Lesson 8
Crystal Structure Models

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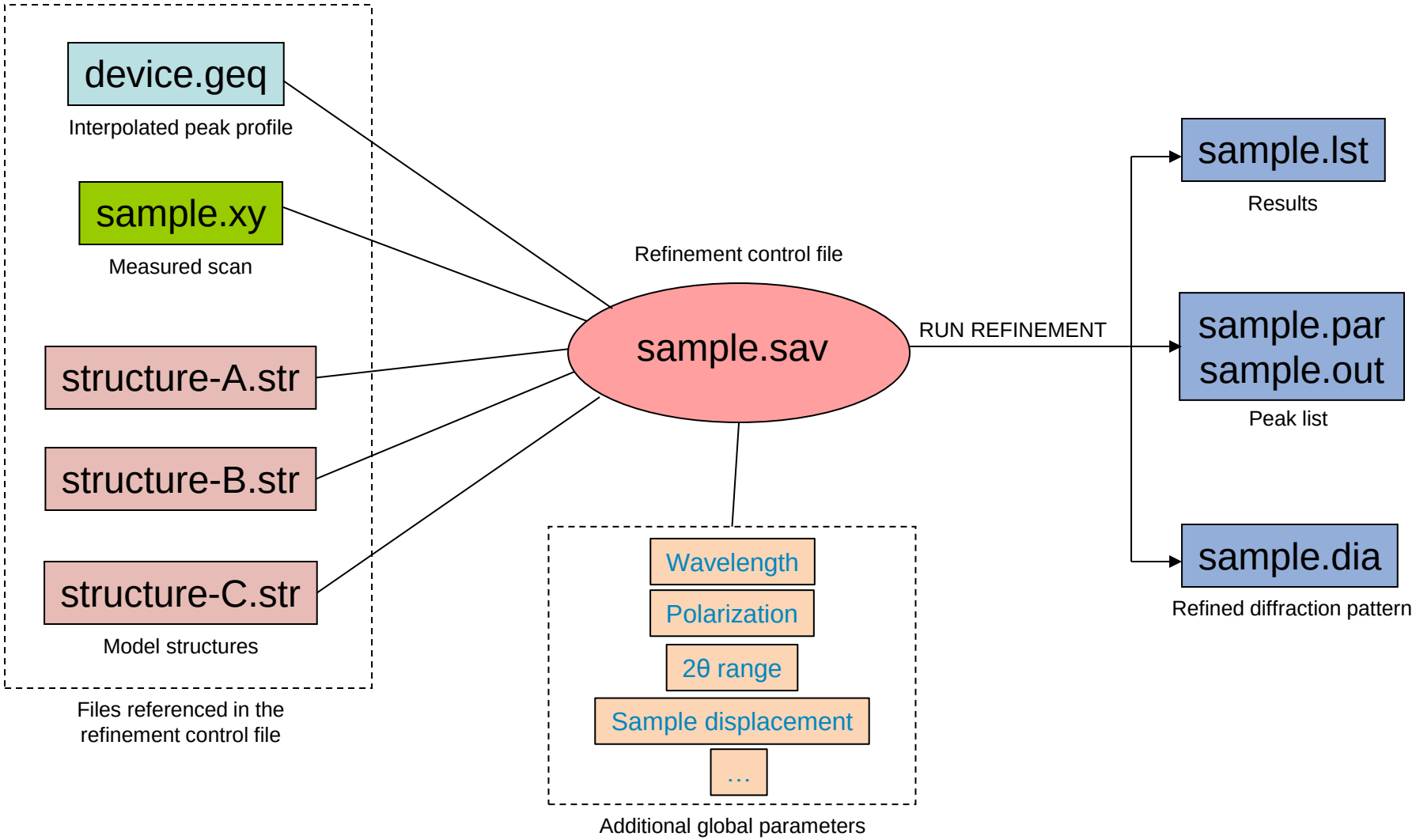
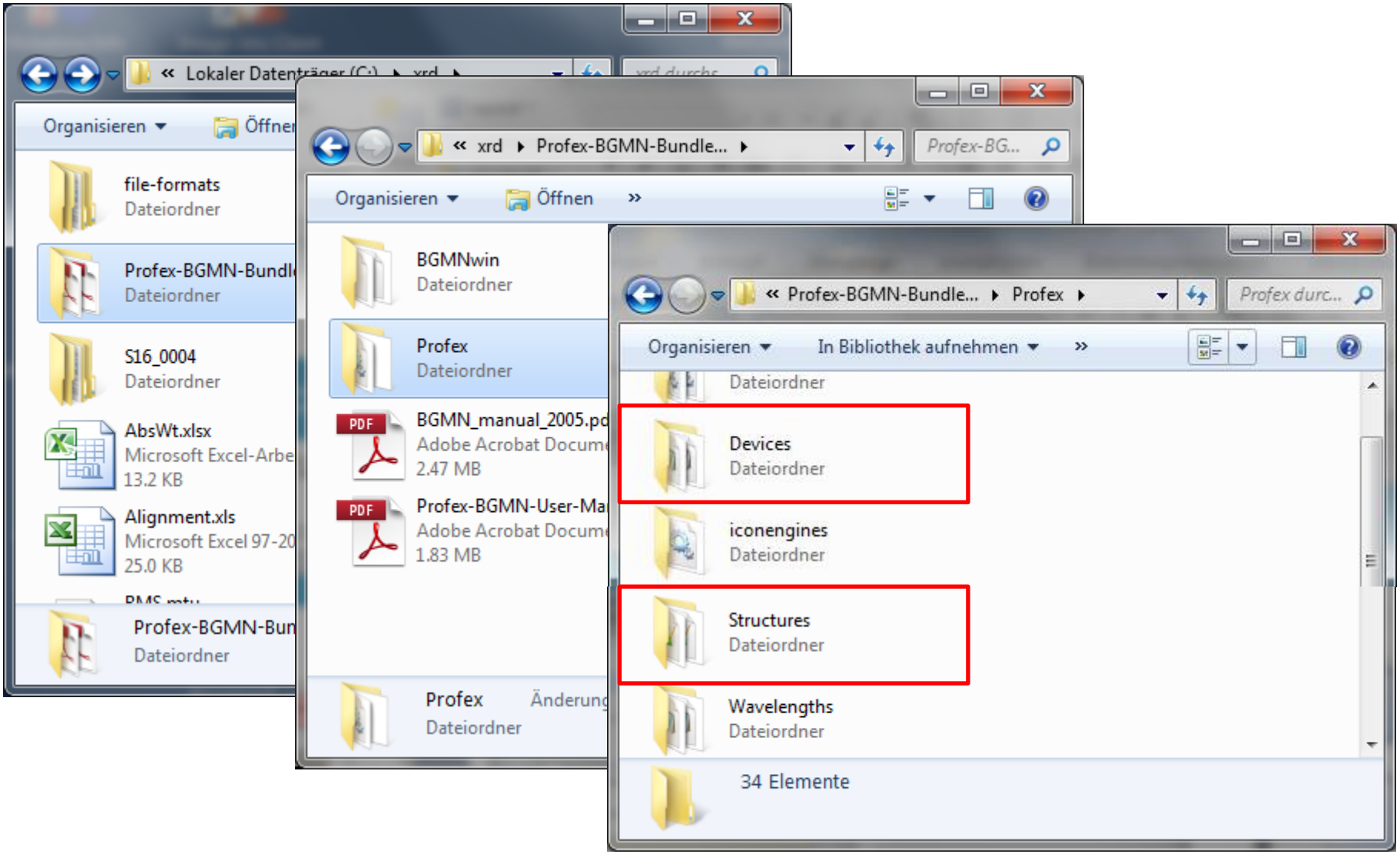
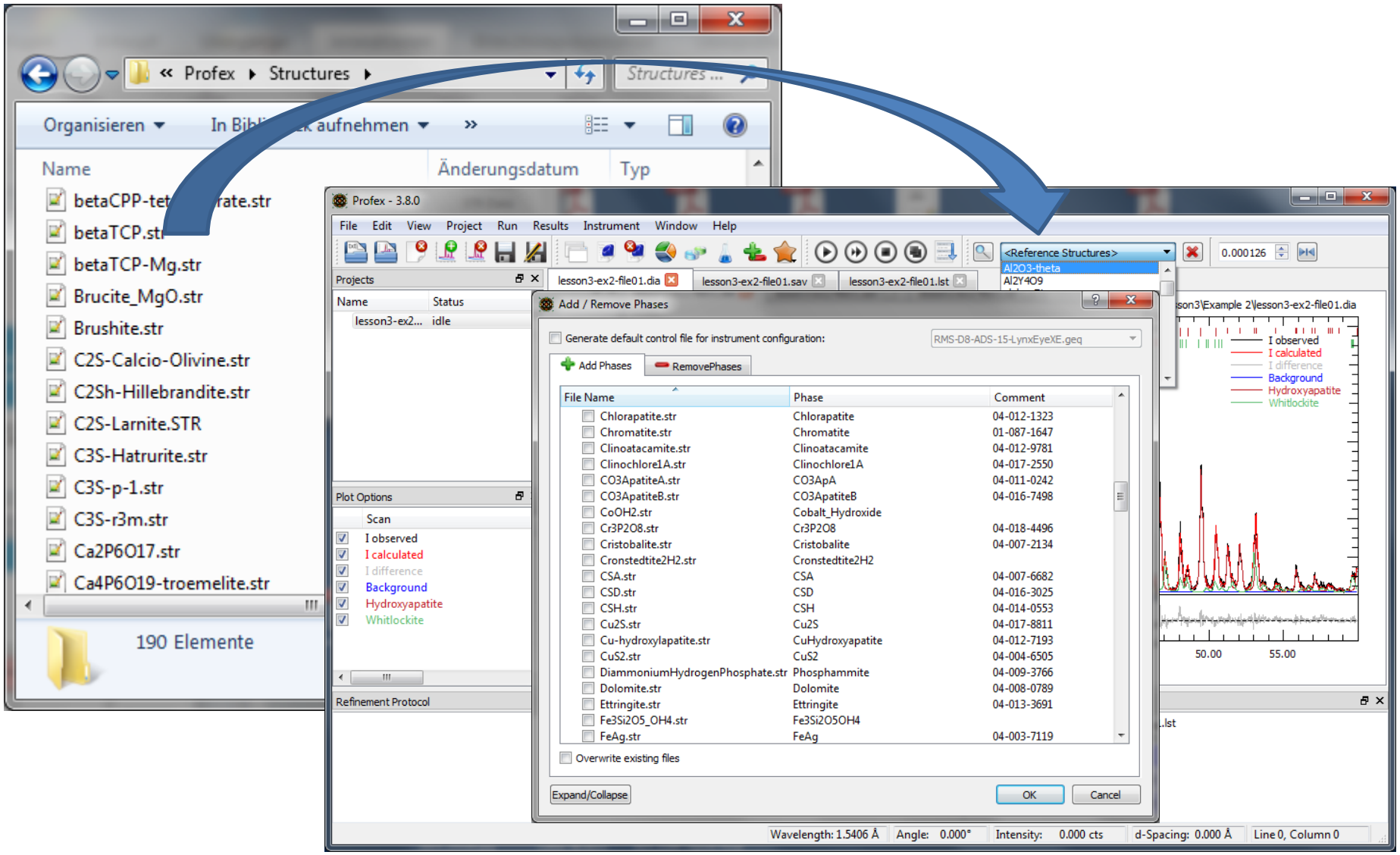
BGMN Project Structure



