

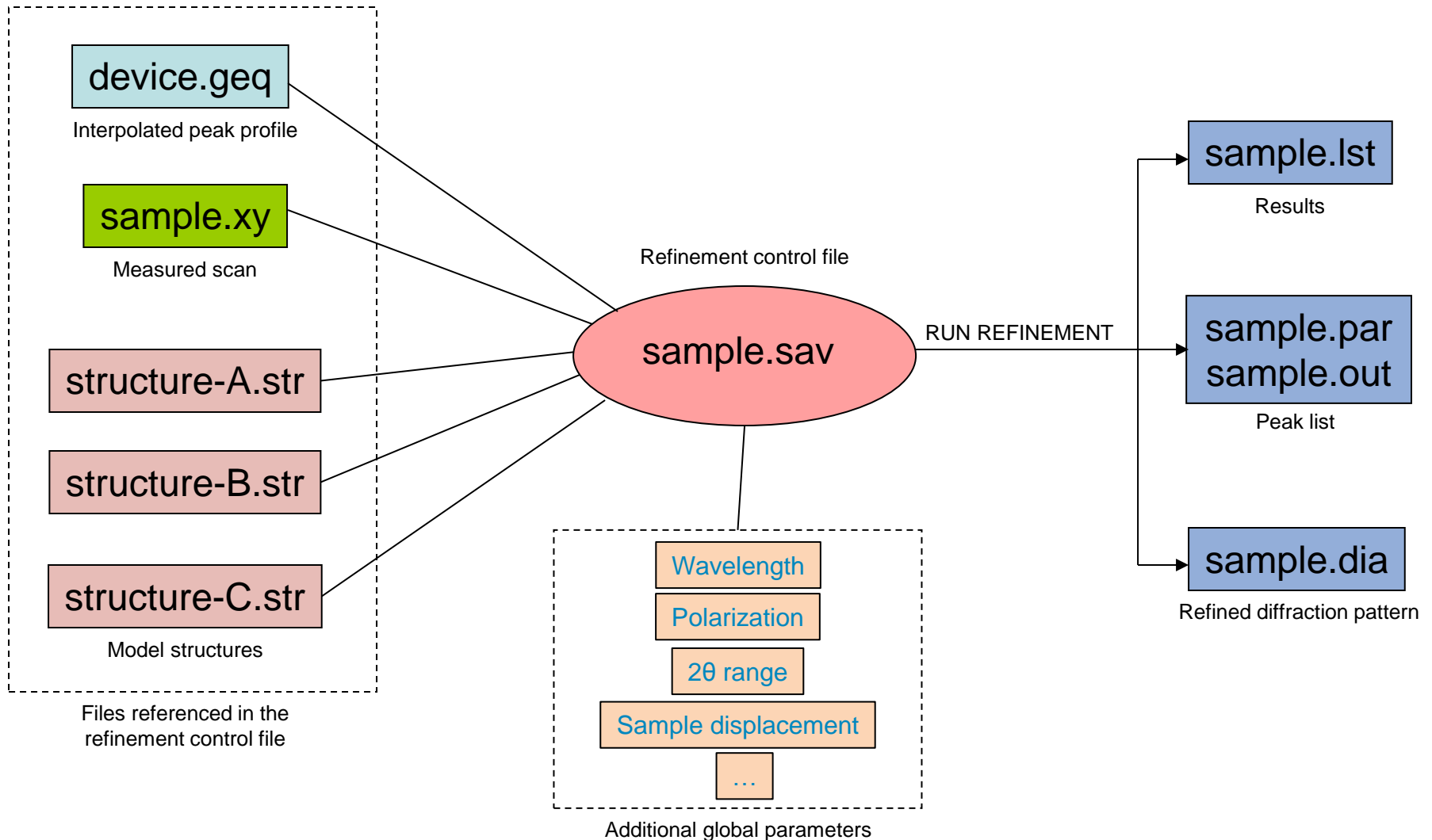
Lesson 8

Crystal Structure Models

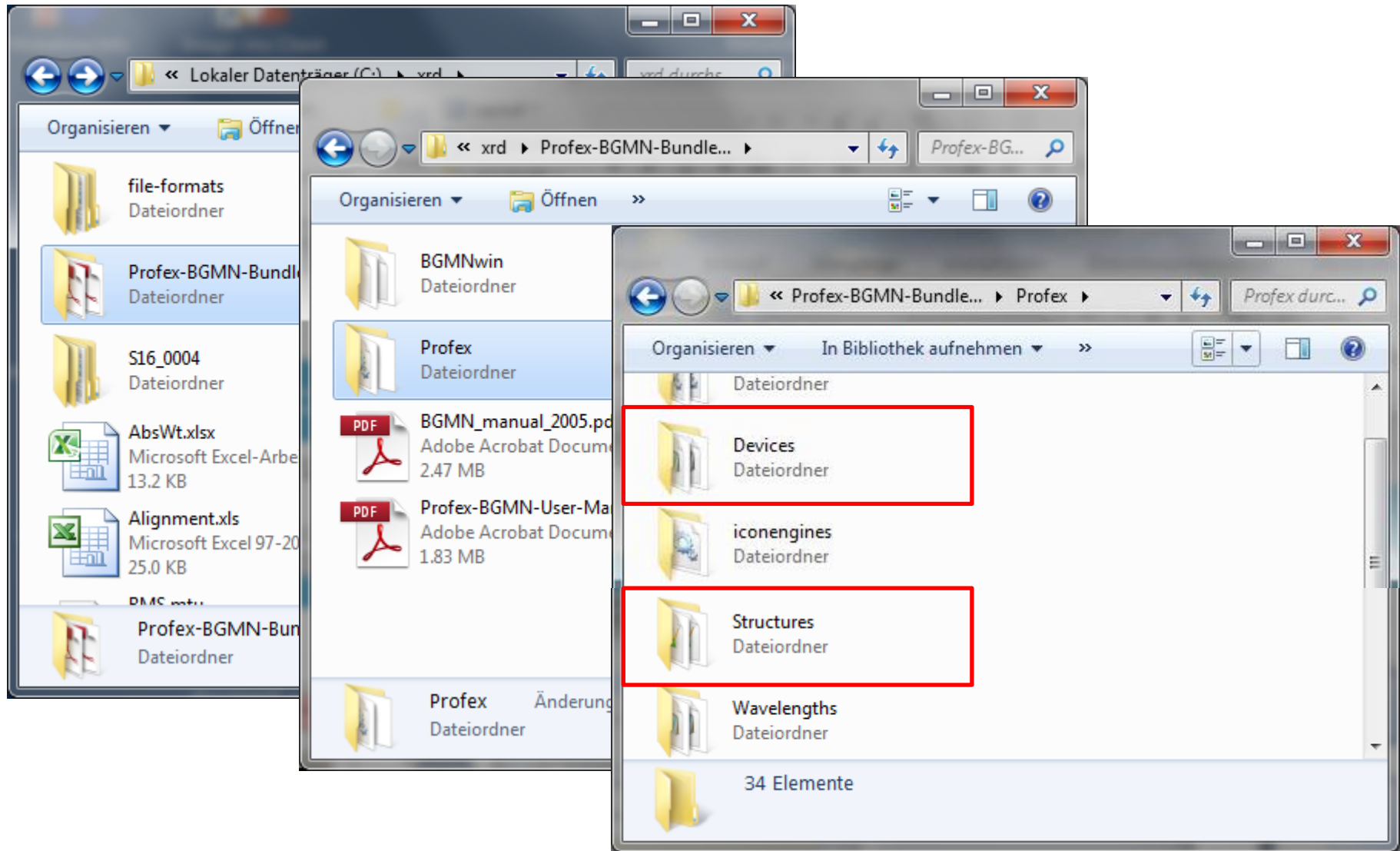


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BGMN Project Structure



Profex Structure and Device File Database



Profex Structure and Device File Database

The screenshot displays the Profex 3.8.0 software interface. The main window shows a list of 190 elements in the 'Structures' folder. A dialog box titled 'Add / Remove Phases' is open, showing a table of phases with columns for File Name, Phase, and Comment. A plot on the right shows observed and calculated data.

File Name	Phase	Comment
<input type="checkbox"/> Chlorapatite.str	Chlorapatite	04-012-1323
<input type="checkbox"/> Chromatite.str	Chromatite	01-087-1647
<input type="checkbox"/> Clinoatacamite.str	Clinoatacamite	04-012-9781
<input type="checkbox"/> Clinochlore1A.str	Clinochlore1A	04-017-2550
<input type="checkbox"/> CO3ApatiteA.str	CO3ApA	04-011-0242
<input type="checkbox"/> CO3ApatiteB.str	CO3ApatiteB	04-016-7498
<input type="checkbox"/> CoOH2.str	Cobalt_Hydroxide	
<input type="checkbox"/> Cr3P2O8.str	Cr3P2O8	04-018-4496
<input type="checkbox"/> Cristobalite.str	Cristobalite	04-007-2134
<input type="checkbox"/> Cronstedtite2H2.str	Cronstedtite2H2	
<input type="checkbox"/> CSA.str	CSA	04-007-6682
<input type="checkbox"/> CSD.str	CSD	04-016-3025
<input type="checkbox"/> CSH.str	CSH	04-014-0553
<input type="checkbox"/> Cu2S.str	Cu2S	04-017-8811
<input type="checkbox"/> Cu-hydroxylapatite.str	CuHydroxylapatite	04-012-7193
<input type="checkbox"/> CuS2.str	CuS2	04-004-6505
<input type="checkbox"/> DiammoniumHydrogenPhosphate.str	Phosphammite	04-009-3766
<input type="checkbox"/> Dolomite.str	Dolomite	04-008-0789
<input type="checkbox"/> Ettringite.str	Ettringite	04-013-3691
<input type="checkbox"/> Fe3Si2O5_OH4.str	Fe3Si2O5OH4	
<input type="checkbox"/> FeAg.str	FeAg	04-003-7119

Plot Options:

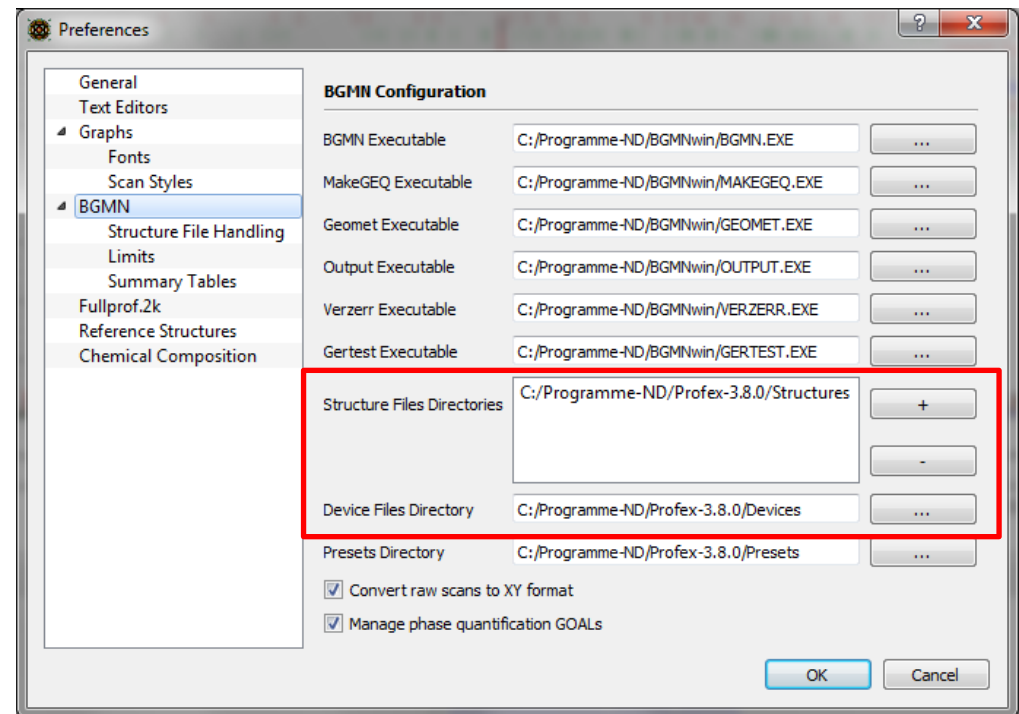
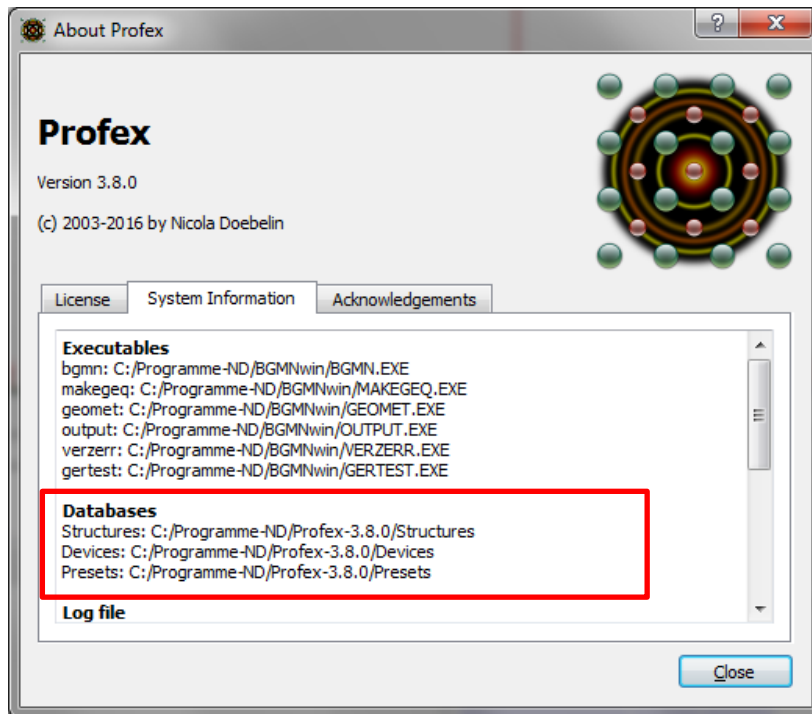
- I observed
- I calculated
- I difference
- Background
- Hydroxyapatite
- Whitlockite

Wavelength: 1.5406 Å Angle: 0.000° Intensity: 0.000 cts d-Spacing: 0.000 Å Line 0, Column 0

Profex Structure and Device File Database

«Help → About Profex...»

«Edit → Preferences... → BGMN»



Databases can be changed to a network share.

→ Structures added by one user become available to others.

Public Structure Databases

- STR files shipped with Profex (created manually by the Profex developer)
- <http://www.bgmn.de/download-structures.html> (created manually by BGMN team)

- Create manually from:
 - ICSD (<http://www.fiz-karlsruhe.de/icsd.html>)
 - PDF-4+ (<http://www.icdd.com/>)
 - American Mineralogist Structure Database (<http://rruff.geo.arizona.edu/AMS/amcsd.php>)
 - Crystallography Open Database COD (<http://www.crystallography.net/>)
 - Cambridge Crystallographic Data Centre (<http://beta-www.ccdc.cam.ac.uk/pages/Home.aspx>)

The screenshot shows a Firefox browser window displaying the American Mineralogist Crystal Structure Database (AMCSD) website. The browser's address bar shows the URL `rruff.geo.arizona.edu/AMS/amcsd.php`. The page title is "American Mineralogist Crystal Structure Database".

The main content area features a search interface with a text input field containing "anatase" and several search criteria labels: **Mineral**, **Author**, **Chemistry Search**, **Cell Parameters and Symmetry**, **Diffraction Search**, and **General Search**. Below these labels are "Search" and "Reset" buttons.

At the bottom of the search interface, there are radio button options for "Logic interface" (AND and OR), "Viewing" (amc long form, amc short form, and cif), and "Download" (amc, cif, and diffraction data).

AMCSD: Downloading CIF Files

AMCSD Search Results

rruff.geo.arizona.edu/AMS/result.php

American Mineralogist Crystal Structure Database

7 matching records for this search.

Anatase

Howard C J, Sabine T M, Dickson F

Acta Crystallographica B47 (1991) 462-468

Structural and thermal parameters for rutile and anatase

Locality: synthetic

_database_code_amcsd 0019093

3.7845 3.7845 9.5143 90 90 90 I4_1/amd

atom	x	y	z	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
Ti	0	0	0	.0052	0	0	.0052	0	.0070
O	0	0	.20806	.0117	0	0	.0027	0	.0072

[Download AMC data \(View Text File\)](#)

[Download CIF data \(View Text File\)](#)

[Download diffraction data \(View Text File\)](#)

[View Jmol 3-D Structure](#)

Anatase

Parker R

Zeitschrift fur Kristallographie 59 (1924) 1-54

Zur Kristallstruktur von Anastas und Rutil. (II. Teil. Die Anastasstruktur).

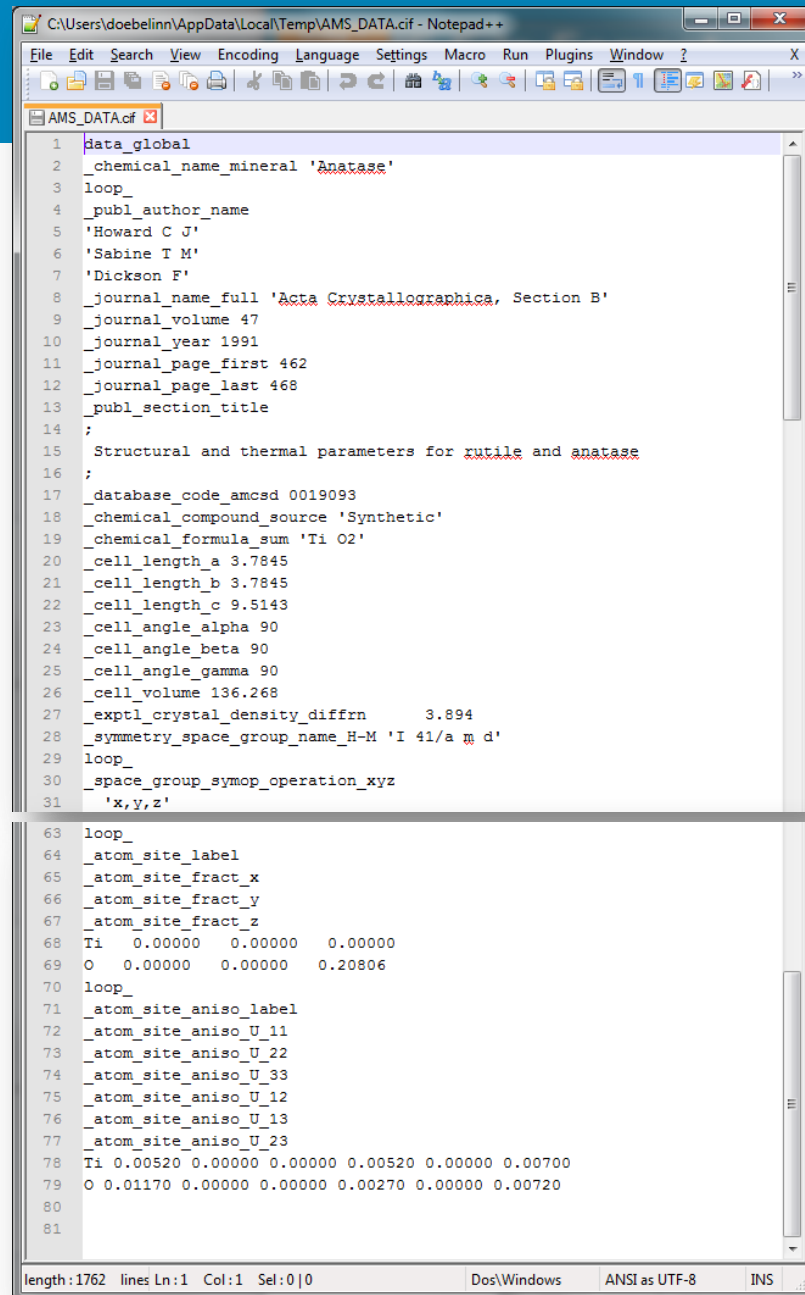
Watch out for high-temp and high-pressure datasets

Download CIF file

CIF File Format

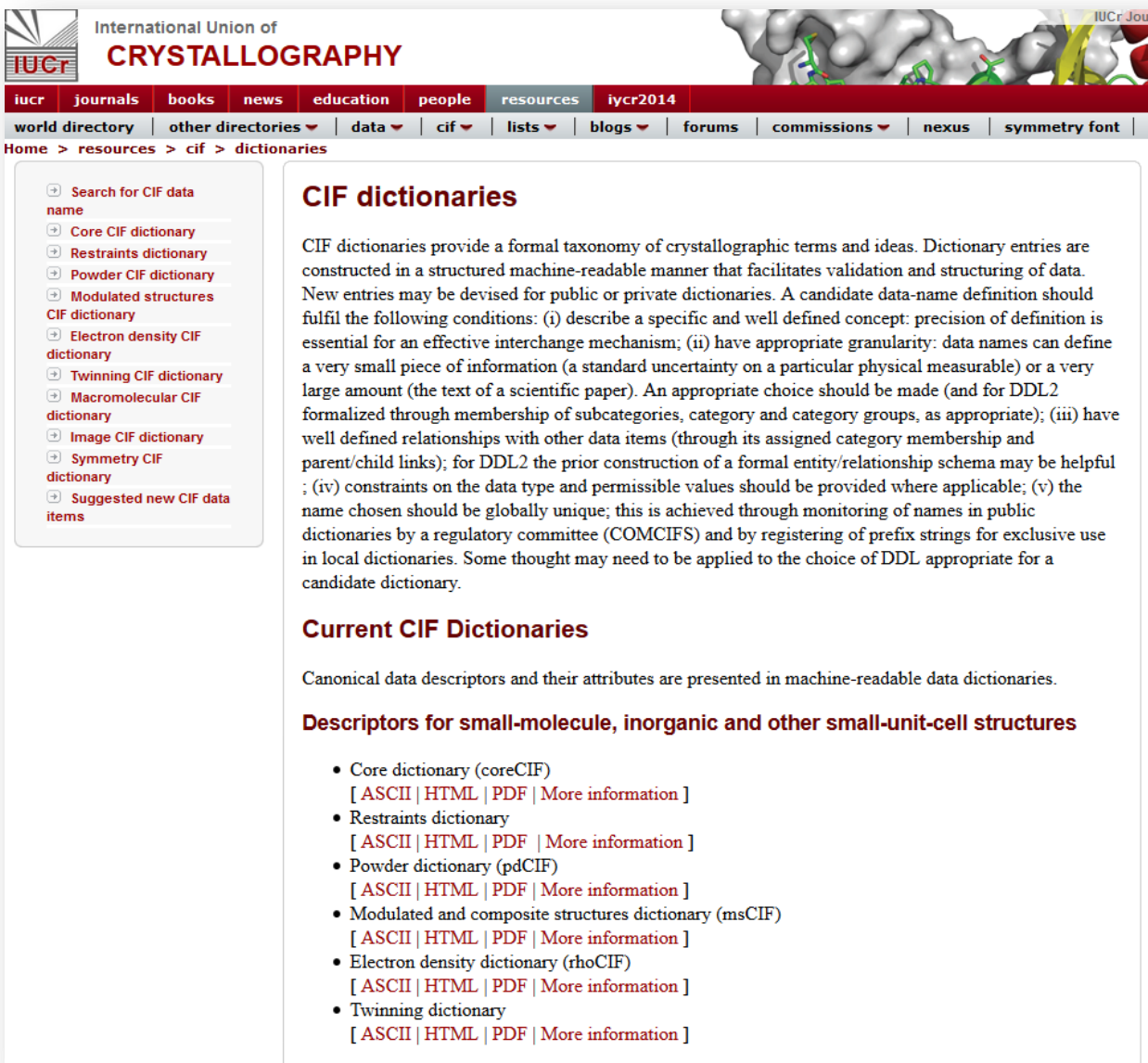
CIF (Crystallographic Information File) Format:

- Standardized file format
- Contains structural information
- Contains references
- Specification available at <http://www.iucr.org>




```
1 data_global
2 _chemical_name_mineral 'Anatase'
3 loop_
4 _publ_author_name
5 'Howard C J'
6 'Sabine T M'
7 'Dickson F'
8 _journal_name_full 'Acta Crystallographica, Section B'
9 _journal_volume 47
10 _journal_year 1991
11 _journal_page_first 462
12 _journal_page_last 468
13 _publ_section_title
14 ;
15 Structural and thermal parameters for rutile and anatase
16 ;
17 _database_code_amcsd 0019093
18 _chemical_compound_source 'Synthetic'
19 _chemical_formula_sum 'Ti O2'
20 _cell_length_a 3.7845
21 _cell_length_b 3.7845
22 _cell_length_c 9.5143
23 _cell_angle_alpha 90
24 _cell_angle_beta 90
25 _cell_angle_gamma 90
26 _cell_volume 136.268
27 _exptl_crystal_density_diffn      3.894
28 _symmetry_space_group_name_H-M 'I 41/a m d'
29 loop_
30 _space_group_symop_operation_xyz
31 'x,y,z'
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60
61
62
63 loop_
64 _atom_site_label
65 _atom_site_fract_x
66 _atom_site_fract_y
67 _atom_site_fract_z
68 Ti 0.00000 0.00000 0.00000
69 O 0.00000 0.00000 0.20806
70 loop_
71 _atom_site_aniso_label
72 _atom_site_aniso_U_11
73 _atom_site_aniso_U_22
74 _atom_site_aniso_U_33
75 _atom_site_aniso_U_12
76 _atom_site_aniso_U_13
77 _atom_site_aniso_U_23
78 Ti 0.00520 0.00000 0.00000 0.00520 0.00000 0.00700
79 O 0.01170 0.00000 0.00000 0.00270 0.00000 0.00720
80
81
```

length : 1762 lines Ln: 1 Col: 1 Sel: 0 | 0 Dos\Windows ANSI as UTF-8 INS



International Union of
CRYSTALLOGRAPHY



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[Home](#) > [resources](#) > [cif](#) > [dictionaries](#)

➤ [Search for CIF data name](#)

➤ [Core CIF dictionary](#)

➤ [Restraints dictionary](#)

➤ [Powder CIF dictionary](#)

➤ [Modulated structures CIF dictionary](#)

➤ [Electron density CIF dictionary](#)

➤ [Twinning CIF dictionary](#)

➤ [Macromolecular CIF dictionary](#)

➤ [Image CIF dictionary](#)

➤ [Symmetry CIF dictionary](#)

➤ [Suggested new CIF data items](#)

CIF dictionaries

CIF dictionaries provide a formal taxonomy of crystallographic terms and ideas. Dictionary entries are constructed in a structured machine-readable manner that facilitates validation and structuring of data. New entries may be devised for public or private dictionaries. A candidate data-name definition should fulfil the following conditions: (i) describe a specific and well defined concept; precision of definition is essential for an effective interchange mechanism; (ii) have appropriate granularity: data names can define a very small piece of information (a standard uncertainty on a particular physical measurable) or a very large amount (the text of a scientific paper). An appropriate choice should be made (and for DDL2 formalized through membership of subcategories, category and category groups, as appropriate); (iii) have well defined relationships with other data items (through its assigned category membership and parent/child links); for DDL2 the prior construction of a formal entity/relationship schema may be helpful; (iv) constraints on the data type and permissible values should be provided where applicable; (v) the name chosen should be globally unique; this is achieved through monitoring of names in public dictionaries by a regulatory committee (COMCIFS) and by registering of prefix strings for exclusive use in local dictionaries. Some thought may need to be applied to the choice of DDL appropriate for a candidate dictionary.

Current CIF Dictionaries

Canonical data descriptors and their attributes are presented in machine-readable data dictionaries.

Descriptors for small-molecule, inorganic and other small-unit-cell structures

- Core dictionary (coreCIF)
[[ASCII](#) | [HTML](#) | [PDF](#) | [More information](#)]
- Restraints dictionary
[[ASCII](#) | [HTML](#) | [PDF](#) | [More information](#)]
- Powder dictionary (pdCIF)
[[ASCII](#) | [HTML](#) | [PDF](#) | [More information](#)]
- Modulated and composite structures dictionary (msCIF)
[[ASCII](#) | [HTML](#) | [PDF](#) | [More information](#)]
- Electron density dictionary (rhoCIF)
[[ASCII](#) | [HTML](#) | [PDF](#) | [More information](#)]
- Twinning dictionary
[[ASCII](#) | [HTML](#) | [PDF](#) | [More information](#)]

Problems with CIF Files

Problems with CIF files:

1. May be (and very often ARE) incomplete
2. May use non-standard atomic settings
3. Must be converted to STR format for BGMN

With Profex:

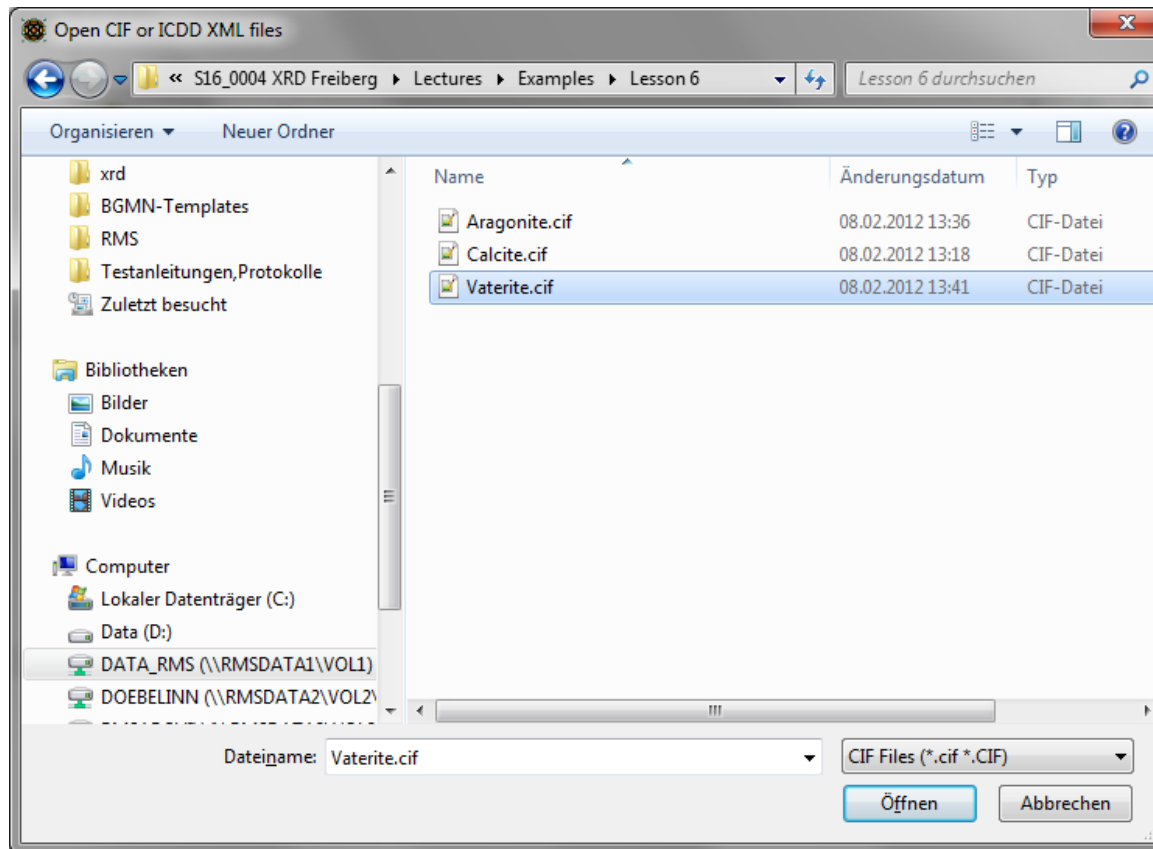
- For complete CIF files: automatic import
- For incomplete CIF files: semi-automatic import



Profex CIF Import

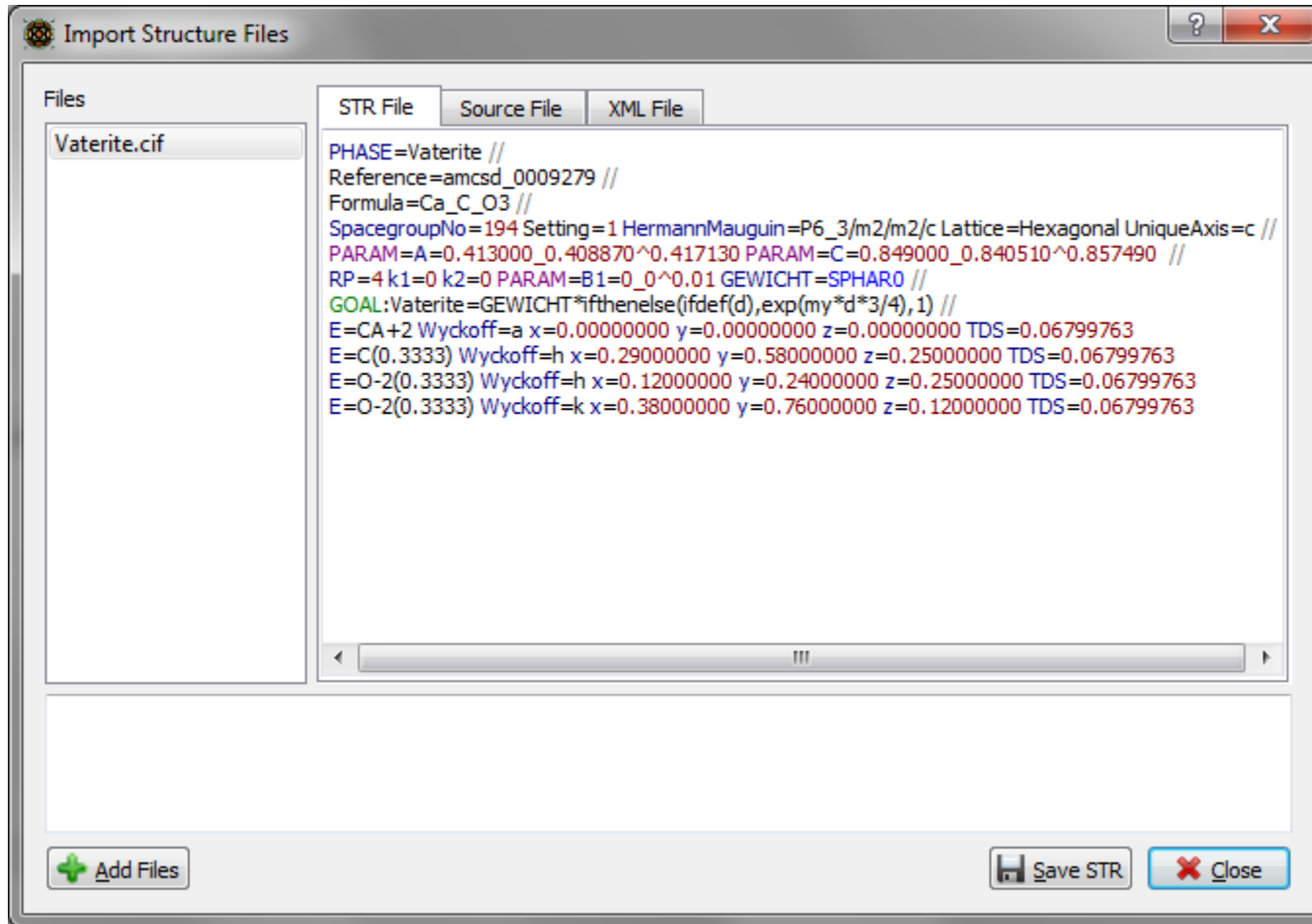
«File → Import Structure File...»

