

SpecsLab Prodigy Reporting

VERSION 1.19

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SPECSTM

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1 Introduction

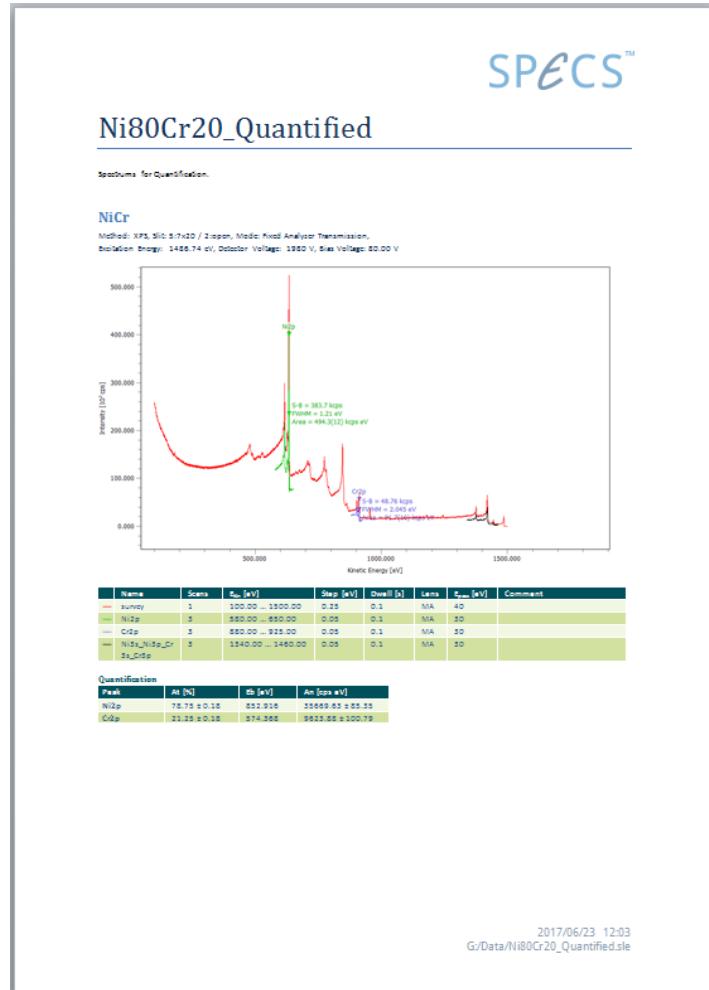
This module requires a license. Without a license only preconfigured standard reports can be used. Please contact SPECS support if you want to obtain a license.

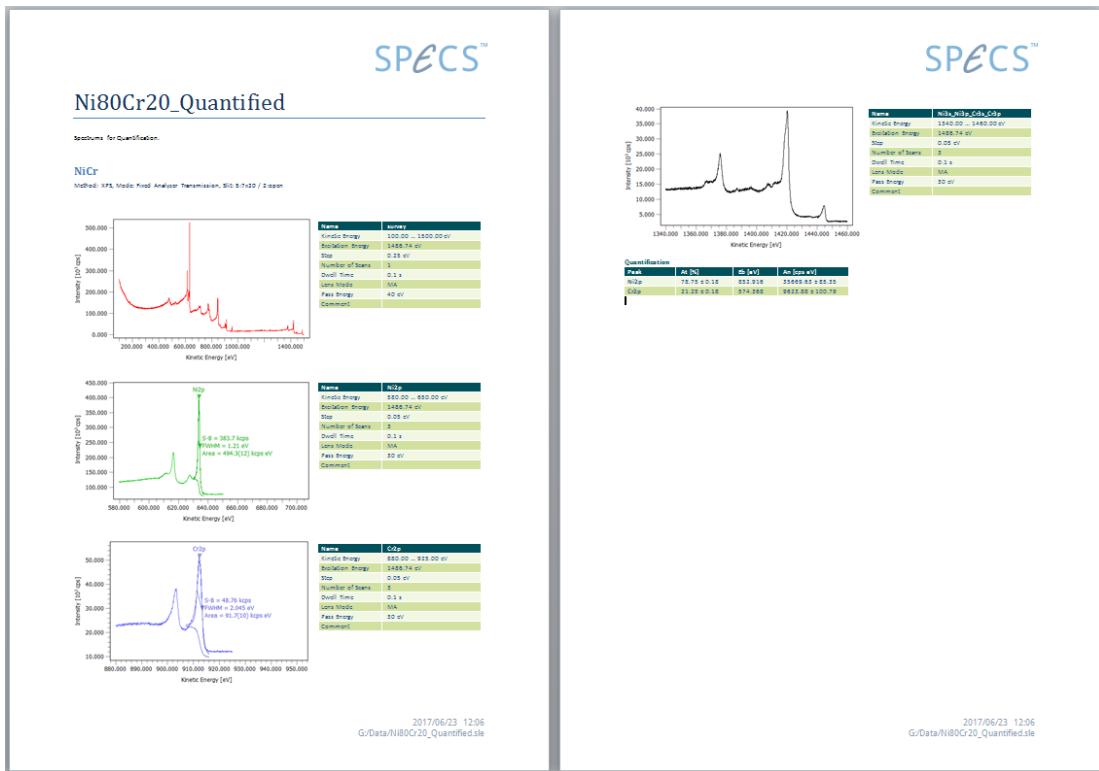
1.1 SpecsLab Prodigy Reporting

The SpecsLab Prodigy Reporting feature allows creating highly configurable reports in both Microsoft Word™ and PDF™ format.

The report templates can be easily written or modified in Microsoft Word™.

It is possible to create a report automatically while an experiment is running or manually after the experiment has finished.





1.2 General Information

- The Report Template itself is a Microsoft Word™ File (docx).
- WordPad (included in Windows™) is sufficient to view created Reports.
- Microsoft Word™ is required to modify a report template.
- Microsoft Word™ is required to create PDF files.

