

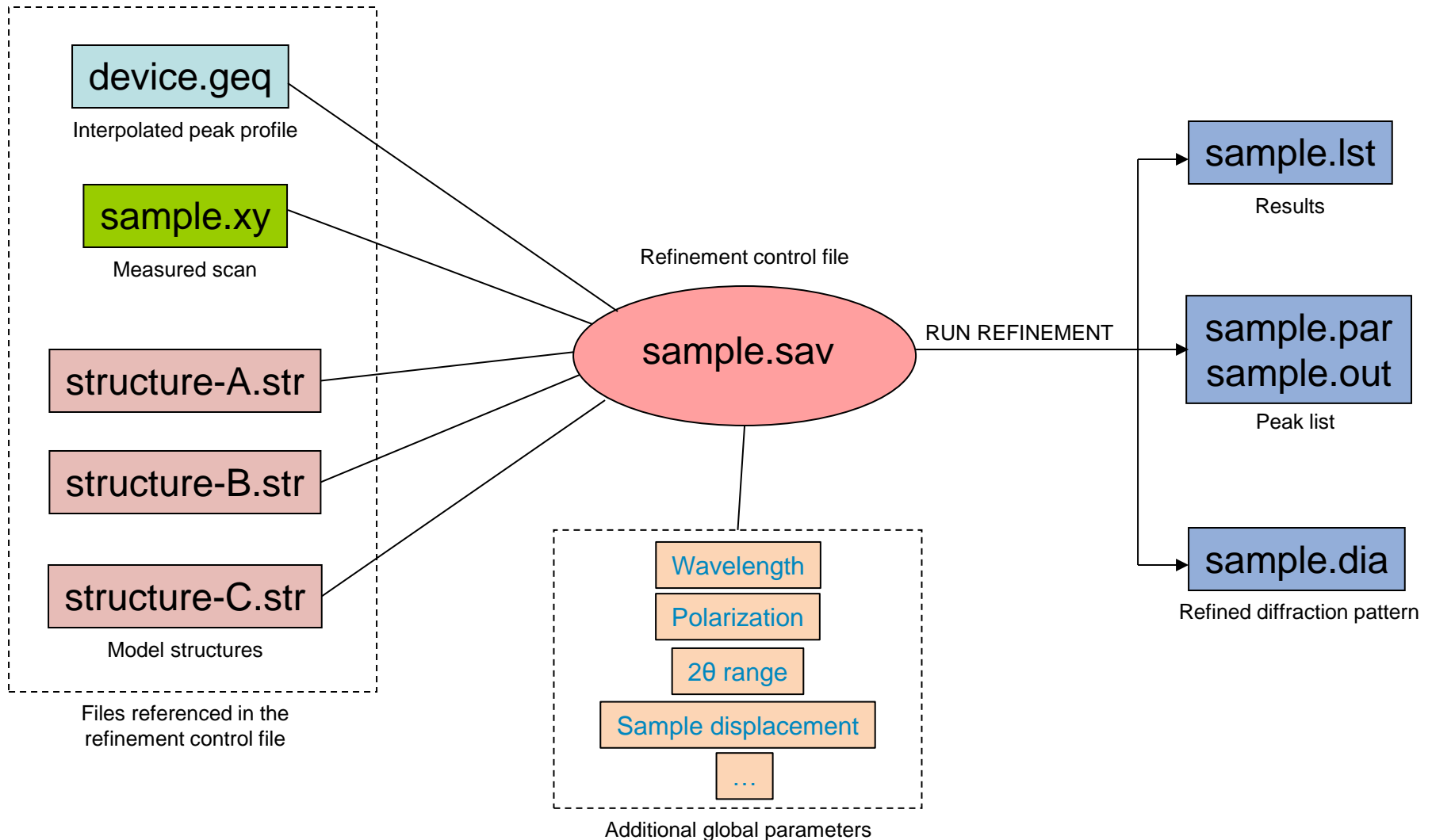
Lesson 6

Crystal Structure Models

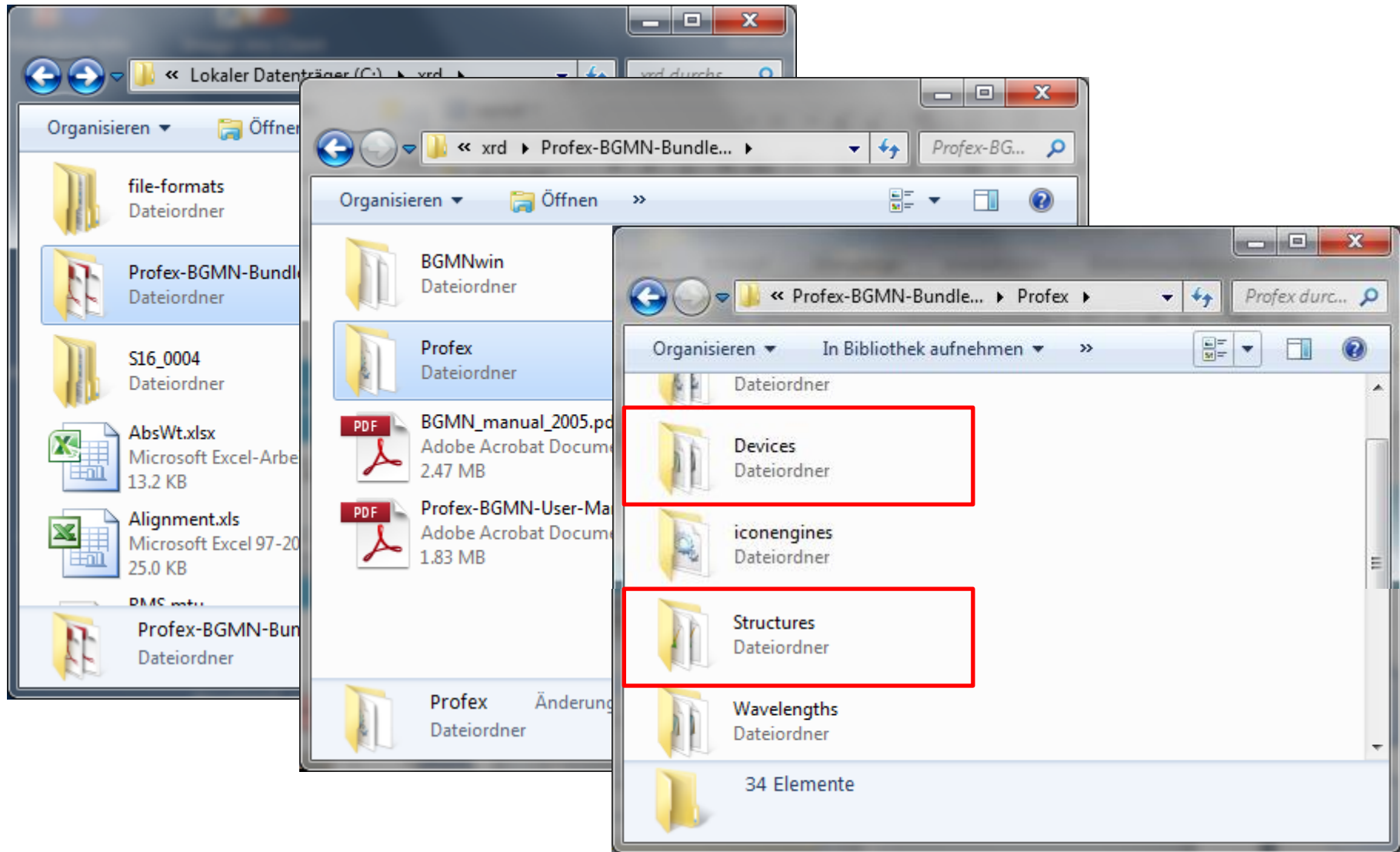


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BGMN Project Structure



Profex Structure and Device File Database



Profex Structure and Device File Database

The screenshot displays the Profex 3.8.0 software interface. On the left, a file browser window shows a directory of structure files (e.g., betaCPP-tetrate.str, betaTCP.str, Brucite_MgO.str) and a folder icon labeled "190 Elemente". A blue arrow points from this folder to the main software window. The main window shows the "Add / Remove Phases" dialog box, which contains a table of phases:

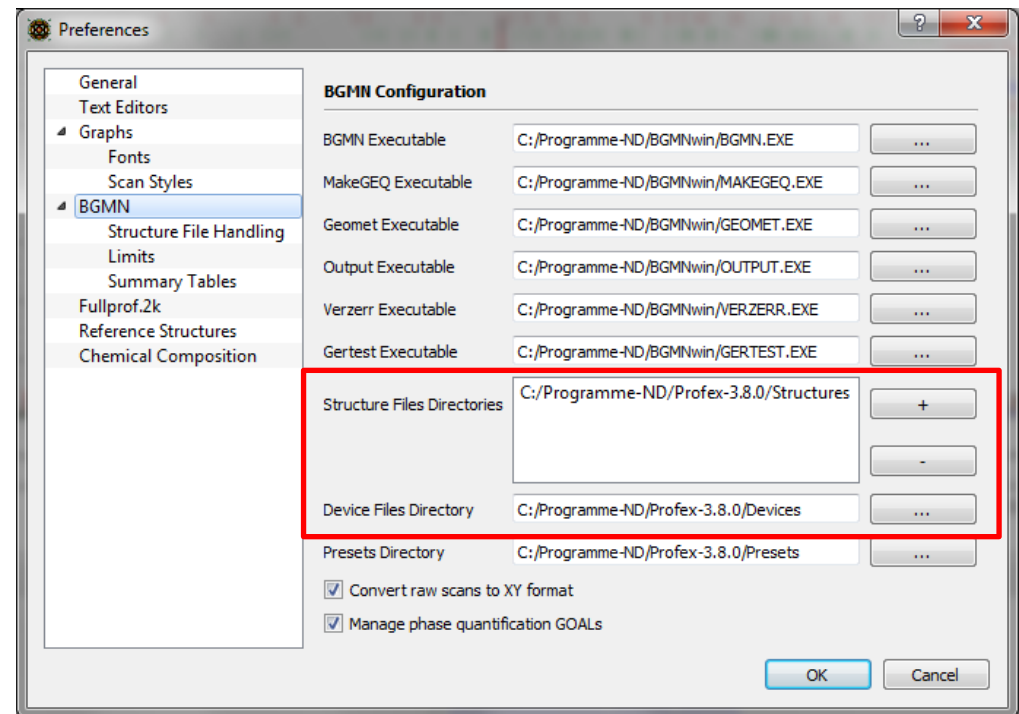
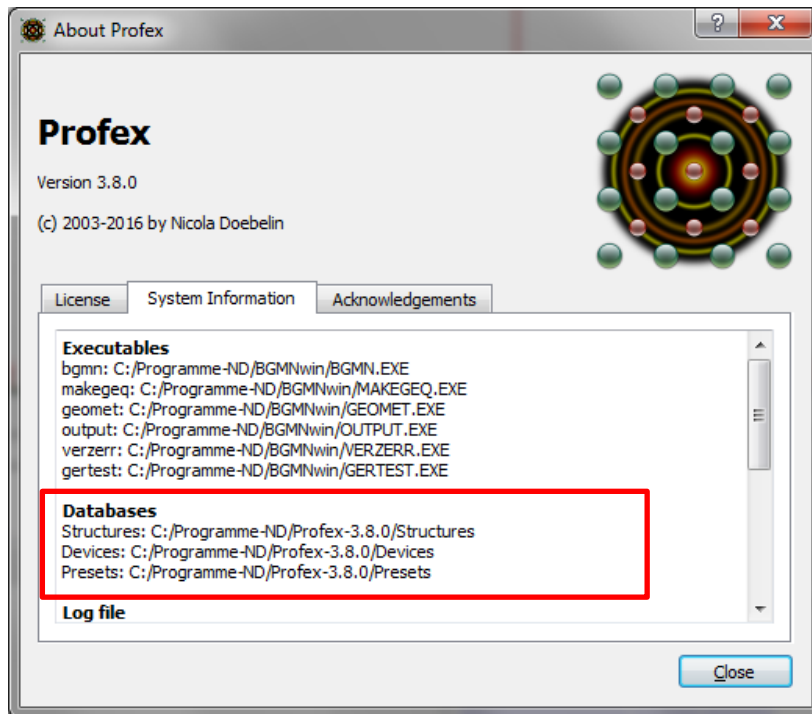
File Name	Phase	Comment
<input type="checkbox"/> Chlorapatite.str	Chlorapatite	04-012-1323
<input type="checkbox"/> Chromatite.str	Chromatite	01-087-1647
<input type="checkbox"/> Clinoatacamite.str	Clinoatacamite	04-012-9781
<input type="checkbox"/> Clinochlore1A.str	Clinochlore1A	04-017-2550
<input 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

Below the table, there are checkboxes for "Overwrite existing files" and "Generate default control file for instrument configuration: RMS-D8-ADS-15-LynxEyeXE.geq". The "Add Phases" button is highlighted. In the background, a plot window shows an XRD pattern with "I observed" (black), "I calculated" (red), "I difference" (blue), "Background" (green), "Hydroxylapatite" (red), and "Whitlockite" (green) overlaid. The x-axis is labeled "50.00" and "55.00".

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 area, there are radio button options for the search logic and viewing format:

- Logic interface**: AND OR
- Viewing** (About [File Formats](#)): amc long form amc short form cif
- Download**: amc cif 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).

! (1924)

Download CIF file

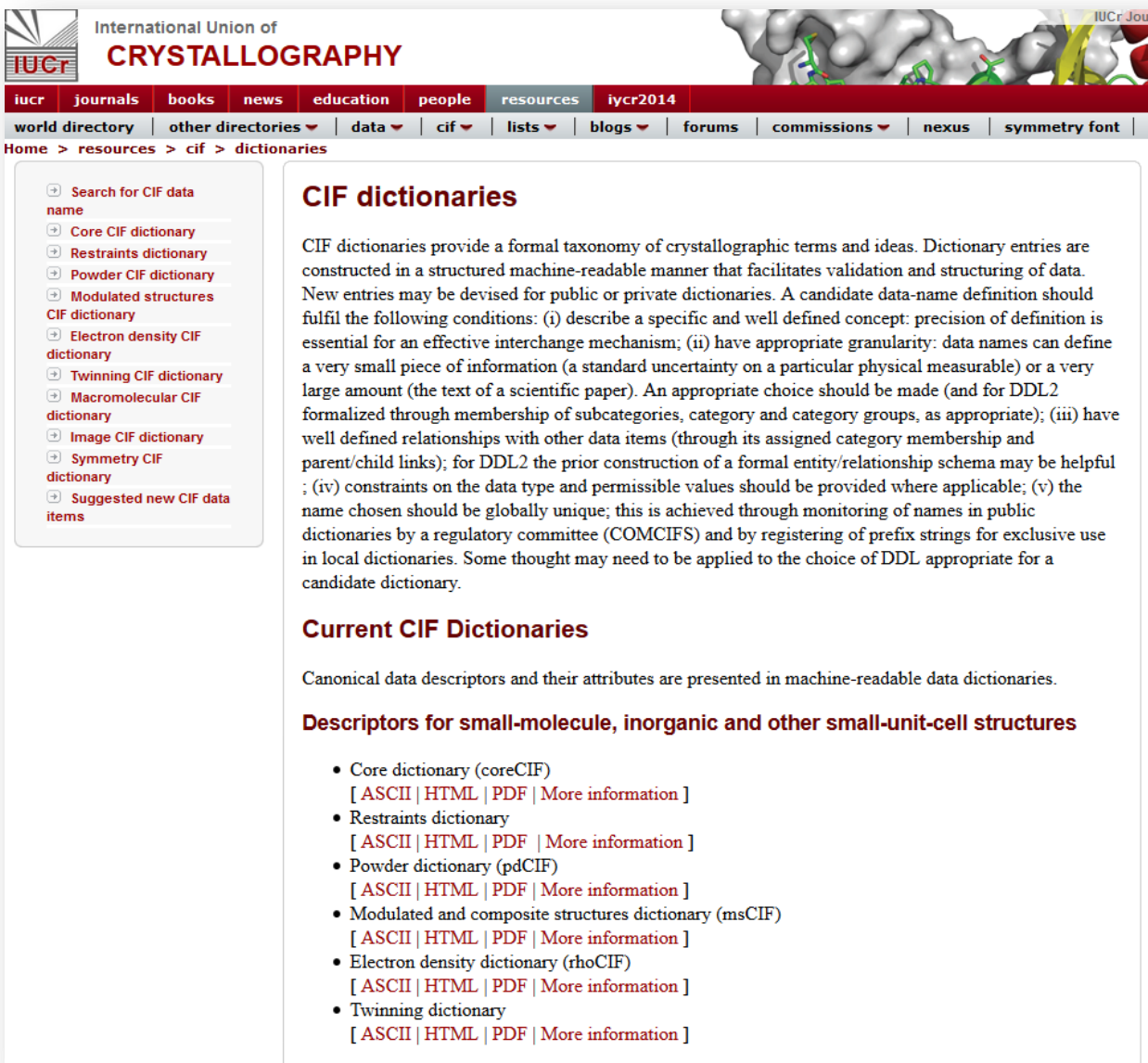
Watch out for high-temp and high-pressure datasets