«Examples/Lesson 6/Vaterite.cif»



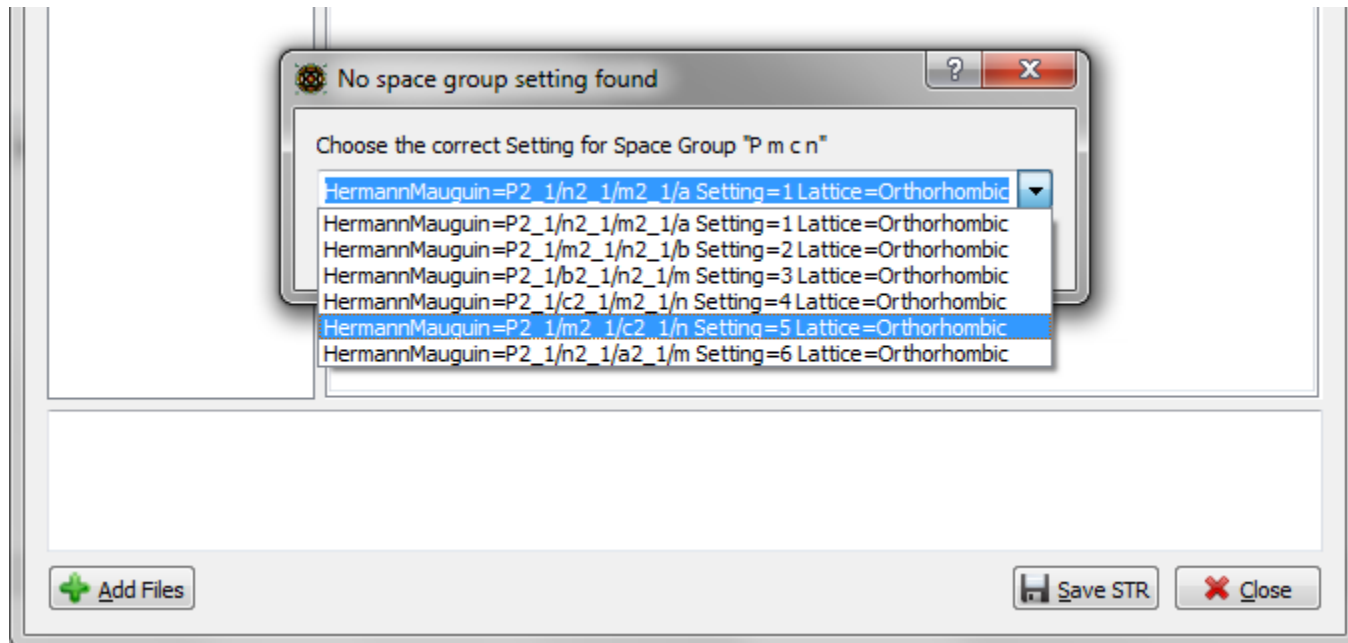
Profex CIF Import

Best Case: No Questions asked = automatic import



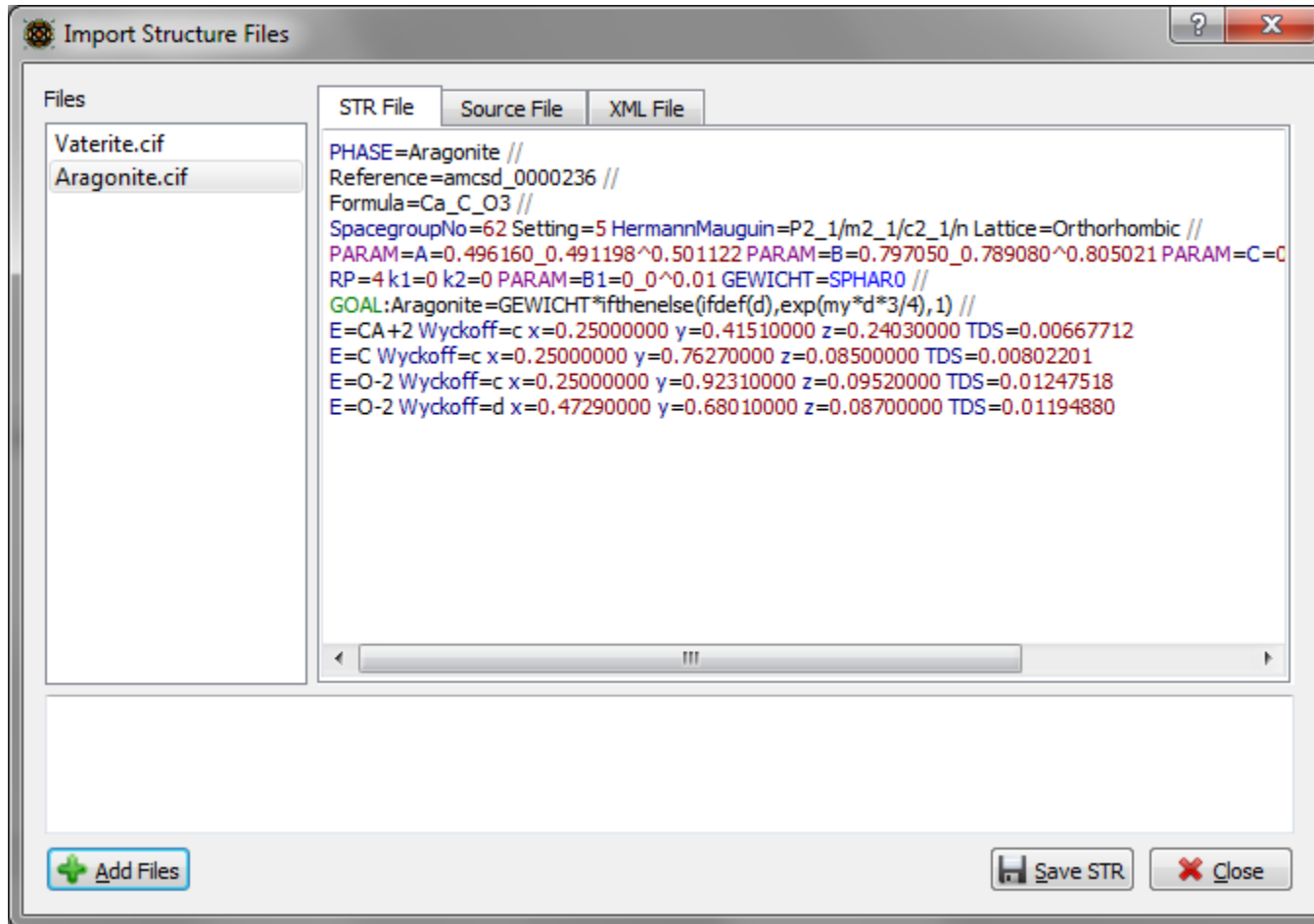
«Save STR» to Structures database directory

«+ Add Files → Aragonite.cif»



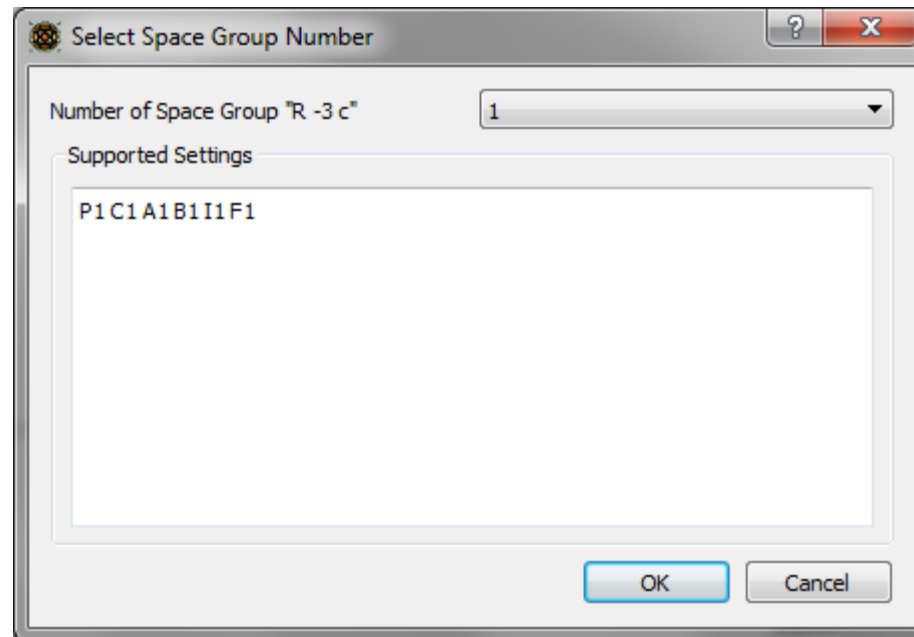
Profex could not assign the CIF HM symbol «P m c n»
to BGMN's full notation.

No further input required



«Save STR» to Structures database directory

«+ Add Files → Calcite.cif»



Space Group Number for «*R -3 c*» is missing.