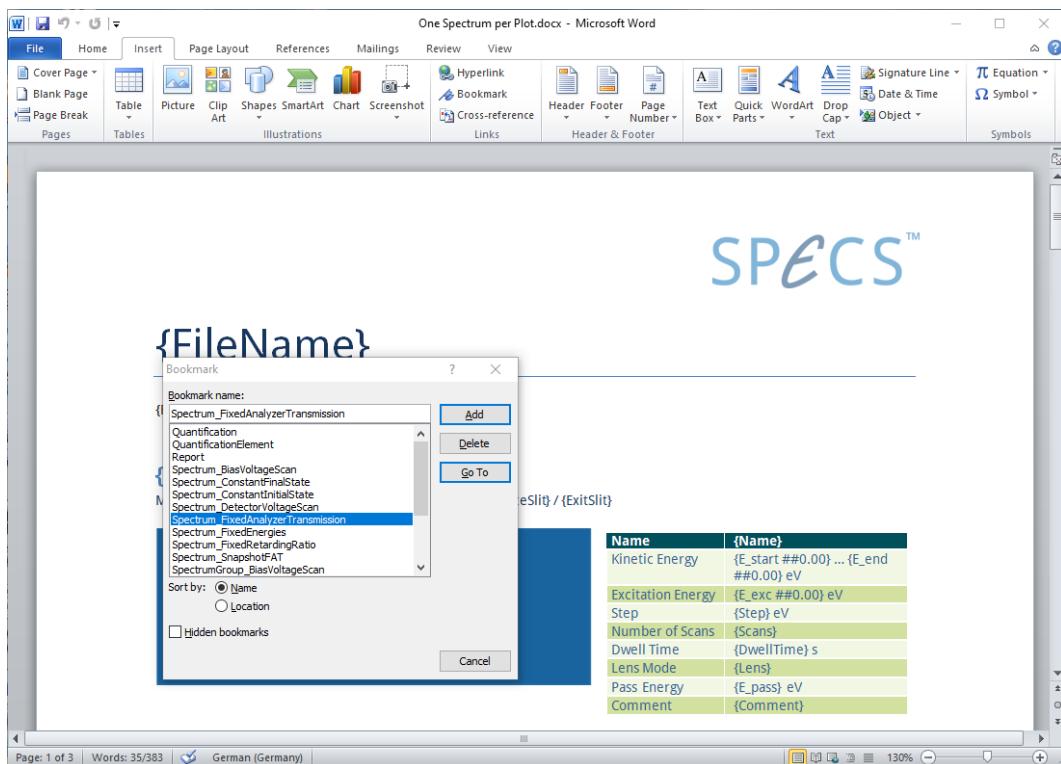
1.3 Template Basics

- The template is based on bookmarks and fields.
- Bookmarks represent SpecsLab Prodigy experiment items like “File”, “Spectrum Group”, “Spectrum”, or “Quantification”.
- Fields are entries within items like “DwellTime” for the acquisition dwell time.
- Bookmarks are used for items which can occur multiple times in a report.
- Fields are elements within these bookmarks which will be replaced.
- Fields and bookmarks are case insensitive.
- Fields must be enclosed in brackets.
- An export traverses the experiment from top to bottom and exports every non-empty item.
- When SpecsLab Prodigy processes “Quantification” or any other item it searches the report template for a bookmark named “Quantification”, pastes the block at the end of the new report file and then replaces all known fields by its values.

1.4 Bookmarks and Fields

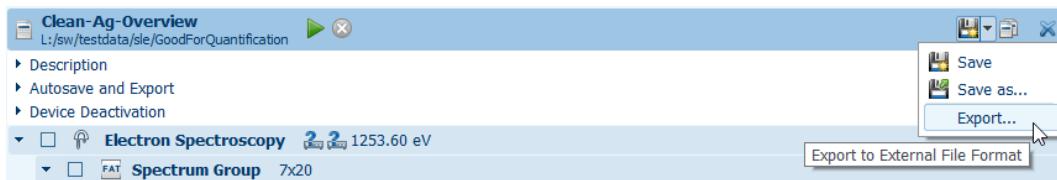
Bookmarks are used to group experiment items. Each bookmark has specific fields which will be replaced by SpecsLab Prodigy when processing the template.

Existing Bookmarks get listed in the Bookmark Dialog which is available in the Insert Ribbon. The “Go To” command highlights the bookmark section.



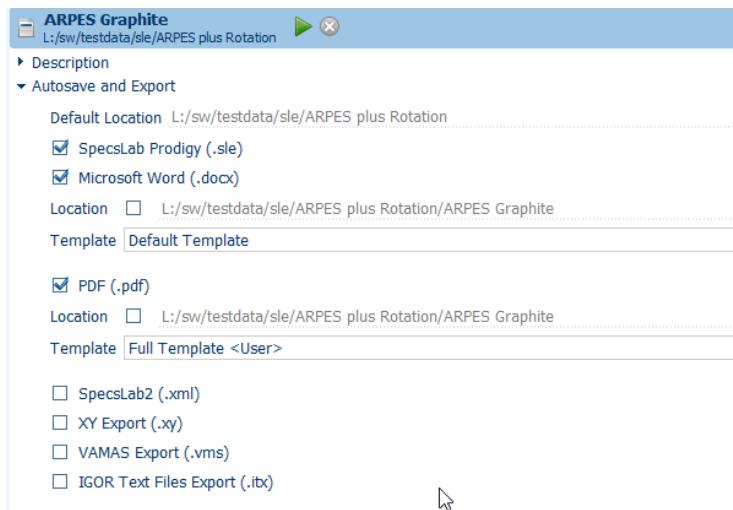
1.5 Using Experiment Templates

It is possible to create a report manually using “Export” in the toolbar of the experiment in the Experiment Editor and selecting Microsoft Word™ (.docx) or .pdf as type.



It is also possible to automatically create the report after the experiment has finished: In the Experiment Editor expand “Autosave and Export” and check Microsoft Word (.docx) or PDF (.pdf). The “Template” drop down menu allows you to select different templates. You can place your own templates in the Folder

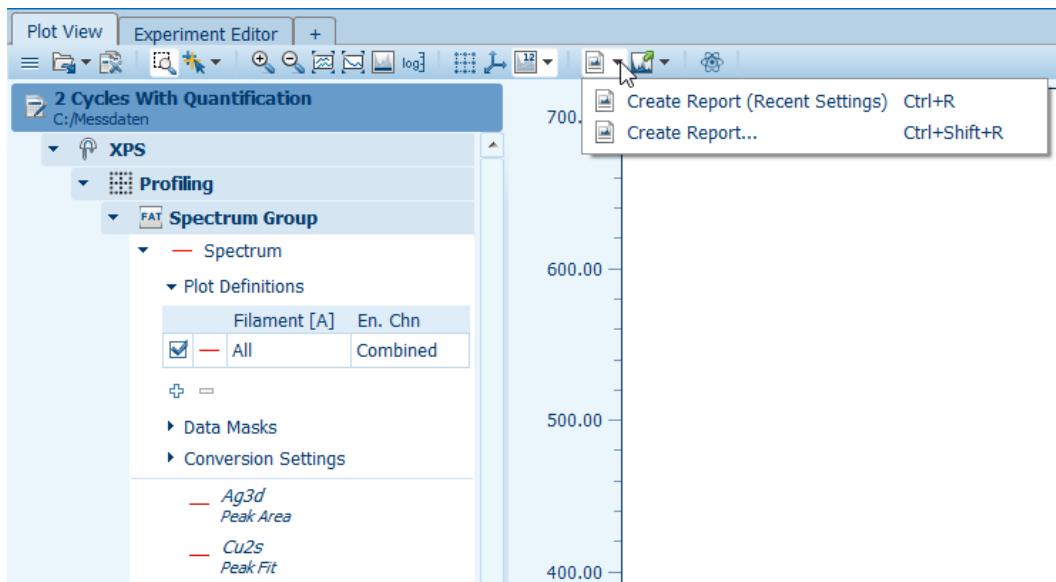
C:\Users\Public\Documents\SpecsLab
Prodigy\ReportingTemplates\Experiment
(Restart of Prodigy is required to use them.)