Profex Structure and Device File Database

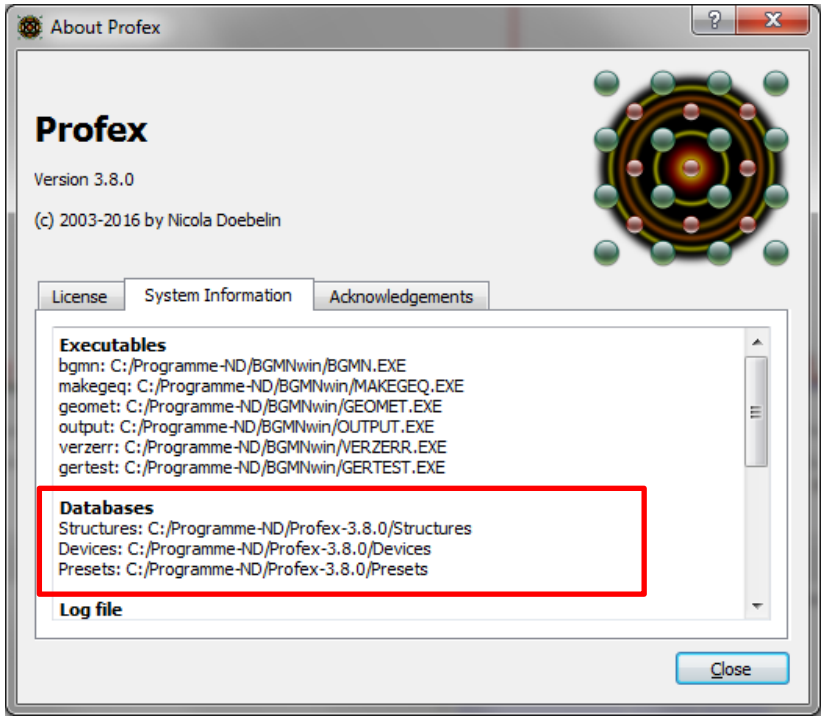


Profex Structure and Device File Database

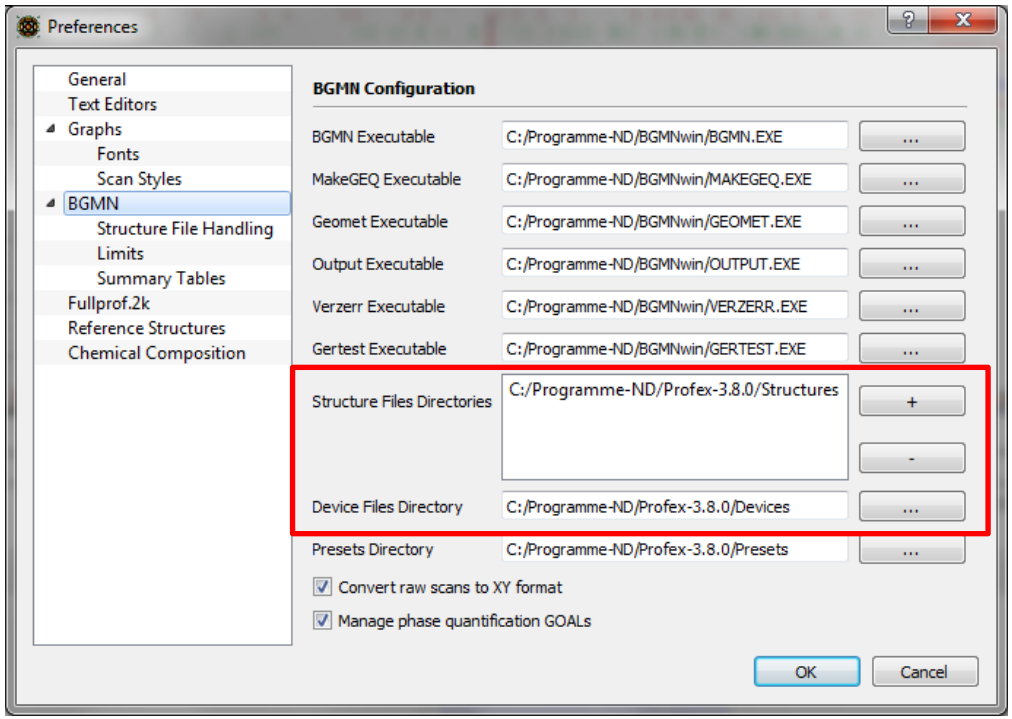


Profex Structure and Device File Database

«Help → About Profex…»



«Edit → Preferences… → BGMN»



Databases can be changed to a network share.

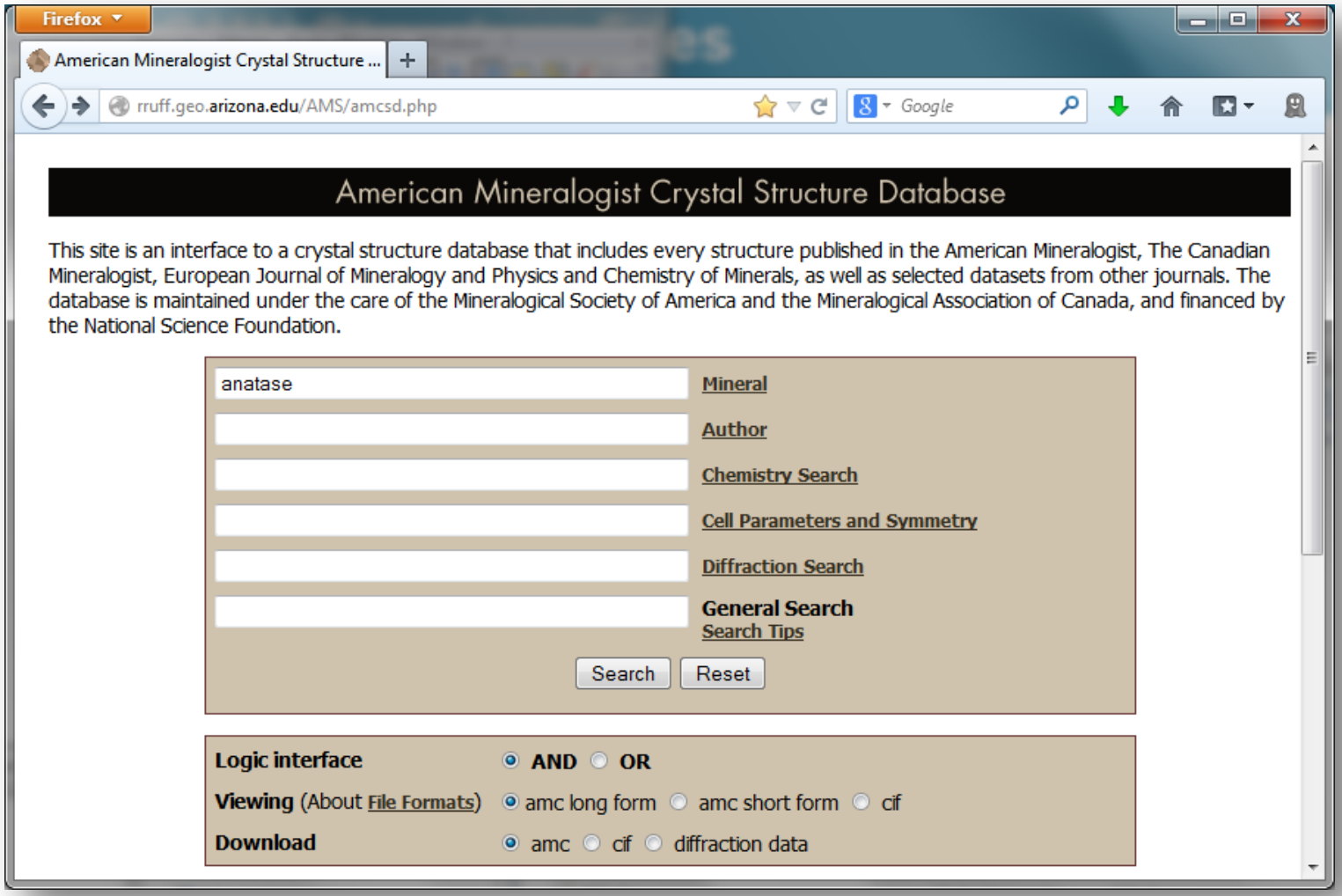
→ Structures added by one user become available to others.

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)