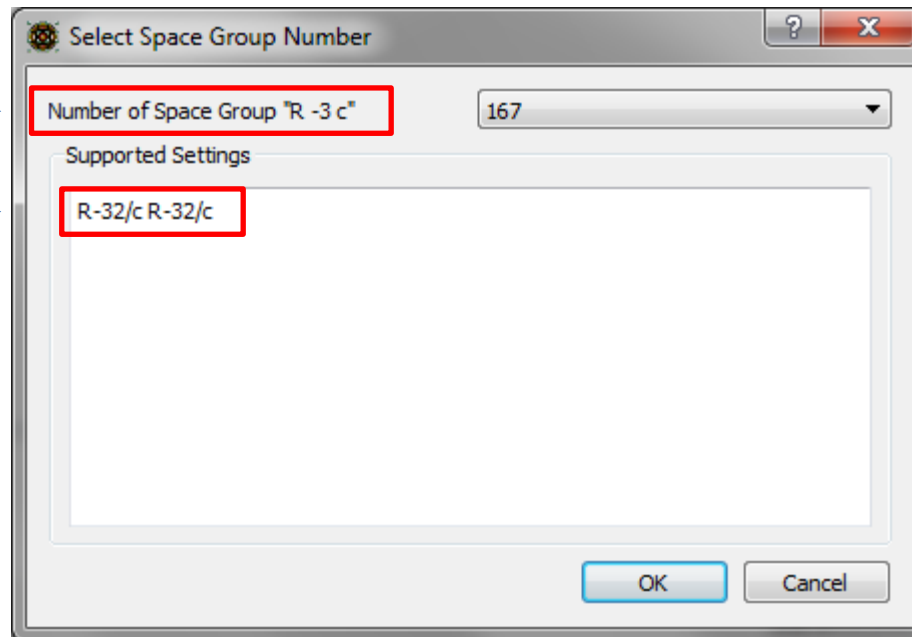
Found elsewhere: 167

Profex CIF Import

BGMN's full notations for SG #167

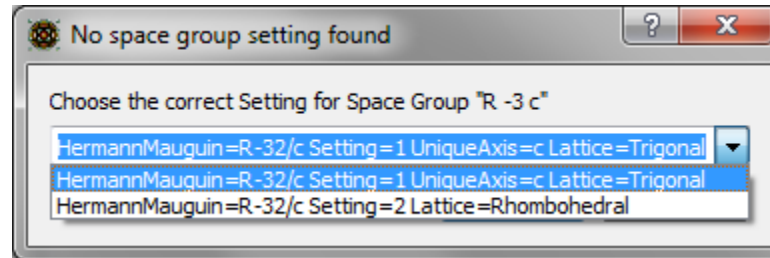
Read from CIF file →

Supported by BGMN →



Seems to match. Click «OK»

BGMN's full notations for SG #167



Two settings for $R-3_2/c$:

- Trigonal
- Rhombohedral

Check CIF file which one is correct
(here: Trigonal)

Warning: Missing Wyckoff symbols

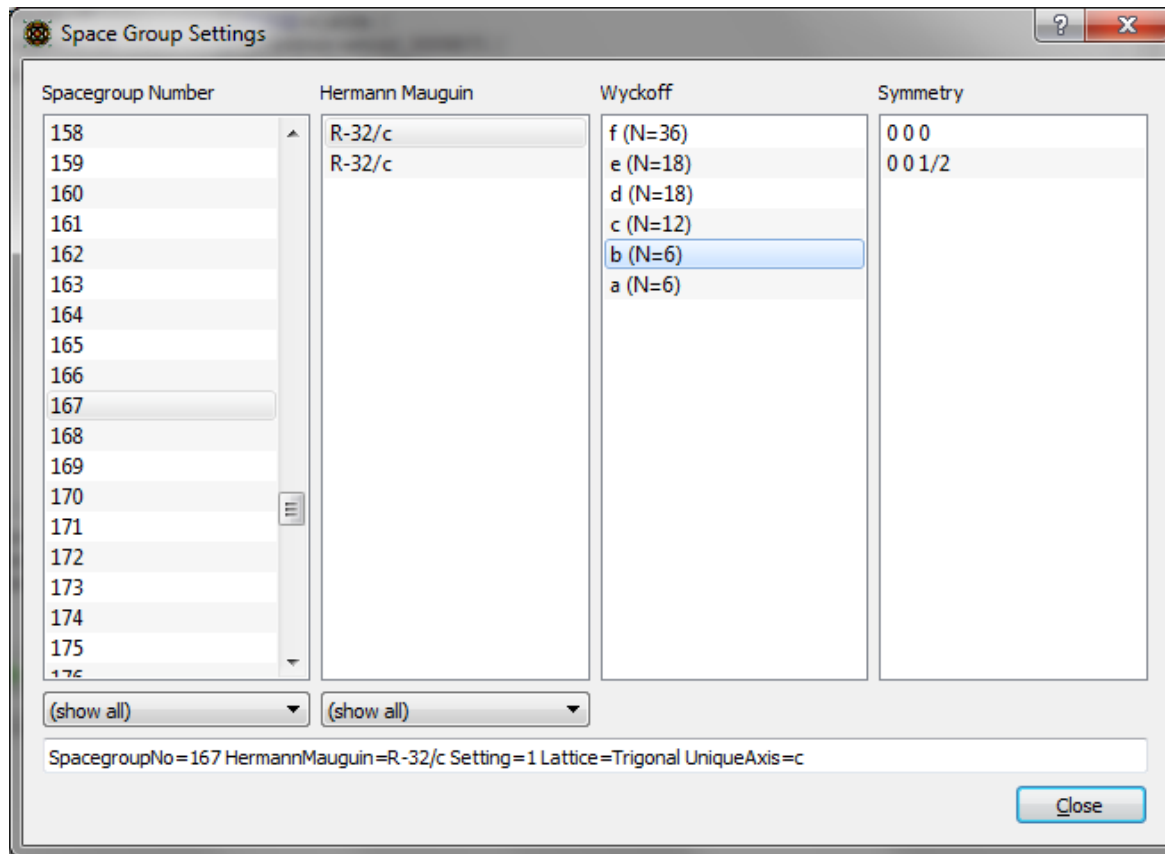
The screenshot shows a software window titled "Import Structure Files" with a file list on the left containing "Vaterite.cif", "Aragonite.cif", and "Calcite.cif". The main area displays the content of a selected CIF file in "STR File" format. The text includes phase information, reference, formula, space group, and atom positions. A red bracket highlights the atom position lines, with the word "Empty!" written below them. A red box at the bottom contains three warning messages: "Warning: No Wyckoff information found for atom number 0.", "Warning: No Wyckoff information found for atom number 1.", and "Warning: No Wyckoff information found for atom number 2." Buttons for "Add Files", "Save STR", and "Close" are visible at the bottom.

```
PHASE=Calcite //
Reference=amcsd_0009873 //
Formula=Ca_C_O3 //
SpacegroupNo=167 Setting=1 HermannMauguin=R-32/c Lattice=Trigonal UniqueAxis=c //
PARAM=A=0.499100_0.494109^0.504091 PARAM=C=1.706200_1.689138^1.723262 //
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.01 GEWICHT=SPHARO //
GOAL:Calcite=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1) //
E=CA Wyckoff= x=0.00000000 y=0.00000000 z=0.00000000 TDS=0.00796938
E=C Wyckoff= x=0.00000000 y=0.00000000 z=0.25000000 TDS=0.00757986
E=O Wyckoff= x=0.25730000 y=0.00000000 z=0.25000000 TDS=0.01306297
```

Empty!

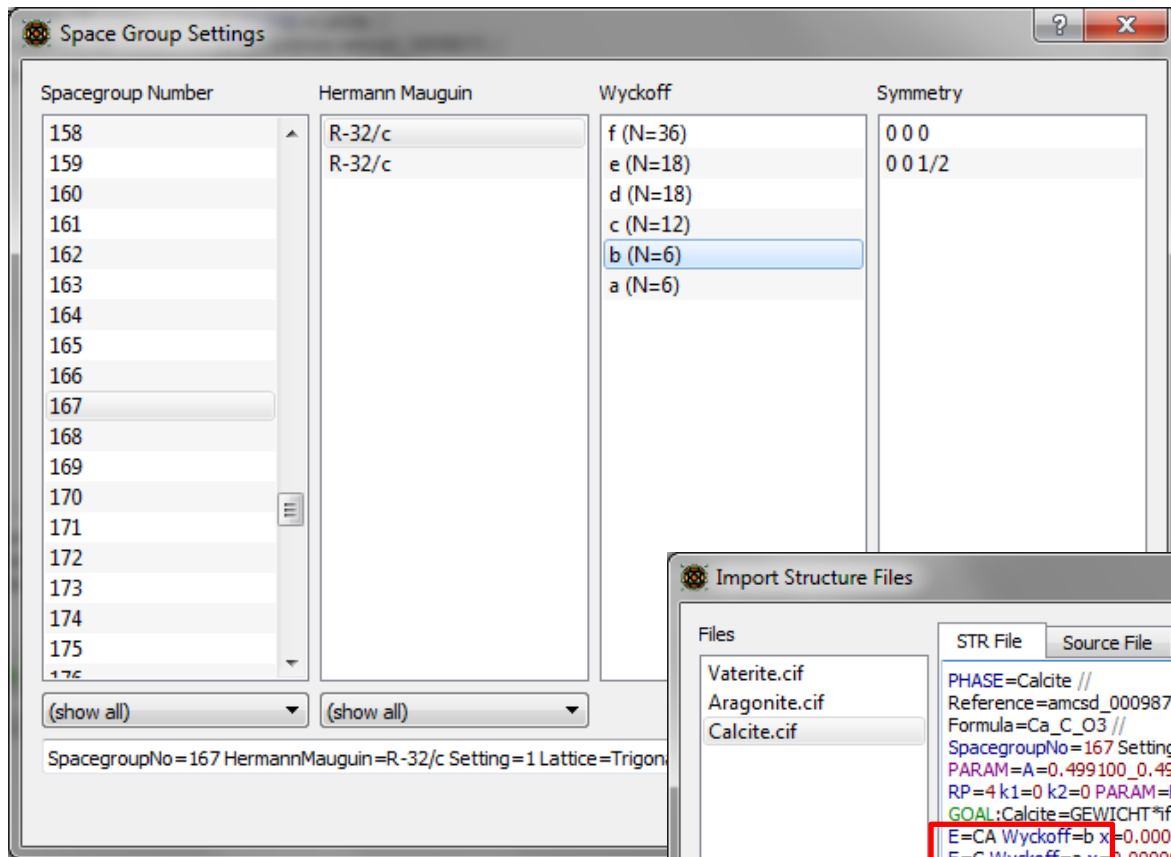
Warning: No Wyckoff information found for atom number 0.
Warning: No Wyckoff information found for atom number 1.
Warning: No Wyckoff information found for atom number 2.

«Help → BGMN SPACEGRP.DAT»



Select Number 167, Trigonal setting, and browse all Wyckoff positions.