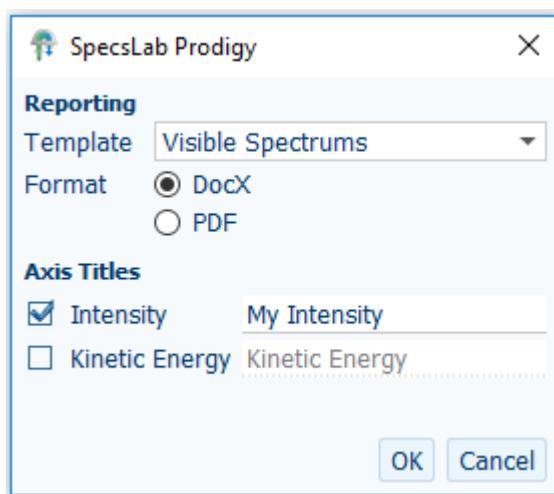
After the experiment has been executed the report will be created.

1.6 Using Plot View/Image View Templates

In Plot View and Image View a report can be created using the toolbar buttons. This report will contain all visible elements and an image of the currently visible plot.



After clicking "Create Report...", a dialog appears which allows to choose the template, the output format and to customize the axis titles:



You can place your own templates in the Folder

C:\ProgramData\SPECS\SpecsLab Prodigy\ReportingTemplates\PlotView\

C:\ProgramData\SPECS\SpecsLab Prodigy\ReportingTemplates\ImageView\

1.7 Creating PDF Files

PDF Files are created using Microsoft Word™ as post processor. In Microsoft Word™ PDF options are configurable as for example the resolution of the document.

1.8 Modifying Templates

It is recommended to modify an existing report template, for example "Full Template.docx". This template contains examples for all spectrum variants and is a good starting point.

Copy one of the existing docx Templates from

C:\Program Files\SPECS\SpecsLab Prodigy\database\ReportingTemplates

to the folder for "User Templates":

C:\ProgramData\SPECS\SpecsLab Prodigy\ReportingTemplates

Open the copied file in Microsoft Word™ and adapt it as desired.

Please note that a restart of SpecsLab Prodigy is required when you add a new template to the user folder before it is visible in "Autosave and Export" and in Plot View/Image View. Changes in the report file will have immediate effect.

2 List of Items (Bookmarks)

2.1 ViewReport

The Bookmark ViewReport is available only in reports from Image View and Plot View. This is necessary since Plot View and Image View can create reports for more than one file.

This bookmark provides the field ViewPicture which reports the currently visible plot with the active axis settings including the current image section. Since the axes of the plot are already configured only the Image Sizing options (see 3.4.1) are available in the “Alt Text” section.

Field	Description	Example
ViewPicture	The currently visible plot/image	See below for Picture Formatting

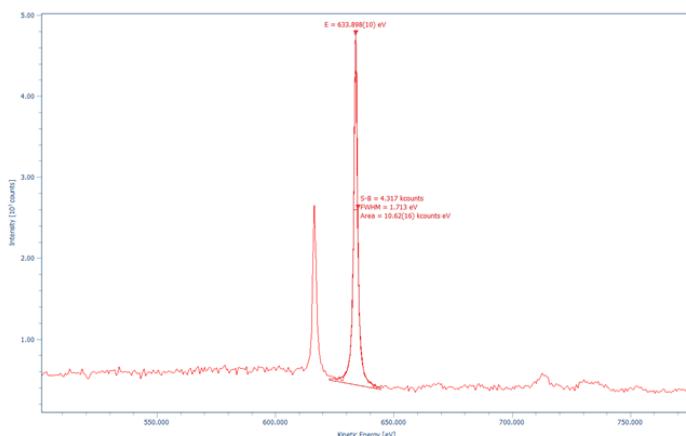
Template snippet:

My Plot View/Image View Report



Results in:

My Plot View/Image View Report



2.2 Report

The “Report” bookmark must always be present and must enclose everything else in experiment report templates. Fields usable in this context are:

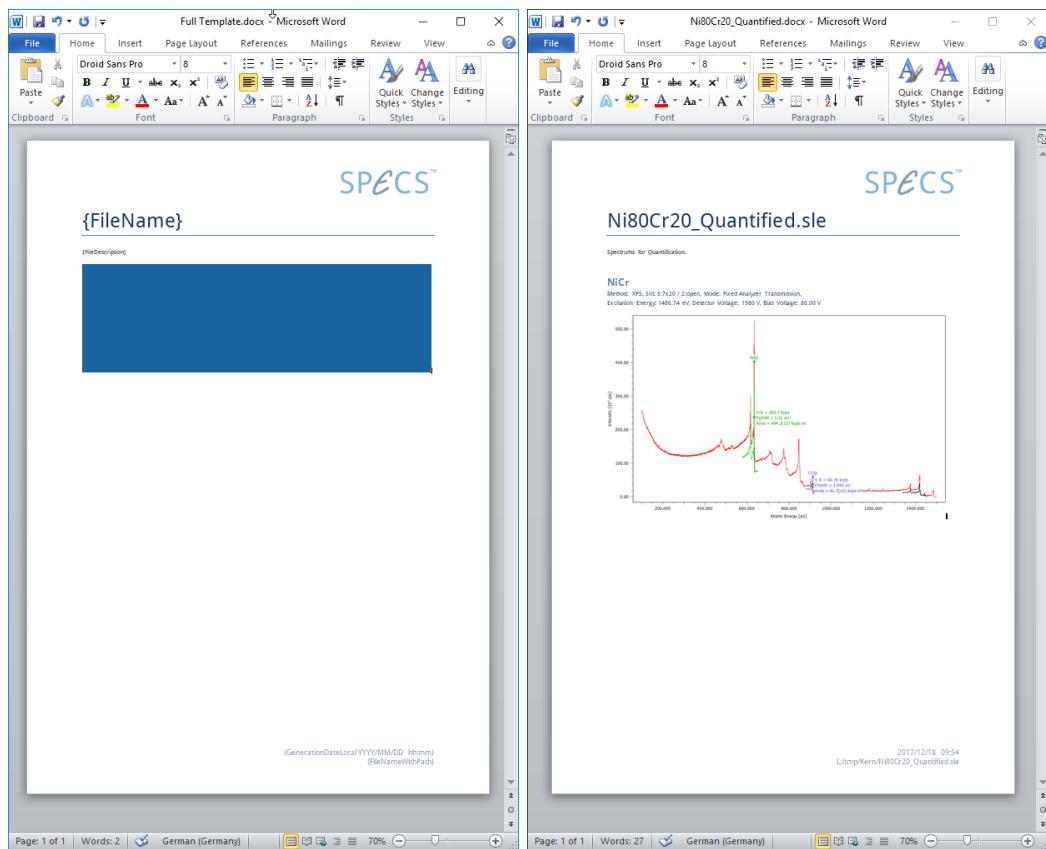
Field	Description	Example / Remark
FileName	Name of the Experimentfile	MyExperiment.sle
FileNameWithoutExtension	Name of the Experimentfile without extension	MyExperiment
FileNameWithPath	Name with Path of the Experimentfile	C:/MyExperiment.sle
UserName	Username of the currently logged on user including domain	SPECS\smith
UserFullName	Name of the logged on user taken from windows user	John Smith
GenerationDateLocal	Generation Date of the report in local time.	26/May/2017 13:09:28 (see below for date formatting)
GenerationDateUTC	Generation Date of the report in UTC time	26/May/2017 12:09:28 (see below for date formatting)
FileDescription	Description of the Experiment set in the Experiment	My description of the experiment.
PlotPicture	Plot of all elements in the experiment	(see below for Picture Formatting)
Meta_*	Additional information with a Meta_ prefix	(usable only in special cases)
SampleHolder_Description	Description of the sample holder set in the Experiment	My description of the sample holder.
SampleHolder_Picture	Sample holder image from the experiment	(use ‘UsePlaceHolderWidth’ for automatic fitting)
Experiment_*	Additional information for the experiment as defined by the user	(only available if defined)

All fields except picture fields can also be used in the header or footer and are available in all other bookmarks as well.

