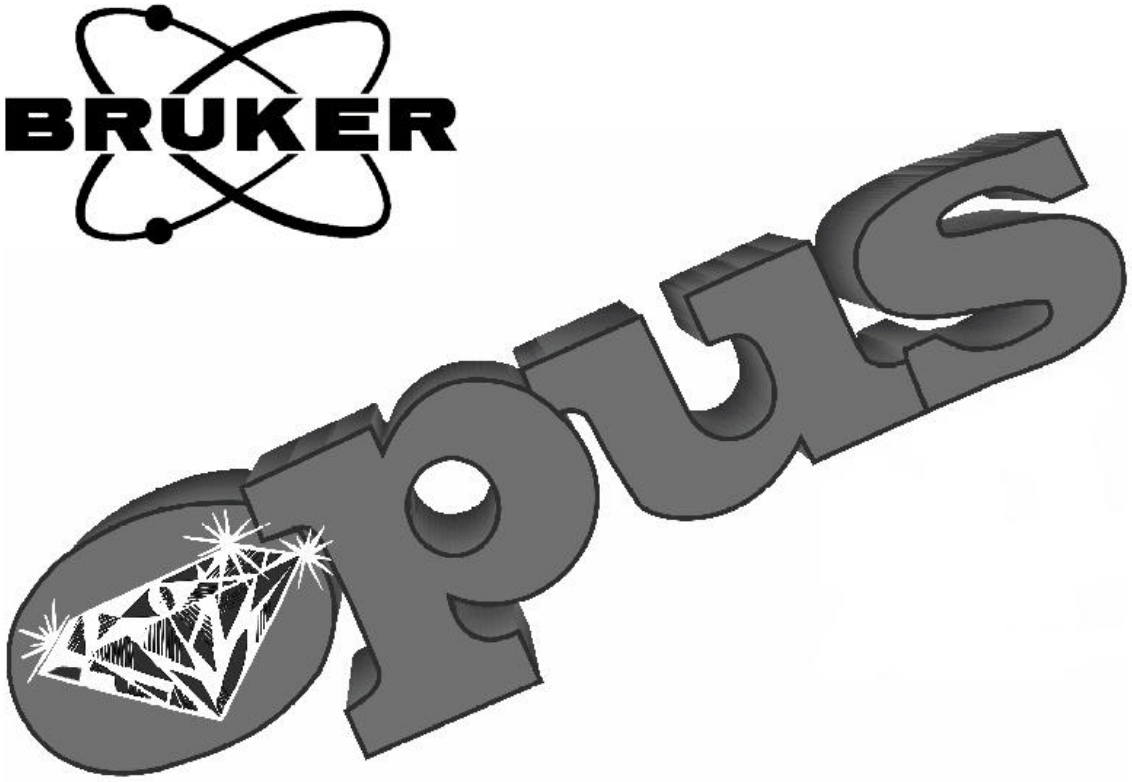
Spectroscopic Software



Configuration of the OPUS-ROUTINE Interface

OPUS/IR

(Version 3)

01/2001

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

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1. General

The configuration of the OPUS-Routine Interface is stored in a text file “ROUTINE.PAR” which is located in the routine root path.
The Routine Setup program can be used to either modify an existing configuration or to set up a new one from scratch. Although it is possible to edit the configuration file manually with any text editor we highly recommend to use the Setup Program to prevent problems. A detailed list of the text entries can be found in the attachment of this manual.

2. Setting up a Routine Configuration

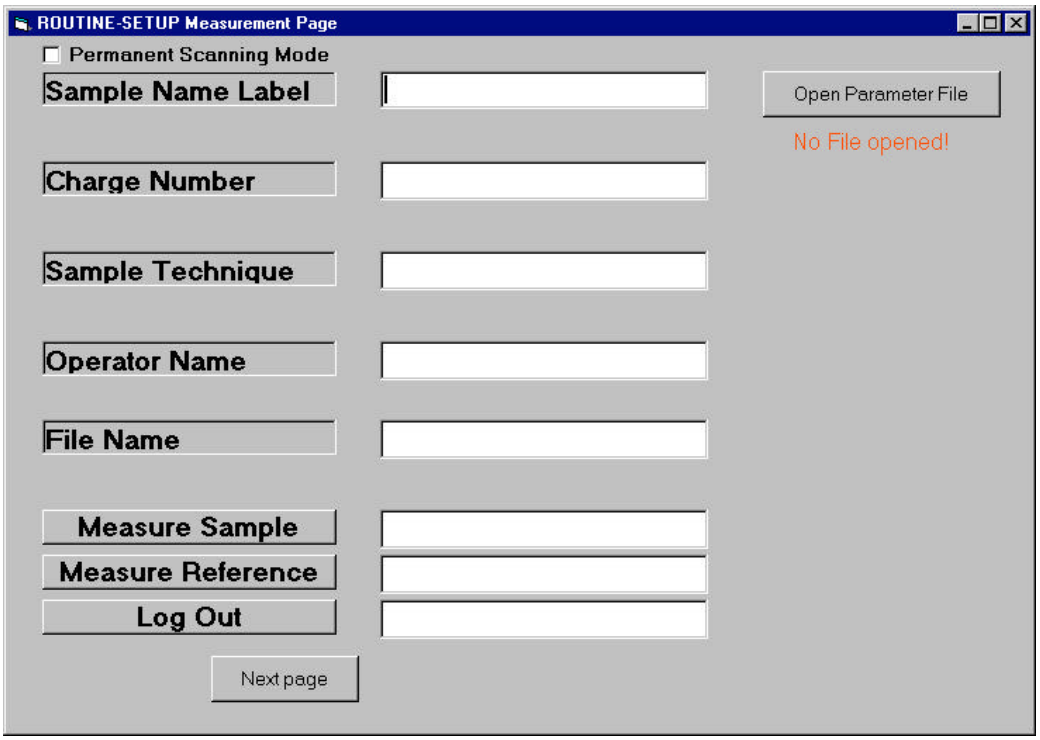
Run the Routine Setup program. The program consists of several pages which can be switched back and force. In the following description we will modify the already specified default configuration and make a German version.

2.1 Measurement Page Setup Part 1

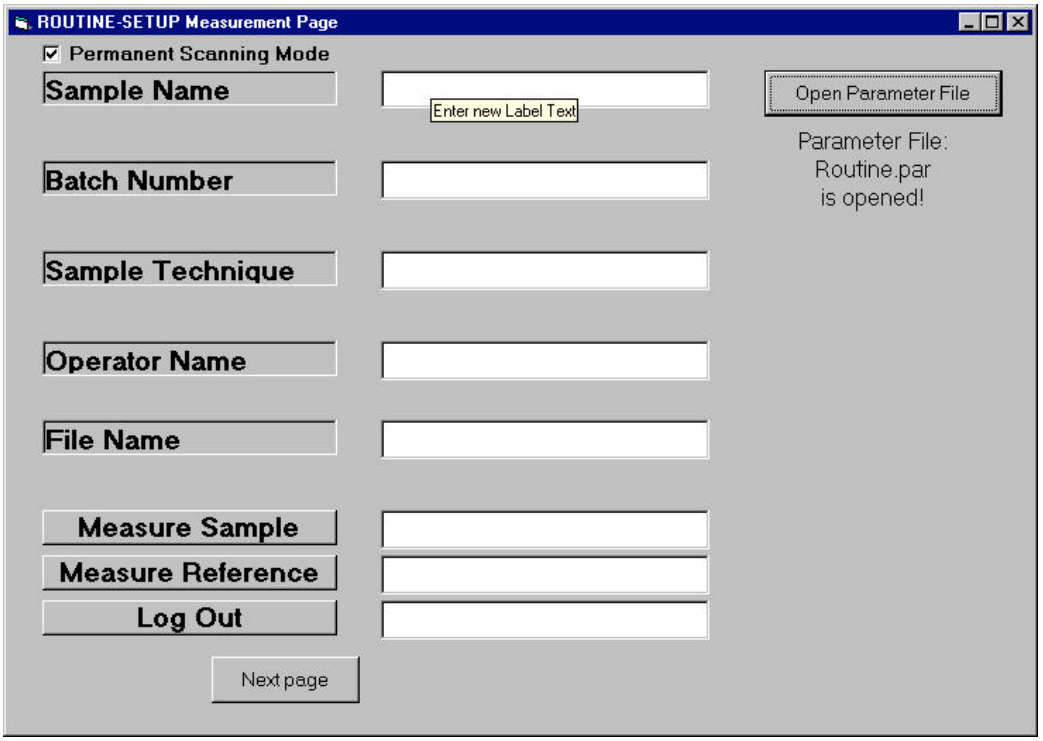
The first setup page for the ROUTINE measurement page is used to specifiy the captions of all labels and buttons on the measurement page.