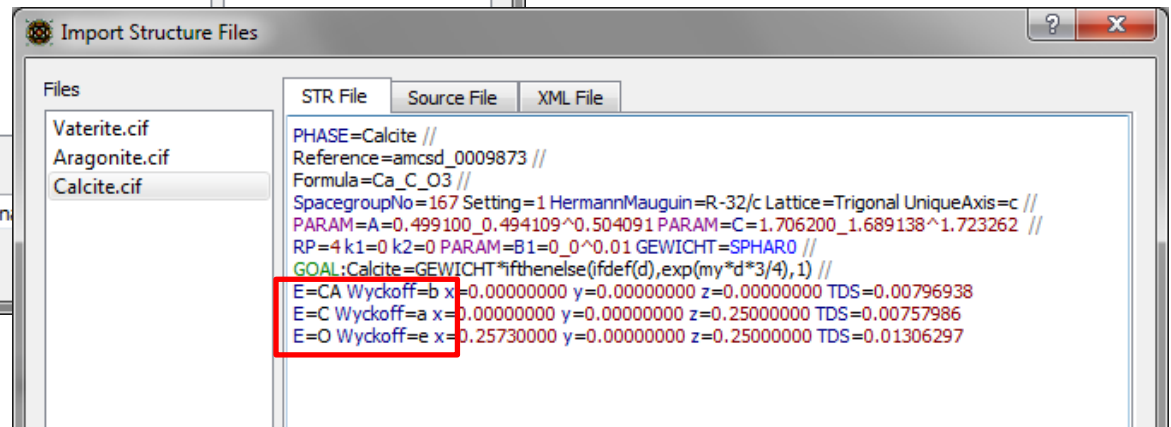
Profex CIF Import



Ca at 0,0,0: Wyckoff=b

C at 0,0,1/4: Wyckoff=a

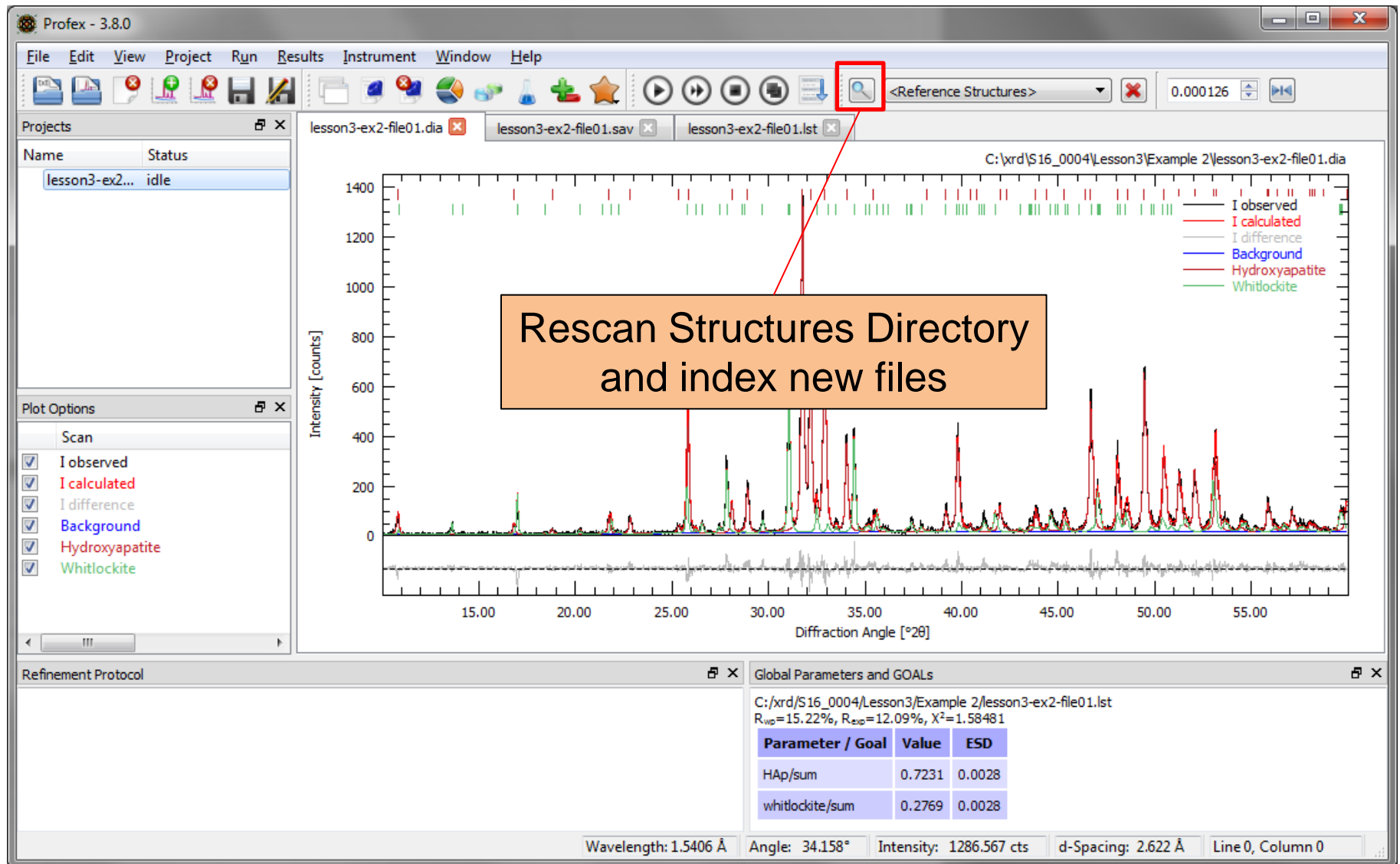
O at x,0,1/4: Wyckoff=e



Fill in manually

“Save STR” to Structure Database directory

Profex CIF Import



Import from ICDD PDF4+ XML Format

Ca (C O3) - 04-007-8659

File Edit PDF Features Plots Window Help

Cu Kα1 1.54056 Å Simulated Profile (Calc-based)

Fixed Slit Intensity Raw Diffraction Data (PD3)

2θ (°)	d (Å)	I	h	k	l	*
23.0554	3.854450	99	0	1	2	
29.4003	3.035460	999	1	0	4	
31.4327	2.843670	21	0	0	6	
35.9728	2.494500	138	1	1	0	
39.4112	2.284430	197	1	1	3	
43.1620	2.094200	145	2	0	2	
47.1167	1.927230	64	0	2	4	
47.5033	1.912440	187	0	1	8	
48.5056	1.875240	205	1	1	6	

Intensity

PDF Experimental Physical Crystal Optical Structure Miscellaneous References Comments

Status: Primary QM: Indexed

Chemical Formula: Ca (C O3)

Structural Formula:

Compound Name: Calcium Carbonate

Mineral Name: Calcite, syn

Common Name:

Save PDF Card

Speichern in: Desktop

Zuletzt verwendet

Desktop

Eigene Dokumente

Computer

Netzwerk

Dateiname: PDF Card - 04-007-8659

Dateityp: ICDD XML Files (*.xml)

Speichern

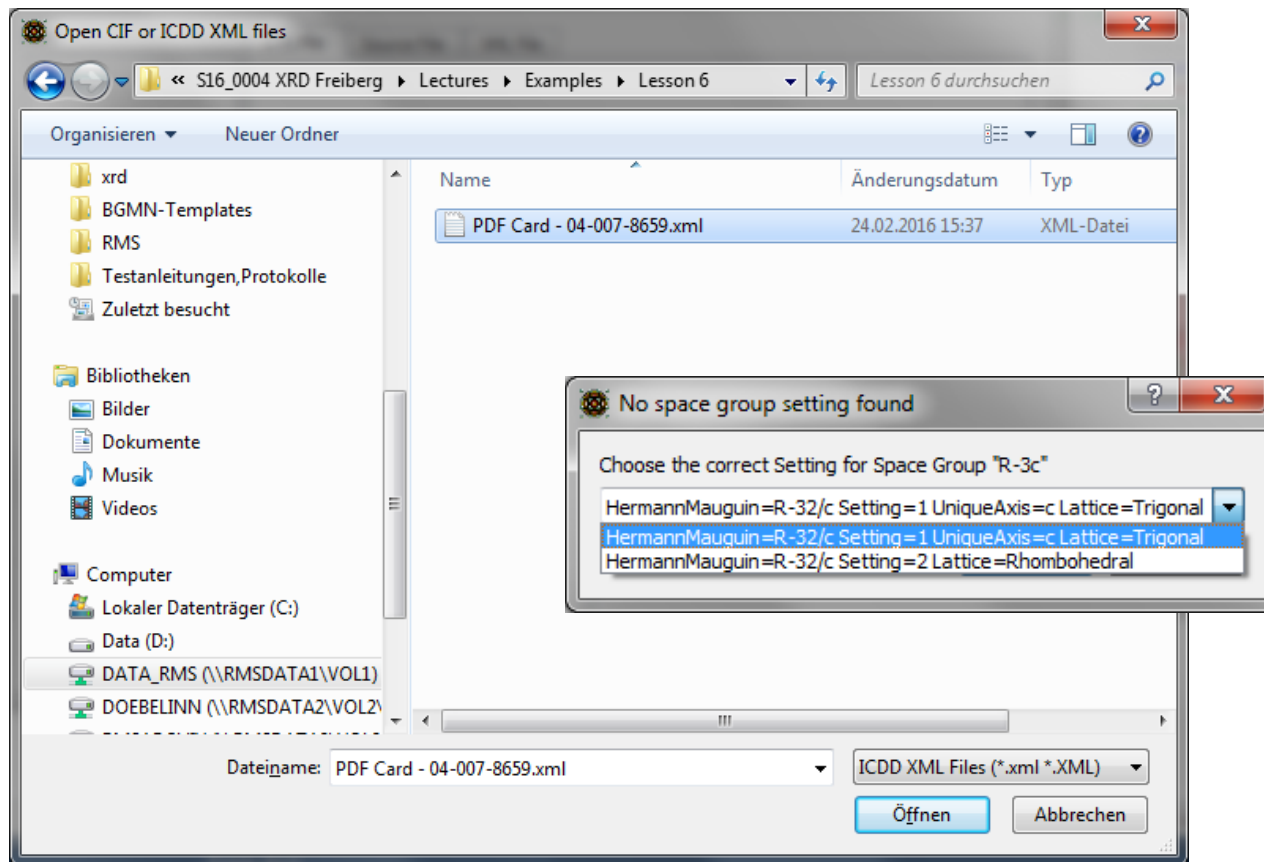
Abbrechen

«File → Save PDF Card»
in «ICDD XML Files» Format

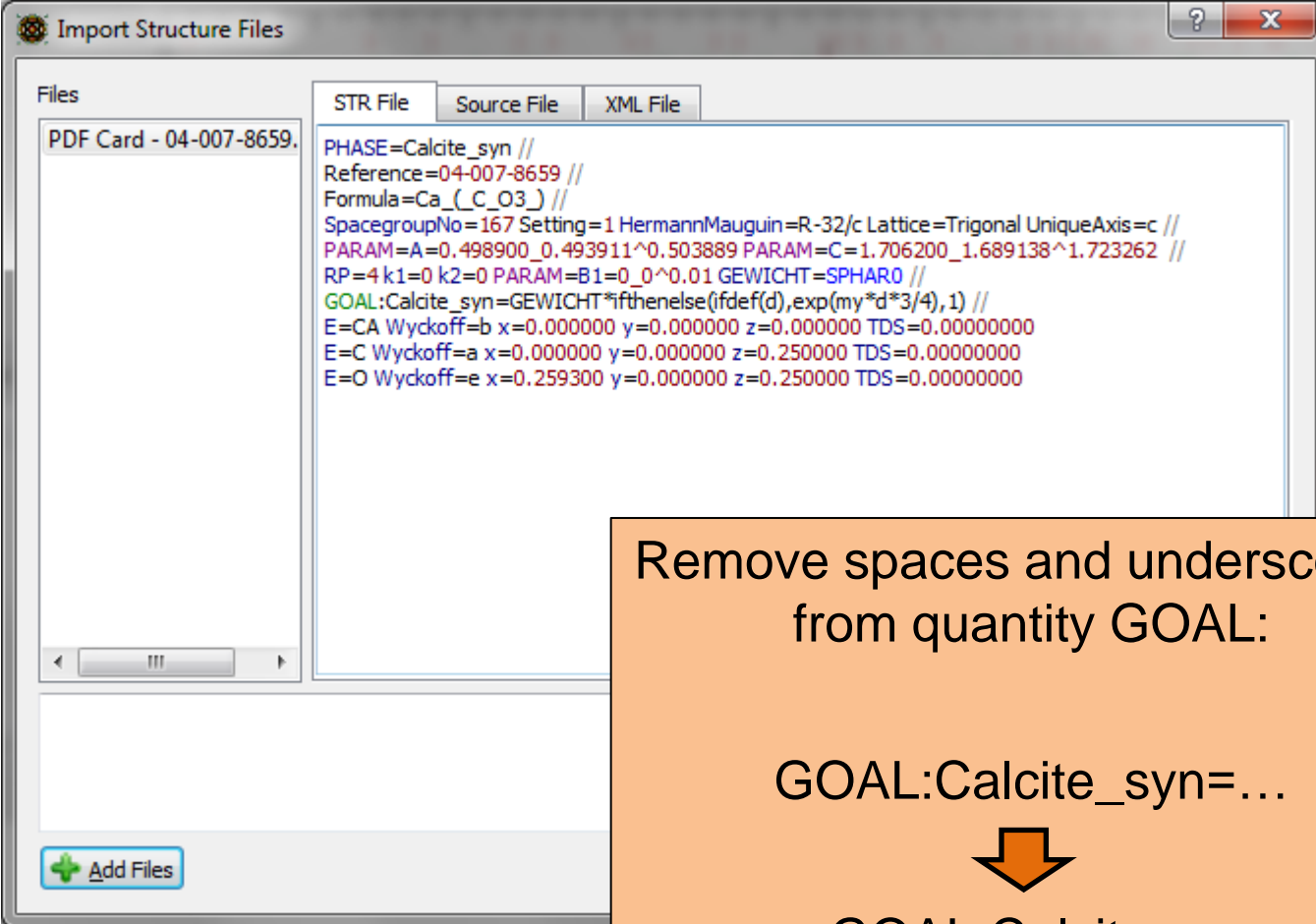
Import from ICDD PDF4+ XML Format

In Profex: «File → Import Structure File...»