‘FileDescription’ and ‘SampleHolder_Description’ can be enclosed in an optional bookmark with the same name to avoid empty lines in the report.

In addition to the individual meta information fields, the entire information can also be specified in a table by using the ‘Experiment_MetaInfo’ bookmark for the table and ‘Experiment_MetaInfoElement’ for each row. Each entry provides the fields ‘Name’ and ‘Value’ or ‘Value_Num’ for textual or numerical values.

The left screenshot shows a part of the template, the right screenshot the result:

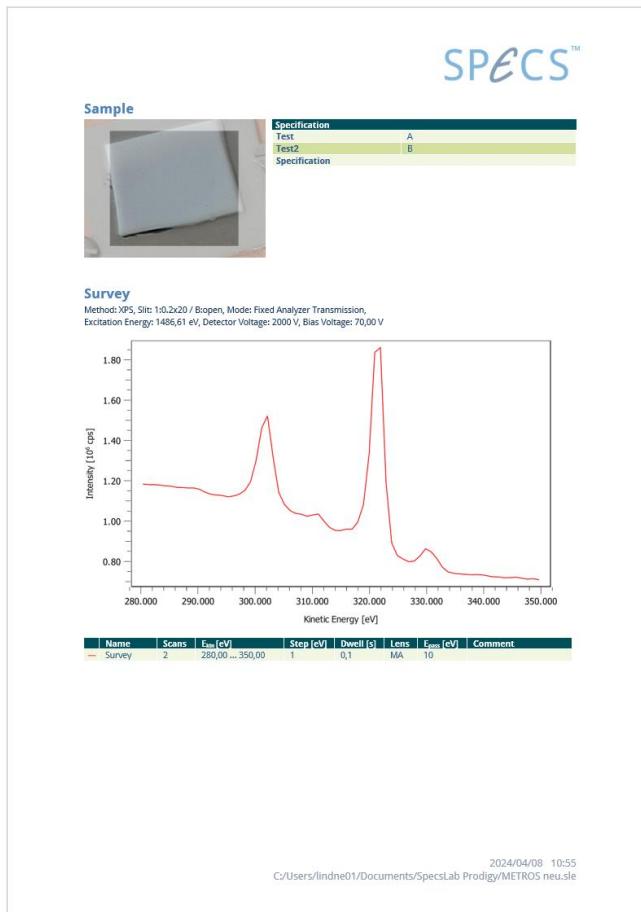


2.3 Sample

The 'Sample' bookmark can be used to insert the name, additional meta information and the image of each sample from the experiment. Fields usable in this context are:

Field	Description	Remark
Sample_Name	Name of the sample	
Sample_Picture	Sample image from the experiment	(use 'UsePlaceholderWidth' for automatic fitting)
Sample_*	Additional information per samples as defined by the user	(only available if defined)

In addition to the individual meta information fields, the entire information can also be specified in a table by using the 'Sample_MetaInfo' bookmark for the table and 'Sample_MetaInfoElement' for each row. Each entry provides the fields 'Name' and 'Value' or 'Value_Num' for textual or numerical values.



2.4 SpectrumGroup_*

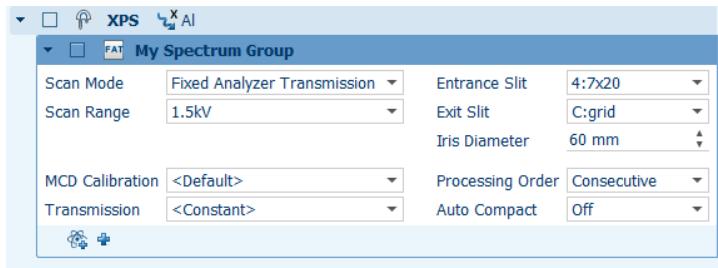
There are cases where it makes sense to have different representations of a “Spectrum Group” with its spectrums depending on the scan mode. For that purpose you can specify different bookmarks:

- SpectrumGroup_FixedAnalyzerTransmission
- SpectrumGroup_FixedEnergies
- SpectrumGroup_SnapshotFAT
- SpectrumGroup_FixedRetardingRatio
- SpectrumGroup_DetectorVoltageScan
- SpectrumGroup_BiasVoltageScan
- SpectrumGroup_ConstantFinalState
- SpectrumGroup_ConstantFinalState
- SpectrumGroup_LogicalVariableScan

The most commonly used is SpectrumGroup_FixedAnalyzerTransmission.

Available fields in the SpectrumGroup_* bookmarks are:

Field	Description	Example
SpectrumGroup	Name of the Spectrum Group	My Spectrum Group
EntranceSlit	Specified Entrance Slit	4:7x20
ExitSlit	Specified Exit Slit	C:grid
ExcitationEnergy	Excitation Energy used in eV	1486.61 (defined by used Source)
Iris	Iris in mm	60
LensVoltage	Range of scan voltage	1.5kV
ScanMode	Used Scan Mode	Fixed Analyzer Transmission
AnalysisMethod	Analysis Method	XPS
U_det	Used Detector Voltage in V	1500
U_bias	Used Bias Voltage in V	81.2
PlotPicture	Plot of all elements in the Spectrum Group	See below
<Name_LineStyle>	Line style of named spectrum, can be used to create legends; spaces in the name must be replaced by underscores	See below
LogicalVariable_name	Name of the scanned variable (only for Logical Variable Scan)	Focus Displacement 1
LogicalVariable_unit	Unit of the scanned variable (only for Logical Variable Scan)	V



Example snippet from the template:

{SpectrumGroup}

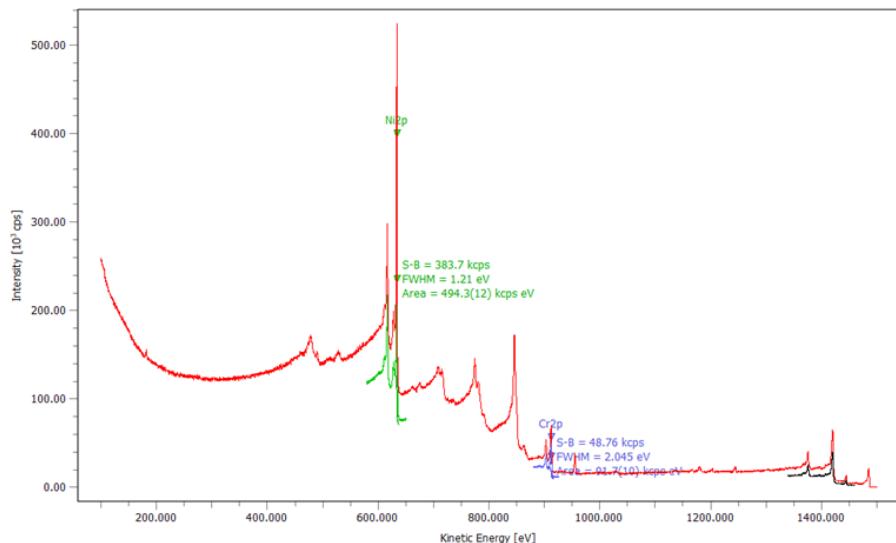
Method: {AnalysisMethod}, Slit: {EntranceSlit} / {ExitSlit}, Mode: {ScanMode},
 Excitation Energy: {ExcitationEnergy ##0.00} eV, Detector Voltage: {U_det##0} V, Bias Voltage: {U_bias ##0.00} V