AMCSD


Firefox
American Mineralogist Crystal Structure ...
rruff.geo.arizona.edu/AMS/amcsd.php
Google
American Mineralogist Crystal Structure Database
This site is an interface to a crystal structure database that includes every structure published in the American Mineralogist, The Canadian Mineralogist, European Journal of Mineralogy and Physics and Chemistry of Minerals, as well as selected datasets from other journals. The database is maintained under the care of the Mineralogical Society of America and the Mineralogical Association of Canada, and financed by the National Science Foundation.
anatase
Mineral
Author
Chemistry Search
Cell Parameters and Symmetry
Diffraction Search
General Search
Search Tips
Search
Reset
Logic interface
AND
OR
Viewing (About File Formats)
amc long form
amc short form
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Download
amc
cif
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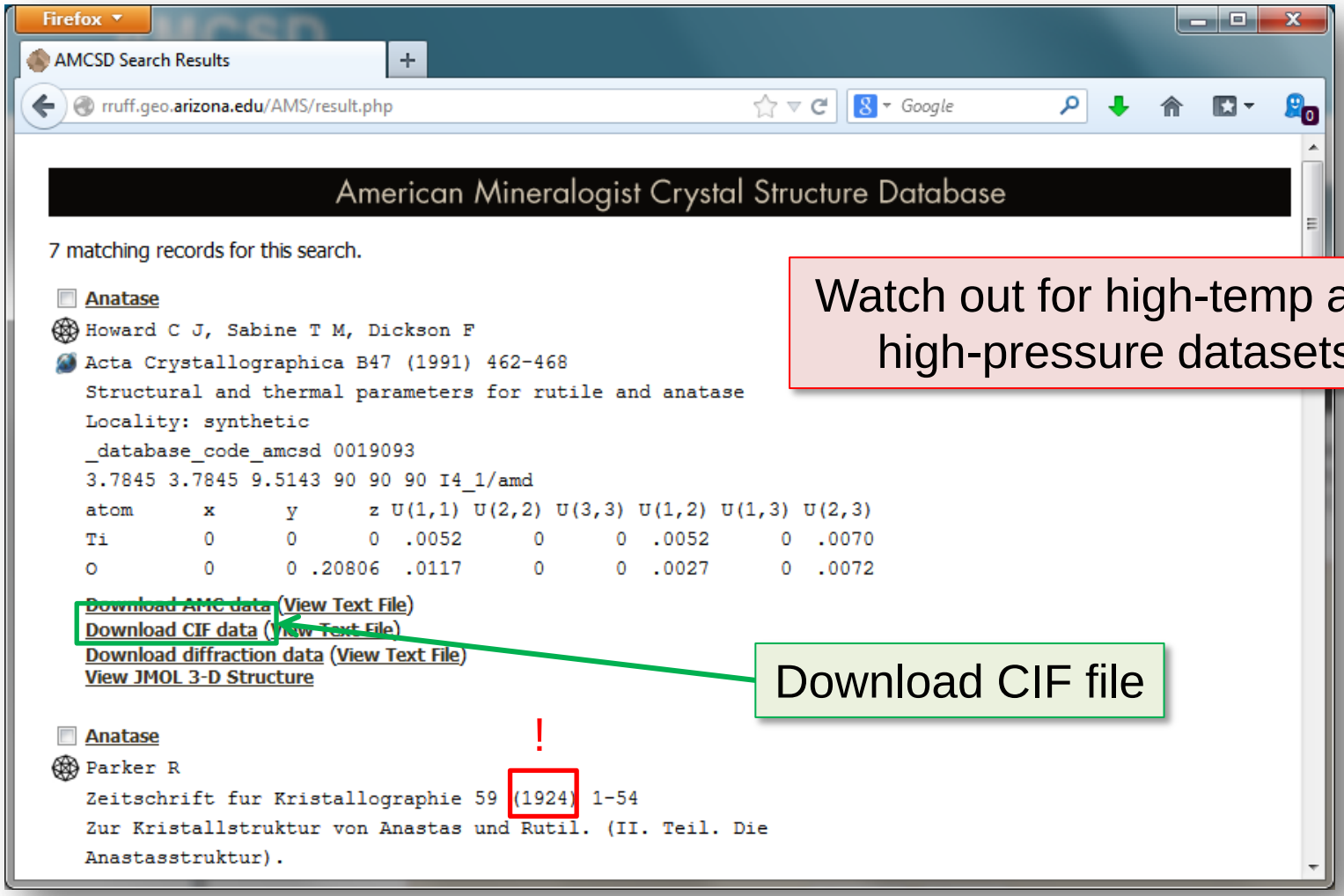
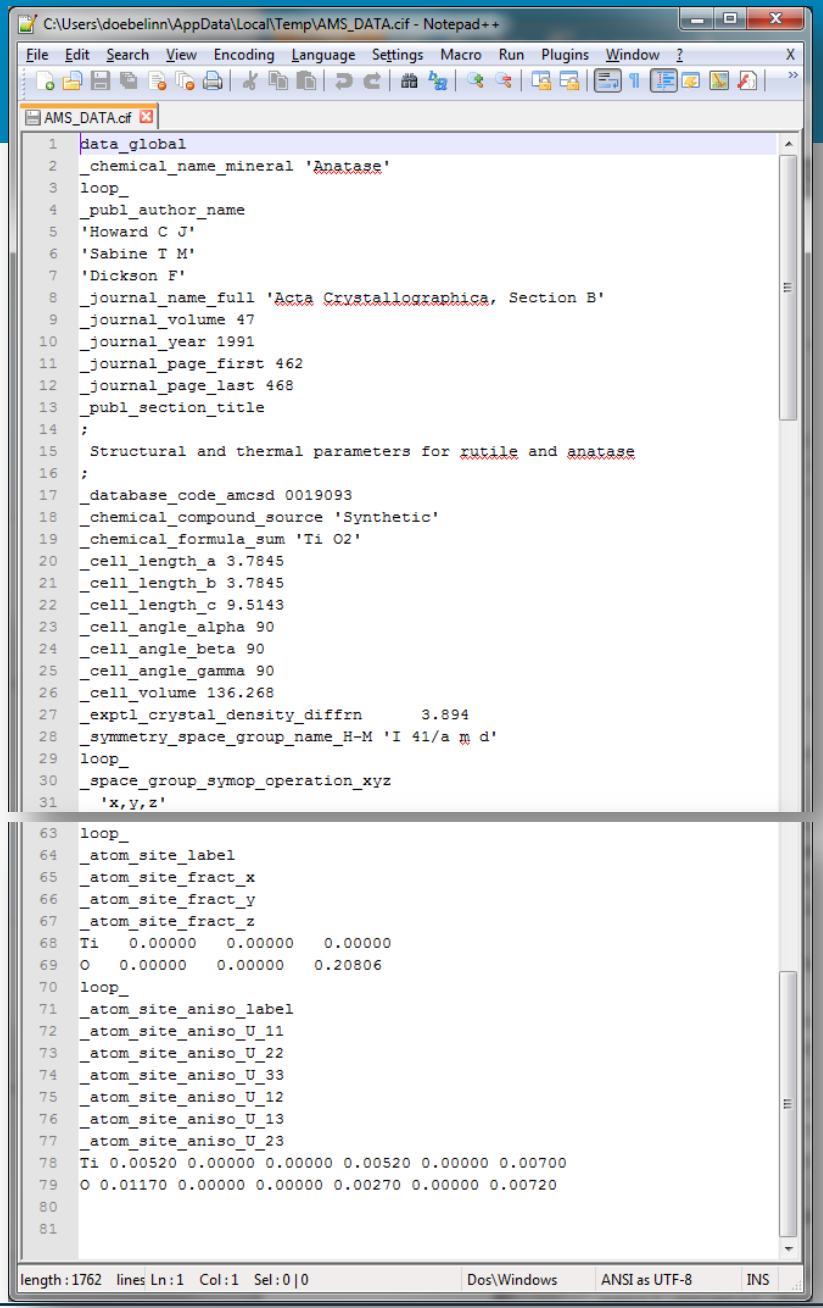
AMCSD: Downloading CIF Files



CIF File Format

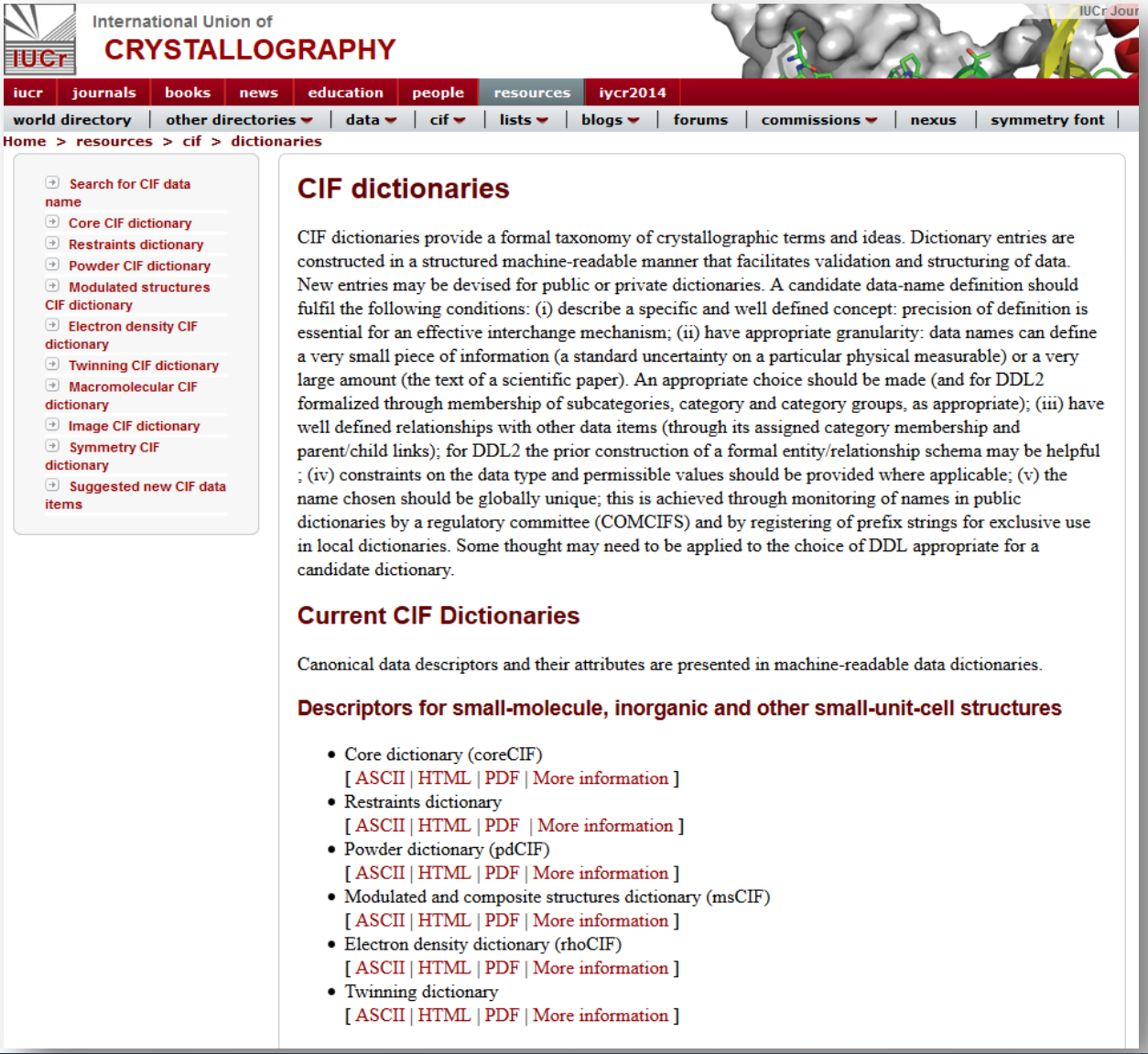
CIF (Crystallographic Information File) Format:

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



CIF Format Specification

http://www.iucr.org/resources/cif/dictionaries



International Union of
CRYSTALLOGRAPHY

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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

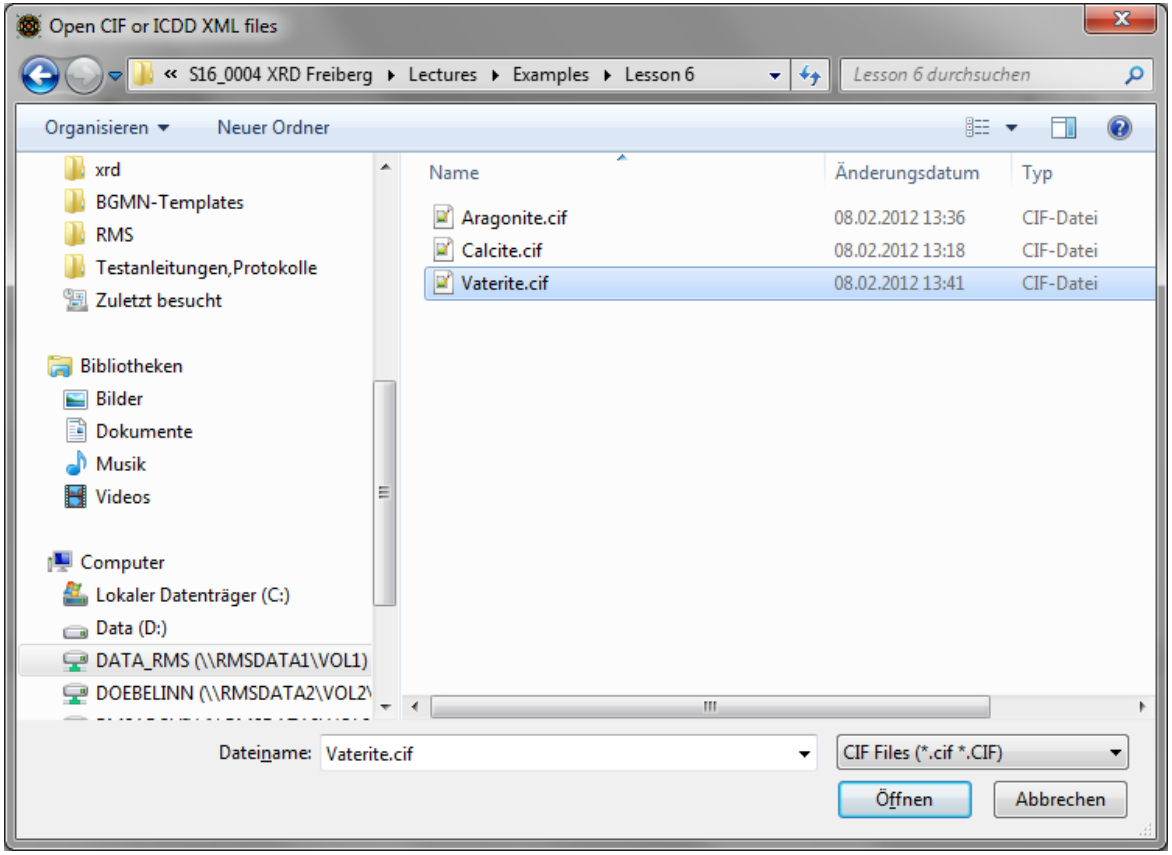
With Profex:

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

Profex CIF Import

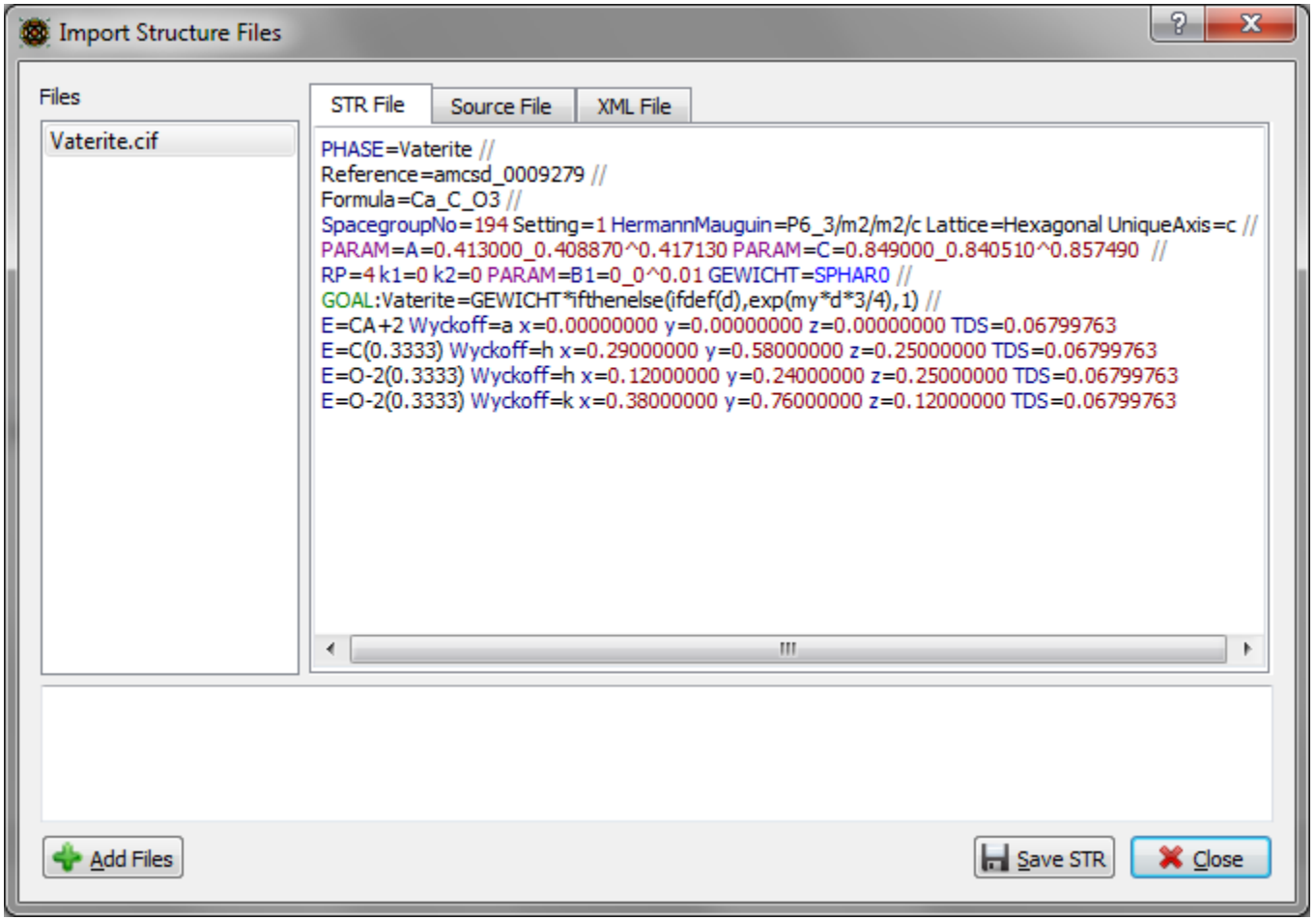
«File → Import Structure File…»

«Examples/Lesson 6/Vaterite.cif»



Profex CIF Import

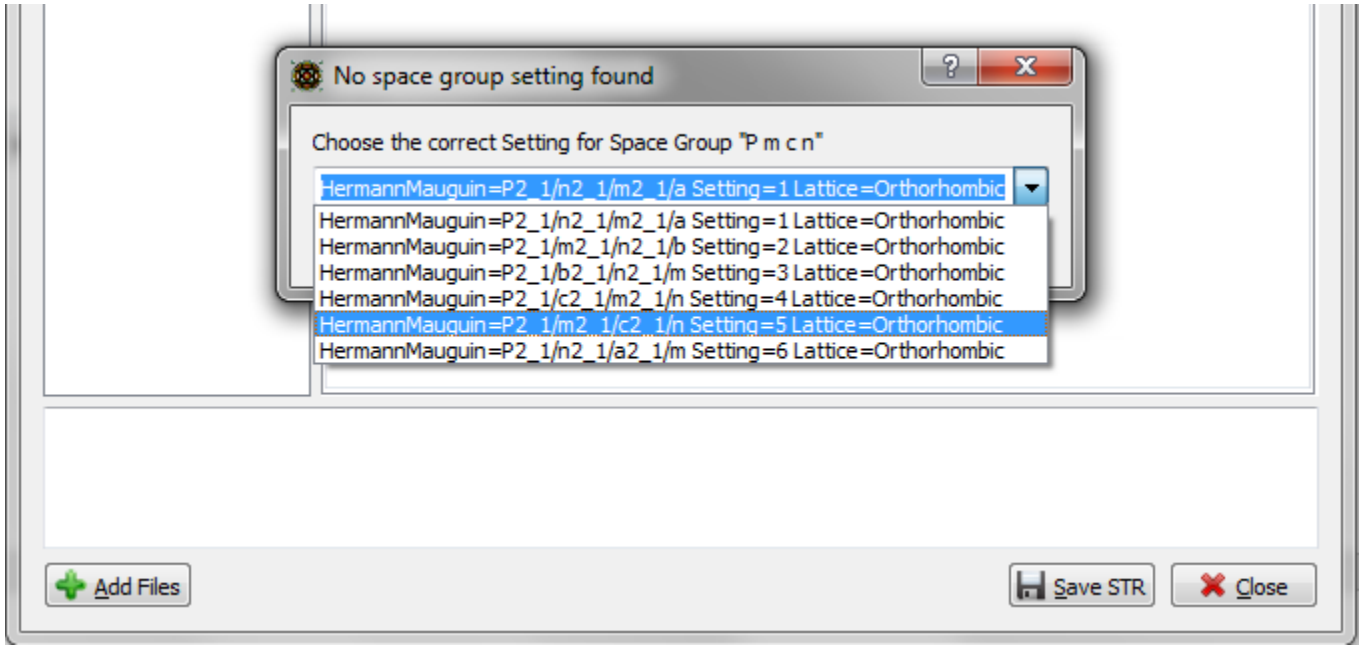
Best Case: No Questions asked = automatic import



«Save STR» to Structures database directory

Profex CIF Import

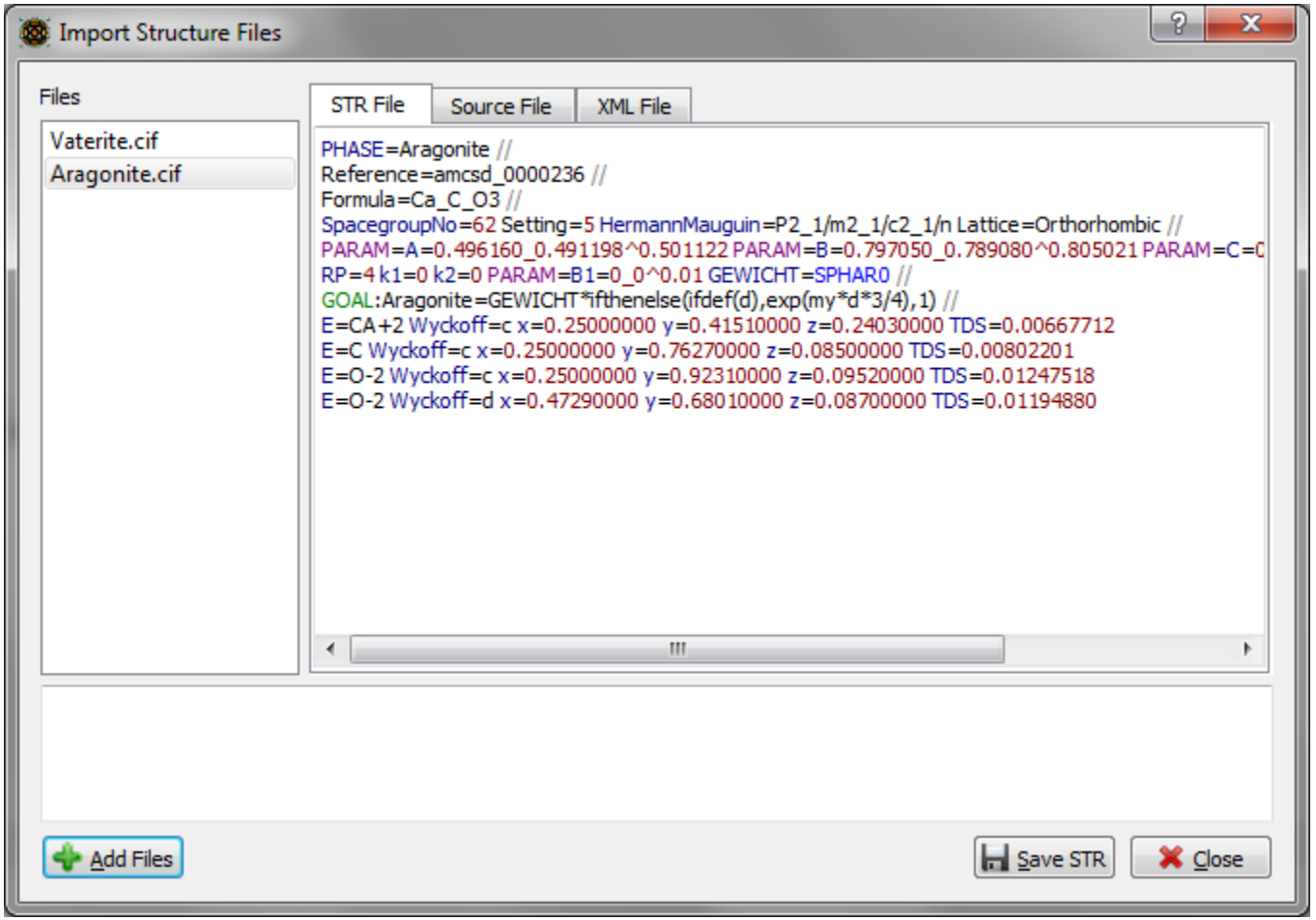
«+ Add Files → Aragonite.cif»



