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Workshop „Rietveld Refinement with Profex“

Lesson 6: Structure and Device Files

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GOALs = „Results“ in BGMN terminology

```
PHASE=Calcite // 04-008-0788
MineralName=Calcite
Formula=Ca_(CO3)
SpacegroupNo=167 HermannMauguin=R-32/c
PARAM=A=0.4991_0.4941^0.5041 PARAM=C=1.7062_1.6891^1.7233
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.01 GEWICHT=SPHAR4
GOAL=GrainSize(1,1,1)
GOAL:Calcite=GEWICHT
E=CA Wyckoff=b x=0.0000 y=0.0000 z=0.0000 TDS=0.00796938
E=C Wyckoff=a x=0.0000 y=0.0000 z=0.2500 TDS=0.00757986
E=O Wyckoff=e x=0.2573 y=0.0000 z=0.2500 TDS=0.01400168
```

Direct GOALs **GOAL=<value>** writes the result and its error to the list file (*.lst)

Indirect GOALs **GOAL:<name>=<value>** assigns <value> to the variable <name>
and exports <name> to the control file (*.sav)

Structure Files: Direct GOALS

Apatite-OH.str

240222-01.lst

```
PHASE=Hydroxyapatite // 01-074-0565
MineralName=Hydroxylapatite
Formula=Ca5_(PO4)3_(OH)
SpacegroupNo=176 HermannMauguin=P6_3/m
PARAM=A=0.9424_0.9330^0.9518 PARAM=C=0.6879_0.6810^0.6948
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.05 GEWICHT=SPHAR4
```

```
GOAL=GrainSize(0,0,1)
```

```
GOAL=GrainSize(1,0,0)
```

```
GOAL:Hydroxyapatite=GEWICHT
```

```
E=CA Wyckoff=f x=0.3333 y=0.6667 z=0.0015 TDS=
E=CA Wyckoff=h x=0.2468 y=0.9934 z=0.2500 TDS=
E=P Wyckoff=h x=0.3987 y=0.3685 z=0.2500 TDS=
E=O Wyckoff=h x=0.3284 y=0.4848 z=0.2500 TDS=
E=O Wyckoff=h x=0.5873 y=0.4651 z=0.2500 TDS=
E=O Wyckoff=i x=0.3437 y=0.2579 z=0.0702 TDS=
E=O(0.5000) Wyckoff=e x=0.0000 y=0.0000 z=0.1
E=H(0.5000) Wyckoff=e x=0.0000 y=0.0000 z=0.0
```

Other examples:

```
// volume of hexagonal unit cell
```

```
GOAL=sqrt(3)*A*A*C/2
```

```
// mass absorption coefficient
```

```
GOAL=10000*my/density
```

```
Local parameters and GOALS for phase Hydroxyapatite
*****
```

```
SpacegroupNo=176
```

```
HermannMauguin=P6_3/m
```

```
XrayDensity=3.120
```

```
Rphase=5.46%
```

```
UNIT=NM
```

```
A=0.9425500+-0.0000033
```

```
C=0.6883876+-0.0000030
```

```
GrainSize(0,0,1)=387+-15
```

```
GrainSize(1,0,0)=379+-10
```

```
GEWICHT=SPHAR4, MeanValue(GEWICHT)=0.161184
```

```
B1=ANISOLIN, MeanValue(B1)=0.00111181, sqrt3(det(B1))=0.00111171
```

```
Atomic positions for phase Hydroxyapatite
```

```
-----
```

```
4 0.3333 0.6667 0.0015 E=(CA(1.000))
```

```
6 0.2468 0.9934 0.2500 E=(CA(1.0000))
```

```
6 0.3987 0.3685 0.2500 E=(P(1.0000))
```

```
6 0.3284 0.4848 0.2500 E=(O(1.0000))
```

```
6 0.5873 0.4651 0.2500 E=(O(1.0000))
```

```
12 0.3437 0.2579 0.0702 E=(O(1.0000))
```

```
4 0.0000 0.0000 0.1950 E=(O(0.5000))
```

```
4 0.0000 0.0000 0.0608 E=(H(0.5000))
```

Structure Files: Indirect GOALS

Apatite-OH.str

```
PHASE=Hydroxyapatite // 01-074-0565
MineralName=Hydroxylapatite
Formula=Ca5_(PO4)3_(OH)
SpacegroupNo=176 HermannMauguin=P6_3/m
PARAM=A=0.9424_0.9330^0.9518 PARAM=C=0.6879_0.6810^0.6948
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.05 GEWICHT=SPHAR4
GOAL=GrainSize(0,0,1)
GOAL=GrainSize(1,0,0)
GOAL:Hydroxyapatite=GEWICHT
E=CA Wyckoff=f x=0.3333 y=0.6667 z=0.0015 TDS=0.00664290
E=CA Wyckoff=h x=0.2468 y=0.9934 z=0.2500 TDS=0.00567436
E=P Wyckoff=h x=0.3987 y=0.3685 z=0.2500 TDS=0.00477426
E=O Wyckoff=h x=0.3284 y=0.4848 z=0.2500 TDS=0.00953535
E=O Wyckoff=h x=0.5873 y=0.4651 z=0.2500 TDS=0.01014069
E=O Wyckoff=i x=0.3437 y=0.2579 z=0.0702 TDS=
E=O(0.5000) Wyckoff=e x=0.0000 y=0.0000 z=0.1
E=H(0.5000) Wyckoff=e x=0.0000 y=0.0000 z=0.0
```

240222-01.sav

Other examples:

```
// volume of hexagonal unit cell
GOAL:VolApatite=sqrt(3)*A*A*C/2
```

```
// mass absorption coefficient
GOAL:MacApatite=10000*my/density
```

```
sum=Hydroxyapatite+Calcite
QHydroxyapatite=Hydroxyapatite/sum
QCalcite=Calcite/sum

GOAL[1]=QHydroxyapatite
GOAL[2]=QCalcite
```

„VolApatite“ and „MacApatite“ are new global variables that can be accessed in the *.sav file.

Structure Files: GOALS

Summary of GOAL implementations:

Code	Accessible in STR file	Written to LST file	Accessible in SAV file
<code>VolApatite=sqrt(3)*A*A*C/2</code>	Yes	No	No
<code>GOAL=sqrt(3)*A*A*C/2</code>	No	Yes	No
<code>GOAL:VolApatite=sqrt(3)*A*A*C/2</code>	Yes	No	Yes
<code>GOAL:VolApatite=sqrt(3)*A*A*C/2</code> <code>GOAL=VolApatite</code>	Yes	Yes	Yes



Structure Files: Site Occupancy Factors and Substitutions

Apatite-OH.str

```
PHASE=Hydroxyapatite // 01-074-0565
MineralName=Hydroxylapatite
Formula=Ca5_(PO4)3_(OH)
SpacegroupNo=176 HermannMauguin=P6_3/m
PARAM=A=0.9424_0.9330^0.9518 PARAM=C=0.6879_0.6810^0.6948
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.05 GEWICHT=SPHAR4
GOAL=GrainSize(0,0,1)
GOAL=GrainSize(1,0,0)
GOAL:Hydroxyapatite=GEWICHT
E=CA Wyckoff=f x=0.3333 y=0.6667 z=0.0015 TDS=0.00664290
E=CA Wyckoff=h x=0.2468 y=0.9934 z=0.2500 TDS=0.00567436
E=P Wyckoff=h x=0.3987 y=0.3685 z=0.2500 TDS=0.00477426
E=O Wyckoff=h x=0.3284 y=0.4848 z=0.2500 TDS=0.00953535
E=O Wyckoff=h x=0.5873 y=0.4651 z=0.2500 TDS=0.01014069
E=O Wyckoff=i x=0.3437 y=0.2579 z=0.0702 TDS=0.01499127
E=O(0.5000) Wyckoff=e x=0.0000 y=0.0000 z=0.1950 TDS=0.00000000
E=H(0.5000) Wyckoff=e x=0.0000 y=0.0000 z=0.0608 TDS=0.02947459
```

Scheme: **E=<scattering factor>(occupancy)**

Examples: **E=CA** is equivalent to **E=CA(1.0)** (fully occupied)
E=SI(0.5) (partially occupied)
E=SI+4(0.5) (ionic scat. fact. partially occupied)
E=(SI(0.75),AL(0.25)) (substitution)

Structure Files: Site Occupancy Factors and Substitutions

Refining Substitutions:

$E = (\text{SI}(0.75), \text{AL}(0.25))$



$E = (\text{SI}(p), \text{AL}(1-p))$ $\text{PARAM}=p=0.75_0^1$

Calcite.str

```
PHASE=Calcite // 04-008-0788
MineralName=Calcite
Formula=Ca_(CO3)
SpacegroupNo=167 HermannMauguin=R-32/c
PARAM=A=0.4991_0.4941^0.5041 PARAM=C=1.7062_1.6891^1.7233
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.01 GEWICHT=SPHAR4
GOAL=GrainSize(1,1,1)
GOAL:Calcite=GEWICHT
E=(CA(p),MG(1-p)) PARAM=p=1_0^1 Wyckoff=b x=0.0000 y=0.0000 z=0.0000 TDS=0.00796938
E=C Wyckoff=a x=0.0000 y=0.0000 z=0.2500 TDS=0.00757986
E=O Wyckoff=e x=0.2573 y=0.0000 z=0.25
```