Results in:

NiCr

Method: XPS, Slit: 5:7x20 / 2:open, Mode: Fixed Analyzer Transmission,
 Excitation Energy: 1486.74 eV, Detector Voltage: 1980 V, Bias Voltage: 80.00 V



Example:

c — / N — / O —

With alternative texts for the images, e.g.: “{C_LineStyle UsePlaceHolderWidth}”

Results in:

c — / N — / O —

2.5 Spectrum_*

As there are cases where it makes sense to have different representations of a Spectrum Group it makes sense to have different representations of Spectrum:

- Spectrum_FixedAnalyzerTransmission
- Spectrum_FixedEnergies
- Spectrum_SnapshotFAT
- Spectrum_FixedRetardingRatio
- Spectrum_DetectorVoltageScan
- Spectrum_BiasVoltageScan
- Spectrum_ConstantFinalState
- Spectrum_ConstantFinalState
- Spectrum_LogicalVariableScan

A Spectrum_* bookmark should be defined within a SpectrumGroup_* bookmark!

Field	Description	Example
Name	Name of the Spectrum	My Spectrum
LineStyle	Picture of Line Style	See below {LineStyle UsePlaceHolderWidth}
AnalysisMethod	Analysis Method	XPS
Lens	Lens Mode	SA
Slit	Entrance and Exit Slit	4:7x20 / C:grid
ScanMode	Scan Mode	Fixed Analyzer Transmission
Scans	Number of Scans	3
DwellTime	Dwell Time ins	0.1
Comment	Comment in Spectrum	My Spectrum Comment
E_bin_start	Binding Energy Start in eV	686.61 (see Excitation Energy)
E_bin_end	Binding Energy End in eV	676.61 (see Excitation Energy)
E_Start	[Kinetic] Start Energy	800
E_end	[Kinetic] End Energy	810
U_bias	Bias Voltage in V	81.2
U_det	Detector Voltage in V	1500
E_exc	Excitation Energy in eV	1486.61
E_kin	Kinetic Energy	
Step	Stepwidth	0.1
Values	Number of acquired values	101
RR	Retarding Ratio	
E_pass	Pass Energy in eV	100
PlotPicture	Picture of the Spectrum	See below

LogicalVariable_name	Name of the scanned variable (only for Logical Variable Scan)	Focus Displacement 1
LogicalVariable_unit	Unit of the scanned variable (only for Logical Variable Scan)	V
LogicalVariable_start	First value of scanned variable (only for Logical Variable Scan)	1.2
LogicalVariable_end	Last value of scanned variable (only for Logical Variable Scan)	3.5

Please note that some fields do not make sense in every context, e.g. RR should only be used for Spectrum_FixedRetardingRatio.

Spectrum Group 7x20												
	Name	Scans	Start (Ekin)	End (Ekin)	Step	Values	Dwell	Lens	Epass	Duration	Acq. Time	Comment
	Spectrum	1	150	1300	1	1151	0.1	MM	30	00:00	8/28/2013 13:42:10	My Comment

Example snippet from the template:

	Name	Scans	E _{kin} [eV]	Step [eV]	Dwell [s]	Lens	E _{pass} [eV]	Comment
	{Name}	{Scans}	{E_start ##0.00} ... {E_end ##0.00}	{Step}	{DwellTime e}	{Lens}	{E_Pass}	{Comment}

Results in:

	Name	Scans	E _{kin} [eV]	Step [eV]	Dwell [s]	Lens	E _{pass} [eV]	Comment
	Spectrum	1	150.00 ... 1300.00	1	0.1	MM	30	My Comment

2.6 Operation_*

This Item is merely a container for OperationElement_*. Each spectrum operation has its own Operation_* item, see the following table for the individual names for each operation.

Operation	Item Name
Arithmetic Mean	Operation_ArithmeticMean
Background	Operation_Background
Dead Time	Operation_DeadTimeCorrection
Despike	Operation_Despike
Fermi Edge	Operation_FermiEdge
Least Squares Gradient	Operation_LeastSquaresGradient
Linear Operation	Operation_LinearOperation
Multi Peak Fit	Operation_MultiPeakFit Operation_MultiPeakFit_OnePerPeak
Noise	Operation_Noise
Peak Area	Operation_PeakArea
Peak Fit	Operation_PeakFit
Peak Identification	Operation_PeakIdentification
Peak FWHM	Operation_SL2PeakFWHM
Peak Location	Operation_SL2PeakLocation
Savitzky Golay Smooth	Operation_SavitzkyGolaySmooth
Smoothing Spline	Operation_SmoothingSpline

An Operation_* item does not have fields on its own, but you can use fields from an embedded OperationElement_* item. These will be filled by the first OperationElement_* item within this Operation_* item. For example, if an operation is displayed in tabular form, this can be used to insert the units for a specific parameter in the column header, as demonstrated in the examples next chapter.

2.7 OperationElement_*

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Spectrum operations are applied on a single spectrum. The configuration of the operations as well as the result can be exported using OperationElement_* items. The individual names for the operations correspond to those of the Operation_* items shown in the previous chapter. Some operations provide additional output which will be described later in specific chapters.

Available fields in every OperationElement_* are:

Field	Description	Example
LineStyle	Picture of Line Style	See below {LineStyle UsePlaceHolderWidth}
SpectrumName	Name of the spectrum the operation is applied on	My Spectrum
OperationName	Name of the operation	My Operation

Operations have configuration- and/or output-parameters. Each parameter is available as field under its specific name. Configuration-parameters are prefixed with config_. If a numerical output parameter has an error and a unit, these will be available separately with postfixes _Error resp. _Unit. Note that whitespaces in parameter names have to be replaced by underscores.

Let's demonstrate this using "Peak Area"-operation as example:

The screenshot shows the configuration dialog for the "Peak Area" operation under the "Ag3d" transition. The "Parameters" section includes a range selector from 389.00 eV to 358.00 eV, and a table of parameters with their values:

Parameter	Value
Transition	Ag3d
Label	
Background Method	Linear
Left background points	1
Right background points	1
Annotation Text	<Transition>Area = <Area:@>

Below the parameters are "Results" showing the calculated area and center values:

Result	Value
Area	(26589.128 ± 849.048) counts eV
Center	(362.318 ± 0.033) eV

A "Styles & Visibility" section is also present.