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

Profex CIF Import

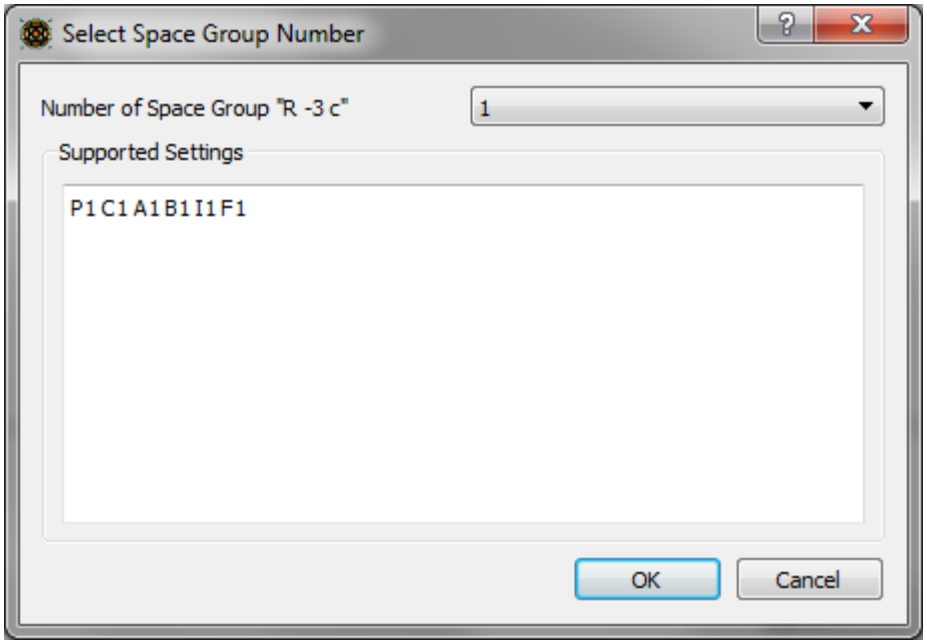
No further input required



«Save STR» to Structures database directory

Profex CIF Import

«+ Add Files → Calcite.cif»



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

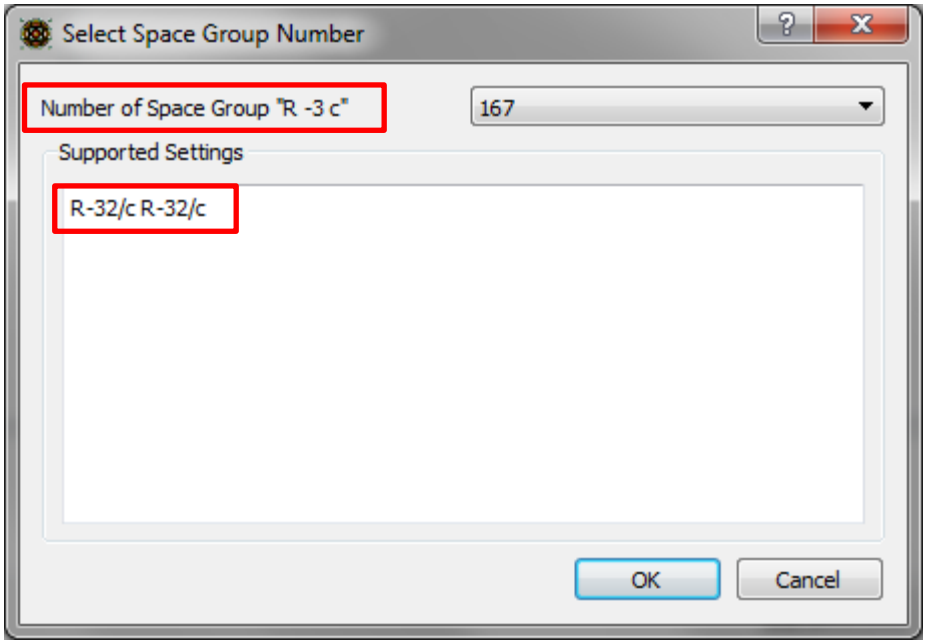
Found elsewhere: 167

Profex CIF Import

BGMN's full notations for SG #167

Read from CIF file →

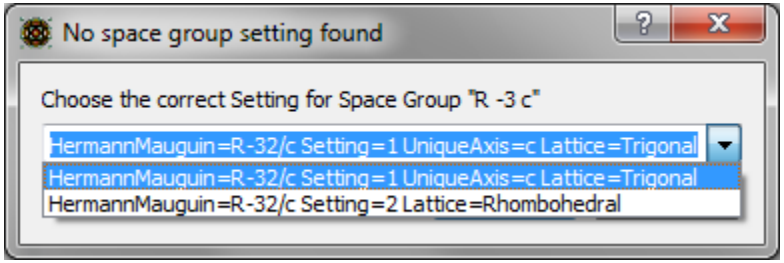
Supported by BGMN →



Seems to match. Click «OK»

Profex CIF Import

BGMN's full notations for SG #167



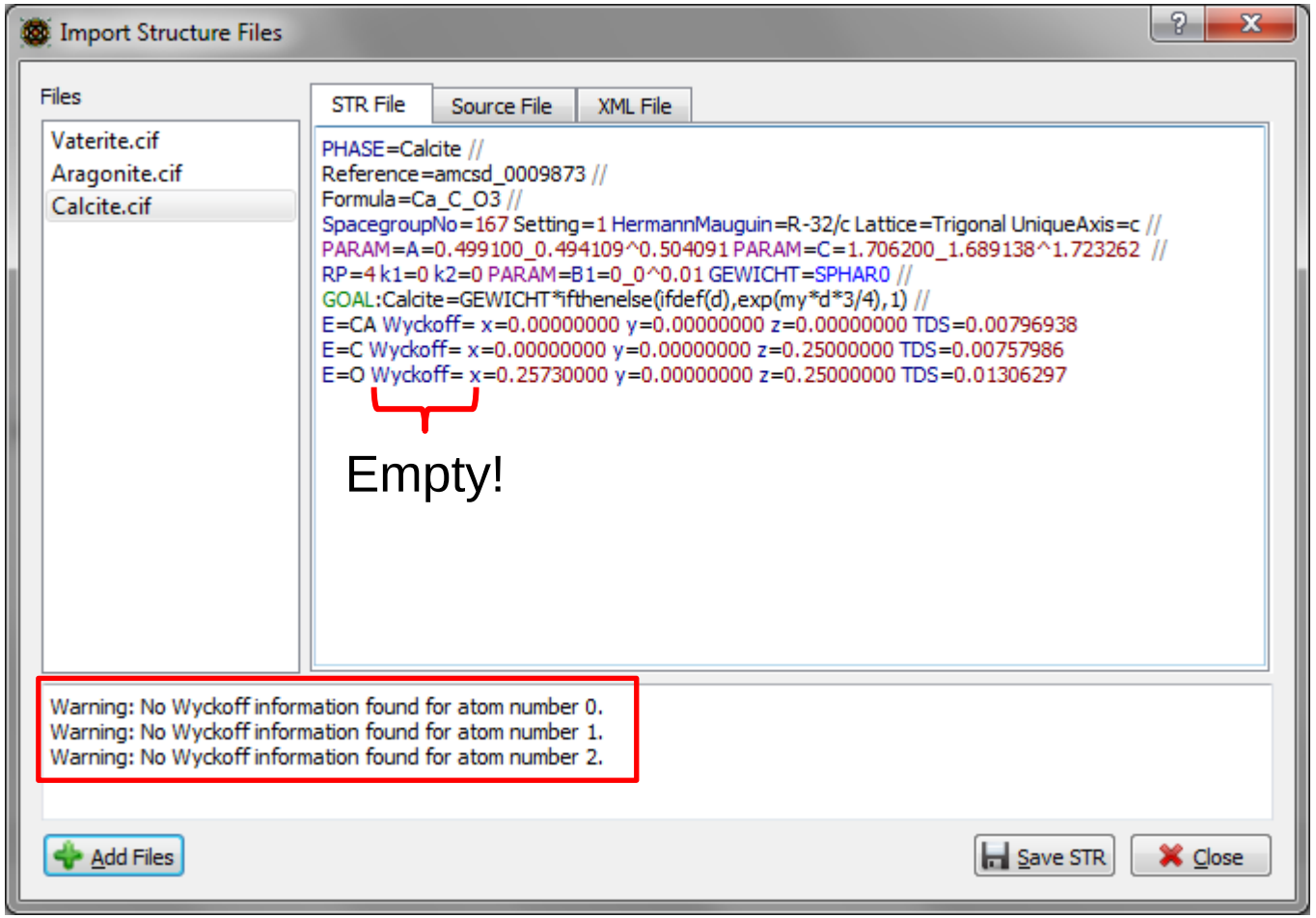
Two settings for $R\text{-}3_2/c$:

- Trigonal
- Rhombohedral

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

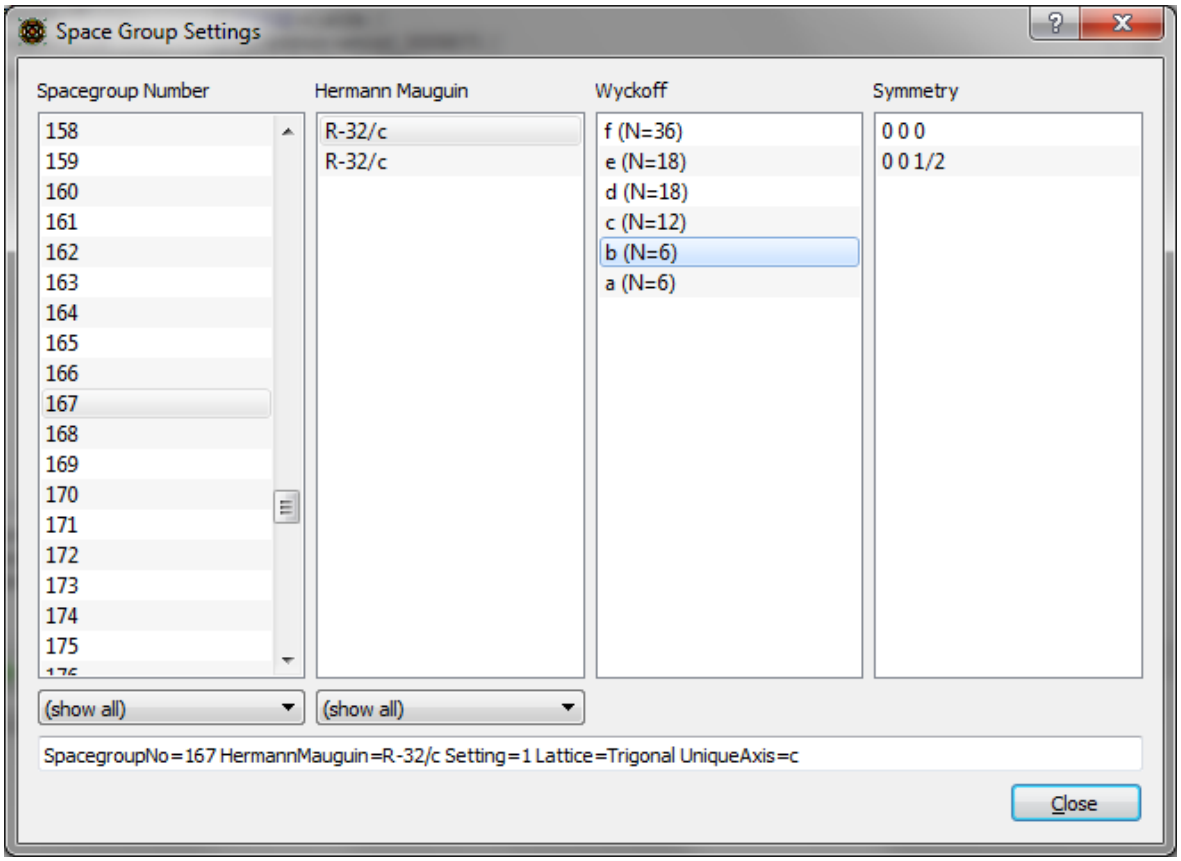
Profex CIF Import

Warning: Missing Wyckoff symbols



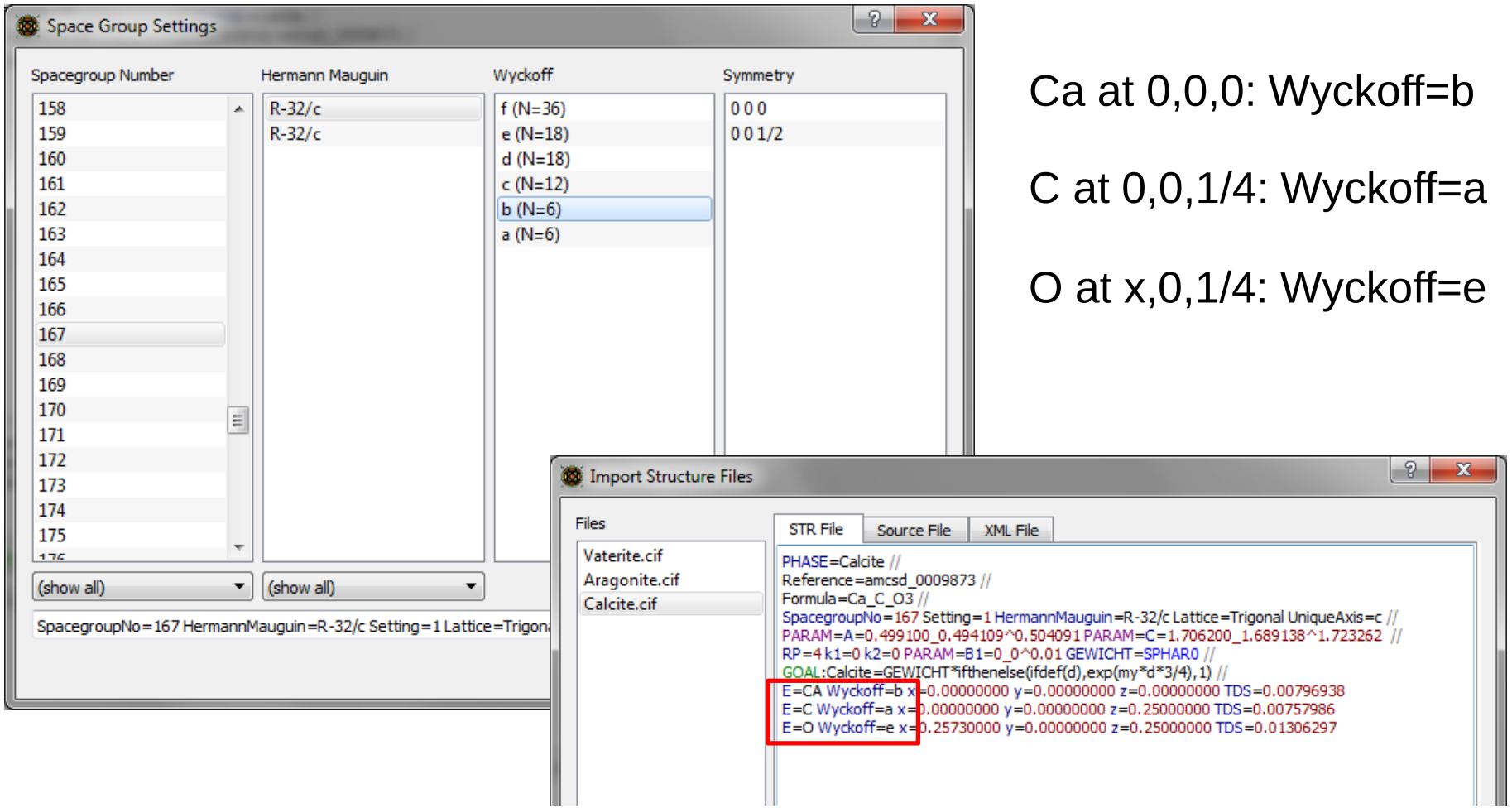
Profex CIF Import

«Help → BGMN SPACEGRP.DAT»