CIF File Format

CIF (Crystallographic Information File) Format:

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

```
C:\Users\doebelln\AppData\Local\Temp\AMS_DATA.cif - Notepad++
File Edit Search View Encoding Language Settings Macro Run Plugins Window ?
AMS_DATA.cif
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'
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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
```



The screenshot shows the IUCr website's CIF dictionaries page. At the top, there is the IUCr logo and the text 'International Union of CRYSTALLOGRAPHY'. A navigation bar contains links for 'iucr', 'journals', 'books', 'news', 'education', 'people', 'resources', and 'iycr2014'. Below this is a secondary navigation bar with links for 'world directory', 'other directories', 'data', 'cif', 'lists', 'blogs', 'forums', 'commissions', 'nexus', and 'symmetry font'. The main content area is titled 'CIF dictionaries' and contains a search box, a list of dictionary categories, and a detailed description of CIF dictionaries. A sidebar on the left lists various CIF dictionaries with expandable arrows. The main text explains the purpose and requirements for CIF dictionaries, followed by a section on 'Current CIF Dictionaries' and a list of descriptors for small-molecule, inorganic, and other small-unit-cell structures.

International Union of
CRYSTALLOGRAPHY

[iucr](#) | [journals](#) | [books](#) | [news](#) | [education](#) | [people](#) | [resources](#) | [iycr2014](#)

[world directory](#) | [other directories](#) | [data](#) | [cif](#) | [lists](#) | [blogs](#) | [forums](#) | [commissions](#) | [nexus](#) | [symmetry font](#)

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:

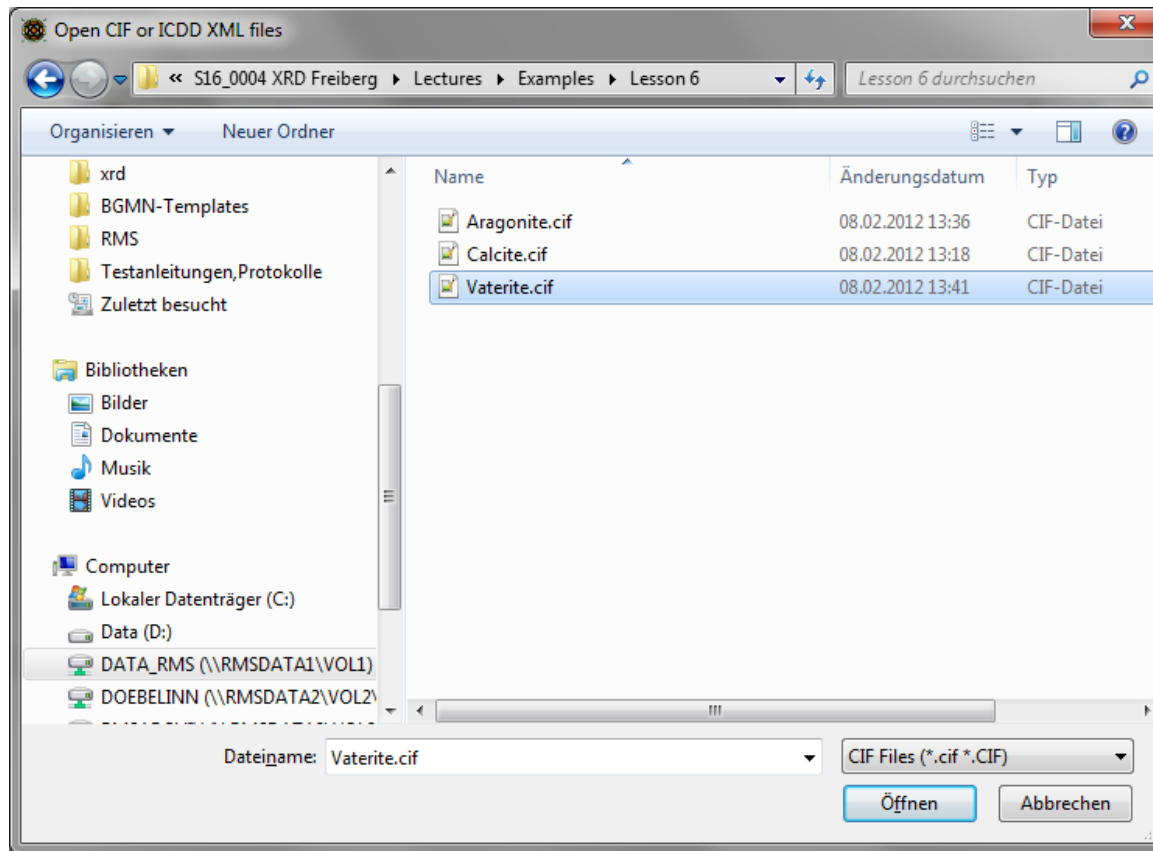
- For complete CIF files: automatic import
- For incomplete CIF files: semi-automatic import