Parameter	Type	Field	Example
Transition	Input	input_Transition	Ag3d
Label	Input	input_Label	Surface
Background Method	Input	input_Background_Method	Linear
Left background points	Input	input_Left_background_points	1
Right background points	Input	input_Right_background_points	1
Annotation Text	Input	input_Annotation_Text	<Transition>Area = <Area:@>
Area	Output (Value)	Area	26589.128
Area	Output (Error)	Area_Error	849.048
Area	Output (Unit)	Area_Unit	counts eV
Center	Output (Value)	Center	362.318
Center	Output (Error)	Center_Error	0.033
Center	Output (Unit)	Center_Unit	eV

Example snippet from the template:

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Peak Area

	Spectrum	Name	Background	Center [[Center_Unit]]	Area [[Area_Unit]]
— {SpectrumName}	{OperationName}	{input_Background_Method}	{Center##0.00} ± {Center_Error##0.00}	{Area ##0.00} ± {Area_Error##0.00}	

Results in:

Peak Area

	Spectrum	Name	Background	Center [eV]	Area [cps eV]
— MySpectrum2	Ag3d	Linear	1124,29 ± 0,03	265891,28 ± 8490,48	

2.7.1 Additional Counts per Second Parameters

All Parameter that are exported with the unit counts get additionally exported as counts per second. Following the Peak Area example from the previous chapter, the following parameters are written in addition to Area, Area_Error and Area_Unit

Parameter	Type	Field	Example
Area	Output (Value)	Area_cps	53178.256
Area	Output (Error)	Area_cps_Error	1698.096
Area	Output (Unit)	Area_cps_Unit	cps eV

2.7.2 Output for Operations with Multiple Cycles

If an operation is applied on a spectrum that is embedded in a profiling, it has multiple results – one for each step in this loop (“cycle”). In this case, a OperationElement_* will be created for each cycle containing the corresponding operations output data. The items output contains two additional fields to distinguish the cycles:

Field	Description	Example
Cycle	Textual description of the cycle	Current=0 A, Filament=1.45 A
SpectrumWithCycle	Name of the spectrum and cycle description in a table-friendly format	Spectrum Current=0 A Filament=1.45 A

Example snippet from the template:

Peak Area

	Spectrum	Name	Background	Center [{{Center_Unit}}]	Area [{{Area_Unit}}]
—	{SpectrumWithCycle}	{OperationName}	{input_Background_Method}	{Center ##0.00} ± {Center_Error ##0.00}	{Area ##0.00} ± {Area_Error ##0.00}

Results in:

Peak Area

	Spectrum	Name	Background	Center [eV]	Area [cps eV]
—	Spectrum Filament=1 A	Ag3d	Linear	314,71 ± 0,00	14357250,18 ± 34030,21
—	Spectrum Filament=2 A	Ag3d	Linear	314,71 ± 0,00	13985037,29 ± 34201,78

2.7.3 Additional Output for “Peak Identification”-Operation

The “Peak Identification”-operation has the same output as the others operations, but it provides an additional item with fields to allow for better access on the identified peaks. This is the PeakID_Peaks item, which acts as container for PeakID_PeakElement items. Each of these items represents one identified peak and can contain three fields:

Field	Description	Example
Peak	Name of the identified peak	Zn2s
Center	Position of the identified peak	291.61
Unit	Unit for “Center” value	eV

Snippet from the Template. The PeakID_Peaks is the table contained in the “Peaks” column, PeakID_PeakElement is one row in this embedded table.

Peak Identification

Spectrum	Name	Peaks
{SpectrumWithCycle}	{OperationName}	{Peak}: {Center} ##.##-{Unit}

Results in:

Peak Identification

Spectrum	Name	Peaks
Spectrum	Peak Identification	Zn2s: 291,61 eV Ce3p3/2: 302,61 eV Th4p1/2: 316,61 eV Np4p: 320,31 eV

2.7.4 Additional Output for “Multi Peak Fit”-Operation

The “Multi Peak Fit”-operation is the only operation with two different items: OperationElement_MultiPeakFit and OperationElement_MultiPeakFit_OnePerPeak. The first version behaves like the other operation items. i.e. one item will be created with all parameters. The second version splits the operation and creates one item per defined peak.

The first version differs from other operations in the parameter naming convention:

- Parameters, that belong directly to a specific peak, are prefixed with Peak_x/ where x represents the peak index (starting at 1) and are postfixed with /Value. Error and Unit of a numerical value are available as parameters with postfix /Value_Error resp. /Value_Unit
- Other parameters are grouped with prefix Baseline/, LM_Parameters/, LM_Result/ and Fit_Result/

Here are some examples:

Field	Example
input_Peak_Function	Voigt
input_Background_Function	Shirley
input_Baseline	Constant
input_LM_Parameters/Max_Iterations	220
input_LM_Parameters/Tolerance	2.22045e-016
input_Baseline/BL_I/Value	0
input_Baseline/BL_I/Value_Unit	cps
input_Baseline/BL_I/Value_Error	0
input_Peak_1/C/Value	0
input_Peak_1/C/Value_Unit	eV
input_Peak_1/C/Value_Error	0
Baseline/BL_I/Value	273336
Baseline/BL_I/Value_Unit	cps
Baseline/BL_I/Value_Error	9.82906e+006
Peak_1/C/Value	1125.68
Peak_1/C/Value_Unit	eV
Peak_1/C/Value_Error	0.033
LM_Result/Termination_State	ReachedMaxIterations
LM_Result/Iterations	200
Fit_Result/ChiSquare	0.0915918
Fit_Result/Reduced_Chisquare	0.00261691
Fit_Result/Abbe_Factor	0.0526526
Fit_Result/Q-Probability	1

Multi Peak Fit

Parameters

Range 602.73 eV 563.19 eV

	Peak 1	Peak 2
Transition	Ag3d3/2	Ag3d5/2
Label		
C	0	0
A	0	0
a	1e-01	0
s	1e-01	0
FL	1	1
FG	1	1
k	0.0075	0.0075

[Add Peak](#) [Remove Peak](#)

Peak Function	Voigt
Background Function	Shirley
Baseline	Constant
BL_I	0
LM Parameters	...

[Apply](#) [Reset](#)

Results

	Peak 1	Peak 2
Transition	Ag3d3/2	Ag3d5/2
Label		
C	912.237	906.797
A	9.26726e+006	135.998
a	0.01	1.3589e-009
s	1e-006	2.95086e-006
FL	3.73518	-82.157
FG	0.94088	23.4238
k	0.0778798	-0.853239

BL_I	835035
Fit Result	...
LM Result	...

[Use Output as Input](#)

Styles & Visibility

<input checked="" type="checkbox"/>	Combined
<input checked="" type="checkbox"/>	Background
<input checked="" type="checkbox"/>	Peak 1
<input checked="" type="checkbox"/>	Peak 2
<input checked="" type="checkbox"/>	Residuum

Snippet from the template:

Multi Peak Fit

Spectrum	Name	Background	Peak 1 Name	Peak 2 Name
{SpectrumWithCycle}	{OperationName}	{input_Background_Function}	{Peak_1/Transition/Value}	{Peak_2/Transition/Value}

Results in:

Multi Peak Fit

Spectrum	Name	Background	Peak 1 Name	Peak 2 Name
Spectrum	Multi Peak Fit	Shirley	Ag3d3/2	Ag3d5/2

The second version of the “Multi Peak Fit”-operation creates one item per peak. All parameters are available as described above, but additionally there is easier access to the parameters for exactly one peak. E.g. for parameter “C”, there are C, C_Unit and C_Error. Additionally, the linestyle-icon for the specific peak is available as LineStylePeak.