240222-01.lst

Atomic positions for phase Calcite

6 0.0000 0.0000 0.0000 **E=(CA(0.9441),MG(0.0559))**
p=0.9441+-0.0055

6 0.0000 0.0000 0.2500 E=(C(1.0000))
18 0.2573 0.0000 0.2500 E=(O(1.0000))

Structure Files: Coupling Parameters

Assumption: Na⁺ substitutes Ca²⁺

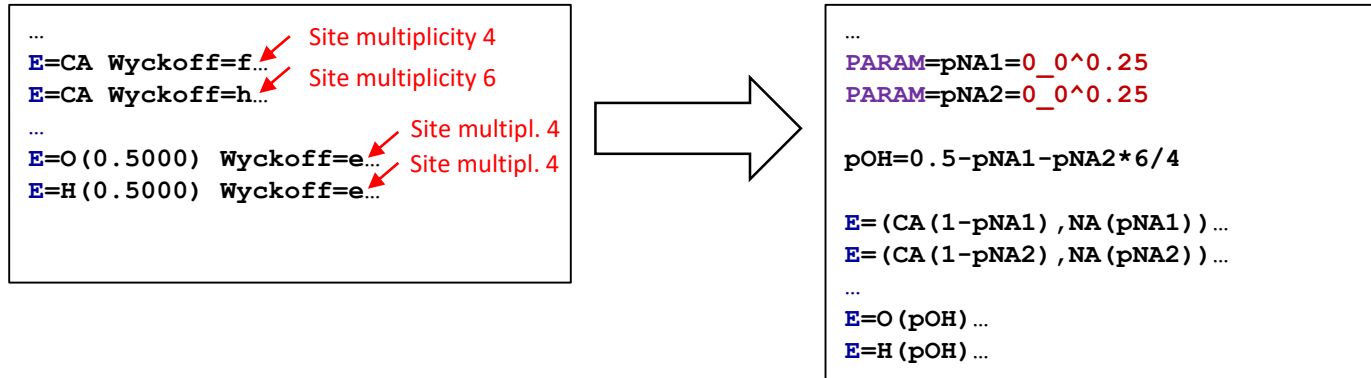
To maintain charge balance, OH⁻ is reduced accordingly

```
PHASE=Hydroxyapatite // 01-074-0565
MineralName=Hydroxylapatite
Formula=Ca5_(PO4)3_(OH)
SpacegroupNo=176 HermannMauguin=P6_3/m
PARAM=A=0.9424_0.9330^0.9518 PARAM=C=0.6879_0.6810^0.6948
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.05 GEWICHT=SPHAR4
GOAL=GrainSize(0,0,1)
GOAL=GrainSize(1,0,0)
GOAL:Hydroxyapatite=GEWICHT
E=(CA(1-p),NA(p)) PARAM=p=0_0^1 Wyckoff=f x=0.3333 y=0.6667 z=0.0015 TDS=0.00664290
E=(CA(1-p),NA(p)) PARAM=p=0_0^1 Wyckoff=h x=0.2468 y=0.9934 z=0.2500 TDS=0.00567436
E=P Wyckoff=h x=0.3987 y=0.3685 z=0.2500 TDS=0.00477426
E=O Wyckoff=h x=0.3284 y=0.4848 z=0.2500 TDS=0.00953535
E=O Wyckoff=h x=0.5873 y=0.4651 z=0.2500 TDS=0.01014069
E=O Wyckoff=i x=0.3437 y=0.2579 z=0.0702 TDS=0.01499127
E=O(0.5000) Wyckoff=e x=0.0000 y=0.0000 z=0.1950 TDS=0.00000000
E=H(0.5000) Wyckoff=e x=0.0000 y=0.0000 z=0.0608 TDS=0.02947459
```


Structure Files: Coupling Parameters

Assumption: Na^+ substitutes Ca^{2+}

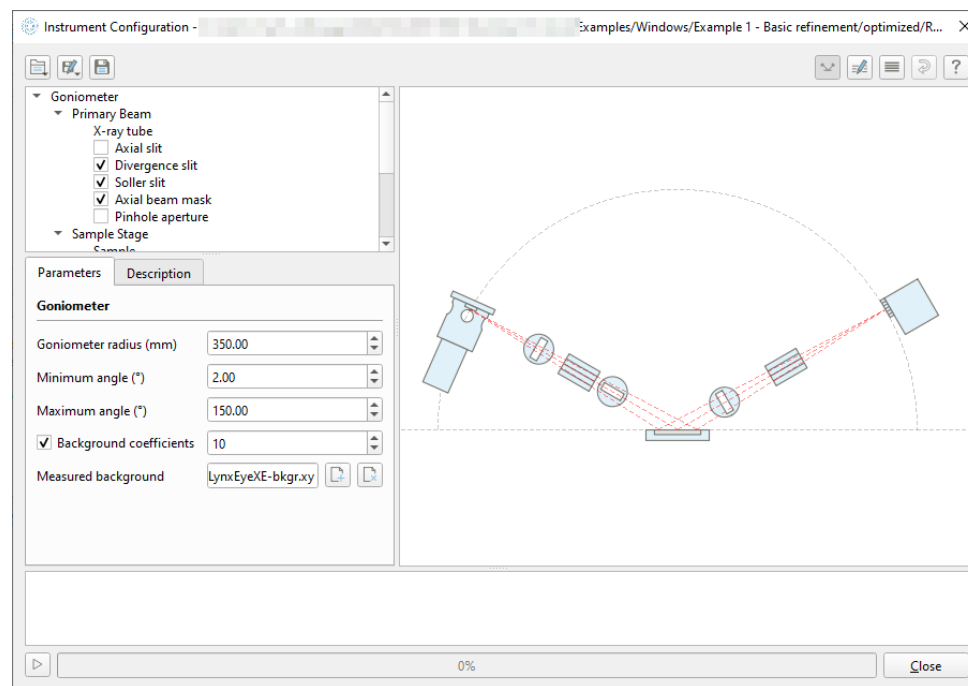
To maintain charge balance, OH^- is reduced accordingly



Parameters used for several atomic sites must be declared **above** the E= lines.

Parameters declared **within** an atomic site (E= line) can only be accessed **within** the site.

Instrument Configuration Files

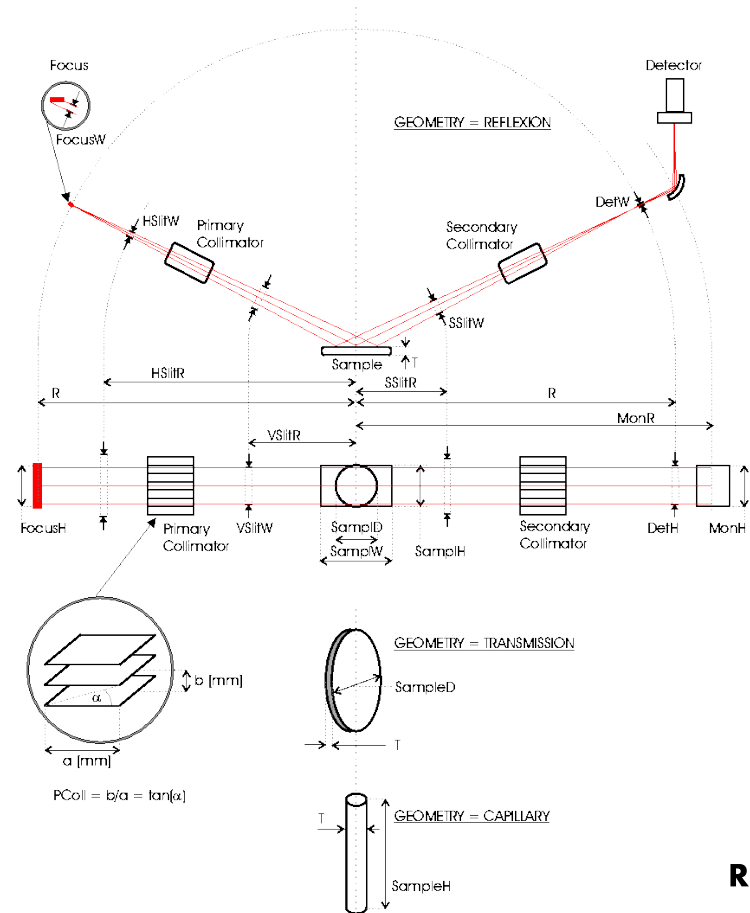
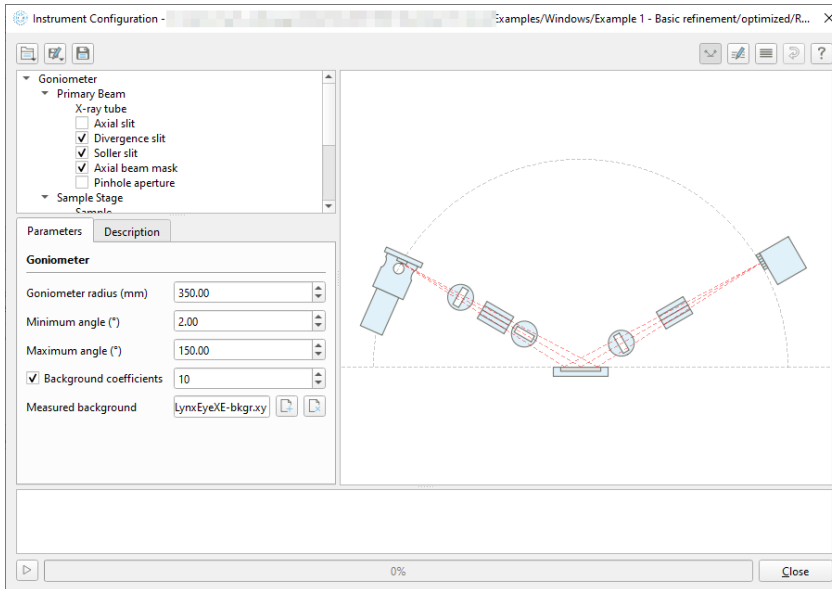