Profex CIF Import

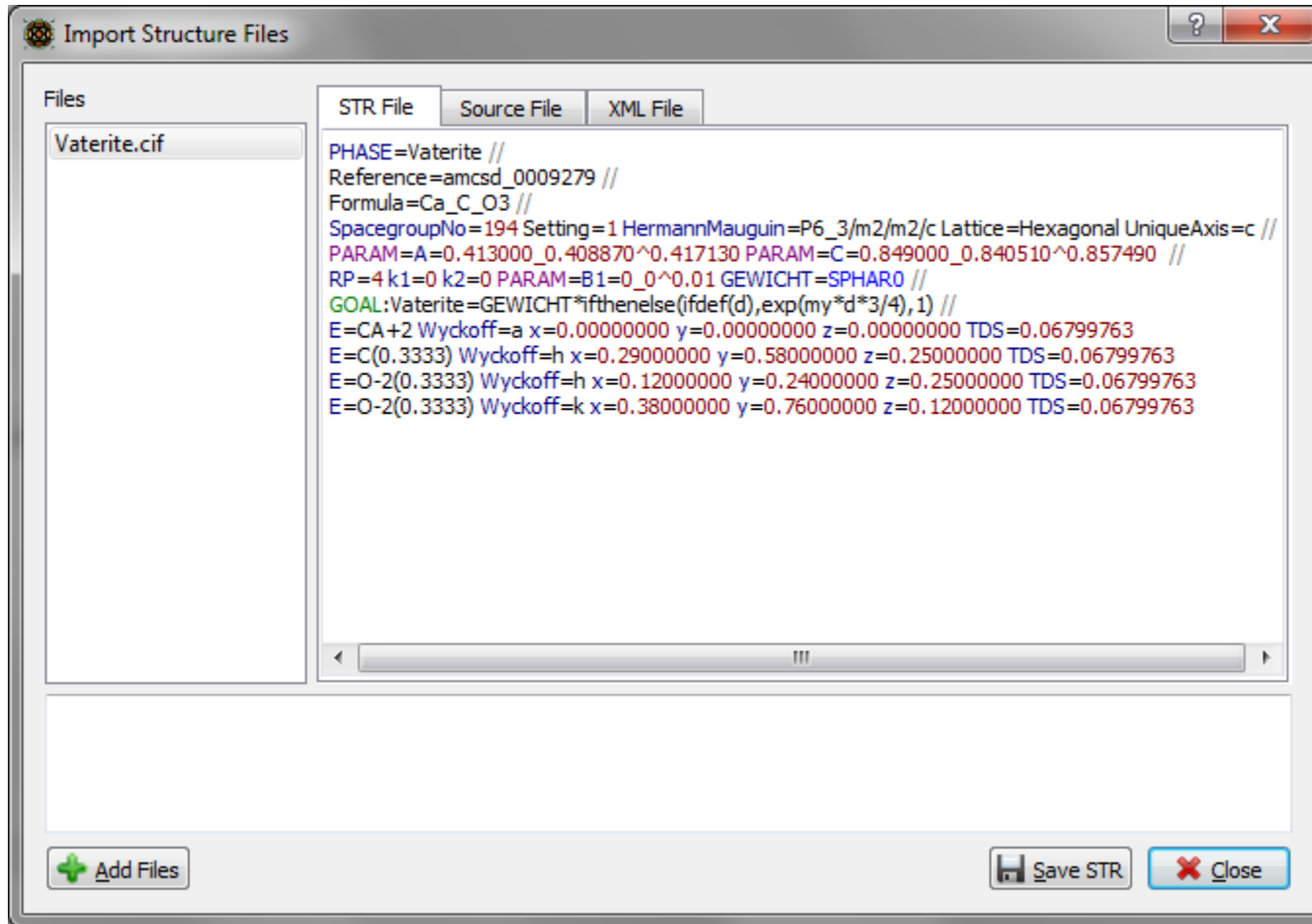
«File → Import Structure File...»

«Examples/Lesson 6/Vaterite.cif»



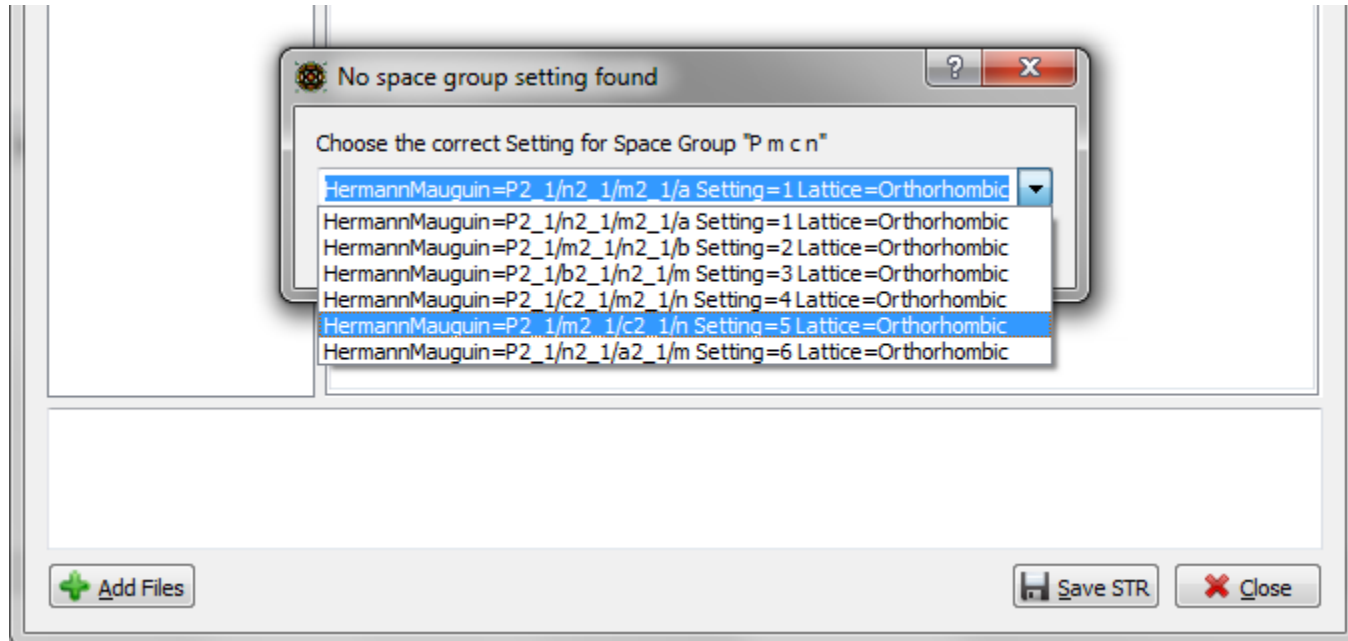
Profex CIF Import

Best Case: No Questions asked = automatic import



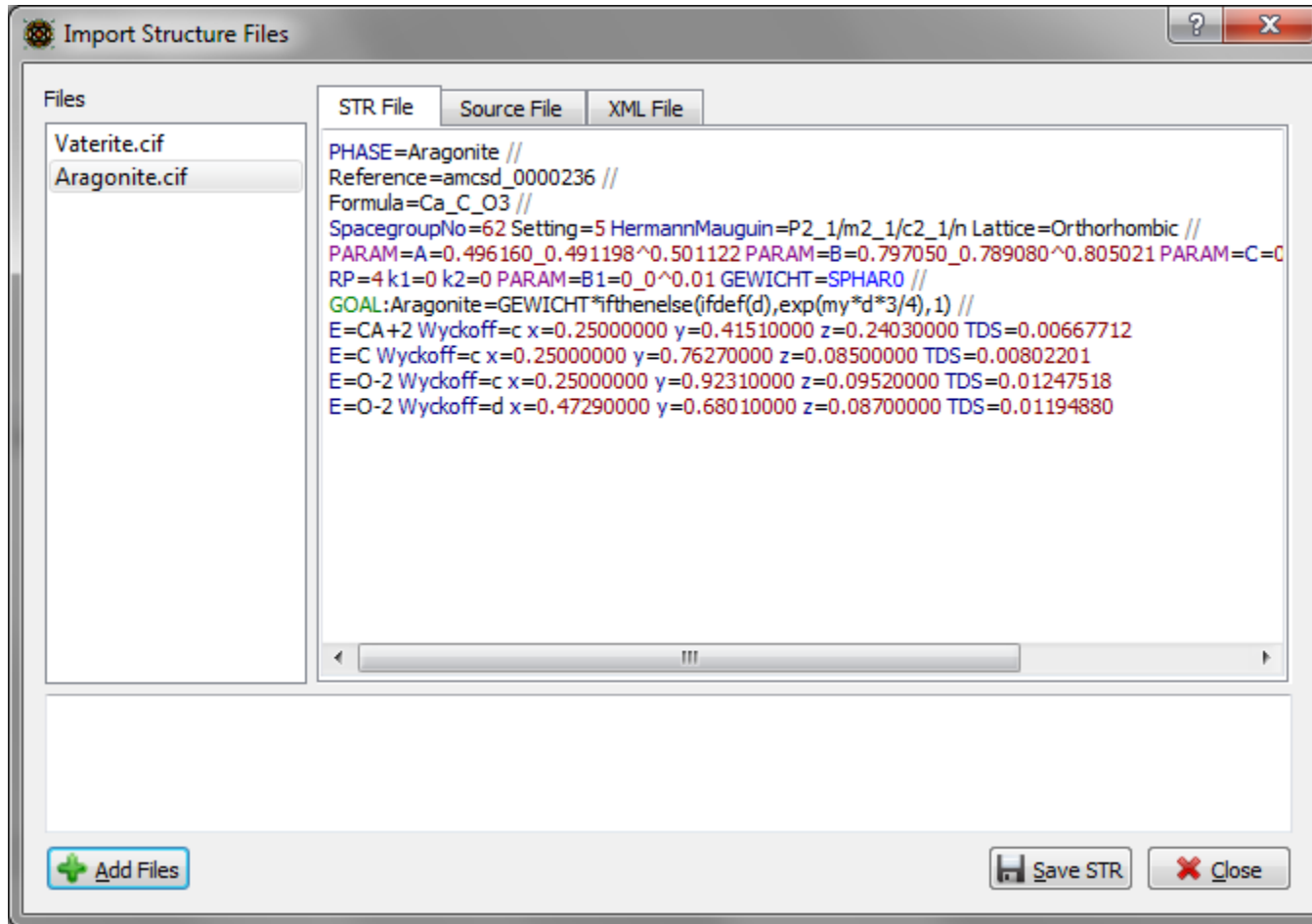
«Save STR» to Structures database directory