The following elements can be specified:

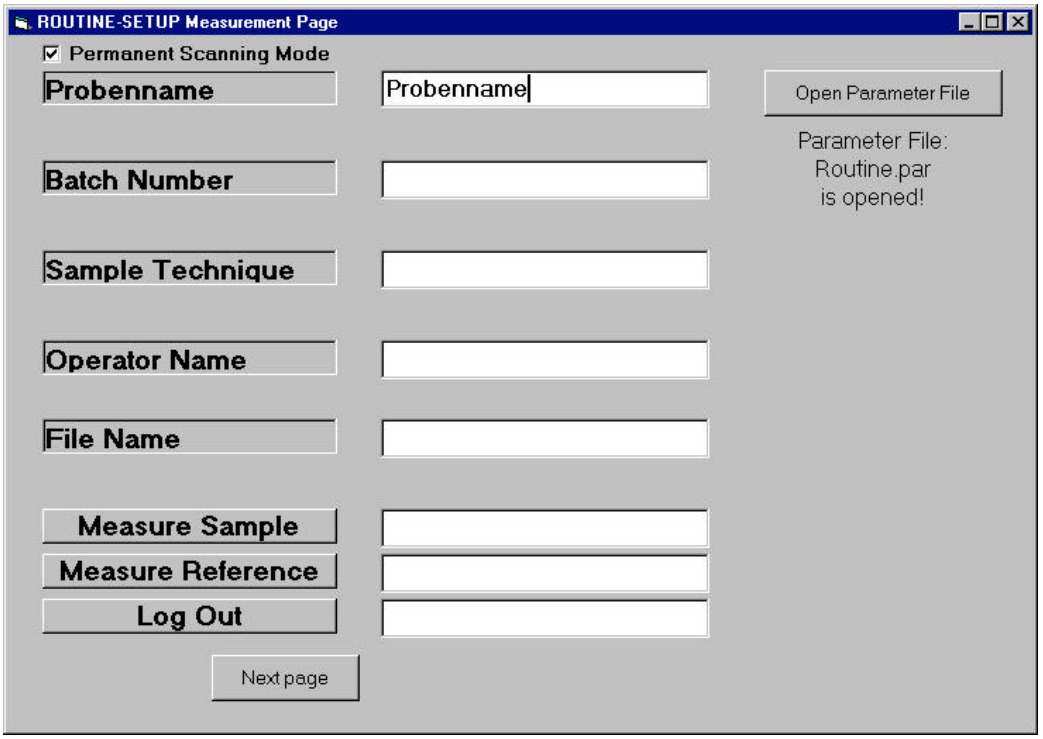
- Text for “Sample Name” Label
- Text for “Charge Number” Label
- Text for “Sample Technique” Label
- Text for “Operator Name” Label
- Text for “File Name” Label
- Text for “Sample Measurement” button
- Text for “Reference Measurement” button
- Text for “Log Out” button



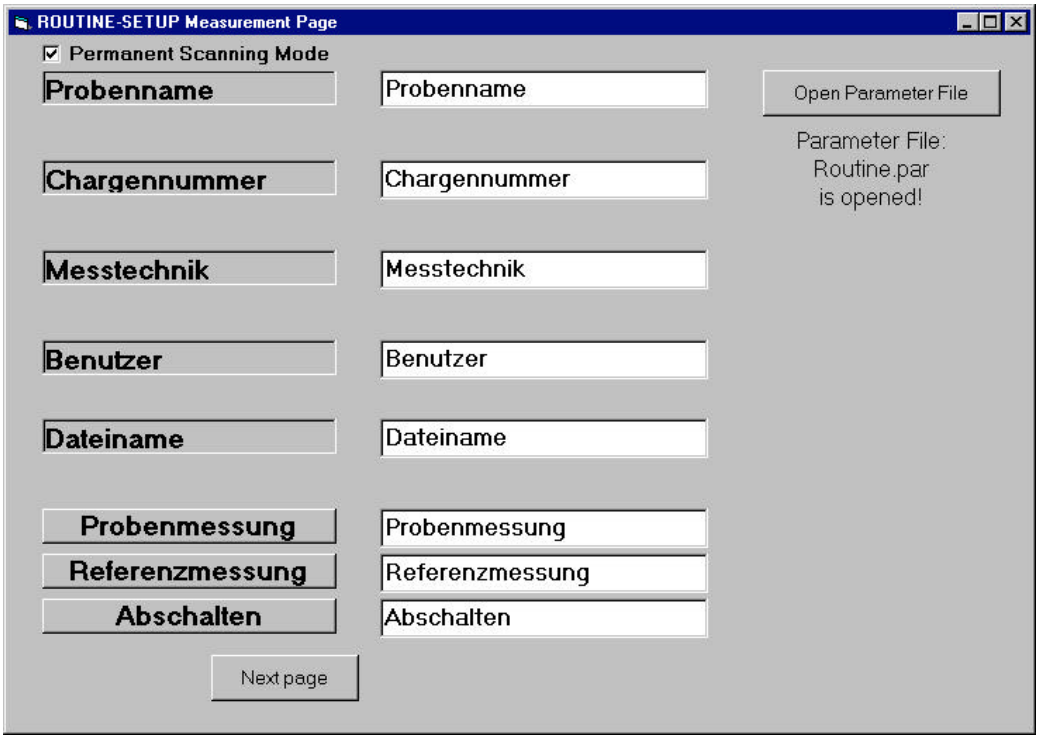
After starting the program the initial page is shown where the captions for labels and buttons can be set. Clicking on the upper right button allows to load any existing parameter file. The next picture shows the first page after loading the ROUTINE.PAR file.



Moving the mouse over the different controls show a short help text as tool tip. To change the text of a label or button simply type the new text in the entry field right from the label or button.



Continue with the rest of the labels and buttons. (If no change is required for one or more labels or buttons you need not enter any text)



Once all entries are done click on the “Next Page” button to advance to the next page.

2.2 Measurement Page Setup Part 2

The second setup page for the ROUTINE measurement page is used to define the sample technique(s) which are offered on the measurement page and the initial contents of all entry fields on that page. It is important to know that these values are directly connected with the sample technique and therefore have to be specified for each sample technique individually.

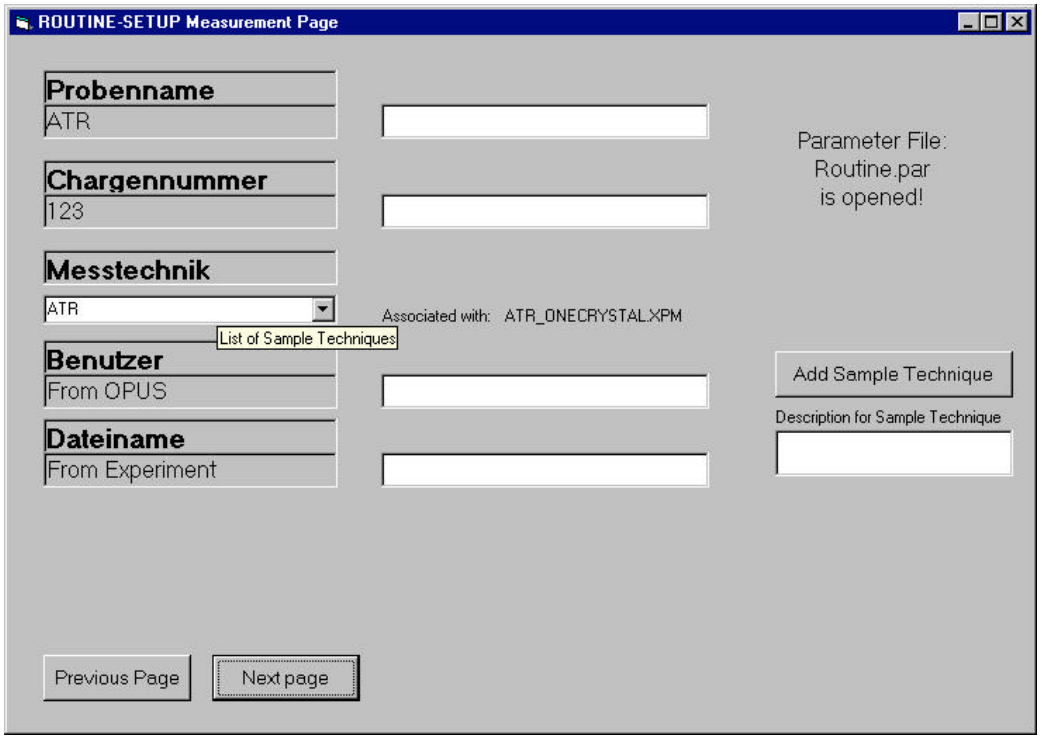
The following elements can be specified:

- Description of the Sample Technique
- Measurement experiment used for the sample technique

For each sample technique the following elements can be specified:

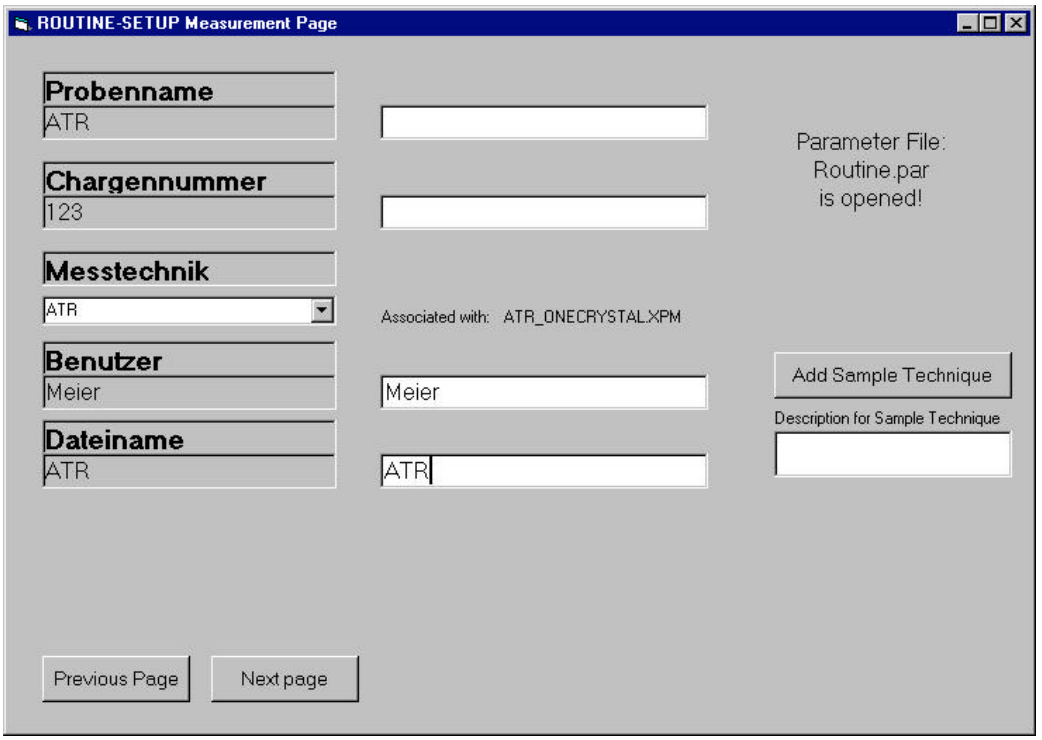
- Initial Sample Name
- Initial Charge Number
- Initial Operator Name (or Keyword “From OPUS”)
- Initial File Name for sample measurements (or Keyword “From Experiment”)

If the keyword “From OPUS” is chosen for the Operator Name the OPUS Login Name will be used.
If the keyword “From Experiment” is chosen for the file name the file name which is specified in the measurement experiment is used.

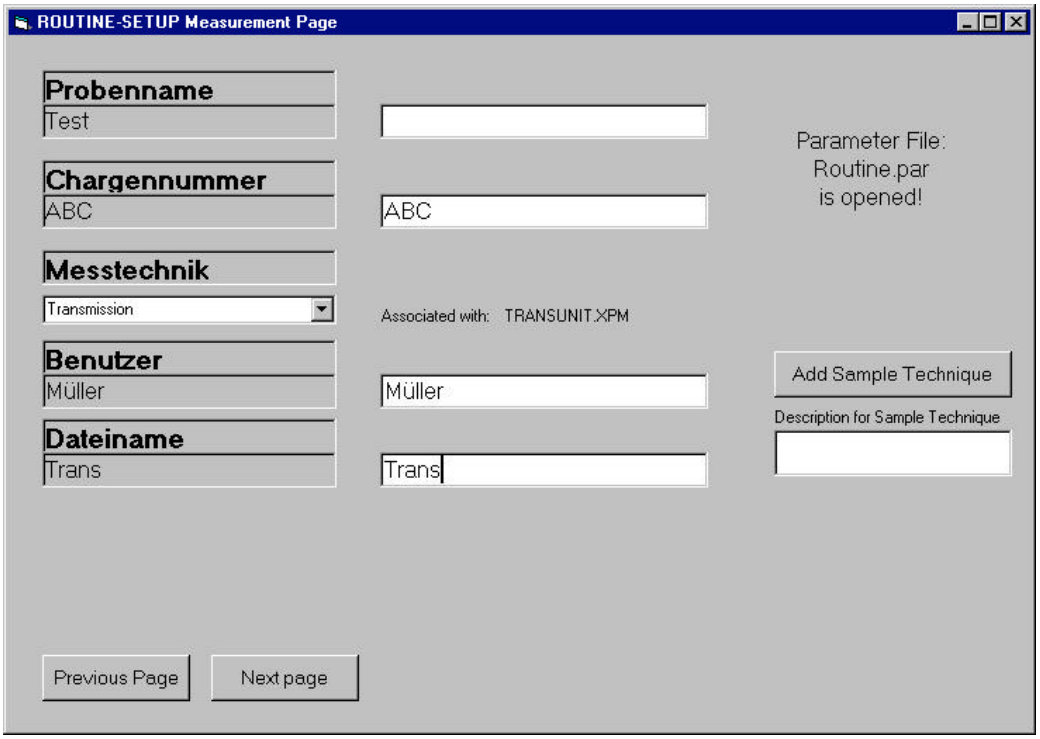


In a first step we will change some of the settings for the available techniques. In the next step we will add a new sample technique.

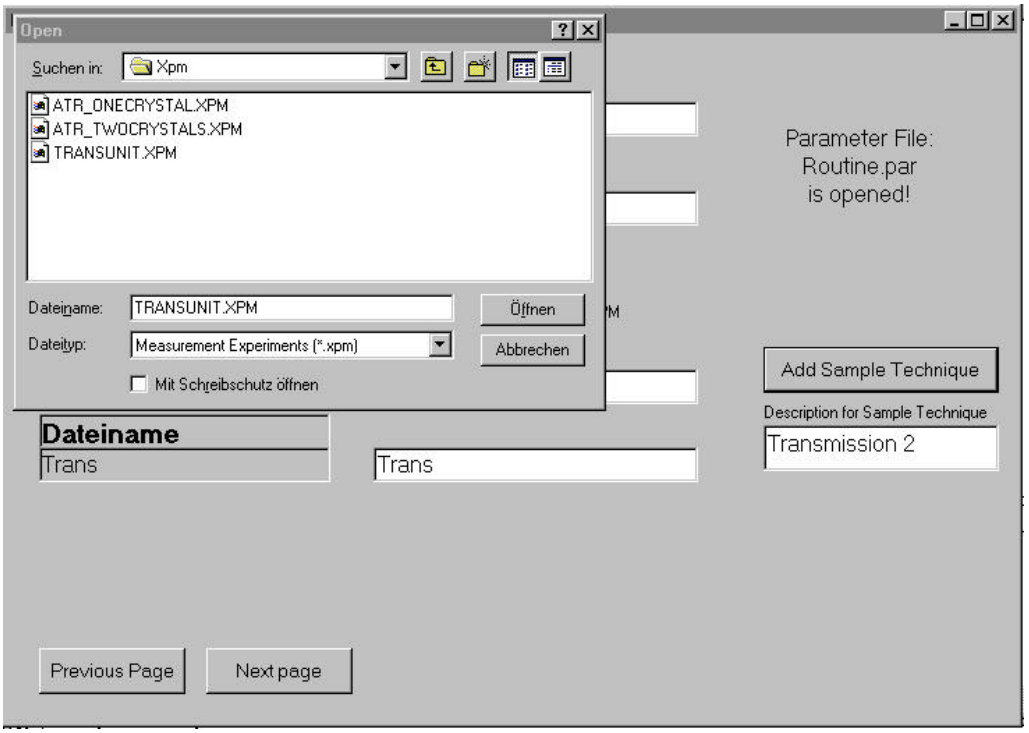
As you can see the fields for the operator name and the file name state the keywords “From OPUS” and “From Experiment”. Alternatively we can also specify our own operator name and file name by entering them in the corresponding entry fields.