«Examples/Lesson 6/Vaterite.cif»



Import from ICDD PDF4+ XML Format



The screenshot shows a software window titled "Import Structure Files". On the left, there is a list of files with "PDF Card - 04-007-8659." selected. On the right, there are tabs for "STR File", "Source File", and "XML File". The "STR File" tab is active, displaying the following text:

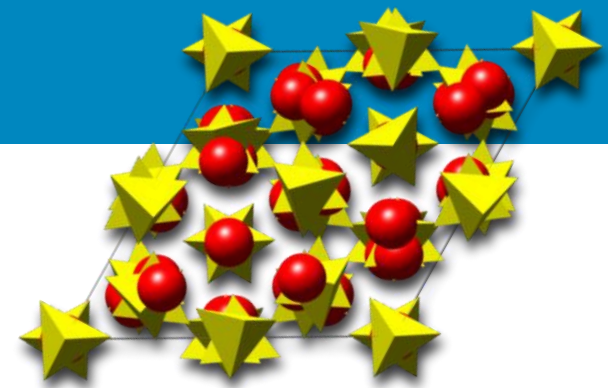
```
PHASE=Calcite_syn //  
Reference=04-007-8659 //  
Formula=Ca_(C_O3) //  
SpacegroupNo=167 Setting=1 HermannMauguin=R-32/c Lattice=Trigonal UniqueAxis=c //  
PARAM=A=0.498900_0.493911^0.503889 PARAM=C=1.706200_1.689138^1.723262 //  
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.01 GEWICHT=SPHARO //  
GOAL:Calcite_syn=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1) //  
E=CA Wyckoff=b x=0.000000 y=0.000000 z=0.000000 TDS=0.00000000  
E=C Wyckoff=a x=0.000000 y=0.000000 z=0.250000 TDS=0.00000000  
E=O Wyckoff=e x=0.259300 y=0.000000 z=0.250000 TDS=0.00000000
```

Below the text editor is an "Add Files" button. An orange callout box is overlaid on the bottom right of the window, containing the following text:

Remove spaces and underscores
from quantity GOAL:

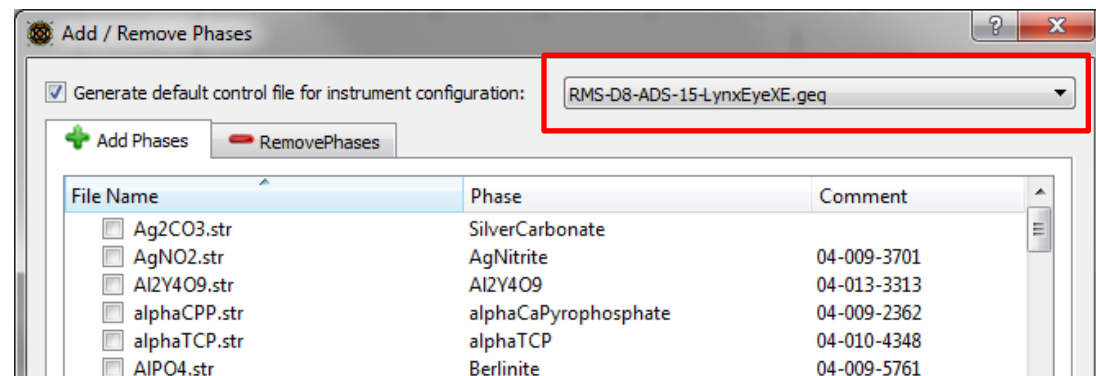
GOAL:Calcite_syn=...
↓
GOAL:Calcite=...

«Save STR» to Structures database directory

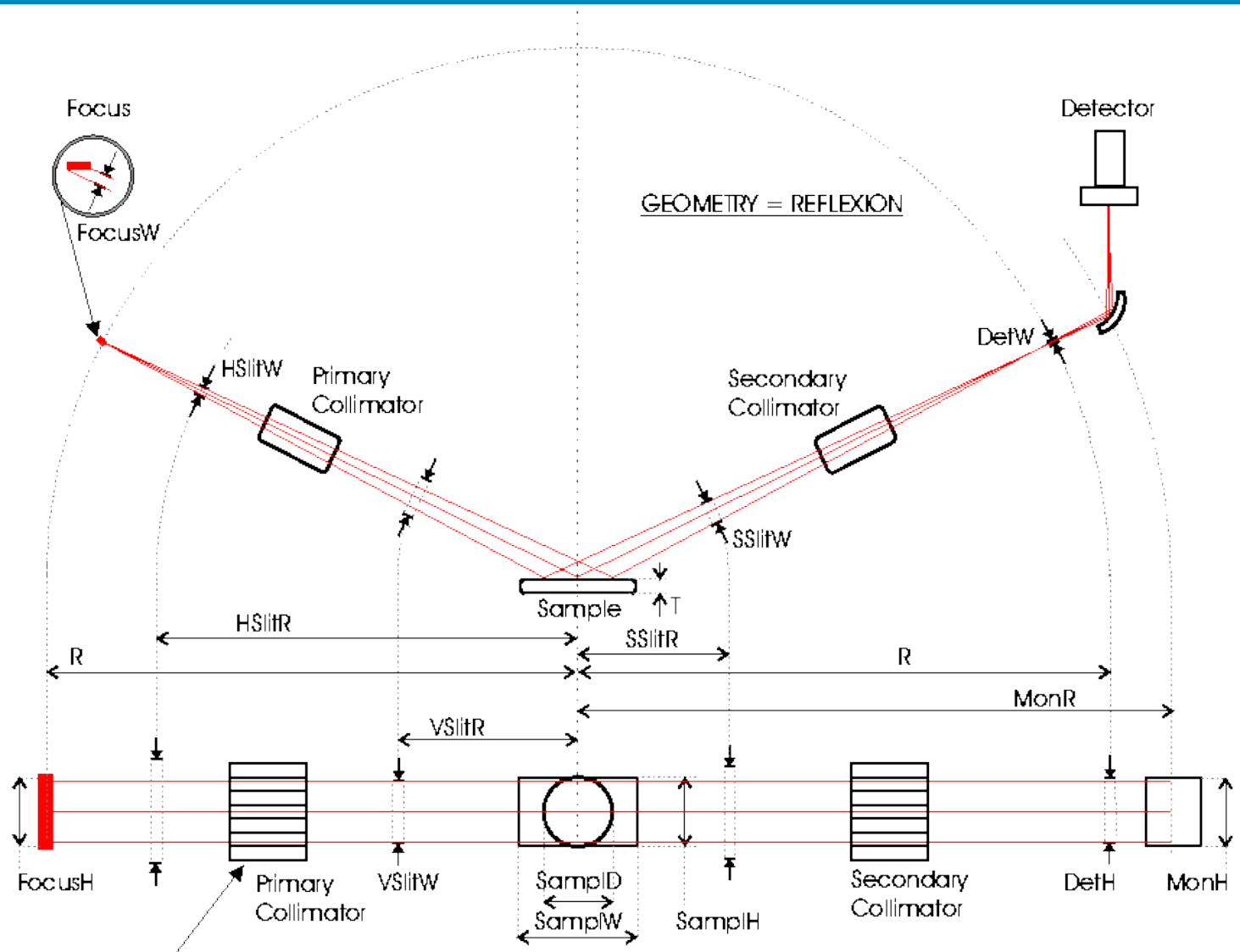


- ▶ If no *.str file is available:
 - ▶ Download CIF file from public database (COD, AMCSD, ICSD)
 - ▶ Or export XML file from PDF-4+ database
 - ▶ → Convert to *.str format with Profex
 - ▶ Fix *.str file manually if necessary
 - ▶ Save to «Structures» directory in Profex-BGMN-Bundle

- BGMN uses Fundamental Parameters Approach (FPA) to model peak shapes
 - Very detailed description of instrument configuration required
 - Wrong Instrument Config = Wrong peak shapes
 - = wrong refinement results (particularly crystallite sizes and micro-strain)
 - = poor fits

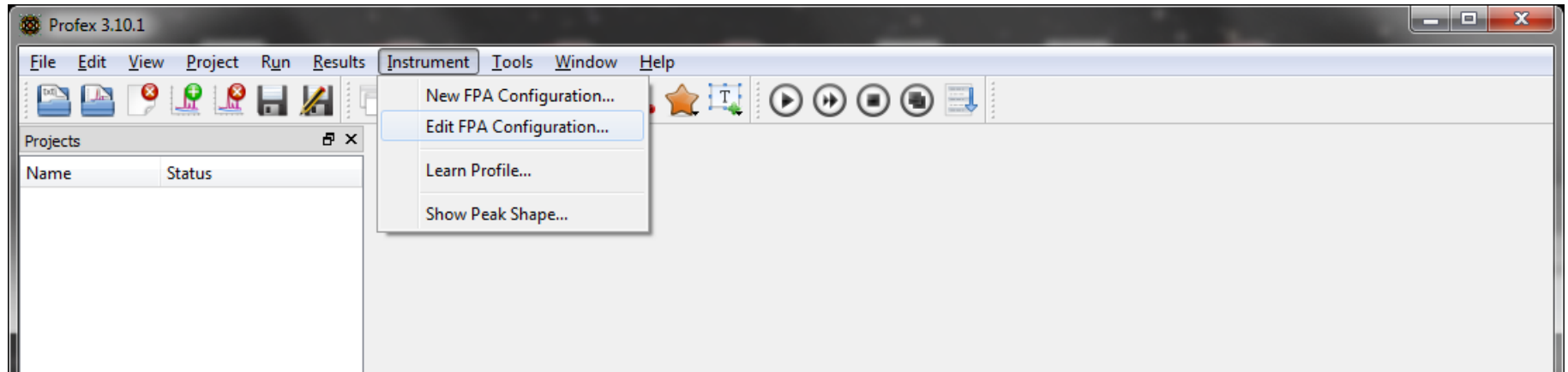


Device Files



<http://www.bgm.de>

- Recommended: Modify an existing instrument configuration



Device Files

The screenshot shows a Windows file explorer window titled "Open Instrument Configuration file". The address bar shows the path: \ll DL > DoebelinN > BGMN-Templates > Devices >. The search bar contains "Devices durchsuchen". The left sidebar shows the navigation pane with "Organisieren" and "Neuer Ordner" options. The main pane displays a list of files and folders:

Name	Änderungsdatum	Typ
unofficial	04.09.2014 13:04	Dateiordner
cubix-ads-10mm.sav	12.02.2014 06:41	SAV-Datei
cubix-ads-15mm.sav	12.02.2014 06:41	SAV-Datei
d2-ssd160-fds-1.sav	04.09.2014 14:59	SAV-Datei
d8-fds-02-LynxEyeXE.sav	12.02.2014 06:41	SAV-Datei
d8-lynxeye-ads-1mm.sav	12.02.2014 06:41	SAV-Datei
d8-lynxeye-fds-02.sav	12.02.2014 06:41	SAV-Datei
d8-lynxeye-fds-05mm.sav	12.02.2014 06:41	SAV-Datei
d8-lynxeye-fds-06mm.sav	12.02.2014 06:41	SAV-Datei
d8-solxe-fds-0600.sav	12.02.2014 06:41	SAV-Datei
d8-solxe-vds-12mm.sav	12.02.2014 06:41	SAV-Datei
INSA-D8-FDS-06-LynxEye.sav	12.02.2014 06:41	SAV-Datei
pw1800-ads-10mm.sav	12.02.2014 06:41	SAV-Datei
pw1800-fds.sav	12.02.2014 06:41	SAV-Datei
Rigaku-Miniflex.sav	12.02.2014 06:42	SAV-Datei

The "Dateiname:" field at the bottom contains "d2-ssd160-fds-1.sav". The file type filter is set to "Configuration Files (*.sav *.SAV)". The "Öffnen" button is highlighted.