Instrument Configuration Files

- Instrument configuration files must **precisely** describe the hardware setup used to measure a dataset.
- Profex includes 70 configurations
- Often customization is necessary

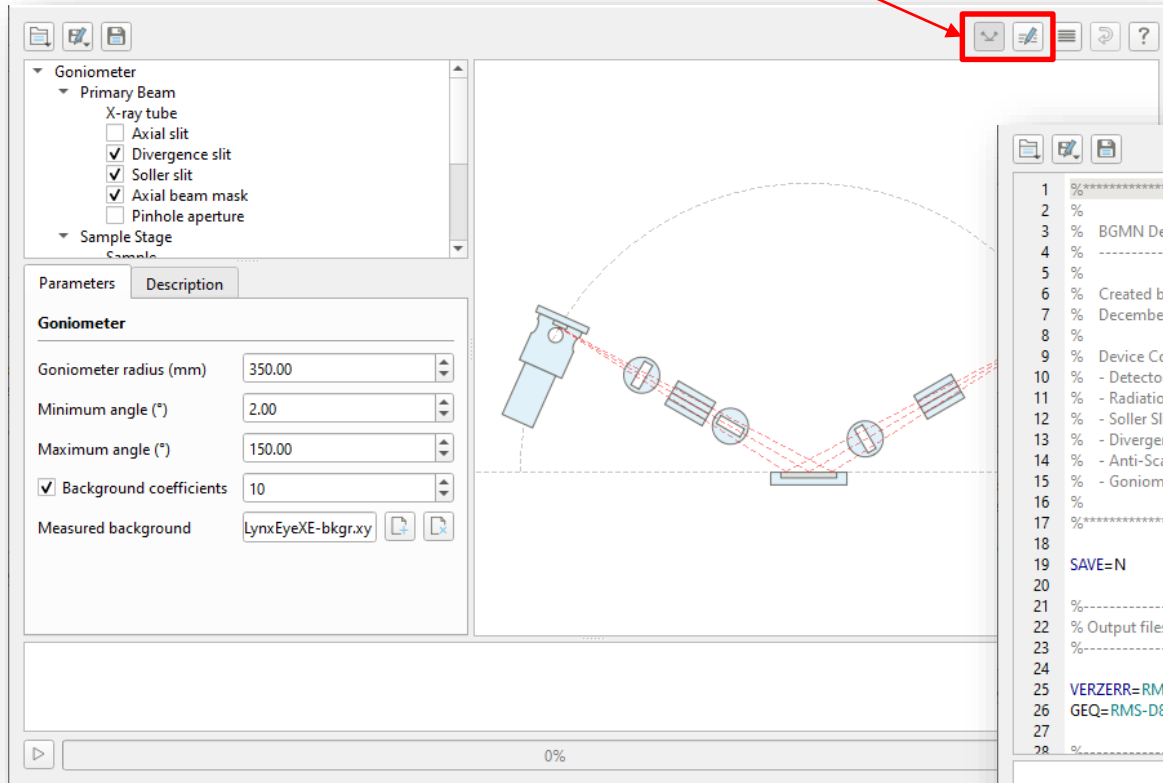
<http://www.bgm.de/raytracing.html>

Profex: Instrument → Edit current FPA configuration

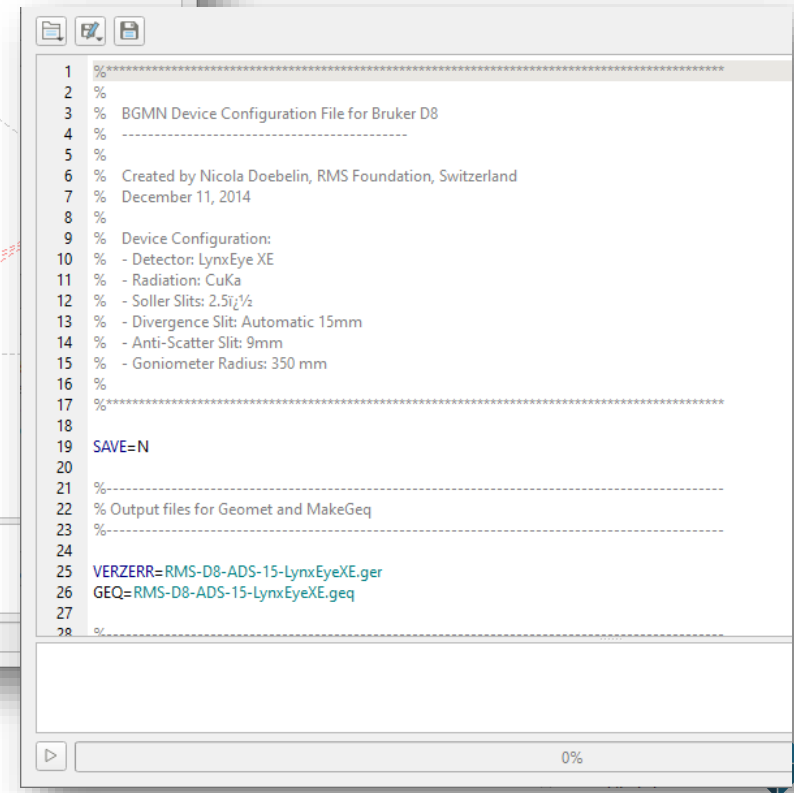


Instrument Configuration Files

Toggle between text editor and graphical editor



Normally the text editor is not needed



Instrument Configuration Files

The screenshot displays a software interface for configuring an instrument. On the left, a tree view under 'Goniometer' shows the 'Primary Beam' section expanded. A red box highlights the 'Axial slit' checkbox, which is unchecked, while 'Divergence slit', 'Soller slit', and 'Axial beam mask' are checked. Below the tree, the 'Parameters' tab is active, showing settings for the 'Divergence slit' module: Mode is 'Variable', Distance from sample (mm) is 250.00, and Irradiated length (mm) is 15.00. On the right, a 3D schematic labeled 'Preview' shows the X-ray beam path through various components, including the X-ray tube, slits, and detector. A red arrow points from the 'Axial slit' checkbox to the schematic, with the text 'Enable/disable modules'. At the bottom of the interface, there is a progress bar at 0% and a 'Close' button.