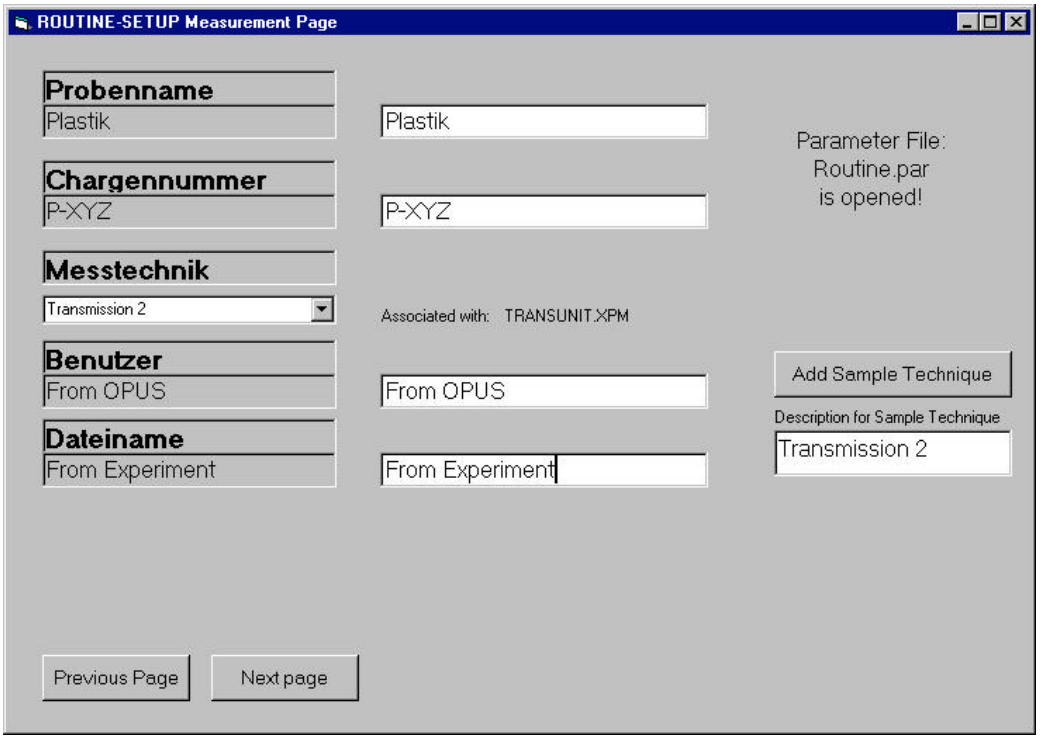
To modify the settings for the next sample technique simply select it from the combo box on the left. All dependant entries will change accordingly and can be modified as already shown.



To add a new sample technique first enter a description in the entry field on the right. Then click on the button “Add Sample Technique” to open a load box where you can choose a measurement experiment. Please note that all measurement experiments to be used for ROUTINE must be stored in the XPM subdirectory of ROUTINE. If you want to use an experiment located in the XPM subdirectory of OPUS you MUST copy or move it to \ROUTINE\XPM first.



Next you must set all entries for this sample technique as well.



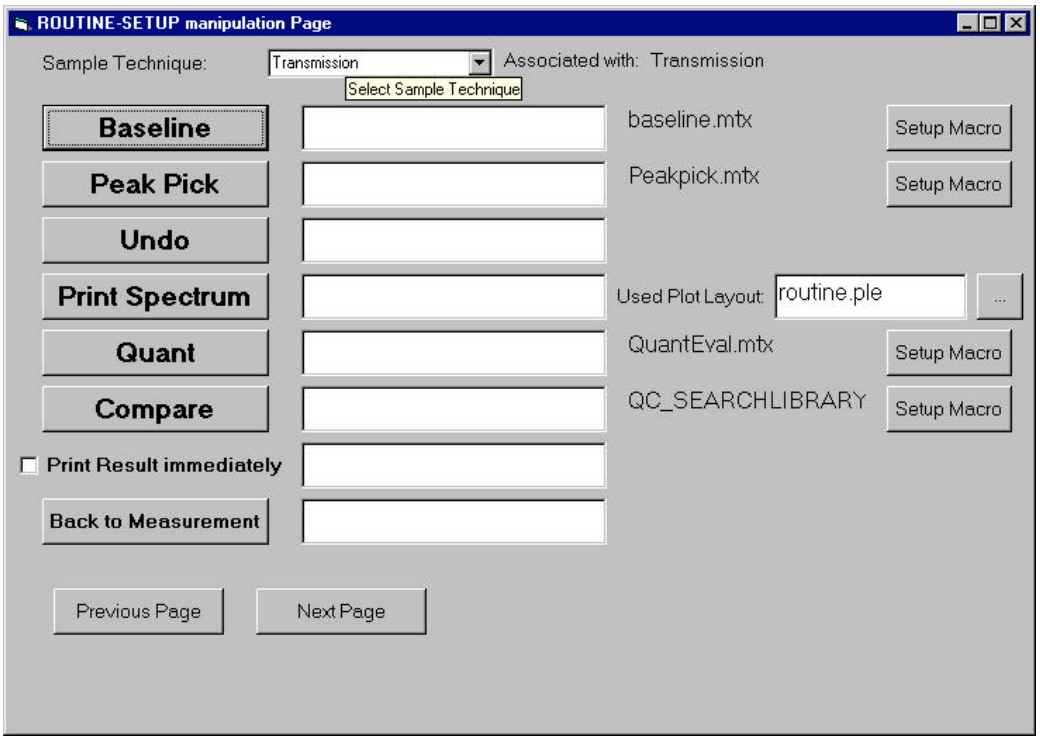
The setup of the measurement page of ROUTINE is now complete. After clicking on “Next Page” button the processing page setup begins.

2.3 Processing Page Setup

The setup page for the ROUTINE processing page is used to define the manipulation and evaluation functions as well as the captions of the controls with predefined functionality. It is important to know that all these values are also directly connected with the sample technique and therefore have to be specified for each sample technique individually.