- Meaningful names were given (model, detector, divergence slit mode, ...)
- Pick one that seems to match your instrument configuration

Device Files

The screenshot shows the 'Instrument Configuration' window for a file named 'd2-ssd160-fds-1.sav'. The main text area contains the following configuration lines:

```
% Detector
%-----
% total detector height (mm)
DetArrayW=12

% height of one strip (mm)
DetW=0.075

% total detector width (mm)
% This value was guessed!
DetH=12

%-----
% Sample holder
%-----

% Note: The diameter was guessed!

% diameter of the sample holder (mm)
```

Below the text area is a control panel with two tabs: 'Control' and 'Output'. The 'Control' tab is active and contains several options:

- Create Template for Refinement Control File
- Tube Emission Profile: CU
- Kbeta Filter / Energy Dispersive Detector / No Filtering
- Monochromator Crystal: 26.60 °theta

The 'Calculations' section on the right has two checked options:

- Raytrace (GEOMET)
- Interpolate (MakeGEQ)

At the bottom of the window, there is a progress bar at 0% and a toolbar with buttons for 'Save As...', 'Save', 'Run', and 'Close'.

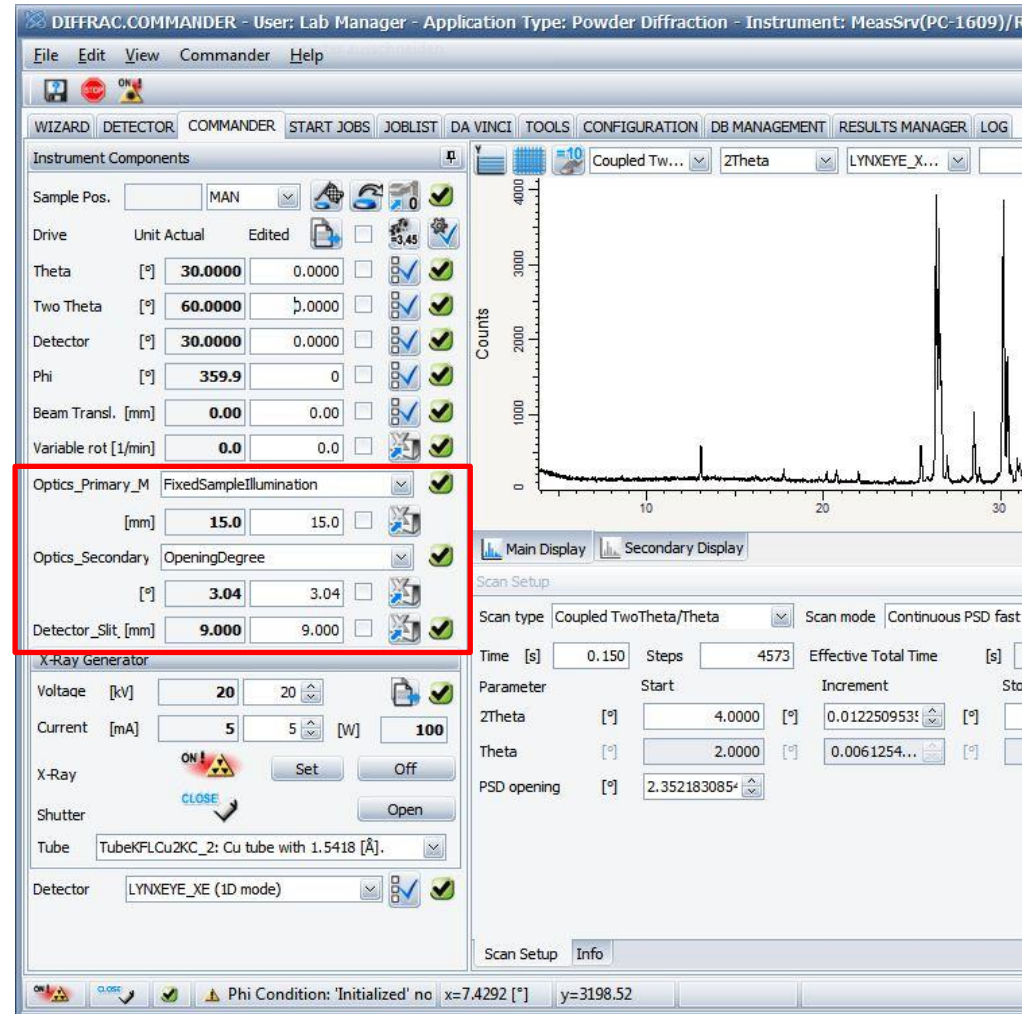
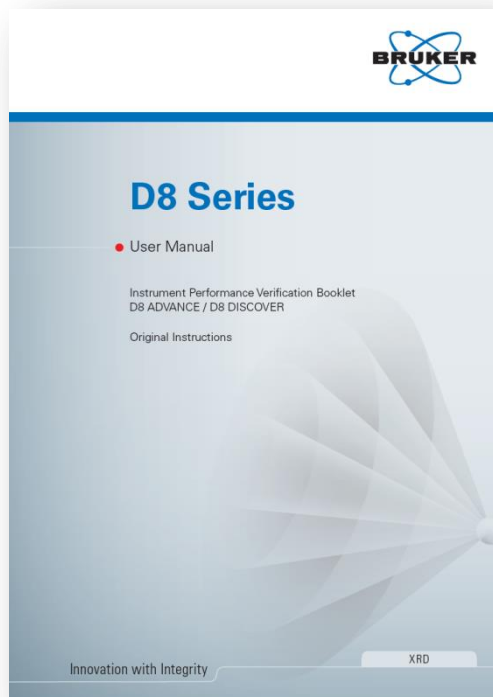
- Verify / modify each line (bundled files are well documented)
- Verify «Control» and «Calculations» options
- If unsure, leave unchanged

- «Save As...» under a new name
- Acknowledge the warning message about file names
- Click «Run»
- Wait for completion

Device Files

Get instrument parameters from:

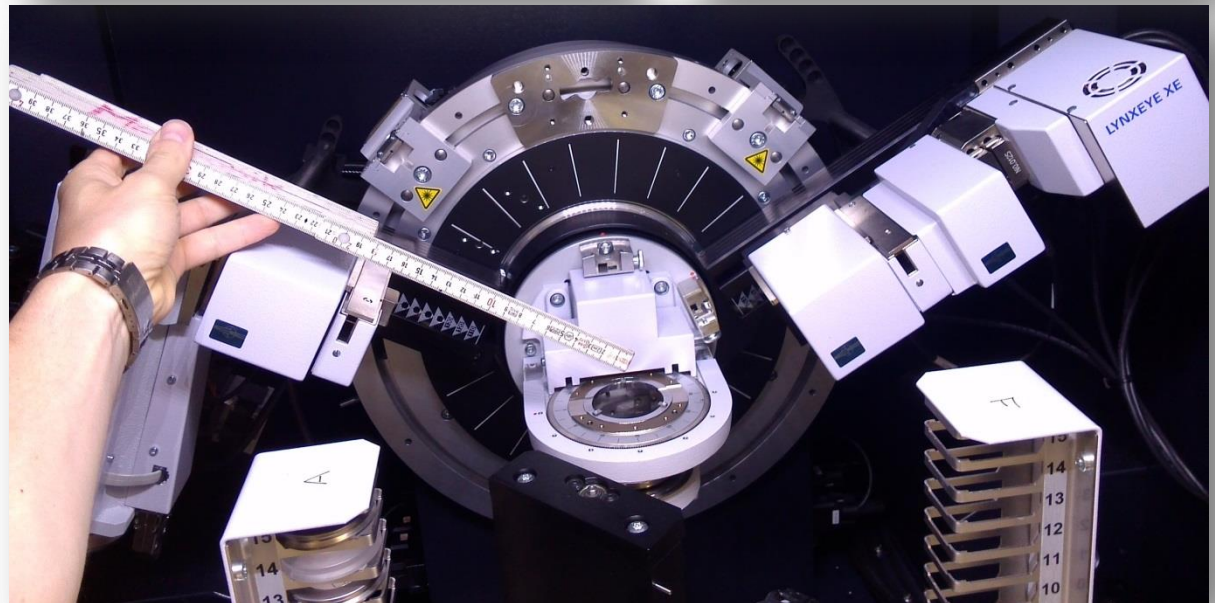
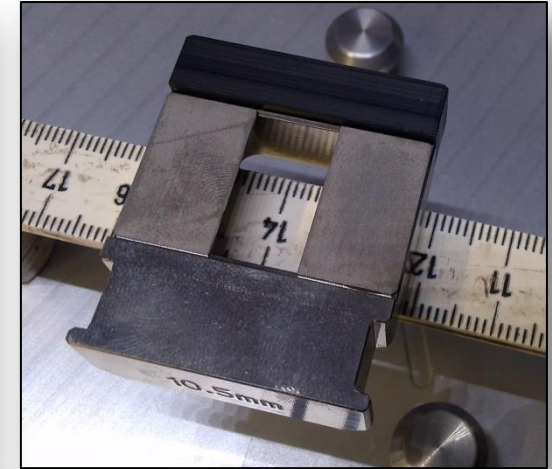
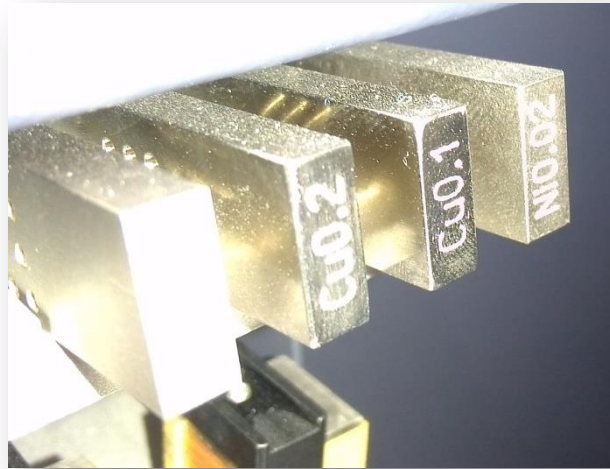
- Measurement software
- Configuration page
- Instrument user manual
- ...



Device Files

...

- labels on apertures
- Or measure!
(better than nothing)



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Creating Instrument Configuration Files



Introduction

The Rietveld refinement software must be able to precisely describe the measured peak shape with a mathematical model to obtain accurate fits of measured diffraction peaks. BGMN uses the fundamental parameters approach (FPA), and thus raytraces the peak shape from the diffractometer's hardware configuration rather than fitting it to a measured reference pattern. Very detailed hardware information must be specified by the user in order to obtain a correct peak shape model. But in return, FPA peak shapes often describe strongly asymmetric peaks at very low diffraction angles more realistically and accurately than generic peak profile functions. FPA peak shapes can also be computed at any 2θ angle, whereas measured peaks of a reference material can only be fitted from the 2θ position of the first peak up. Extrapolation to lower angles introduces increasingly severe error.