«+ Add Files → Aragonite.cif»



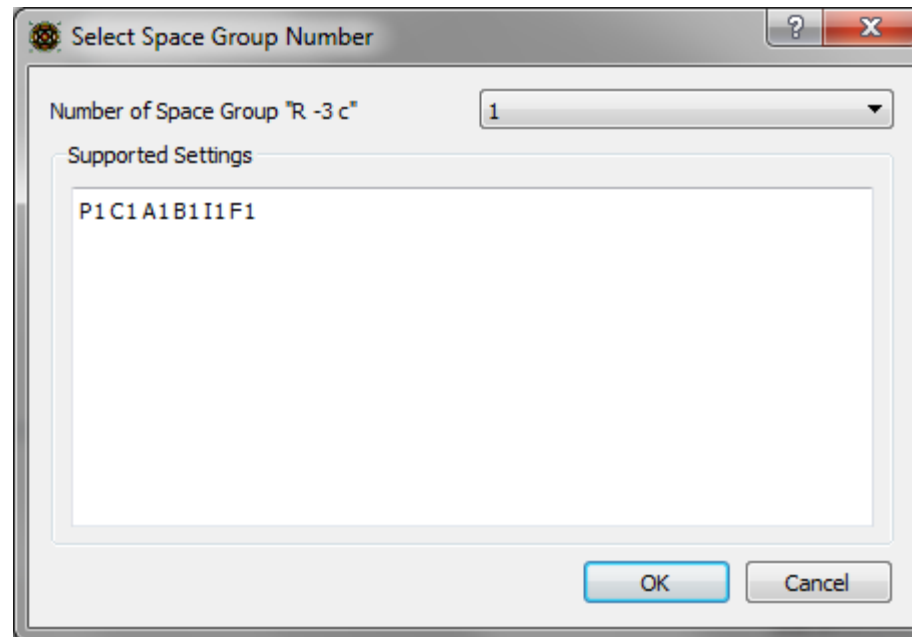
Profex could not assign the CIF HM symbol «P m c n»
to BGMN's full notation.

No further input required



«Save STR» to Structures database directory

«+ Add Files → Calcite.cif»



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

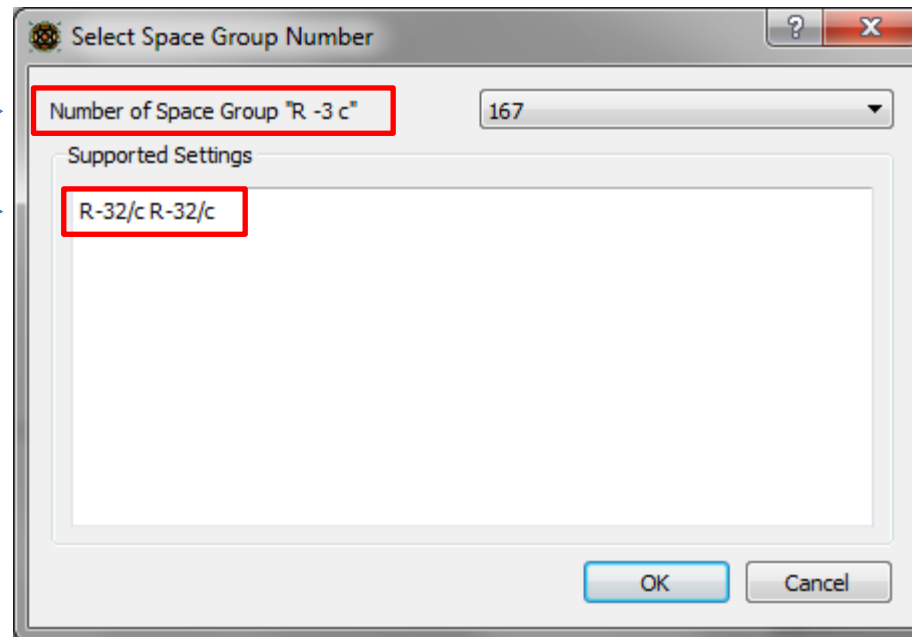
Found elsewhere: 167

Profex CIF Import

BGMN's full notations for SG #167

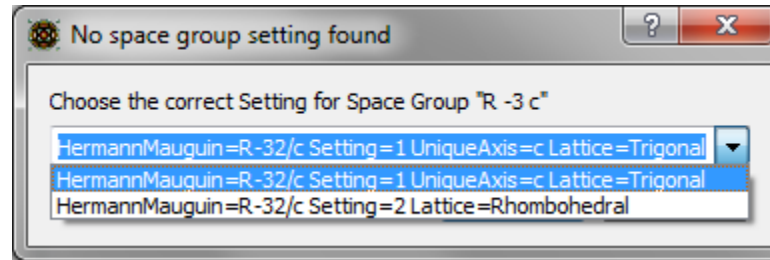
Read from CIF file →

Supported by BGMN →



Seems to match. Click «OK»