Field	Example
input_Peak_Function	Voigt
input_Background_Function	Shirley
input_Baseline	Constant
input_LM_Parameters/Max_Iterations	220
input_LM_Parameters/Tolerance	2.22045e-016
input_Baseline/BL_I/Value	0
input_Baseline/BL_I/Value_Unit	cps
input_Baseline/BL_I/Value_Error	0
input_C	0
input_C_Unit	eV
input_C_Error	0
Baseline/BL_I/Value	273336
Baseline/BL_I/Value_Unit	cps
Baseline/BL_I/Value_Error	9.82906e+006
C	1125.68
C_Unit	eV
C_Error	0.033
LM_Result/Termination_State	ReachedMaxIterations
LM_Result/Iterations	200
Fit_Result/ChiSquare	0.0915918
Fit_Result/Reduced_Chisquare	0.00261691
Fit_Result/Abbe_Factor	0.0526526
Fit_Result/Q-Probability	1

Snippet from the template:

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Multi Peak Fit

	Spectrum	Name	Background	Transition	Center [{C_Unit}]	Area [{A_Unit}]
—	{SpectrumWithCycle}	{OperationName}	{input_Background_Function}	{Transition}	{C ##0.00} ± {C_Error} ##0.00}	{A ##0.00} ± {A_Error} ##0.00

Results in:

Multi Peak Fit

	Spectrum	Name	Background	Transition	Center [eV]	Area [cps eV]
—	Spectrum	Multi Peak Fit	Shirley	Ag3d3/2	912,24 ± 0,01	9267261,38 ± 64138,04
—	Spectrum	Multi Peak Fit	Shirley	Ag3d5/2	906,80 ± 0,28	136,00 ± 73,38

2.8 Quantification

The Quantification bookmark is the base for QuantificationElement and QuantificationPeaks.

Field	Description	Example
Quantification	Name of Quantification	My Quantification
Cycle	Textual description of the cycle	Cycle=3, Etch Time=60 s
<Cycle_Etch_Time_[s]>	Value of specified cycle; spaces in the cycle must be replaced by underscores	90

Snippet from the template:

{Quantification} {Cycle}

Results in:

Quantification Cycle=3, Etch Time=90 s

Alternative example:

{Quantification} (Sputter Duration: {Cycle_Etch_Time_[s]} s)

Results in:

Quantification (Sputter Duration: 90 s)

2.9 QuantificationElement

For every element of quantification following fields are available:

Element, Transition, Label, Transmission, Sensitivity, AngularAsymmetry, BindingEnergy, CrossSection, Asymmetry, IMFP, Transmission, Percentage, Percentage_Error, Area, Area_Error, RelativeError, NormalizedArea, NormalizedArea_Error

For further details see Quantification Documentation.

Lens 1												
Peak	at%	Eb [eV]	σ [Mb]	β [a.u.]	L [a.u.]	λ [nm]	Q [a.u.]	s [norm.]	A [cps eV]	An [cps eV]	$\Delta A/A [\%]$	
<input checked="" type="checkbox"/> O1s	12.08 ± 0.49	538.48	0.04	2.00	1.00	2.46	243894.88	2.47	14198.41	0.02	4.50	
<input checked="" type="checkbox"/> C1s	63.49 ± 0.59	291.67	0.01	2.00	1.00	2.91	248376.08	1.00	30736.60	0.12	1.42	
<input checked="" type="checkbox"/> N1s	22.28 ± 0.48	405.80	0.02	2.00	1.00	2.71	247983.84	1.67	18008.94	0.04	2.41	
<input checked="" type="checkbox"/> Si2p	2.15 ± 0.13	107.26	0.01	1.03	1.00	3.24	245156.89	0.91	930.60	4.18e-03	6.14	

Show Details 

Example snippet from the template:

{Quantification}												
Peak	At [%]	Eb [eV]	σ [Mb]	β	L	λ [nm]	Q	s	A [cps eV]	An [cps eV]	$\Delta A/A [\%]$	
{Element}{Transition} {Percentage} ± {Percentage_Error}	{BindingEnergy} {CrossSection} {Asymmetry} {IMFP} {Transmission} {Sensitivity}	{Area} {NormalizedArea} {RelativeError}	{Area_Error} {NormalizedArea_Error}									

Results in:

Quantification

Peak	At [%]	Eb [eV]	σ [Mb]	β	L	λ [nm]	Q	s	A [cps eV]	An [cps eV]	$\Delta A/A [\%]$
Ni2p	78.75 ± 0.18	852.92	0.30	1.45	1.00	1.83	1.00	13.86	494311.70 ± 1182.78	35669.63 ± 85.35	0.24
Cr2p	21.25 ± 0.18	574.37	0.16	1.43	1.00	2.39	1.00	9.53	91704.37 ± 960.39	9623.88 ± 100.79	1.05

2.10 QuantificationPeaks

QuantificationPeaks are used if there is a need to report only special elements that are known before.

Field	Description	Example
<Element/Transition_Percentage>	Percentage of Peak, e.g. C1s_Percentage	72.11
<Element/Transition_Percentage_Error>	Percentage Error of Peak, e.g. C1s_Percentage_Error	0.01
Quantification	Name of Quantification	

Quantification

Peak	at%
<input checked="" type="checkbox"/> Ni2p	78.75 ± 0.18
<input checked="" type="checkbox"/> Cr2p	21.25 ± 0.18
<input type="checkbox"/> C1s	nan

Show Details 

Example snippet from template:

The {Quantification} result for **Ni2p** is {Ni2p_Percentage ###0.00} % (\pm {Ni2p_Percentage_Error ###0.00}) and **Cr2p** has {Cr2p_Percentage ###0.00} % (\pm {Cr2p_Percentage_Error ###0.00}).

Results in:

The **Quantification** result for **Ni2p** is **78.75 %** (\pm 0.18) and **Cr2p** has **21.25 %** (\pm 0.18).

2.11 Photo

33

Use the bookmark Photo to embed the camera pictures taken during the experiment.

Field	Description	Example
PhotoName	Name of the Photo element	Sample Capture

All captured images along with their meta-data are then exported for the bookmark PhotoData.

2.11.1 PhotoData

Each PhotoData item contains the following fields:

Field	Description	Example
Camera	Name of the camera	Camera 45°
CaptureTimeUTC	Time the image was taken, in universal time	2019/04/09 11:33:01
CaptureTimeLocal	Time the image was taken, in local time	2019/04/09 12:33:01
Cycle	Textual description of the cycle	x=-20mm, y=10mm
Image	The captured image	

Example snippet from template:

{PhotoName}

Description	Capture
{Camera}	
{CaptureTimeLocal YYYY/MM/DD hh:mm:ss}	
{Cycle}	

Results in:

Sample Capture

Description	Capture
Camera 45°	
2019/04/09 11:32:53	
x=-20 mm, y=-10 mm, z=31.245 mm	

2.12 AuditTrailEntry

When an Experiment is executed a protocol is written into the experiment file which can be exported.