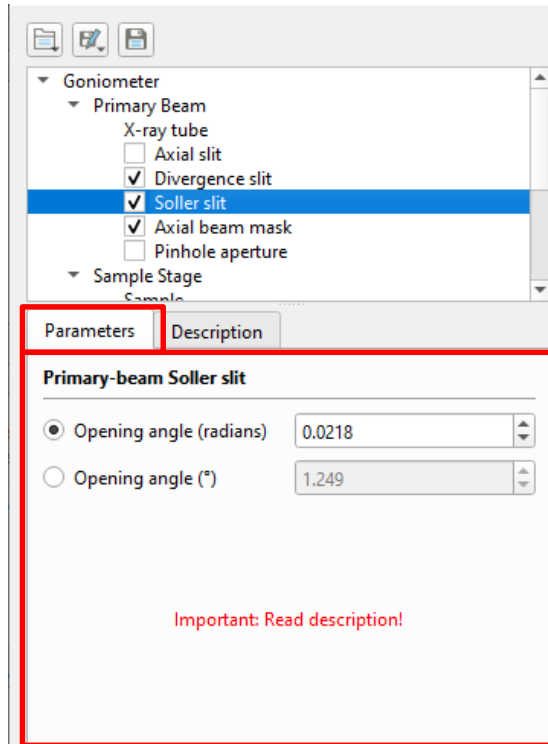
Enable/disable modules

Configure modules

Preview

Instrument Configuration Files

Each configuration page has a „Description“ page with detailed information



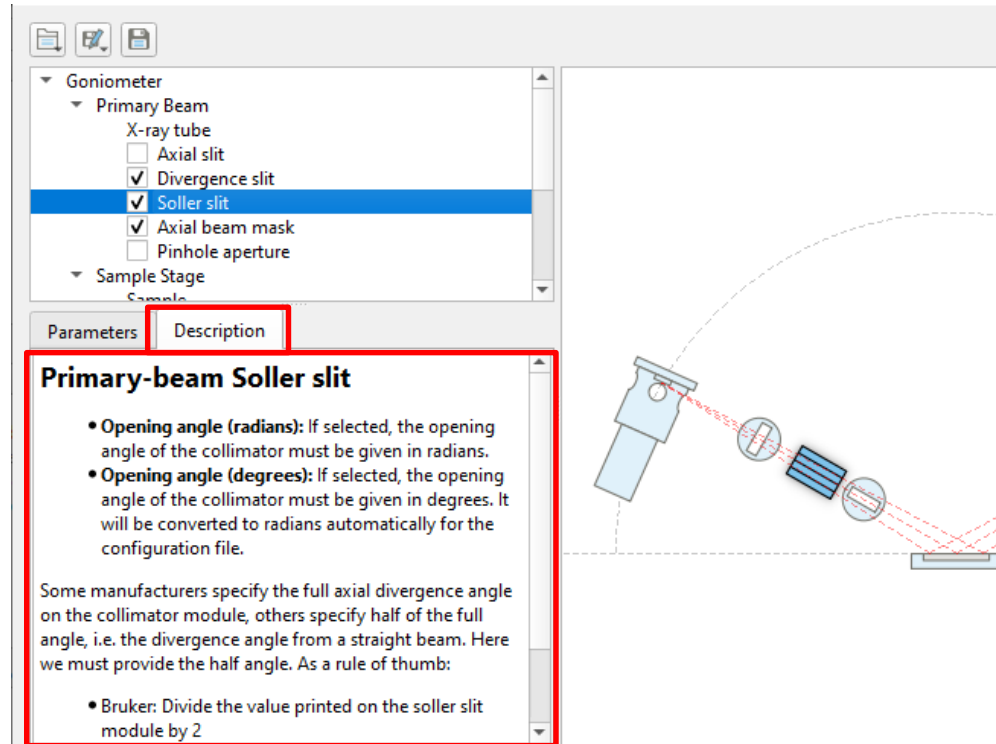
The screenshot shows the 'Parameters' tab for the 'Primary-beam Soller slit' configuration. The tree view on the left shows the following structure:

- Goniometer
 - Primary Beam
 - X-ray tube
 - Axial slit
 - Divergence slit
 - Soller slit
 - Axial beam mask
 - Pinhole aperture
- Sample Stage
 - Sample

The 'Parameters' tab contains the following settings:

- Primary-beam Soller slit**
- Opening angle (radians)
- Opening angle (°)

Important: Read description!



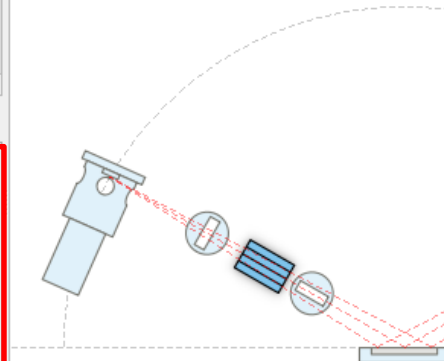
The screenshot shows the 'Description' tab for the 'Primary-beam Soller slit' configuration. The tree view on the left is identical to the 'Parameters' tab. The 'Description' tab contains the following text:

Primary-beam Soller slit

- **Opening angle (radians):** If selected, the opening angle of the collimator must be given in radians.
- **Opening angle (degrees):** If selected, the opening angle of the collimator must be given in degrees. It will be converted to radians automatically for the configuration file.

Some manufacturers specify the full axial divergence angle on the collimator module, others specify half of the full angle, i.e. the divergence angle from a straight beam. Here we must provide the half angle. As a rule of thumb:

- **Bruker:** Divide the value printed on the soller slit module by 2



The diagram illustrates the X-ray beam path through the Soller slit. It shows an X-ray tube on the left emitting a beam (red dashed lines) that passes through a series of collimator modules (blue and grey) and a Soller slit (blue and grey). The beam then hits a sample on the right. The Soller slit is shown as a series of parallel slits that filter the beam.

Instrument Configuration Files: Recommended Workflow

1. Enable / disable the modules according to the instrument setup

The screenshot displays a software interface for configuring an X-ray instrument. On the left, a tree view under 'Goniometer' shows the following components and their status:

- Primary Beam
 - X-ray tube
 - Axial slit
 - Divergence slit
 - Soller slit
 - Axial beam mask
 - Pinhole aperture
- Sample Stage
 - Sample

Below the tree view, the 'Parameters' tab is active for the 'Primary-beam Soller slit'. It shows two options for the opening angle:

- Opening angle (radians): 0.0218
- Opening angle (°): 1.249

A red text warning is present: **Important: Read description!**

The main window contains a schematic diagram of the X-ray beam path. Red dashed lines represent the beam path from the X-ray tube through various slits and masks to the sample and detector. A semi-circular dashed line indicates the goniometer's range of motion.

At the bottom of the window, there is a progress bar showing 0% and a 'Close' button.

Instrument Configuration Files: Recommended Workflow

2. Go through all modules from Tube to Detector and enter the correct settings

The screenshot displays the configuration software for an X-ray diffractometer. On the left, a tree view shows the 'Goniometer' section expanded to 'Primary Beam', with the following settings:

- X-ray tube
- Axial slit
- Divergence slit
- Soller slit
- Axial beam mask
- Pinhole aperture

Below the tree view, the 'Parameters' tab is active for the 'Primary-beam Soller slit' module:

Parameters	Description
<input checked="" type="radio"/> Opening angle (radians)	0.0218
<input type="radio"/> Opening angle (°)	1.249

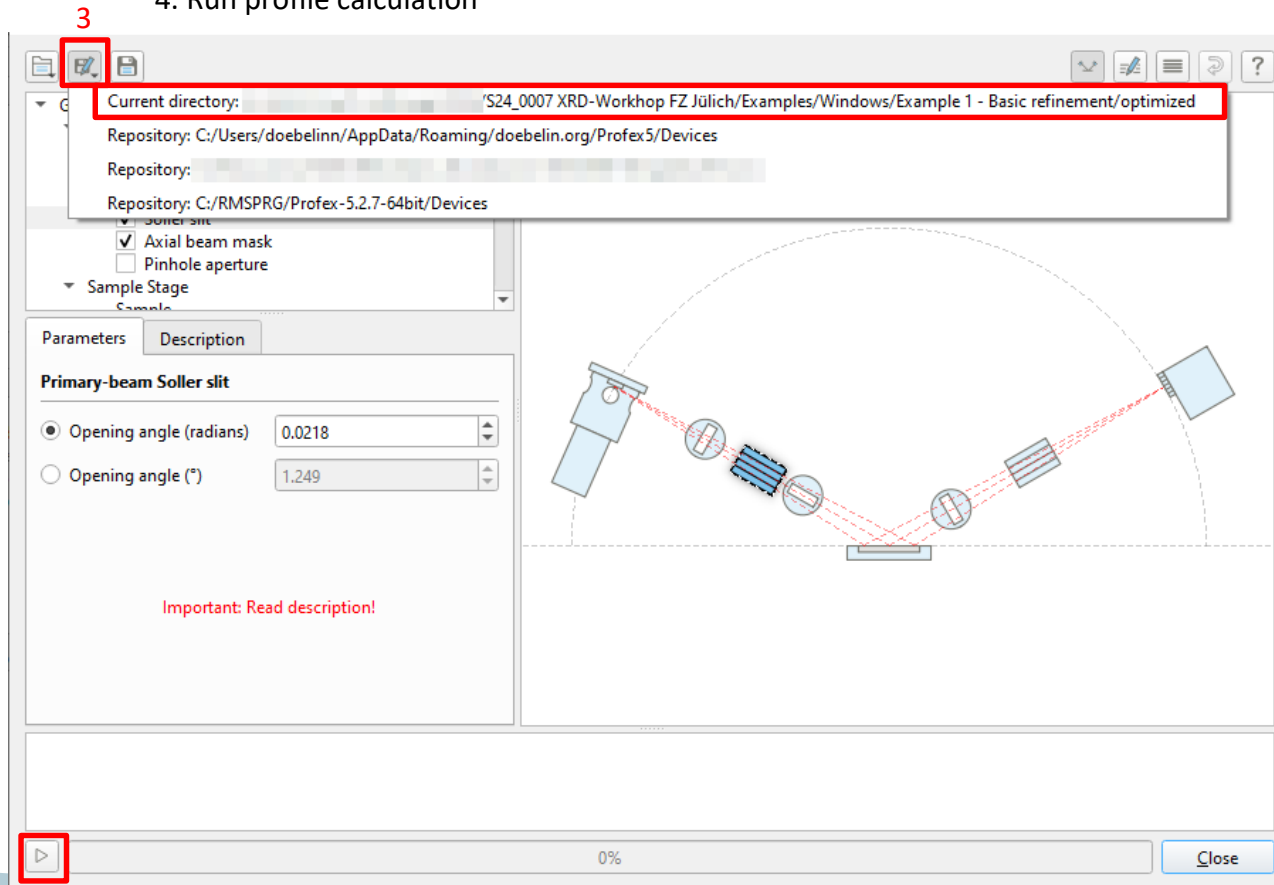
A red text warning is present: **Important: Read description!**

The central diagram illustrates the X-ray path from the tube through various slits and masks to the detector. A large red arrow indicates the direction of the primary beam.