BGMN's full notations for SG #167

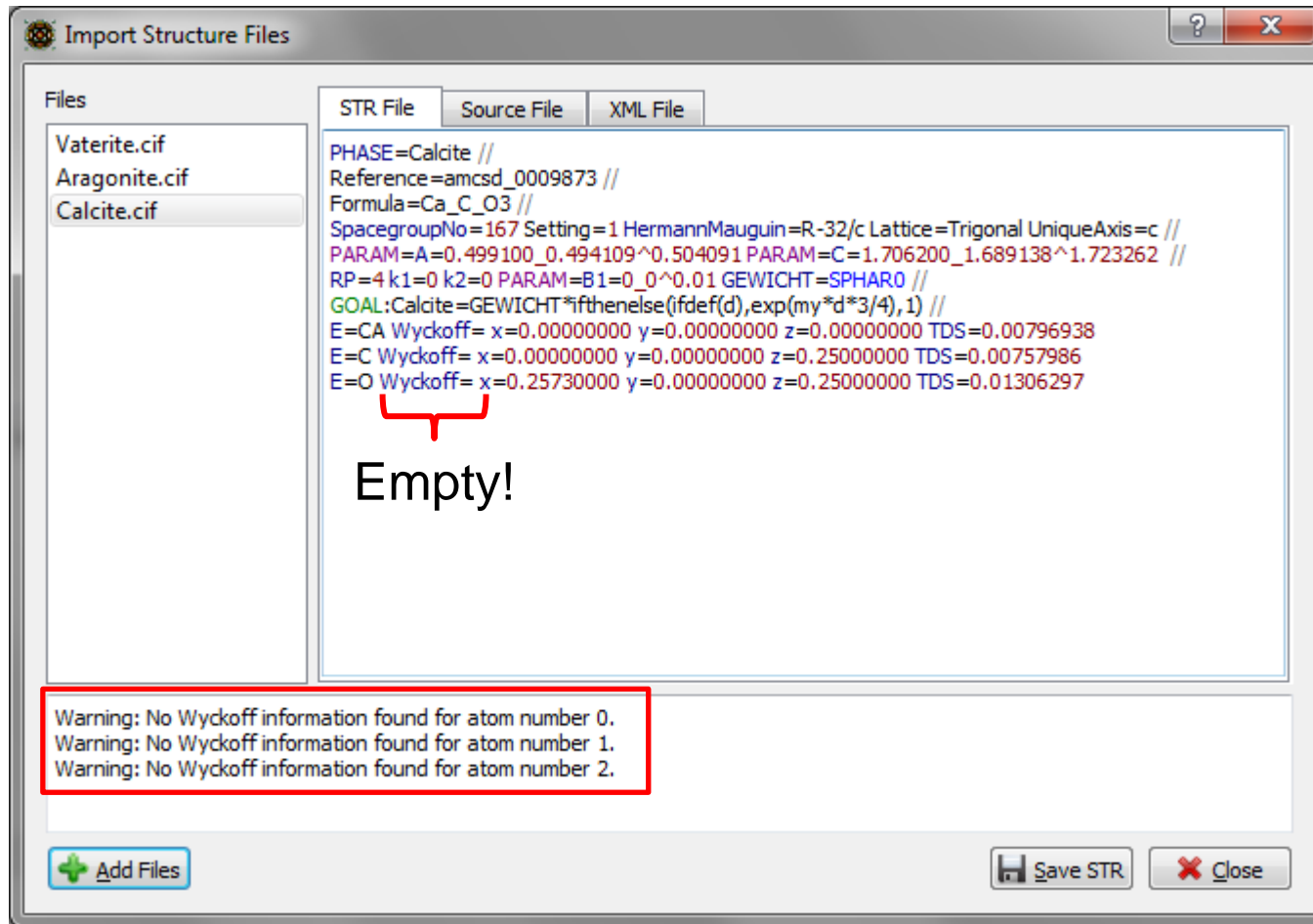


Two settings for $R-3_2/c$:

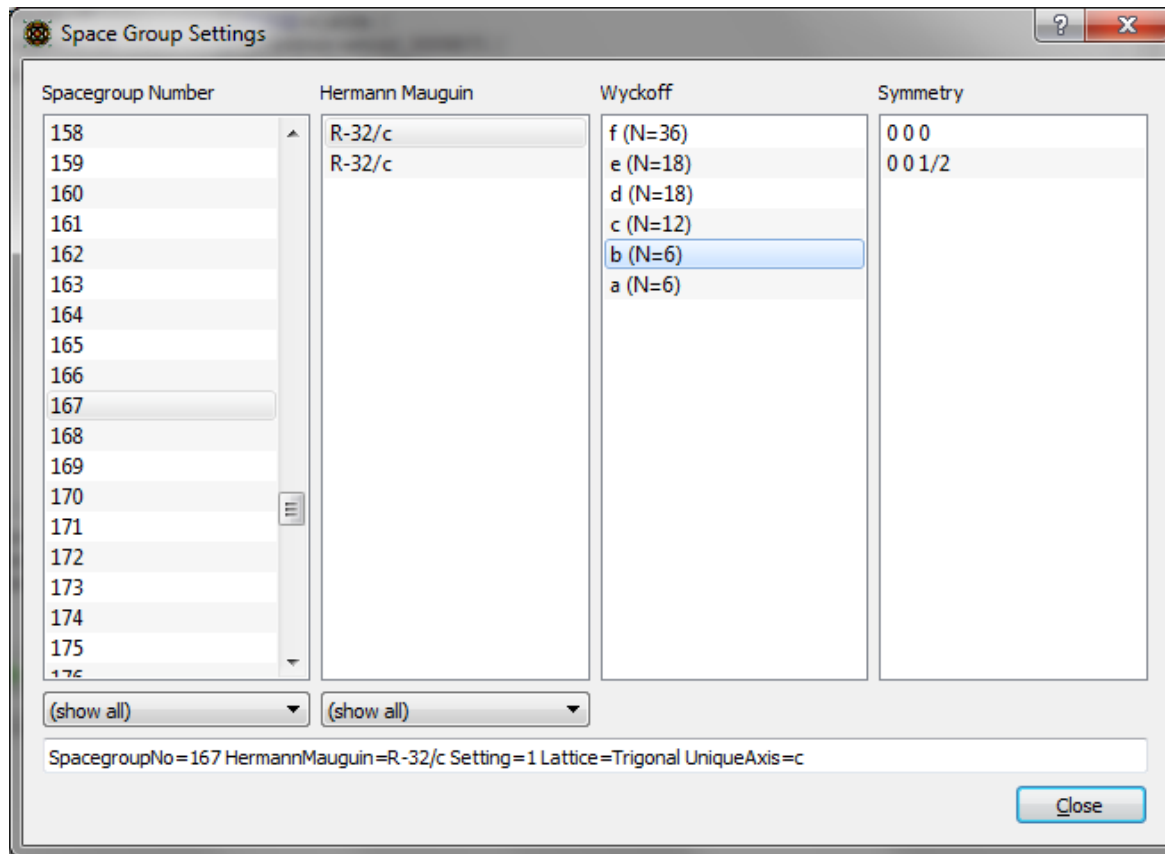
- Trigonal
- Rhombohedral

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

Warning: Missing Wyckoff symbols

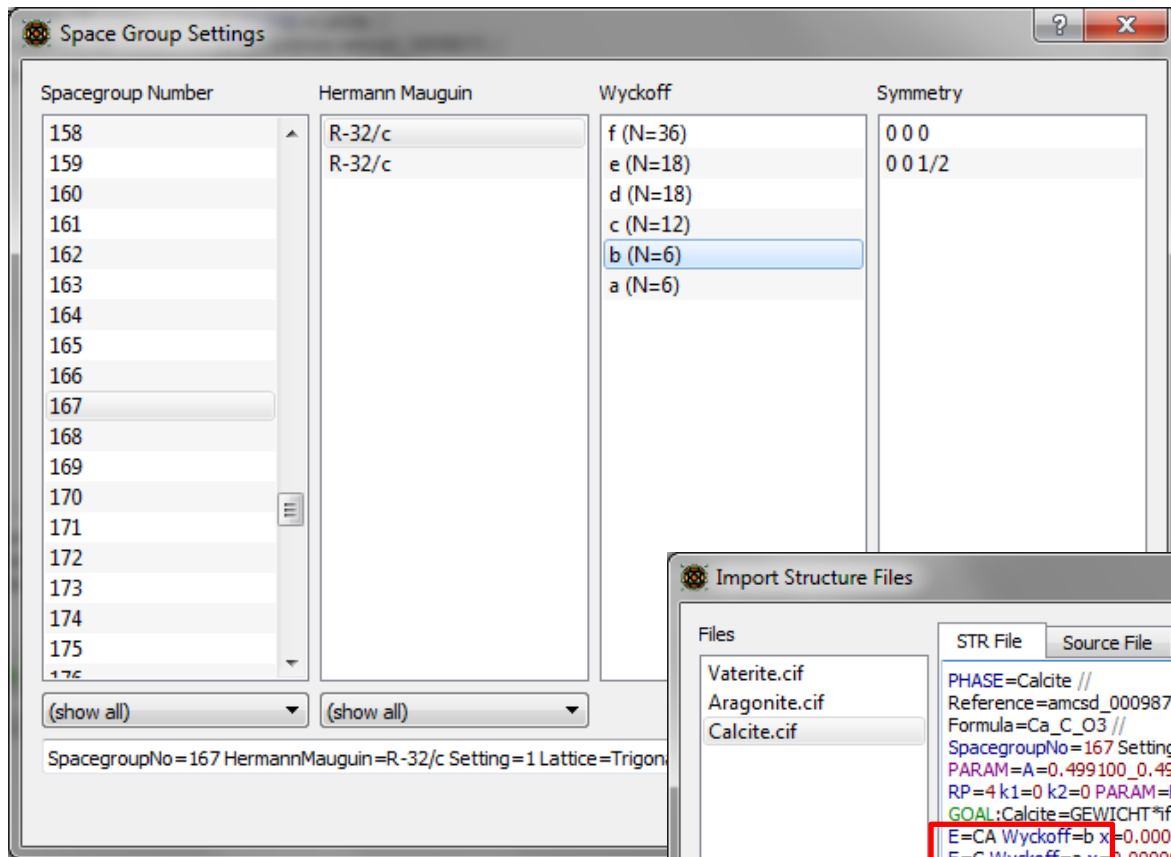


«Help → BGMN SPACEGRP.DAT»