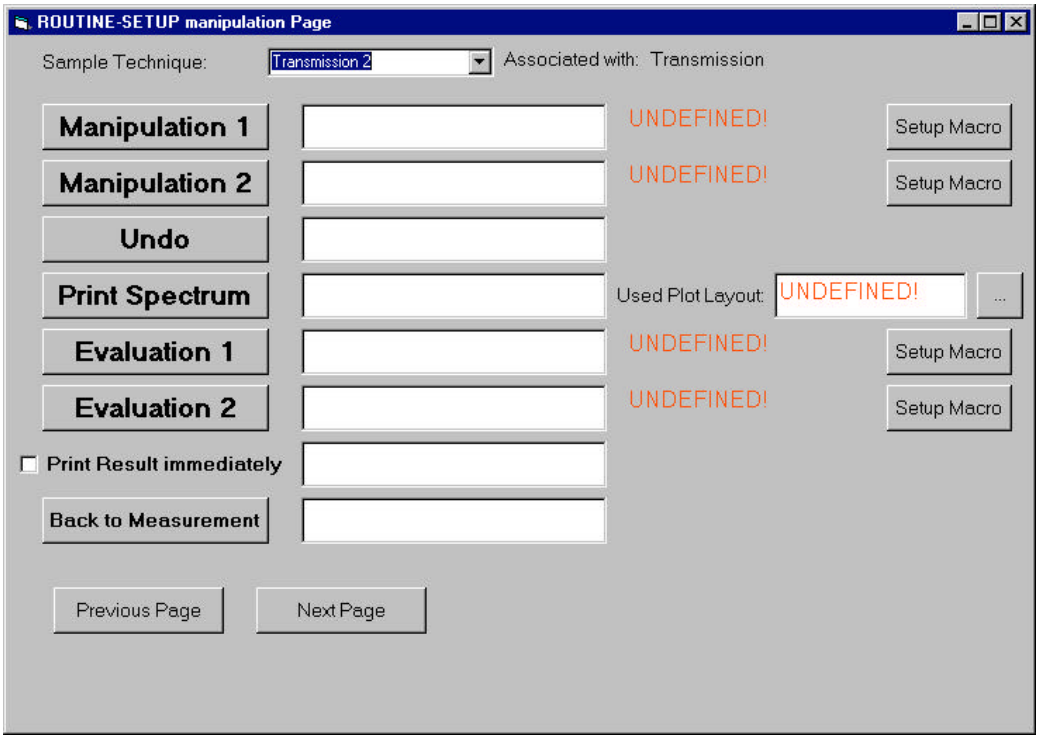
The following elements can be specified:

- Text for the two “Manipulation Function” buttons
- Macros and macro parameters for the two manipulation functions
- Text for the “Undo” button (Functionality is predefined)
- Text for the “Print Spectrum” button (Functionality is predefined)
- Plot Layout for the “Print Spectrum” Function
- Text for the two “Evaluation Function” buttons
- Macros and macro parameters for the two evaluation functions
- Text for the “Print Result immediately” check box (Functionality is predefined)
- Text for the “Back to Measurement” button (Functionality is predefined)



The page shows the buttons and a check box of the ROUTINE processing page. The two manipulation functions and the two evaluation functions show the associated macros right from the input fields and buttons to select and setup the macros. For the Print Spectrum function the plot layout can be selected.

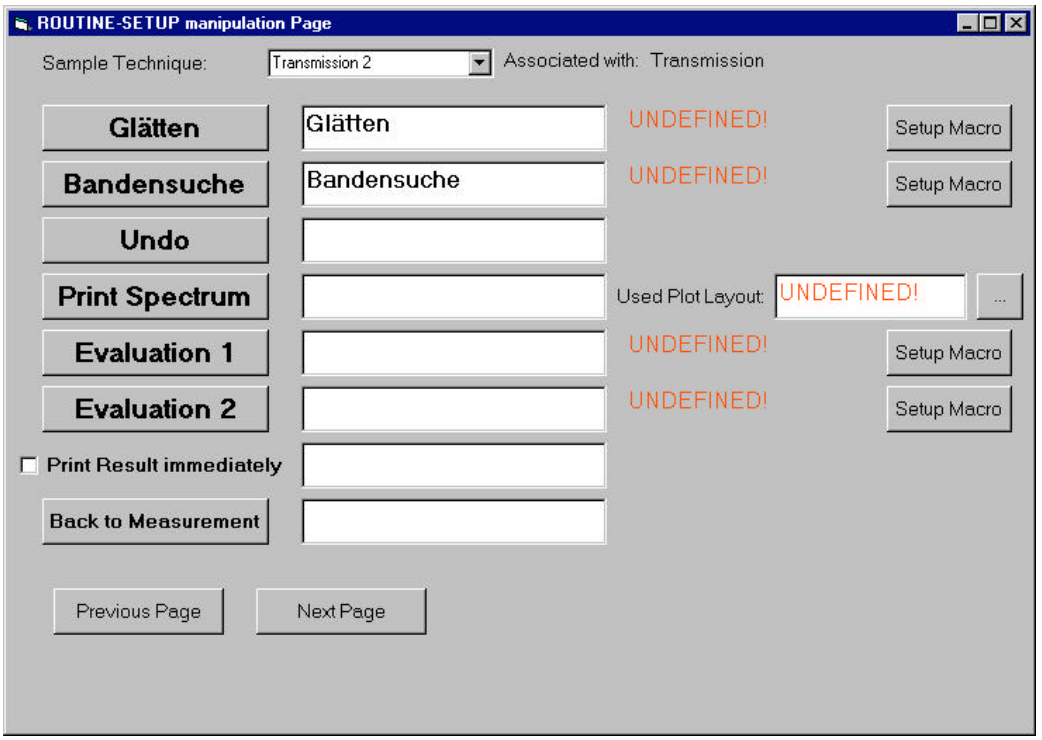
In our example we will keep the functions for the two already existing sample techniques unchanged but we have to specify all settings for the new technique which we have added on the previous page. Therefore as the first step we select the new technique from the combo box at the top of the page.



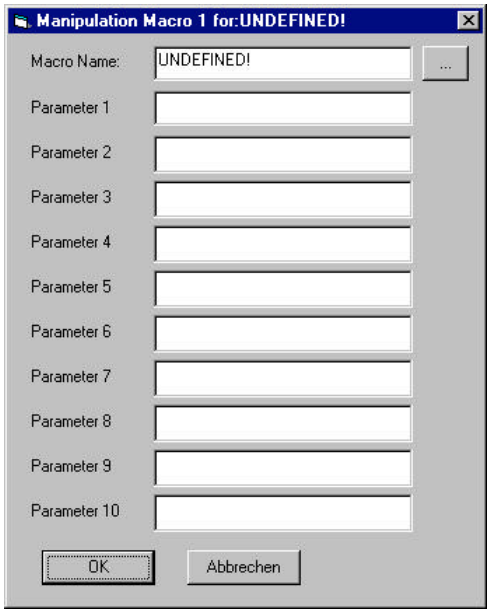
The buttons show the default captions and it is clearly indicated that neither the macros nor the plot layout are yet defined.

Besides the standard functions we only want to specify the two manipulation functions but not the evaluation functions. During executions only those functions are visible for which macros are specified.

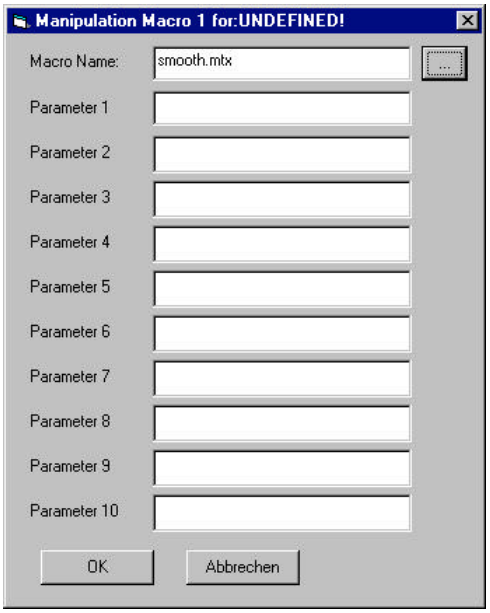
First we enter the button captions as on the other pages by simply typing in the new captions in the entry fields right from the buttons.