At the bottom of the window, there is a play button, a progress indicator at 0%, and a 'Close' button.

Instrument Configuration Files: Recommended Workflow

3. Save configuration under a new name in current project directory
4. Run profile calculation



Instrument Configuration Files: Recommended Workflow

In case of errors, check messages

Parameters Description

Primary-beam Soller slit

Opening angle (radians) 0.0218

Opening angle (°) 1.249

Important: Read description!

```
zweiTheta=90.0000 N=8 GSUM=2.29713e+00  
zweiTheta=135.0000 N=6 GSUM=3.02202e+00  
zweiTheta=148.0000 N=7 GSUM=3.15155e+00
```

39% Close

Instrument Configuration Files: Recommended Workflow

The screenshot displays the Profex 5.2.7 software interface. The main window shows a list of instrument configuration files. The file `VERZERR=RMS-D8-ADS-15-LynxEyeXE.geq` is highlighted with a red box and an arrow pointing to it. A text box on the right side of the interface contains the instruction: "Change instrument name to new configuration name and run test refinement".

The interface also shows the following components:

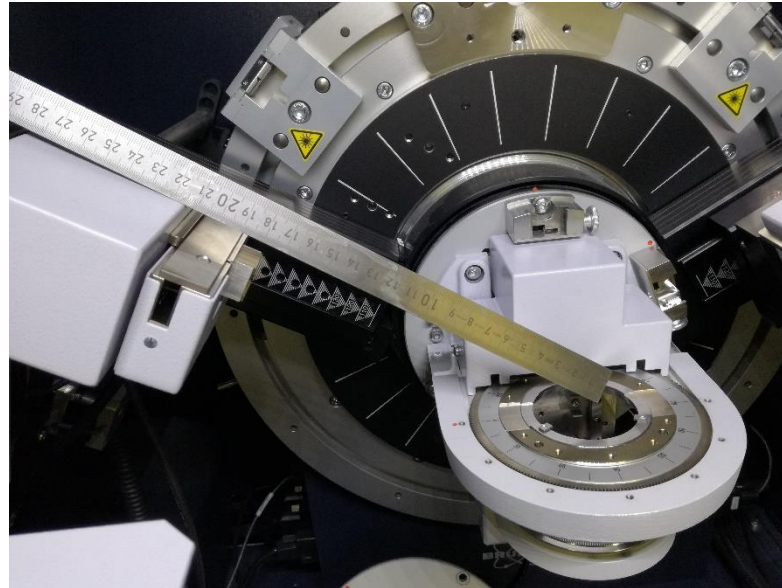
- Projects:** A table with columns for Name, Status, Iteration, and χ^2 . The project "Example_1" is listed with a status of "idle".
- Plot Options:** A table with columns for Scan and Vertical Offset. The options are checked for "I observed", "I calculated", "I difference", "Background", "Hydroxyapatite", and "Calcite".
- Refinement Protocol:** A section for defining the refinement protocol.
- Refined Parameters:** A table showing the results of the refinement process.

Parameter	Value	ESD
▼ Statistics		
Rwp	5.80	
Rexp	4.89	
χ^2	1.41	
GoF	1.19	
Background Coefficients	10	
▼ Global GOALS		
QHydroxyapatite	0.4991	0.0024
QCalcite	0.5009	0.0024
▶ Local GOALS		

At the bottom of the interface, the status bar shows the following information: `G:\Auftr_Proj\S-Auftraege\2024\S24_0007 XRD-Workhop FZ Jülich\E 1 Project $\lambda = 1.54060 \text{ \AA}$ $2\theta = 0.000^\circ$ $I = 0.000 \text{ cts}$ $d = 0.000 \text{ \AA}$ Line: 1, Column: 33`

Instrument Configuration Files: Where to get Information

- ▶ Instrument control software
- ▶ Original data processing software
- ▶ XML file formats: Open in text editor or web browser
- ▶ Old school: Take measurements



Instrument Configuration Files: Where to get Information

Instrument control software (DIFFRAC.MEASUREMENTCENTER, DataCollector, etc.)

DIFFRAC.WIZARD - Benutzer: Lab Manager - Applikations Typ: Pulverdiffraktion - Instrument: MeasSrv(PC-17XRD)/RMS Foundation

Datei Editieren Ansicht Wizard Hilfe

WIZARD DETECTOR COMMANDER START JOBS JOBLIST DA VINCI TOOLS CONFIGURATION DB MANAGEMENT RESULTS MANAGER LOG

DAVINCI

XRD BASIC

Methode #1

DAVINCI

XRD setup

VCT/VSS

Sequenzen

Sequenzen

XY Positionen

XY Positionen

Justage verfeinern

Kamera

Profile

Einstellungen

Tabelleneditor

Grafische Anzeige

Optionen

Optionen

Primärer Strahlengang Radius 350

1 ✓

TubeMount TubeKFLCu2KC_2

2 ✓

Optics_Primary_Mot... FixedSampleillum...

3 ✓

SlitMount No Slit 10.5 [mm] ...

4 ✓

SollerMount Axial Soller 2.5 [°]...

Sekundärer Strahlengang Radius 350

1 ✓

LYNXEYE_XE LYNXEYE_XE (1D Mod...

2 ✓

DetectorOpticsMount2 Filter_Ni_LowBeta 18 [...]

3 ✓

DetectorOpticsMount1 Slit_open_2 18 [mm] 18 ...

4 ✓

Detector_Slit_Motorized Slitwidth 9 [mm]

5 ✓

SollerMount Axial Soller 2.5 [°] 2.5 [°]

6 ✓

SlitMount No Slit 10.5 [mm] 10.5 [...]

7 ✓

Optics_Secondary_Motoriz... OpeningDegree

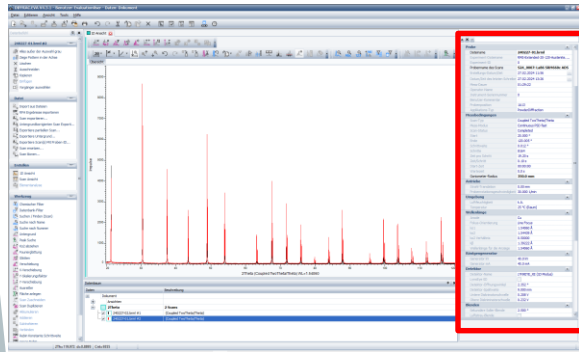
Probenwechsler

1 ✓

AUTOCHANGER

Instrument Configuration Files: Where to get Information

Original data processing software (DIFFRAC.EVA, HighScore etc.)



Probe	
Dateiname	240227-01.brml
Experiment-Dateiname	RMS-Extended-20-120-Austenite....
Experiment-ID	0
Probenname des Scans	524_0007: LaB6 SRM660c ADS
Erstellungs-Datum/Zeit	27.02.2024 11:56
Datum/Zeit des letzten Schreibe	27.02.2024 13:26
Mess-Dauer	01:29:22
Operator-Name	
Instrument-Seriennummer	0
Benutzer-Kommentar	
Probenposition	1A13
Applikations-Typ	PowderDiffraction
Messbedingungen	
Scan-Typ	Coupled TwoTheta/Theta
Mess-Modus	Continuous PSD fast
Scan-Status	Completed
Start	20.000 °
Ende	120.005 °
Schrittweite	0.012 °
Schritte	8164
Zeit pro Schritt	19.20 s
Zeit/Schritt	0.10 s
Start-Zeit	00:00:00
Wartezeit	0.0 s
Goniometer-Radius	350.0 mm

Antriebe	
Strahl-Translation	0.00 mm
Probenrotationsgeschwindigkeit	30.000 1/min
Umgebung	
Luftfeuchtigkeit	k.A.
Temperatur	25 °C (Raum)
Wellenlänge	
Anode	Cu
Fokus-Orientierung	Line Focus
ko1	1.54060 Å
ko2	1.54439 Å
ko2 Verhältnis	0.50000
kβ	1.39222 Å
Wellenlänge für die Anzeige	1.54060 Å
Röntgenergenerator	
Generator kV	40.0 kV
Generator mA	40.0 mA
Detektor	
Detektor-Name	LYNXEYE_XE (1D Modus)
LynxEye 0D	<input type="checkbox"/>
Detektor-Öffnungswinkel	2.352 °
Detektor-Spaltweite	9.000 mm
Untere Diskriminatorschwelle	0.208 V
Obere Diskriminatorschwelle	0.232 V
Blenden	
Sekundäre Soller-Blende	2.500 °
Luftstreu-Blende	<input type="checkbox"/>
Divergenz-Blende	15.000 mm
Streustrahl-Blende	3.030 °
Blenden-Modus	Variabel
Simul. Blenden-Modus	
Korrekturen	