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

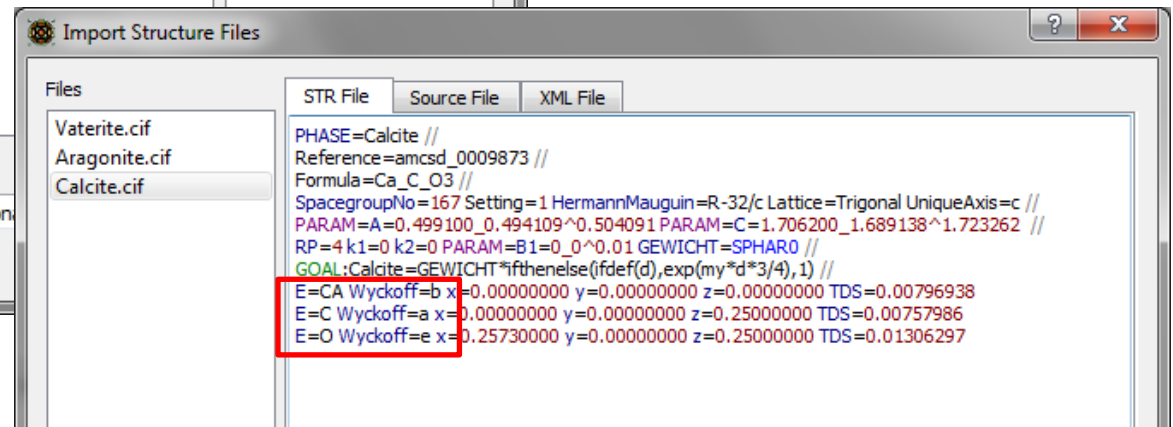
Profex CIF Import



Ca at 0,0,0: Wyckoff=b

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

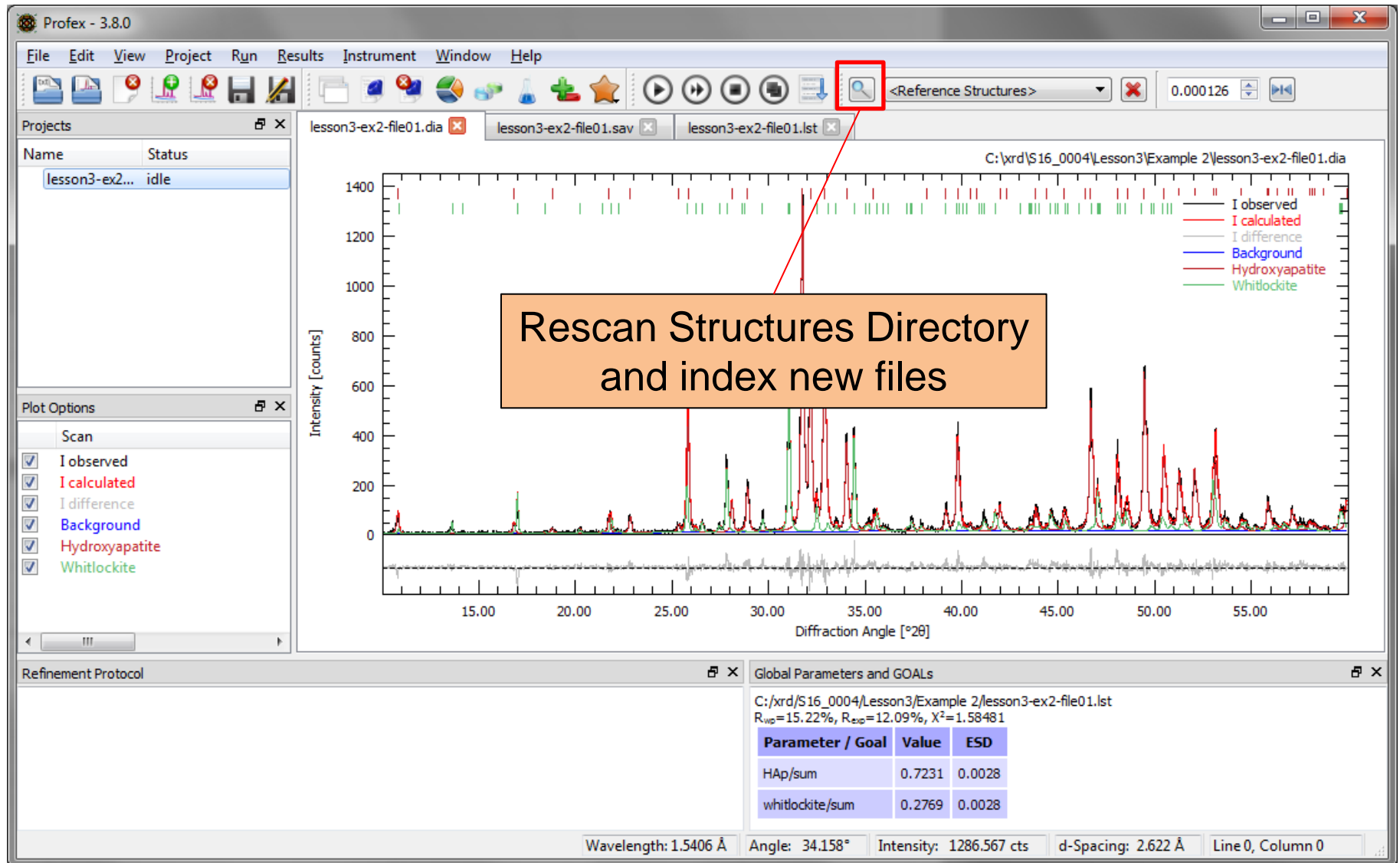
O at x,0,1/4: Wyckoff=e



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

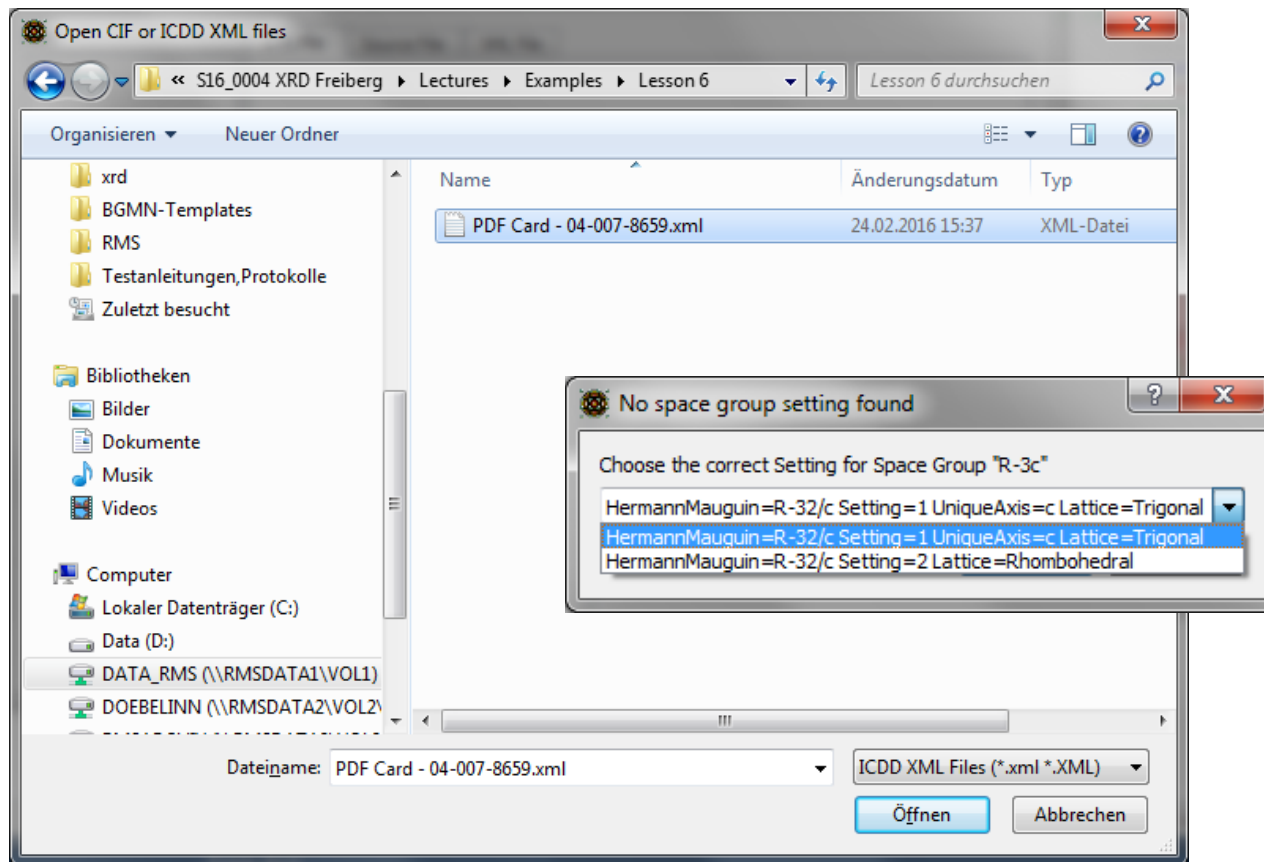
Abbrechen

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

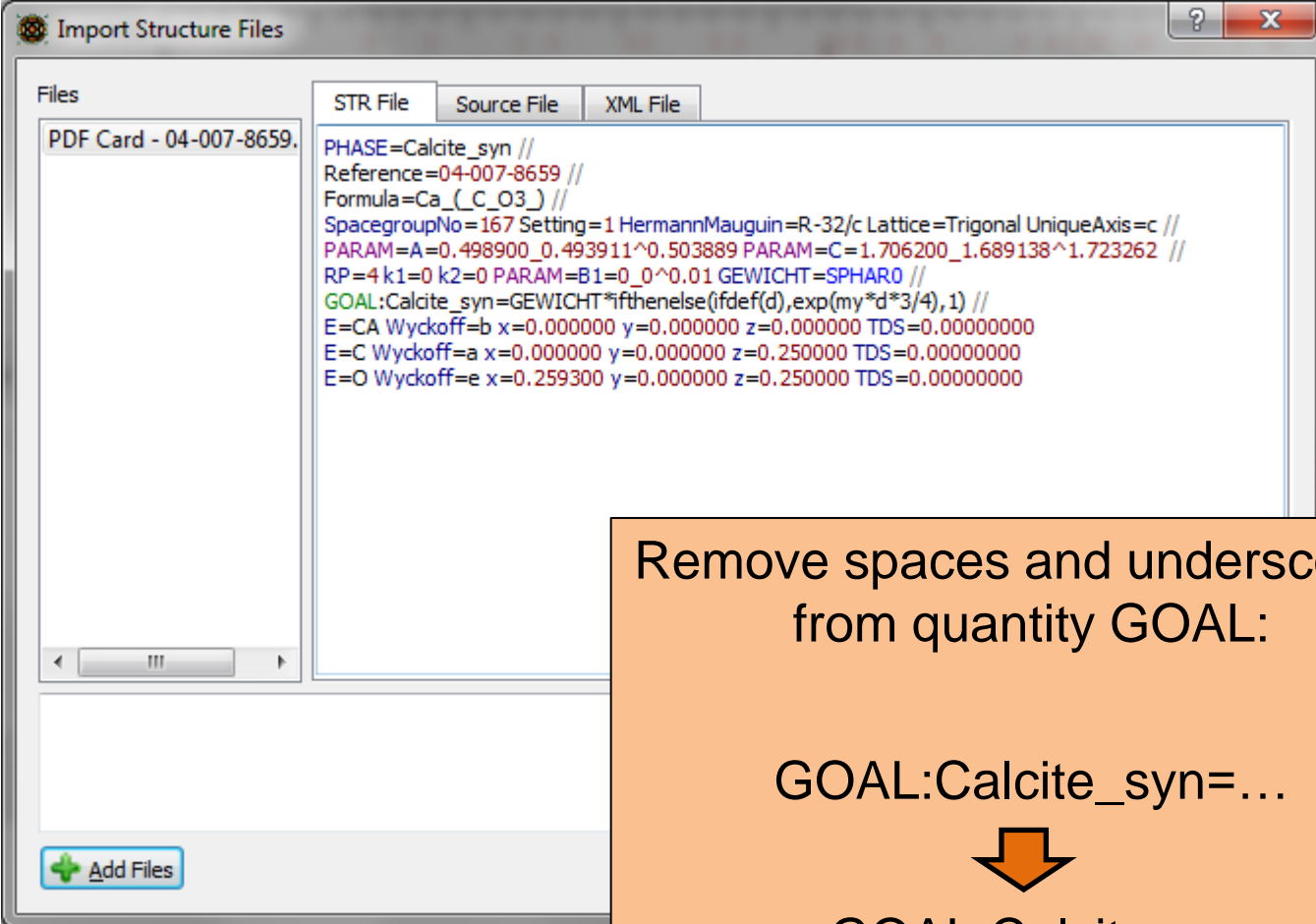
Import from ICDD PDF4+ XML Format

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:

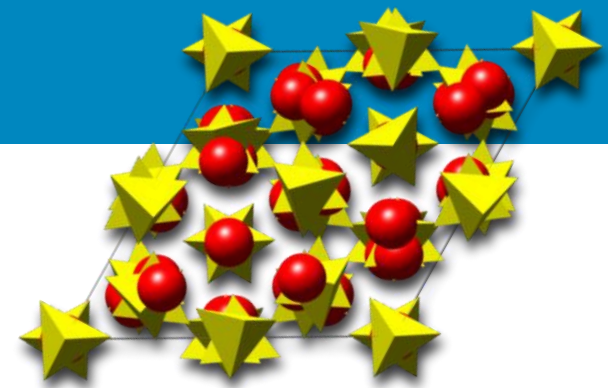
```
PHASE=Calcite_syn //  
Reference=04-007-8659 //  
Formula=Ca_(C_O3) //  
SpacegroupNo=167 Setting=1 HermannMauguin=R-32/c Lattice=Trigonal UniqueAxis=c //  
PARAM=A=0.498900_0.493911^0.503889 PARAM=C=1.706200_1.689138^1.723262 //  
RP=4 k1=0 k2=0 PARAM=B1=0_0^0.01 GEWICHT=SPHARO //  
GOAL:Calcite_syn=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1) //  
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