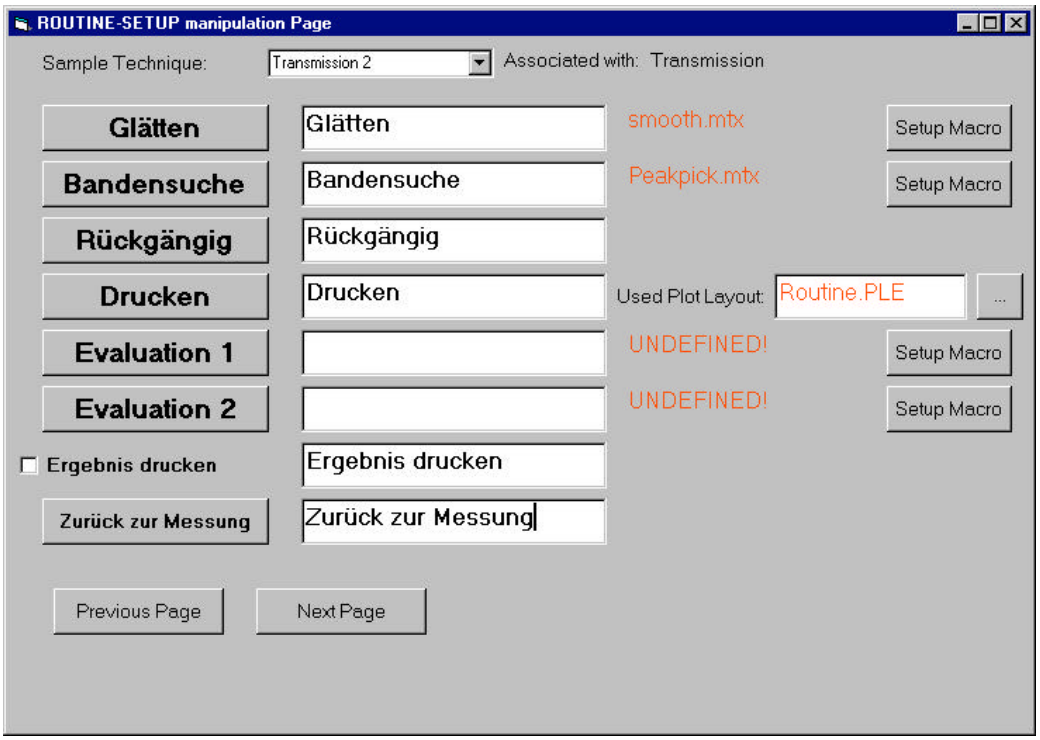
Next we click on the "Setup Macro" button of the first manipulation function. A separate dialog opens where you can select the macro to be executed and eventually required additional parameters to be passed to the macro.



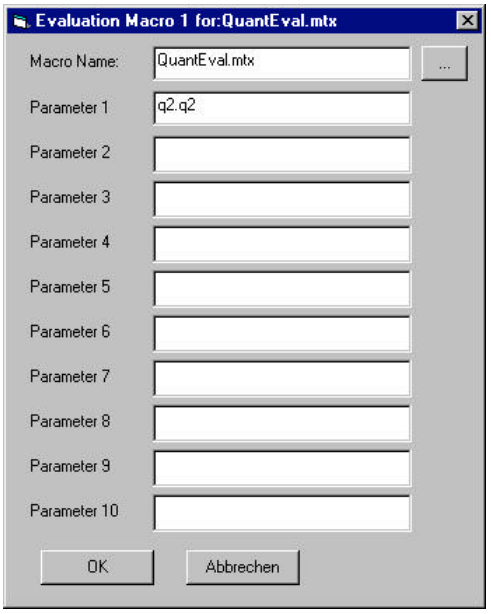
The macros which are used by routine require a special interface which is described later in this manual. The file ID of the previously measured sample spectrum is always passed to all the macro and the print report flag to the evaluation macros.
All macros must be placed in the macro subdirectory of ROUTINE. Macros which have been stored in a different directory must be copied or moved to the \ROUTINE\MACRO path prior to running routine. You can either type in just the name of the macro or select it from the macro path by clicking on the browse button in the upper right corner. We choose the macro "SMOOTH.MTX" which is delivered with the standard configuration. This macro does not require additional parameters.



After clicking on OK the macro name is shown in the first manipulation line. We do the same for the second manipulation function, change the captions of the remaining buttons and controls (except the two evaluation buttons) and choose the plot layout file “ROUTINE.PLE” which can be found in the ROUTINE root path.



A good example for passing additional parameters to a macro is the quantitative analysis which is one of the evaluation functions for the “Transmission” sample technique. In this case the name of the QUANT method is passed to the macro thus giving you the possibility to use the same macro for different types of measurements.



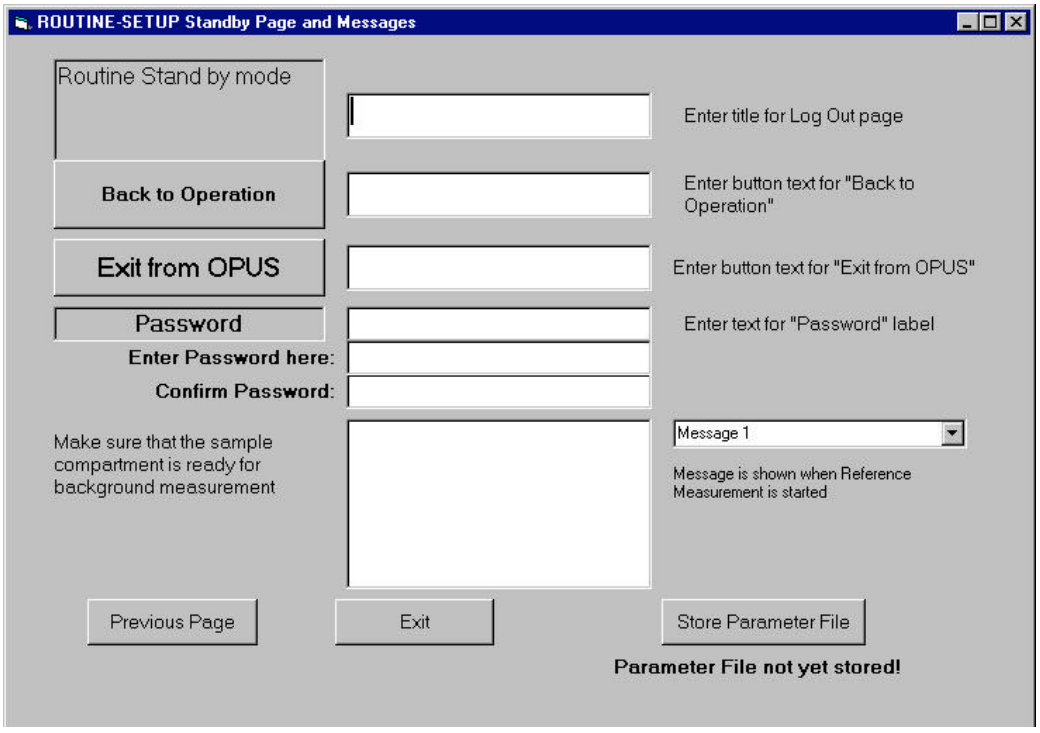
After having set all processing page entries click on the “Next Page” button to proceed to the last page.

2.4 Log Out Page and Messages Setup

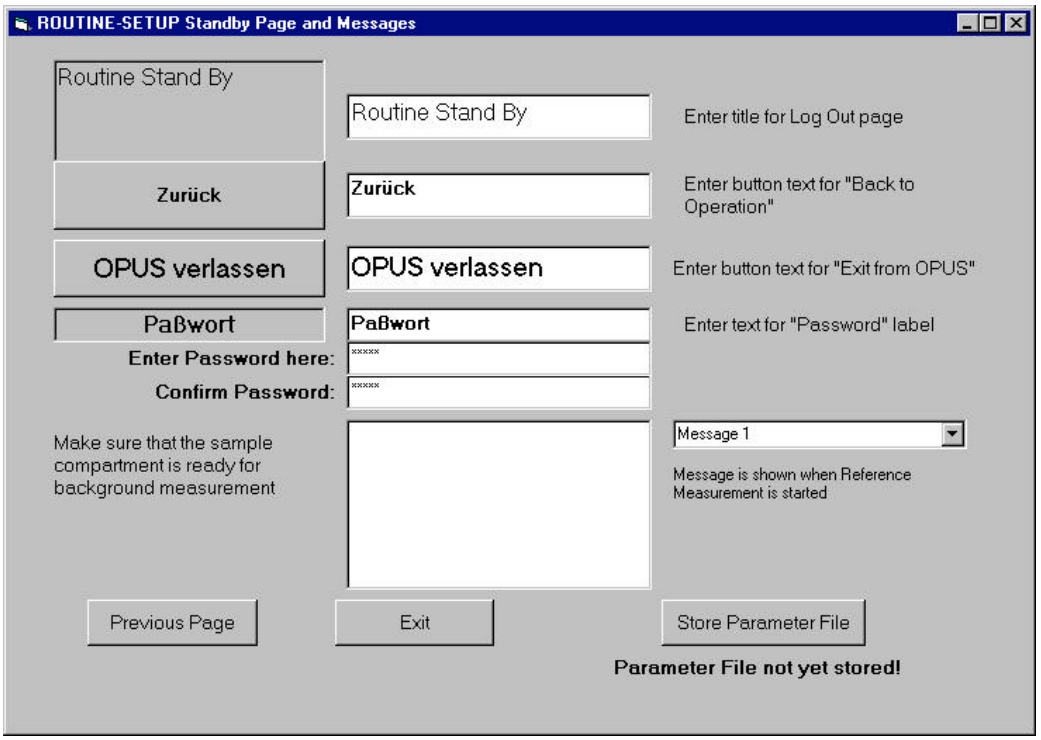
The Log Out page of ROUTINE is used to temporarily shut down the system or to exit from OPUS. Re-entering the ROUTINE interface requires a password. The setup for this page allows to specify title and button caption of this page as well as the password and the text of some messages given by the system during operation.