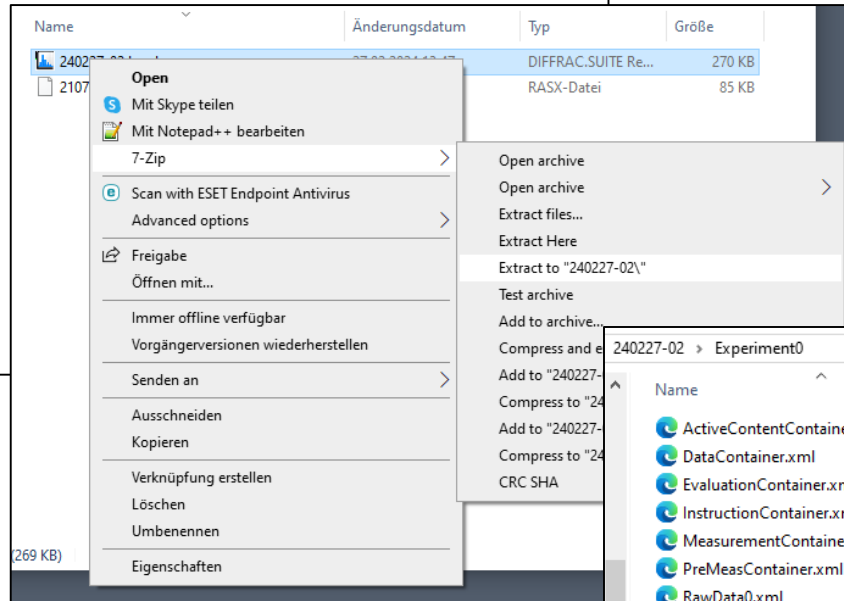
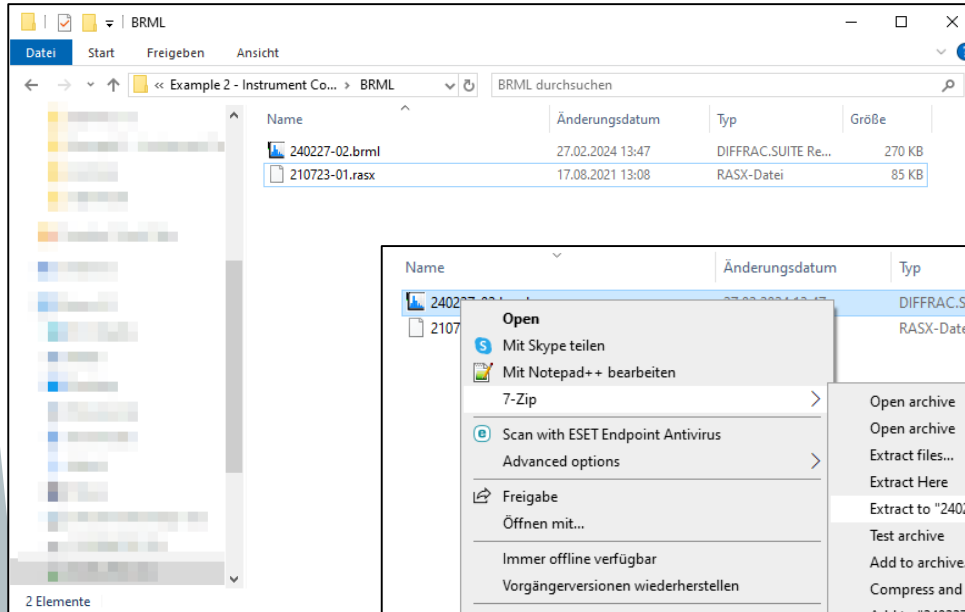
Instrument Configuration Files: Where to get Information

XML file formats: Open in text editor or web browser (XRDML)

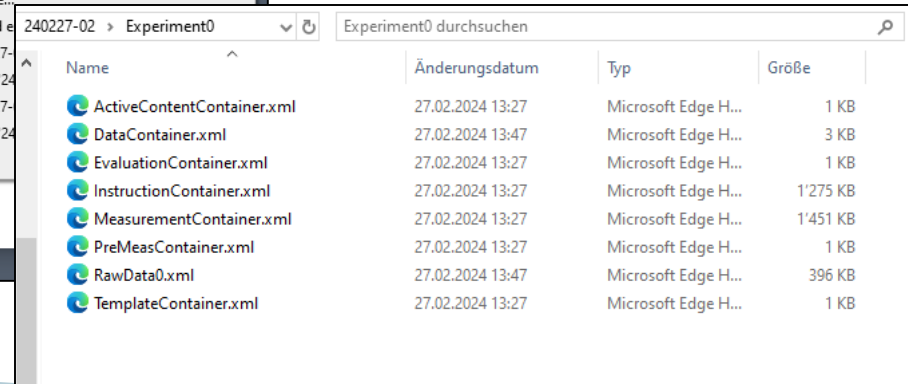
```
<xrdMeasurement measurementType="Scan" status="Completed">
  <usedWavelength intended="K-Alpha 1">
    <kAlpha unit="Angstrom">1.5405980</kAlpha>
    <kAlpha2 unit="Angstrom">1.5444260</kAlpha2>
    <kBeta unit="Angstrom">1.3922499</kBeta>
    <ratioKAlpha2KAlpha>0.500</ratioKAlpha2KAlpha>
  </usedWavelength>
  <incidentBeamPath>
    <radius unit="mm">200.00</radius>
    <xRayTube id="1010041" name="Empyrean Cu LFF (9430 033 7300x) DK0">
      <tension unit="kV">45</tension>
      <current unit="mA">40</current>
      <anodeMaterial>Cu</anodeMaterial>
      <focus type="Line">
        <length unit="mm">12.0</length>
        <width unit="mm">0.4</width>
        <takeOffAngle unit="deg">6.0</takeOffAngle>
      </focus>
    </xRayTube>
    <sollerSlit id="21010002" name="Soller 0.04 rad.">
      <opening unit="rad">0.0400</opening>
    </sollerSlit>
    <mask id="22080003" name="Inc. Mask Fixed 15 mm (MPD/MRD)">
      <width unit="mm">11.6</width>
    </mask>
    <divergenceSlit id="22010012" name="Prog. Div. Slit" xsi:type="automaticDivergenceSlitType">
      <irradiatedLength unit="mm">10.000</irradiatedLength>
      <offset unit="mm">0.000</offset>
    </divergenceSlit>
  </incidentBeamPath>
  <sampleMovement xsi:type="spinningSampleMovementType">
    <spinnerRevolutionTime unit="seconds">1.0</spinnerRevolutionTime>
  </sampleMovement>
</xrdMeasurement>
```

Instrument Configuration Files: Where to get Information

Compressed XML file formats: Extract and open in text editor or web browser (BRML, RASX)