Each AuditTrailEntry consists of the following fields:

Field	Description	Example
Time	Time the event occurred	2017/12/12 1:23:40
Category	Category of the event	Acquisition
Level	Severity of the event	Info
User	User that produced the event or system	SPECS\test
Message	Event Description	Execution of '2017-11-23_14h41m10s 1' started.

Example snippet from template:

Time	Category	Level	User	Message
{Time DD MMM YYYY hh:mm:ss}	{Category}	{Level}	{User}	{Message}

Results in:

Time	Category	Level	User	Message
15/09/2017 14:00:03	Acquisition	Info	<System>	Execution of '1 2017-09-15_15h57m11s' started.
15/09/2017 14:00:19	Acquisition	Info	<System>	Acquiring O1s (Scan: 1/1)

3 Field Types

There are four formats used for fields: Text, Numbers, Dates and Pictures.

3.1 Text

Text Fields are enclosed in {}-Brackets. For example, a field named comment must be written as

{Comment}

in the template.

3.2 Number

Numbers can be written in text fields. More control over how many decimal digits get printed is available using number fields. Number fields can be defined in the Microsoft Excel format.

{Values ##0.00}

This formatting will show values with two decimal digits. It is required to use the American number format in the template. In the report the local number format will be used.

3.3 Datetime

Date/Time formats also use the Microsoft Excel™ datetime formats.

{GenerationDateLocal YYYY/MMMM/DD hh:mm:ss}

Will appear in the template as 2017/January/12 12:13:15

3.4 Picture

To include plot pictures in the report it is necessary to have a place holder picture in the report template. It is recommended to set the width of image in Word and configure the reporting facility to set the height according to the exported image.

This is configurable in the "Alt Text" section of the picture.

{Picure UsePlaceHolderWidth}

3.4.1 Image Sizing

There are four sizing directives available.

UsePlaceHolderWidth (recommended)

Keeps the place holder picture width and calculates the height according to the default width/height ratio.

UsePlaceHolderHeight

Keeps the place holder picture height and calculates the width according to the default width/height ratio.

UseImageFileSize

Resizes the inserted picture to the image file width and height and is the default format if no format is entered.

UsePlaceHolderSize

Keeps the place holder picture width and height.

3.4.2 LineStyle

For showing the line style of a spectrum use an image like the one below and set the "Alt Text" to

```
{LineStyle UsePlaceHolderWidth}  
results in:
```

—

3.4.3 PlotPicture

Plot Pictures are highly configurable. The following Options are available:

Option	Description	Example
width_cm	Width in cm of the target picture	width_cm=15.5
height_cm	Height in cm of the target picture	height_cm=9.2
fontsize	Size of axis labels and annotations	fontsize=8
xAxis	Type of xAxiS. See below	xAxis=BindingEnergy
yAxis	Type of yAxiS, see below	yAxis=CountsPerSecond
Operations	Show/Hide Operations	operations=no
Spectrums	Show Hide Spectrums	spectrums=yes
CycleFilter	Select a specific cycle for display	CycleFilter=Etch_Time_[s]:60

Valid x-axis types are: BindingEnergy, KineticEnergy, ExcitationEnergy, Sample, DetectorVoltage, BiasVoltage

y-axis types are: Counts , CountsPerSecond , at

Example snippet from the template:



```
{PlotPicture|width_cm=15.5|height_cm=9.2|fontsize=8|xAxis=KineticEnergy|yAxis=CountsPerSecond|Operations=Yes UseImageFileSize}
```

The result is similar to the screenshots of the previous pages.

Alternative Example when a quantification on a depth profile is created:

Depth Profile 0.2x20

- C
- N
- O
- Ti

Quantification

- System Geometry
- IMFP Settings
- Calculation Settings

Cycle: Cycle=1, Etch Time=0 s

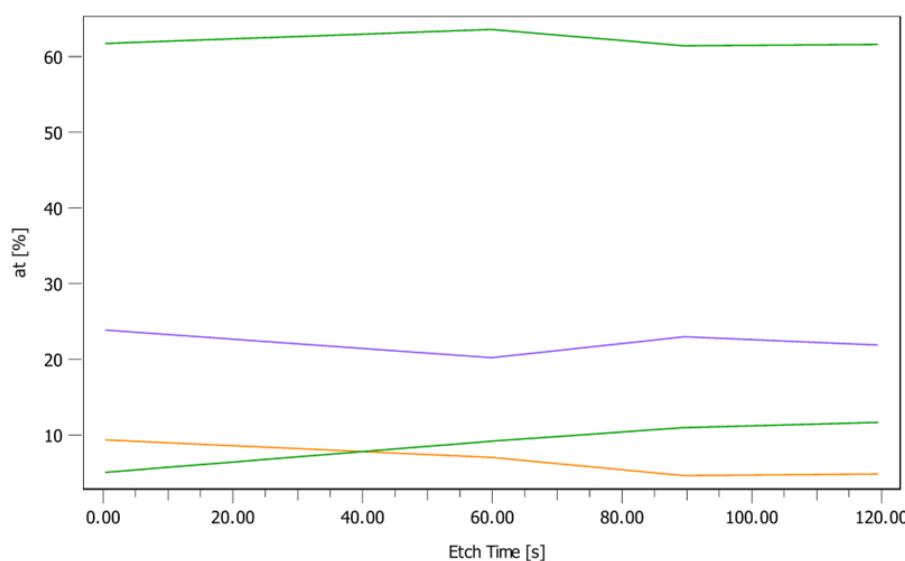
Cycle	Etch Time [s]
1	0
	0
	60
	90
	120

Peak	at%
C1s	61.74 ± 1.11
N1s	9.34 ± 1.08
O1s	23.86 ± 0.71
Ti2p	5.07 ± 0.3

Show Details

```
{PlotPicture|width_cm=15.4|height_cm=9.24|xAxis=Etch_Time_[s]|yAxis=at|GroupOperations=Yes UseImageFileSize}
```

Results in:



4 Version History

1.0 (2017-12-20)

- First fully documented version

1.01 (2018-02-09)

- Changed definition of image size from pixel to cm

1.1 (2018-03-23)

- Added documentation for spectrum operations

1.12 (2018-06-26)

- Added FileNameWithoutExtension

1.13 (2018-09-04)

- Added field “fontsize” for PlotPicture

1.14 (2019-02-06)

- Added information that PDF resolution is configurable in Microsoft Word™

1.15 (2021-06-22)

- Removed reference to Layer in QuantificationElement

1.16 (2023-04-13)

- Added documentation for Photo item

1.17 (2024-01-25)

- Added group operations plots (e.g. Depth Profile Quantification)
- Added specific cycle selection for a PlotPicture element
- Added specific cycle value selection
- Added specific line style selection of spectrum

1.18 (2024-04-11)

- Added documentation for SampleNode item

1.19 (2024-06-03)

- Added documentation for Logical Variable Scan