The following elements can be specified:

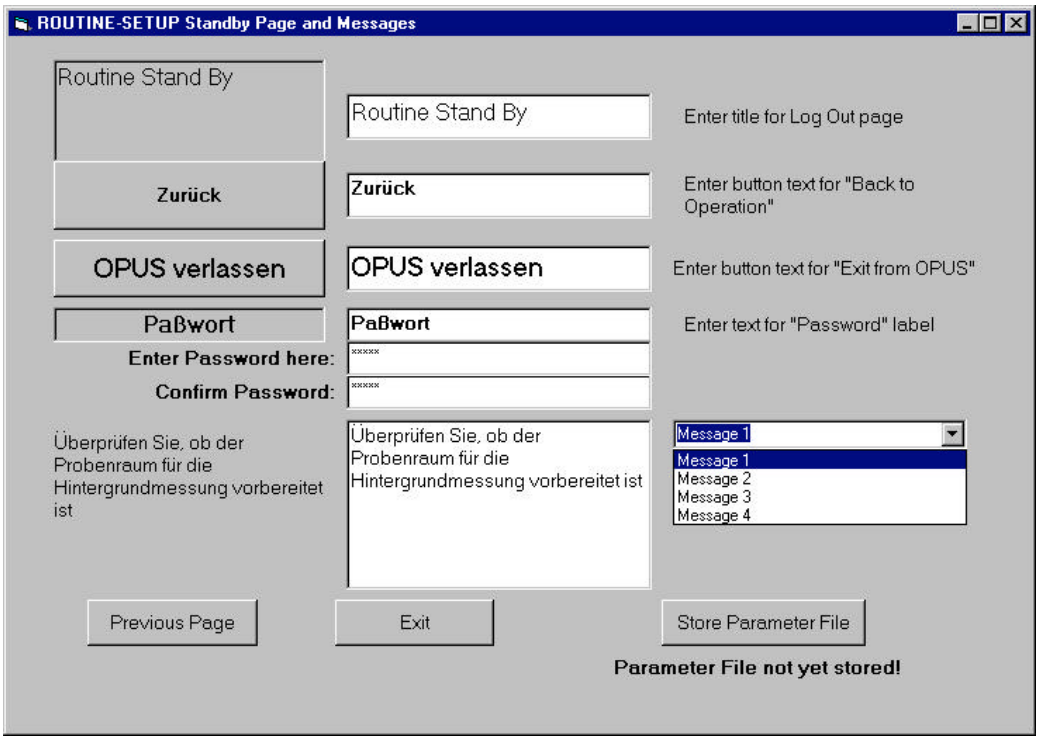
- Title of the Log Out page
- Caption of the “Back to Operation” button
- Caption of the “Exit from OPUS” button
- Text for the “Password” label
- The password itself with confirmation
- A selection of messages



As on the other setup pages the new texts can be entered in the entry fields for the different controls. The password itself and its confirmation is not shown but each character is replaced by a star.



To enter the message texts choose the message to be changed from the combo box. A short description shows the action required to show the message during operation. Enter the new text in the large entry field and advance to the next message. Keeping one of the message entries empty will suppress this message during operation. To get an empty message entry type in a single character and erase it immediately with the “Backspace” key on your keyboard.



To store the changes click on the “Store Parameter File” button. You can either choose to overwrite an existing file or to create a new parameter file. Keep in mind that if you choose a name different from “ROUTINE.PAR” you need to copy or rename it before it can be used by ROUTINE.

3. Structure of a Macro

As already mentioned macros to be used with ROUTINE have to follow certain standards. A master macro in the \ROUTINE\MACRO path can be used to write your own macros quite easily. This macro “MASTER.MTX” already supplies all necessary elements for the ROUTINE calling convention.
Note that all macros must be stored in the \ROUTINE\MACRO directory.

The following documentation shows all required variables and code parts.

The following variables must be present:

STRING <OPUSPath>='';	recommended Variable for the base OPUS path
STRING <ROUTINEPath>='';	recommended Variable for the base ROUTINE path
BOOL <Error> = FALSE;	Error flag top be set within the macro
NUMERIC <File> = 0;	internal file number, this number is passed automatically when the macro is started. This variable has to be used instead of a filevariable in all OPUS functions
BOOL <PrintFlag> = FALSE;	Flag for evaluation macros. This flag is represents the status of the “Print Result immediately” checkbox on the processing page of ROUTINE
STRING <InputPar1>='';	A sequence of 12 additional input parameters
STRING <InputPar2>='';	Any additional values needed for the macro can
STRING <InputPar3>='';	be passed in these parameters
STRING <InputPar4>='';	
STRING <InputPar5>='';	
STRING <InputPar6>='';	
STRING <InputPar7>='';	
STRING <InputPar8>='';	
STRING <InputPar9>='';	
STRING <InputPar10>='';	
STRING <InputPar11>='';	
STRING <InputPar12>='';	
STRING <Status> = '';	The status to be returned to ROUTINE. Set this variable to “OK” if the macro was successful otherwise set it to “NOT OK”
STRING <ErrorOut> = '';	If an error occurs an error text can be passed back which will be shown in a message
STRING <ReturnPar1>='';	*A sequence of return parameters. If at least the*

STRING <ReturnPar2>='';
STRING <ReturnPar3>='';
STRING <ReturnPar4>='';
STRING <ReturnPar5>='';
STRING <ReturnPar6>='';
STRING <ReturnPar7>='';
STRING <ReturnPar8>='';
STRING <ReturnPar9>='';
STRING <ReturnPar10>='';
STRING <ReturnPar11>='';
STRING <ReturnPar12>='';

first parameter is not empty a message box will be shown in ROUTINE with all lines. If the first parameter is empty no message will be shown at all e.g. if the result shall only be printed out..

The following command lines are required in the program section of the macro:

A User Dialog reading all possible input parameters. Note that the first two parameters are passed automatically and need not be specified separately.

UserDialog ('0', STANDARD, FILE:<File>, EDIT:'<PrintFlag>', EDIT:'<InputPar1>', EDIT:'<InputPar2>', EDIT:'<InputPar3>', EDIT:'<InputPar4>', EDIT:'<InputPar5>', EDIT:'<InputPar6>', EDIT:'<InputPar7>', EDIT:'<InputPar8>', EDIT:'<InputPar9>', EDIT:'<InputPar10>', EDIT:'<InputPar11>', EDIT:'<InputPar12>');

The next two lines are optional although highly recommended to write system independent macros.

<OPUSPath> = GetOpusPath();
<ROUTINEPath> = '<OPUSPath>\ROUTINE';

The necessary OPUS Function should be called now using standard command syntax. Use the variable <File> which is passed from the ROUTINE automatically. Error checking should be done as well. In case of an error set the error flag and (optionally) write some error messabge into the variable <ErrorOut>. Depending on the error in most cases you should skip the rest of the macro.

OpusFunctionXYZ ([<File>], {Parameters}); (Syntax example!)
If (MACROERROR, .EQ., TRUE);
<Error> = TRUE;
<ErrorOut> = 'OPUS Function XYZ returned an Error'
Goto (End);
Endif ();

If an evaluation function had been called read the results from the report block into the different output variables. Up to 12 lines can thus be returned to ROUTINE

<ReturnPar2> = FromReportMatrix ([<File>:Spec/Report], Report, Subreport, Row, Column); (Syntax example!)