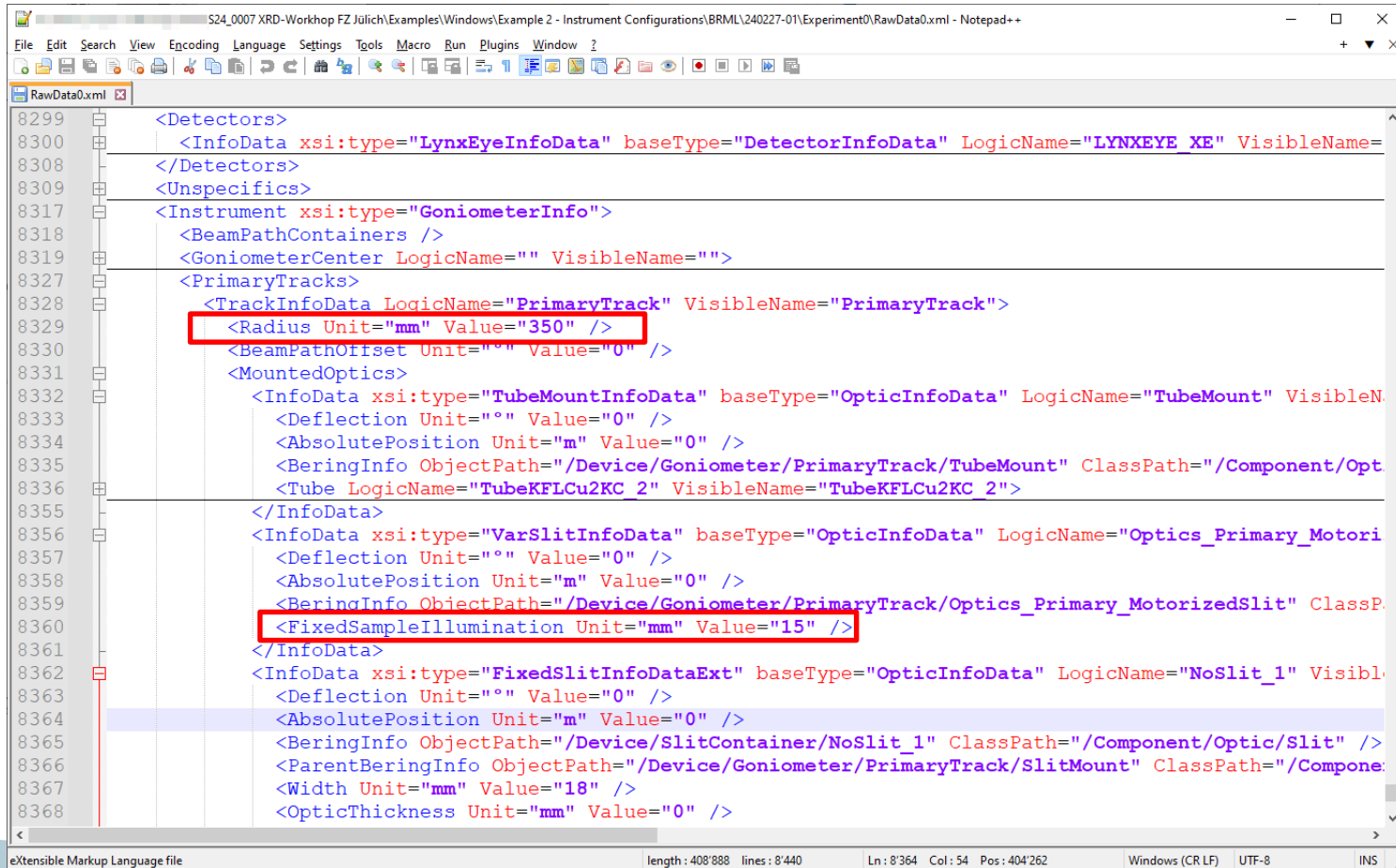


or rename to *.zip before extracting the archive



Instrument Configuration Files: Where to get Information

Bruker BRML: Open file „RawData0.xml“

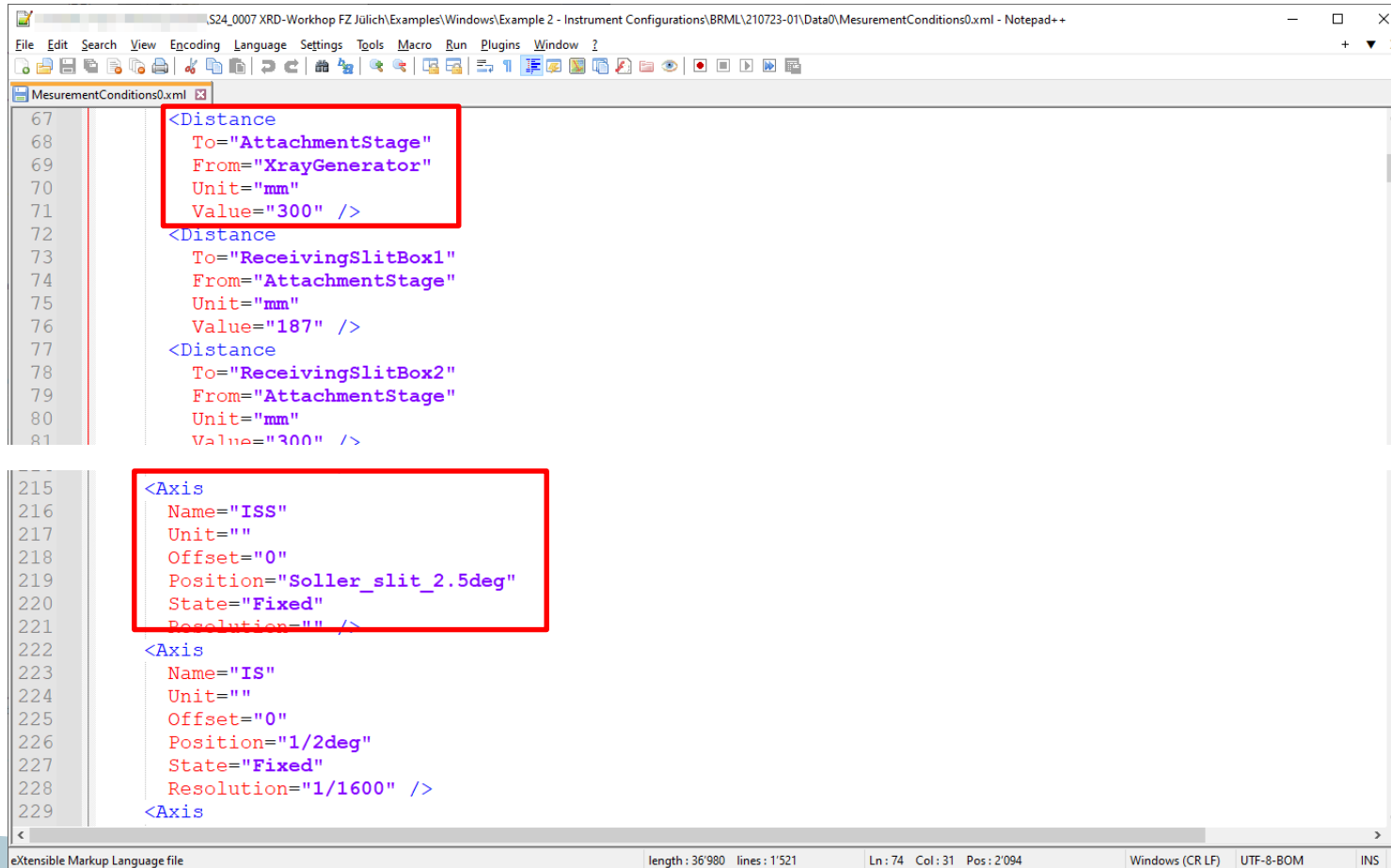


```
8299 <Detectors>
8300 <InfoData xsi:type="LynxEyeInfoData" baseType="DetectorInfoData" LogicName="LYNXEYE_XE" VisibleName=
8308 </Detectors>
8309 <Unspecifics>
8317 <Instrument xsi:type="GoniometerInfo">
8318 <BeamPathContainers />
8319 <GoniometerCenter LogicName="" VisibleName="">
8327 <PrimaryTracks>
8328 <TrackInfoData LogicName="PrimaryTrack" VisibleName="PrimaryTrack">
8329 <Radius Unit="mm" Value="350" />
8330 <BeamPathOffset Unit="" Value="0" />
8331 <MountedOptics>
8332 <InfoData xsi:type="TubeMountInfoData" baseType="OpticInfoData" LogicName="TubeMount" VisibleN
8333 <Deflection Unit="" Value="0" />
8334 <AbsolutePosition Unit="m" Value="0" />
8335 <BeringInfo ObjectPath="/Device/Goniometer/PrimaryTrack/TubeMount" ClassPath="/Component/Opt
8336 <Tube LogicName="TubeKFLCu2KC 2" VisibleName="TubeKFLCu2KC 2">
8355 </InfoData>
8356 <InfoData xsi:type="VarSlitInfoData" baseType="OpticInfoData" LogicName="Optics_Primary_Motori
8357 <Deflection Unit="" Value="0" />
8358 <AbsolutePosition Unit="m" Value="0" />
8359 <BeringInfo ObjectPath="/Device/Goniometer/PrimaryTrack/Optics_Primary_MotorizedSlit" ClassP
8360 <FixedSampleIllumination Unit="mm" Value="15" />
8361 </InfoData>
8362 <InfoData xsi:type="FixedSlitInfoDataExt" baseType="OpticInfoData" LogicName="NoSlit_1" Visibl
8363 <Deflection Unit="" Value="0" />
8364 <AbsolutePosition Unit="m" Value="0" />
8365 <BeringInfo ObjectPath="/Device/SlitContainer/NoSlit_1" ClassPath="/Component/Optic/Slit" />
8366 <ParentBeringInfo ObjectPath="/Device/Goniometer/PrimaryTrack/SlitMount" ClassPath="/Compone
8367 <Width Unit="mm" Value="18" />
8368 <OpticThickness Unit="mm" Value="0" />
```

eXtensible Markup Language file length: 408'888 lines: 8'440 Ln: 8'364 Col: 54 Pos: 404'262 Windows (CR LF) UTF-8 INS

