*

To reset to the default interface copy the file DEFAULT.PAR

COPY DEFAULT.PAR ROUTINE.PAR

If you want to run the ROUTINE interface immediately when starting OPUS do the following:

- create a link to OPUS on your desktop.
- In the "Properties" dialog add the following command line arguments:

/SCRIPT=[OpusBasePath]\ROUTINE\ROUTINE1.obs [OpusBasePath]\ROUTINE\ROUTINE.ows

If you want to modify one of the supplied parameter files or design your own interface please refer to the "Routine Setup" Manual.

1.3 Setting up an OPUS-ROUTINE Start Icon

- Open the explorer and change top the OPUS directory.
- Drag the OPUS.EXE file onto the desktop to create a link to OPUS.
- Right click on the link and open the properties dialog.
- The command line in the upper edit field should look like this :
E:\OPUS_NT\opus.exe (drive and path will differ depending on your system)
- Add the following command arguments right after the above line:
/NO_VIEWMAXIMIZE=ON /SCRIPT=e:\opus_nt\routine\routine.obs (the drive and path have to be modified according to your system)
- The complete line should now look like:

E:\OPUS_NT\opus.exe/NO_VIEWMAXIMIZE=ON /SCRIPT=e:\opus_nt\routine\routine.obs

- Exit from the properties dialog

1.4 Starting OPUS with the ROUTINE interface

Double click on the OPUS icon which you have set up as described above. Login as usual. The Routine interface will start automatically.

If you did not create a special OPUS Icon on the desktop start OPUS as usual. Login as usual. Open the VB-Script ROUTINE.OBS in the ROUTINE subdirectory.

1.5 Exit from OPUS

Before you can exit from OPUS you must switch to the Standby mode by clicking the Log Out button of the ROUTINE dialog.

2. Working with ROUTINE

ROUTINE has two different operation pages, the first for measurement and the second for manipulation/evaluation of measured data.

Note: The following description is based on the default ROUTINE interface. If you are using a different setup the texts for buttons, entry fields and also the functions may be different.

2.1 Page 1

You can enter a **Sample Name** and an additional **Batch Number** for the sample to be measured. The **Sample Technique** can be chosen from a dropdown list. The **Operator Name** is taken from the OPUS Login and can be changed if required. The field **File Name** shows the basic name for all measured sample spectra.

Note: Default settings of **Sample Name** and **File Name** are individually pre-set for each sample technique.

When the Routine interface is started the first time the **Measure Sample** Button is inactive until a new reference spectrum has been measured by clicking on **Measure Reference**. It is also set to inactive whenever a new sample technique is chosen from the **Sample Technique** dropdown list.

As soon as a new reference is measured the program starts scanning single sample Scans and displays the resulting spectra automatically.

Insert a sample and you can immediately observe the sample spectrum. To measure a sample click on **Measure Sample**. Depending on the current state of the system it can take a few seconds until the sample measurement starts. When the sample spectrum is ready the program automatically switches to the second page of the ROUTINE interface.

2.2 Page 2

File Name and **Sample Name** show you the real file name and sample name of the measured sample.

The upper two buttons are mainly reserved for manipulation functions. The type of functions (e.g. Baseline and Peak Pick) depends on the selected sample technique.

The **Undo** button below these two buttons allows you to restore the original measured spectrum after manipulation.

Print Spectrum prints the spectrum. It uses the plot layout specified for the selected sample technique.

The next two buttons allow to run evaluation functions. . The type of functions (e.g. Compare and Quant) also depend on the selected sample technique. Both functions can optionally print the result or show it in Message.

Back to Measurement stores the current sample and returns to the first page for measuring the next sample.

The **Log Out** button is available on both pages and is used to switch the system to standby mode. All activities are stopped and OPUS can be terminated if required. A click on **Back to Operation Mode** opens a login dialog. After typing the password OPUS returns to the first page of ROUTINE.

3. Configurations delivered with this version of ROUTINE

The parameter file "ROUTINE.PAR" contains parameters for 3 different sample techniques:

1. ATR (one crystal)

- Experiment file: ATR_ONECRYSTAL.XPM
- Manipulation function: Smooth
- FirstEvaluation function: Compare
- SecondEvaluation function: Quant 2

2. ATR (two crystals)

- Experiment file: ATR_TWOCRYSTALS.XPM
- Manipulation function: Baseline correction
- FirstEvaluation function: Compare
- SecondEvaluation function: Quant 2

3. Transmission Unit

- Experiment file: TRANSUNIT.XPM
- Manipulation function: Baseline correction
- FirstEvaluation function: Quant 2
- SecondEvaluation function: Compare