If an evaluation function had been called handle the printout of the result in the next few lines. Check the print flag which is also automatically passed fromROUTINE and which represents the status of the “Print Result immediately” check box.

```
If (<PrintFlag>, .EQ., TRUE);
REM Insert Print Statement here
Else ();
REM Set the return variables to show the result in a message
 <ReturnPar1> = 'This is the Header of the Result Report';
 <ReturnPar3> = 'This may be any explaining text';
Endif ();
```

Mark the exit code with the label End (see also comments on error checking above). Set the <Status> variable depending on the result of the operation to either “OK” or “NOT OK”. If not already done you can optionally return an error message in <ErrorOut>

```
Label (End);
If (<Error>, .EQ., FALSE);
<Status> = 'OK';
Else();
<Status> = 'ERROR';
If (‘<ErrorOut>’, .EQ., ‘’);
<ErrorOut> = 'Optional Error Message';
Endif ();
Endif ();
```

The last line in the macro **must** be the dialog with **all** return parameters

```
UserDialog ('0', STANDARD, EDIT:'<Status>', EDIT:'<ErrorOut>',
EDIT:'<ReturnPar1>', EDIT:'<ReturnPar2>', EDIT:'<ReturnPar3>',
EDIT:'<ReturnPar4>', EDIT:'<ReturnPar5>', EDIT:'<ReturnPar6>',
EDIT:'<ReturnPar7>', EDIT:'<ReturnPar8>', EDIT:'<ReturnPar9>',
EDIT:'<ReturnPar10>', EDIT:'<ReturnPar11>', EDIT:'<ReturnPar12>');
```

For further information you can also check the macros already supplied with ROUTINE.

4. Example of a Parameter File

```
ServiceInterval=-1
InstrumentTest=NO
PermanentScanningMode=YES
OperatorButton=Operator Name
SampleNameButton=Sample Name
ChargeNumberButton=Batch Number
SampleTechniqueButton=Sample Technique
FileNameButton=File Name
MeasureSampleButton=Measure Sample
MeasureReferenceButton=Measure Reference
LogOutButton=Log Out
NrSampleTechniques=2
SampleTechnique.1=Transmission
XpmDatei.1=TRANSUNIT.XPM
FileName.1=From Experiment
OperatorName.1=From OPUS
ChargeNumber.1=123
SampleName.1=Test
SampleTechnique.2=ATR
XpmDatei.2=ATR_ONECRYSTAL.XPM
FileName.2=From Experiment
OperatorName.2=From OPUS
ChargeNumber.2=123
SampleName.2=ATR
FirstManipulation.Caption.1=Baseline
FirstManipulation.Macro.1=baseline.mtx
FirstManipulation.Macro.1.NrPara=0
SecondManipulation.Caption.1=Peak Pick
SecondManipulation.Macro.1=Peakpick.mtx
SecondManipulation.Macro.1.NrPara=0
FirstEvaluation.Caption.1=Quant
FirstEvaluation.Macro.1=QuantEval.mtx
FirstEvaluation.Macro.1.NrPara=2
FirstEvaluation.Macro.1.Para.1=path
FirstEvaluation.Macro.1.Para.2=q2.q2
SecondEvaluation.Caption.1=Compare
SecondEvaluation.Macro.1=QC_SEARCHLIBRARY.MTX
SecondEvaluation.Macro.1.NrPara=0
Print.Caption.1=Print Spectrum
PrintResult.Caption.1=Print Result immediately
PrintPLE.1=routine.ple
BackToMeas.Caption.1=Back to Measurement
UndoButton=Undo
FirstManipulation.Caption.2=Smooth
FirstManipulation.Macro.2=smooth.mtx
FirstManipulation.Macro.2.NrPara=0
SecondManipulation.Caption.2=Peak Pick
SecondManipulation.Macro.2=Peakpick.mtx
SecondManipulation.Macro.2.NrPara=0
```

FirstEvaluation.Caption.2=Compare
FirstEvaluation.Macro.2=QC_SEARCHLIBRARY.MTX
FirstEvaluation.Macro.2.NrPara=0
SecondEvaluation.Caption.2=
SecondEvaluation.Macro.2=
SecondEvaluation.Macro.2.NrPara=0
Print.Caption.2=Print Spectrum
PrintResult.Caption.2=Print Result immediately
PrintPLE.2=Routine.PLE
BackToMeas.Caption.2=New Measurement
UndoButton=Undo
LogoutTitle=Routine Stand by mode
LogoutEndButton=Back to Operation
ExitButton=Exit from OPUS
Password.Title=Password
Password.Contents=
Message.1=Make sure that the sample compartment is prepared for the reference measurement!
Message.2=A new reference measurement is necessary!
Message.3=Please remove the sample and clean the sample compartment!
Message.4=Illegal password, retry!

5. Syntax of the entries in the parameter file

Keyword	Comment	Type of entry
ServiceInterval	Not yet used	
InstrumentTest	Perform Instrument Test when started or after return from Log Out	"YES", "NO"
PermanentScanningMode	Operation mode for Permanent Scanning Mode	"YES", "NO"
OperatorButton	Text for Operator Name Label	Text
SampleNameButton	Text for Sample Name Label	Text
ChargeNumberButton	Text for Charge Number Label	Text
SampleTechniqueButton	Text for Sample Technique Label	Text
FileNameButton	Text for File Name Label	Text
MeasureSampleButton	Text for Measure Sample Button	Text
MeasureReferenceButton	Text for Measure Reference Button	Text
LogOutButton	Text for Log Out Button (on page 1 and 2)	Text
NrSampleTechniques	Number of sample techniques used	Number
SampleTechnique.n	Description of Sample Technique number n	Text
XpmDatei.n	Experiment file used for Sample Technique number n	File name with extension
FileName.n	Initial file name for Sample Technique number n	Text or "From Experiment"
OperatorName.n	Initial operator name for Sample Technique number n	Text or "From OPUS"
ChargeNumber.n	Initial charge number for Sample Technique number n	Text
SampleName.n	Initial sample name for Sample Technique number n	Text
Print.Caption.n	Text for Print Button for Sample Technique number n	Text
PrintResult.Caption.n	Text for Print Result check box for Sample Technique number n	Text
PrintPLE.n	Plot Layout file name for Sample Technique number n	File name with extension
BackToMeas.Caption.n	Text for Back to Measurement Button for Sample Technique number n	Text
FirstManipulation.Caption.n	Text for first manipulation button for Sample Technique number n	Text
FirstManipulation.Macro.n	Macro for first manipulation for Sample Technique number n	File name with extension
FirstManipulation.Macro.n.NrPara	Number of Parameters for first manipulation macro	Number
FirstManipulation.Macro.n.Para.m	Parameter m for first manipulation macro	Text

SecondManipulation.Caption.n	Text for second manipulation button for Sample Technique number n	Text
SecondManipulation.Macro.n	Macro for second manipulation for Sample Technique number n	File name with extension
SecondManipulation.Macro.n.NrPara	Number of Parameters for second manipulation macro	Number
SecondManipulation.Macro.n.Para.m	Parameter m for second manipulation macro	Text
FirstEvaluation.Caption.n	Text for first evaluation button for Sample Technique number n	Text
FirstEvaluation.Macro.n	Macro for first evaluation for Sample Technique number n	File name with extension
FirstEvaluation.Macro.n.NrPara	Number of Parameters for first evaluation macro	Number
FirstEvaluation.Macro.n.Para.m	Parameter m for first evaluation macro	Text
SecondEvaluation.Caption.n	Text for second manipulation button for Sample Technique number n	Text
SecondEvaluation.Macro.n	Macro for second manipulation for Sample Technique number n	File name with extension
SecondEvaluation.Macro.n.NrPara	Number of Parameters for second manipulation macro	Number
SecondEvaluation.Macro.n.Para.m	Parameter m for second manipulation macro	Text
LogoutTitle	Title of Log Out page	Text
LogoutEndButton	Text for Back to Operation Mode button	Text
Exit Button	Text for Exit from OPUS button	Text
Password.Title	Text for Password label	Text
Password.Contents	Password	Crypted text
Message.n	Text for message n	Text