Instrument Configuration Files: Where to get Information

Rigaku RASX: Open file „MeasurementConditions0.xml“

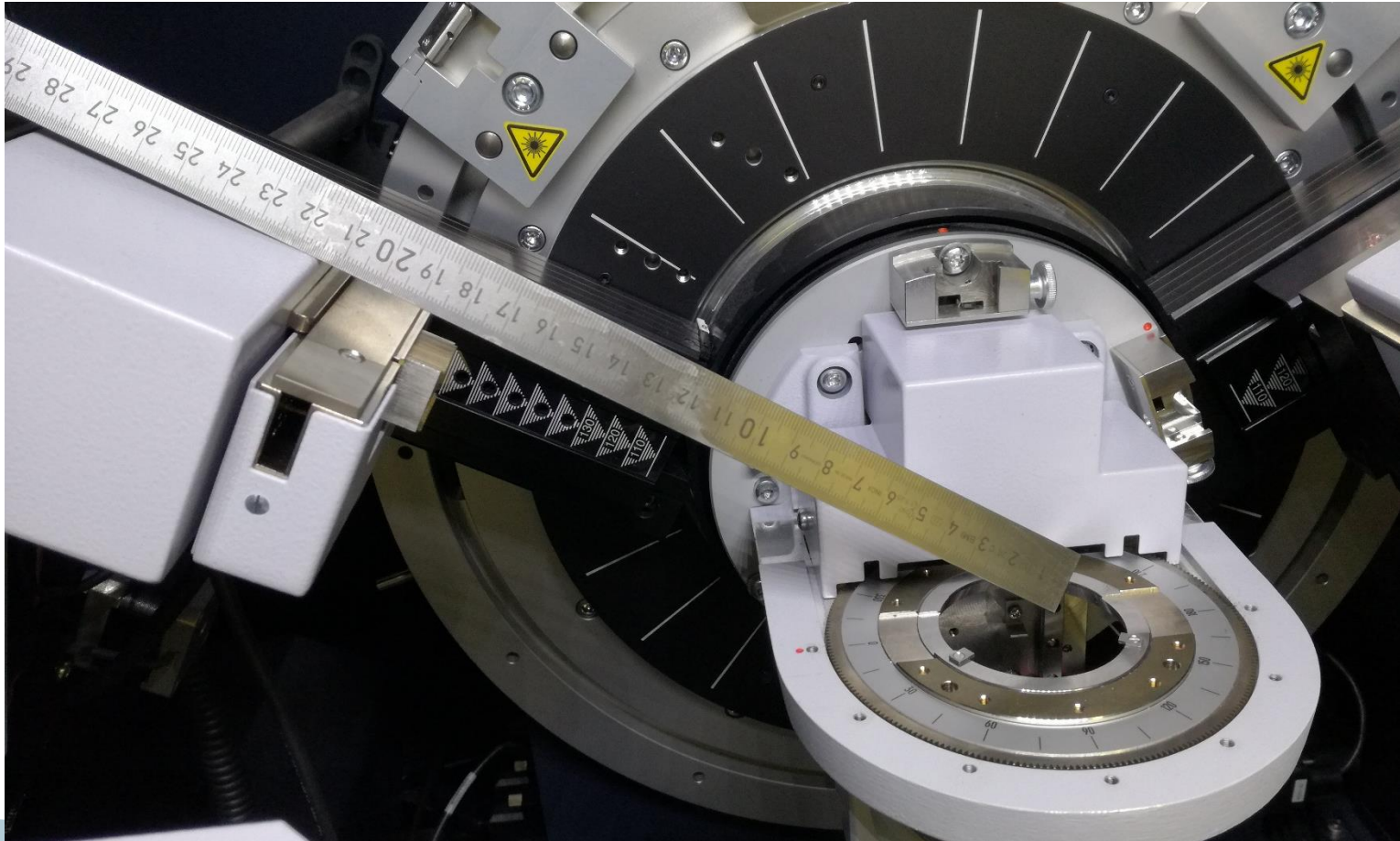


```
67 <Distance
68   To="AttachmentStage"
69   From="XrayGenerator"
70   Unit="mm"
71   Value="300" />
72 <Distance
73   To="ReceivingSlitBox1"
74   From="AttachmentStage"
75   Unit="mm"
76   Value="187" />
77 <Distance
78   To="ReceivingSlitBox2"
79   From="AttachmentStage"
80   Unit="mm"
81   Value="300" />
...
215 <Axis
216   Name="ISS"
217   Unit=""
218   Offset="0"
219   Position="Soller_slit_2.5deg"
220   State="Fixed"
221   Resolution="" />
222 <Axis
223   Name="IS"
224   Unit=""
225   Offset="0"
226   Position="1/2deg"
227   State="Fixed"
228   Resolution="1/1600" />
229 <Axis
```

eXtensible Markup Language file length: 36'980 lines: 1'521 Ln: 74 Col: 31 Pos: 2'094 Windows (CR LF) UTF-8-BOM INS

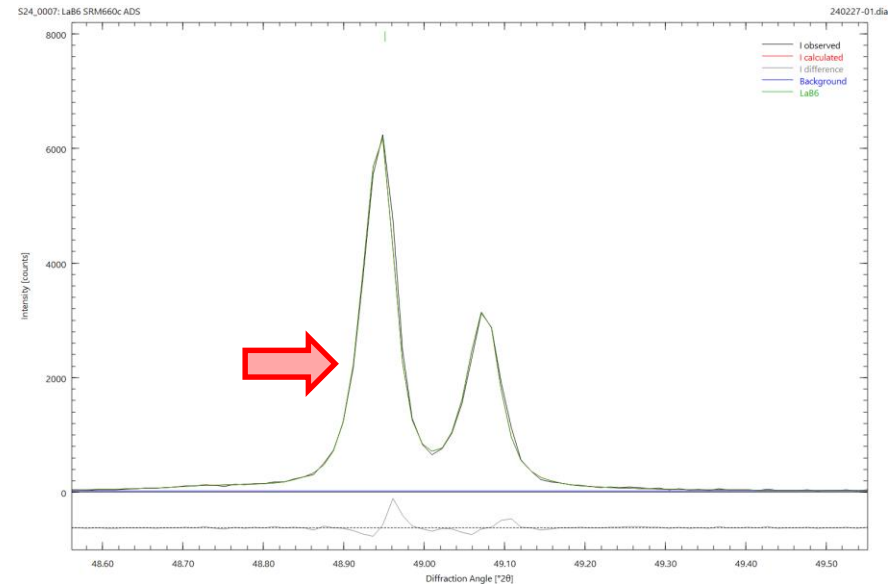
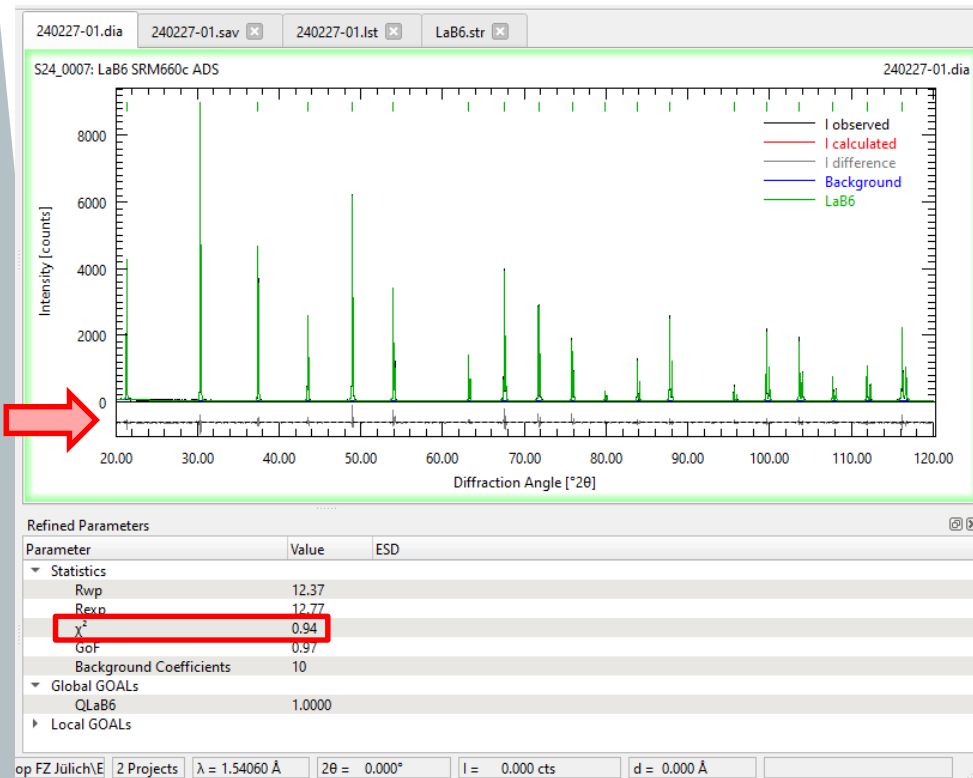
Instrument Configuration Files: Where to get Information

If all other options failed: Take measurements



Instrument Configuration Files

Always verify new instrument configuration files by refining a reference sample (preferably LaB6 NIST SRM 660)



Structure and Device Files: Summary

- Structure files:
 - Use GOAL= to write additional results to the *.LST file
 - Use GOAL: to export variables to the *.SAV file for further computations
 - BGMN expression interpreter allows to implement custom calculations (e.g. substitution models)

- Device files:
 - Must accurately represent the true instrument configuration
 - Get information from:
 - Measurement software
 - Original data processing software
 - XML scan files
 - Take measurements
 - Verify with reference measurement