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

Profex CIF Import



Ca at 0,0,0: Wyckoff=b

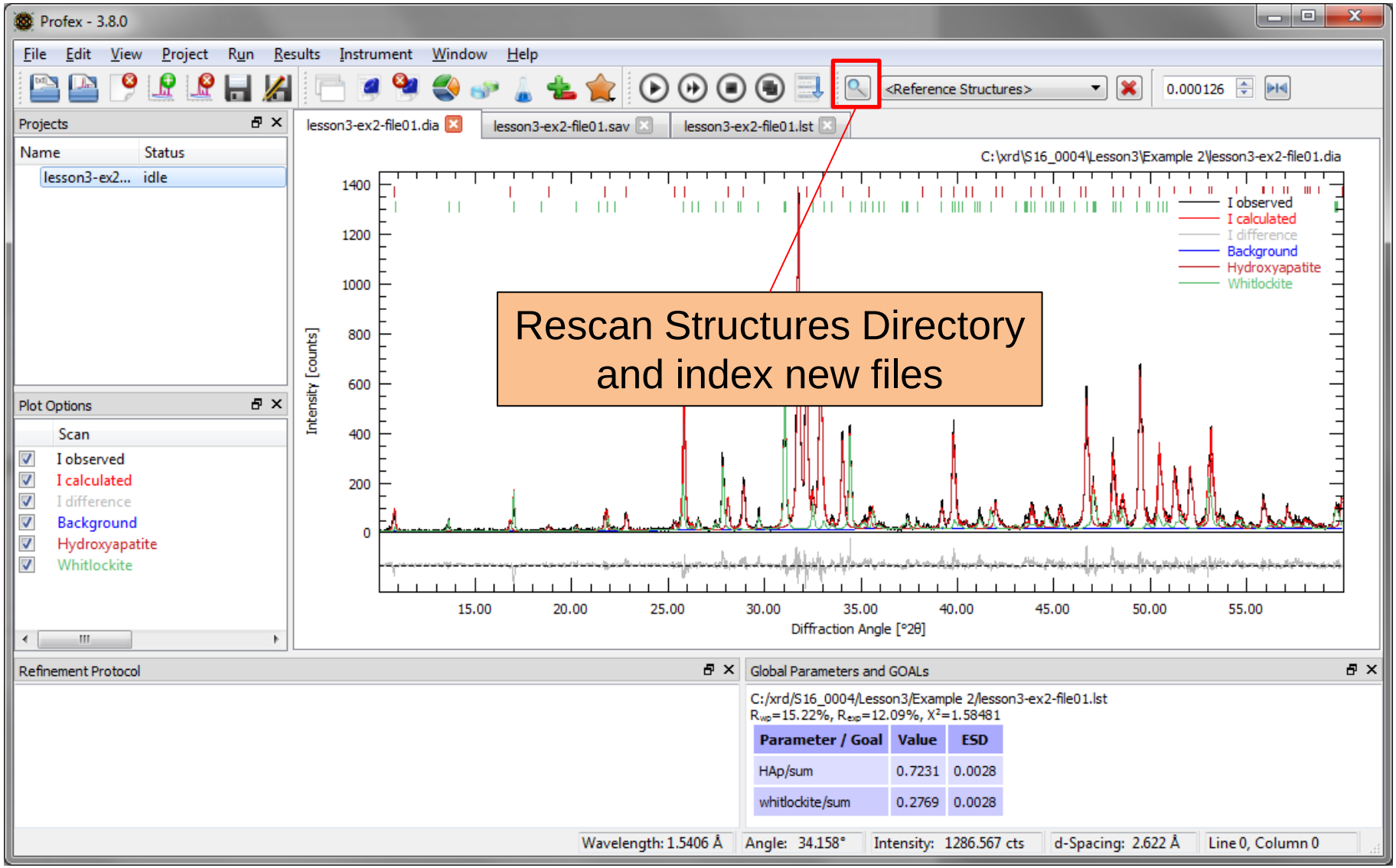
C at 0,0,1/4: Wyckoff=a

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

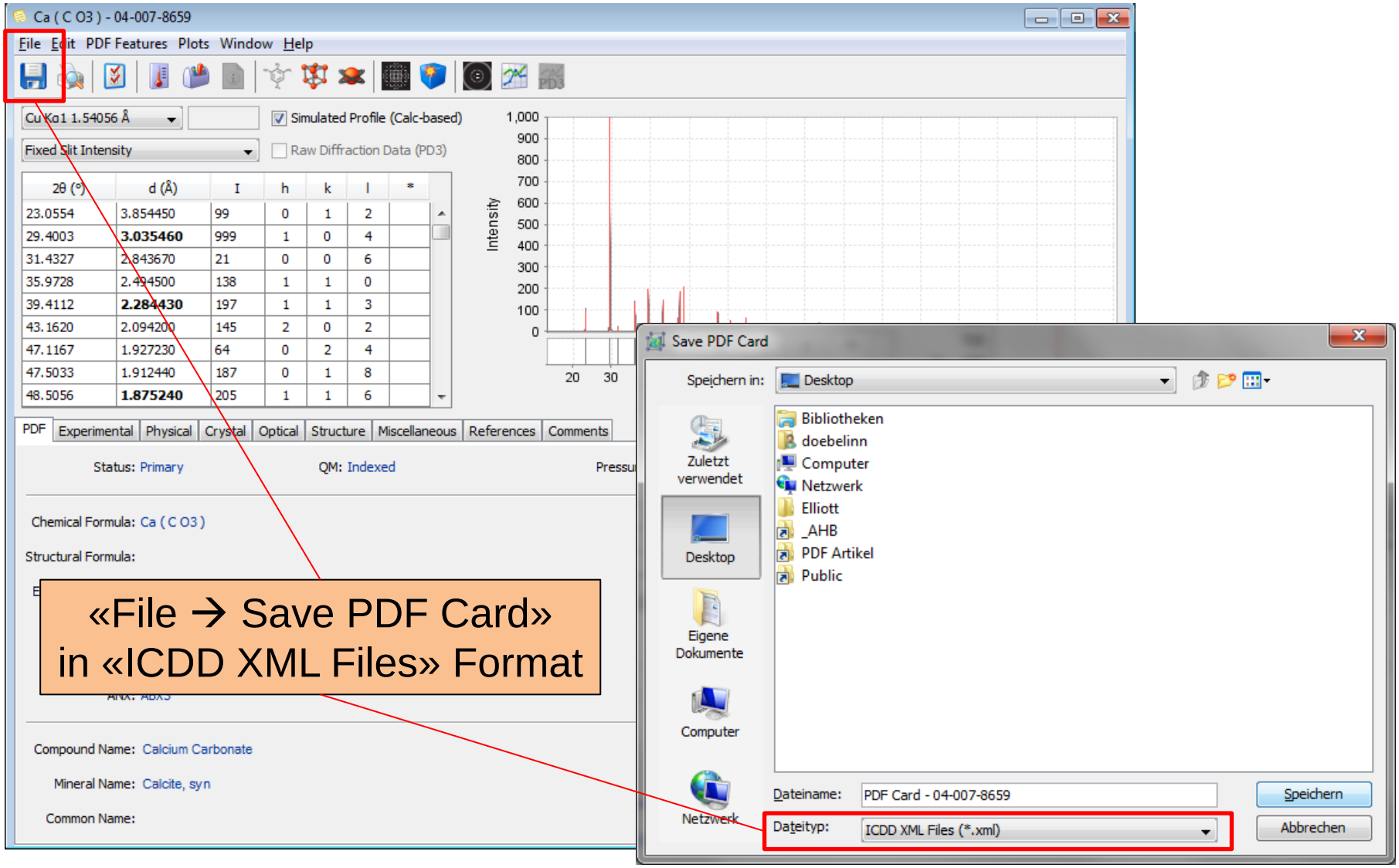
Fill in manually

“Save STR” to Structure Database directory

Profex CIF Import



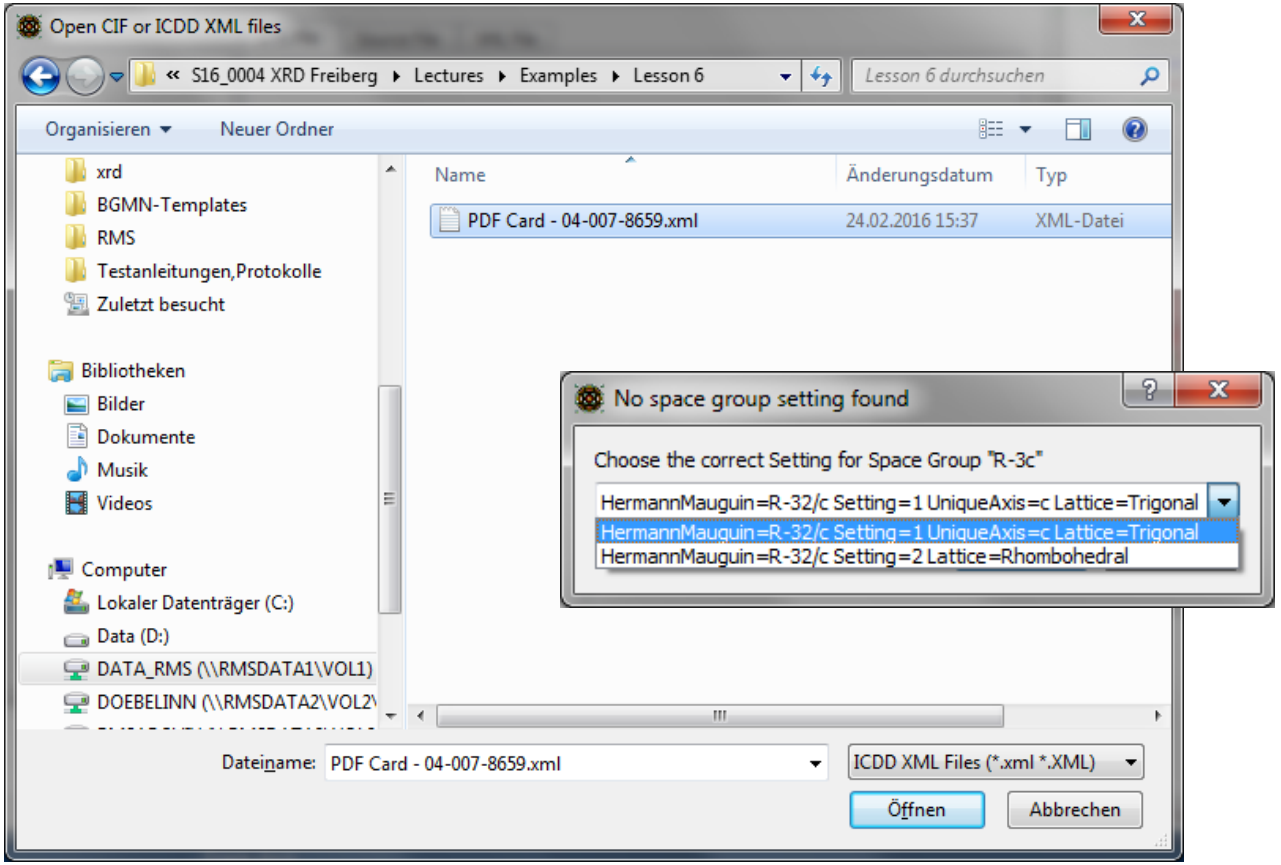
Import from ICDD PDF4+ XML Format



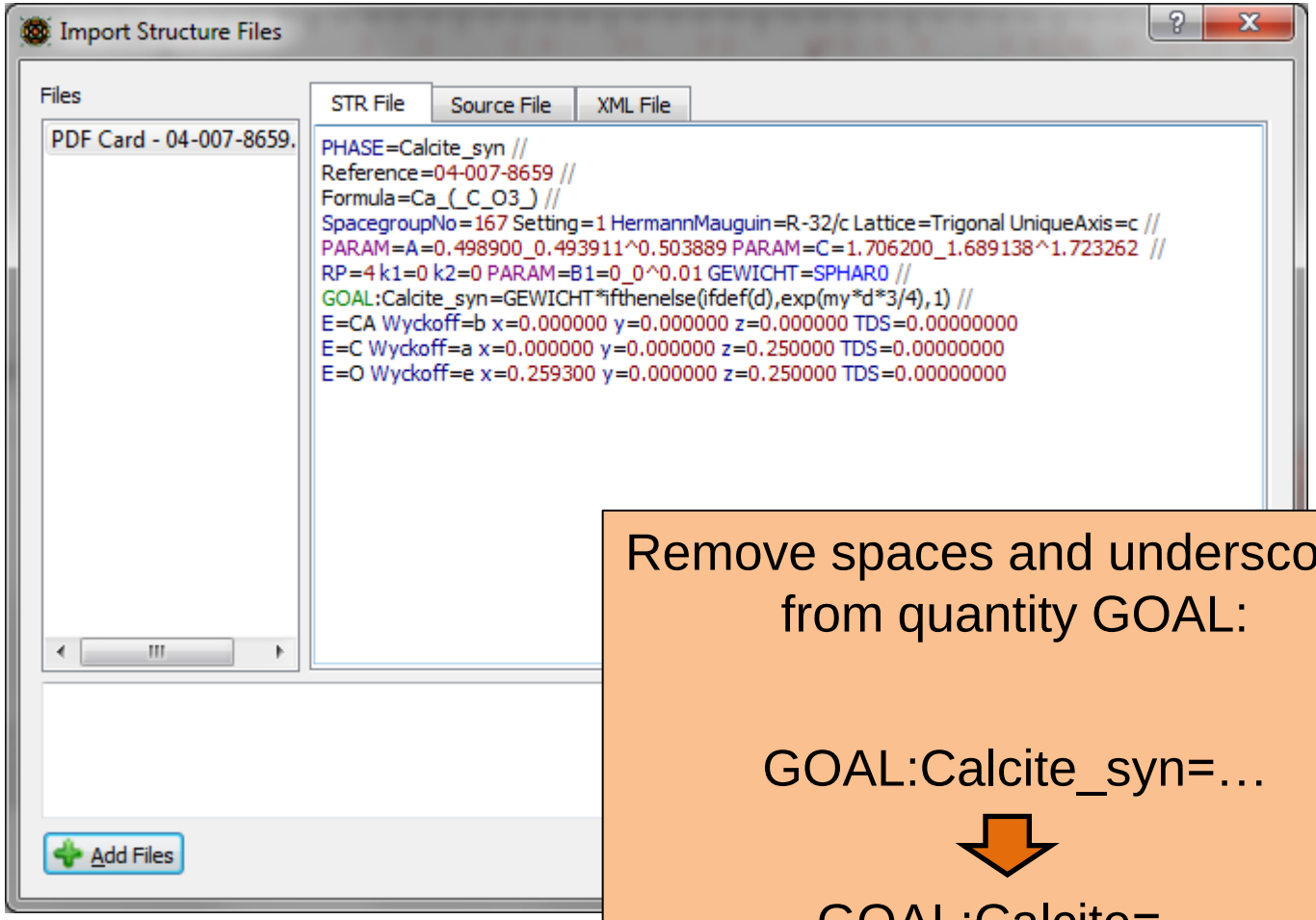
Import from ICDD PDF4+ XML Format

In Profex: «File → Import Structure File…»

«Examples/Lesson 6/Vaterite.cif»



Import from ICDD PDF4+ XML Format



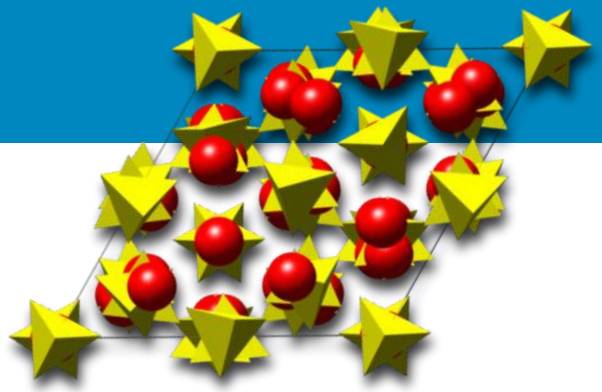
Remove spaces and underscores from quantity GOAL:

GOAL:Calcite_syn=…

GOAL:Calcite=…

«Save STR» to Structures database directory

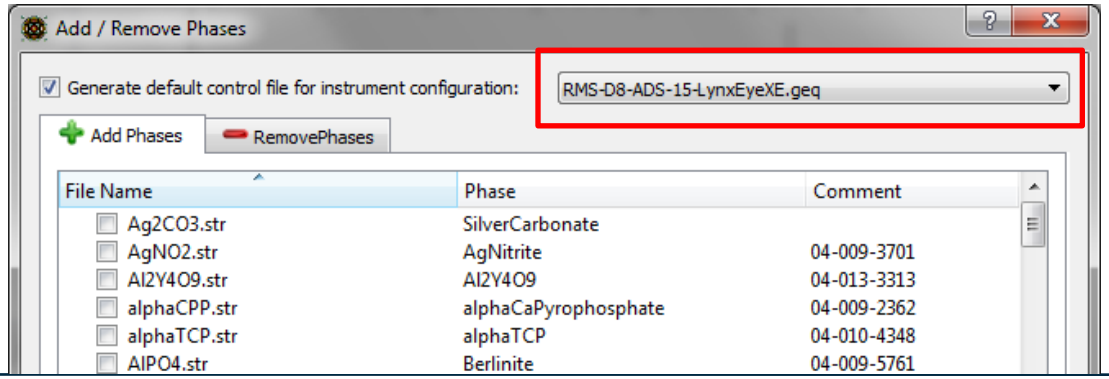
Summary: STR Files



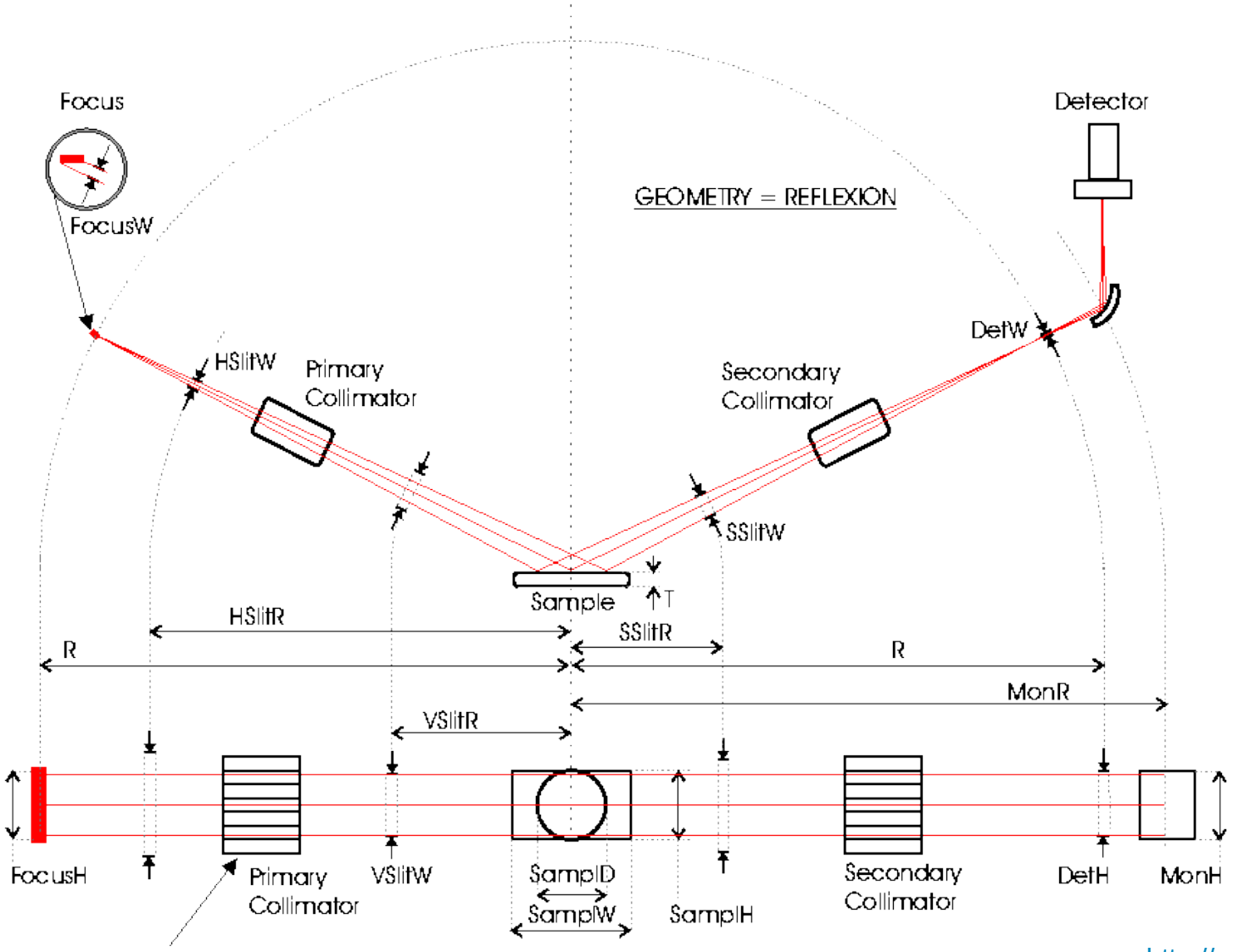
- If no *.str file is available:
  - Download CIF file from public database (COD, AMCSD, ICSD)
  - Or export XML file from PDF-4+ database
  - → Convert to *.str format with Profex
  - Fix *.str file manually if necessary
  - Save to «Structures» directory in Profex-BGMN-Bundle

Device Files

- 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



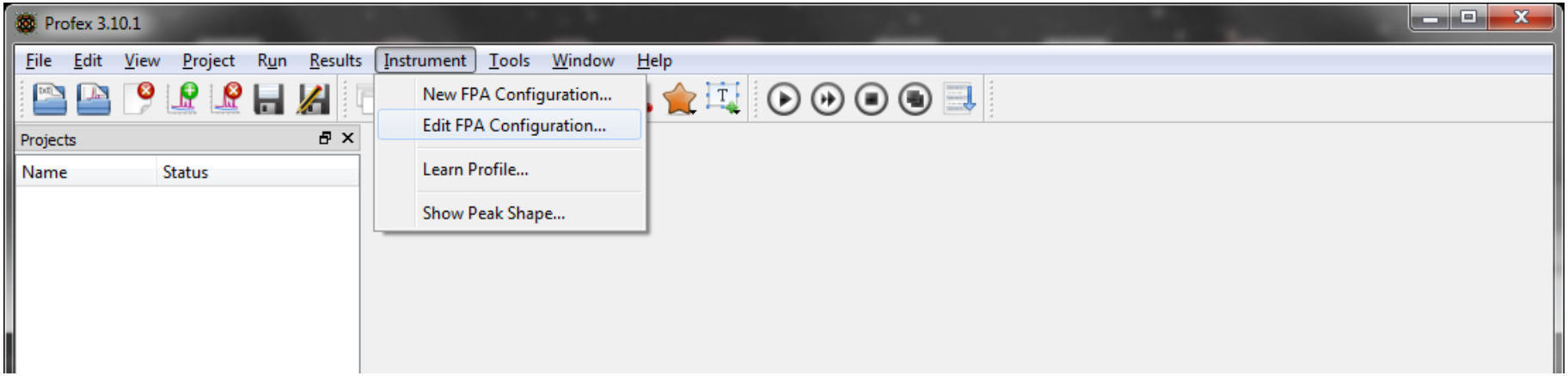
Device Files



http://www.bgmn.de

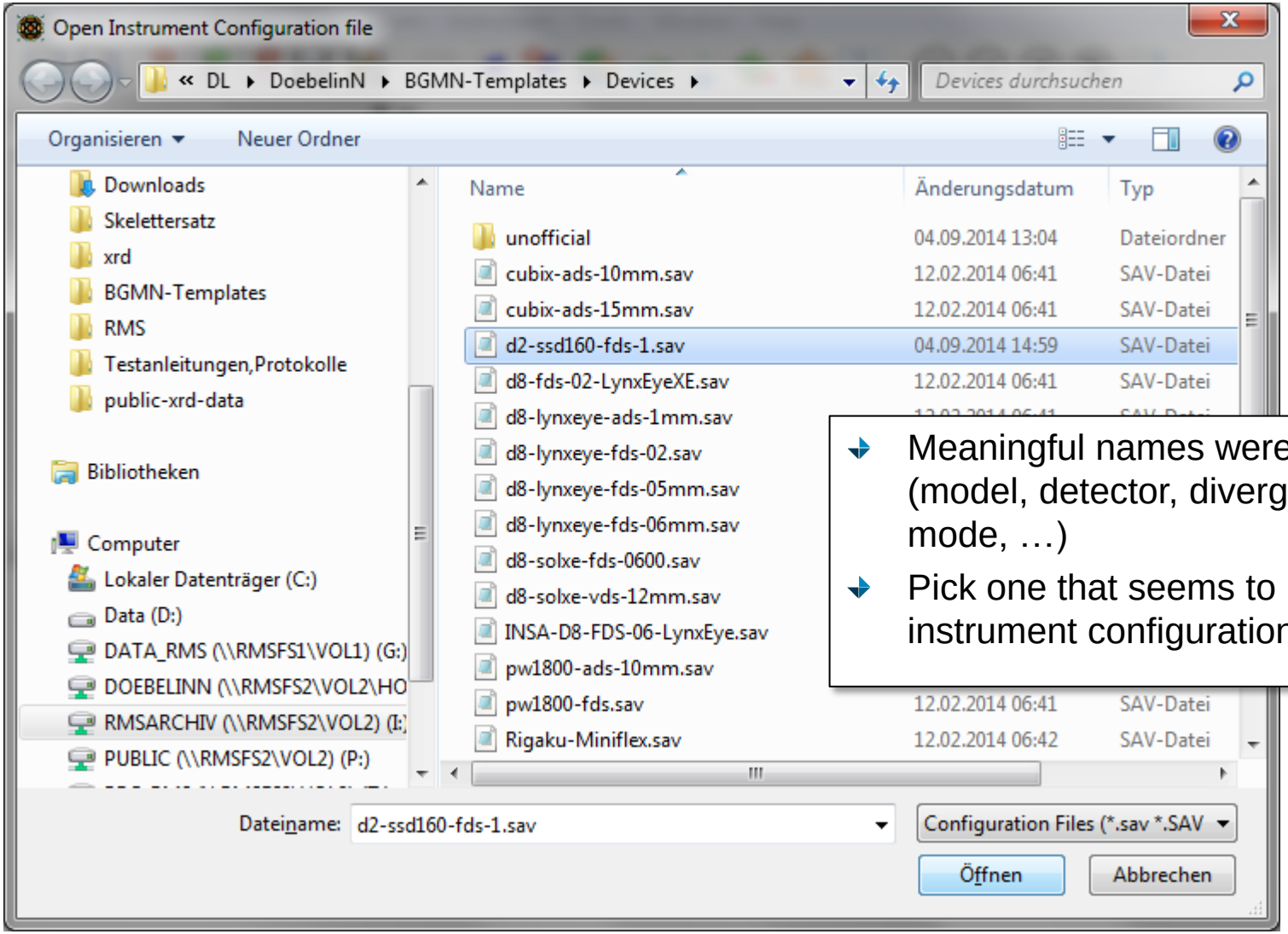
Device Files

- Recommended: Modify an existing instrument configuration



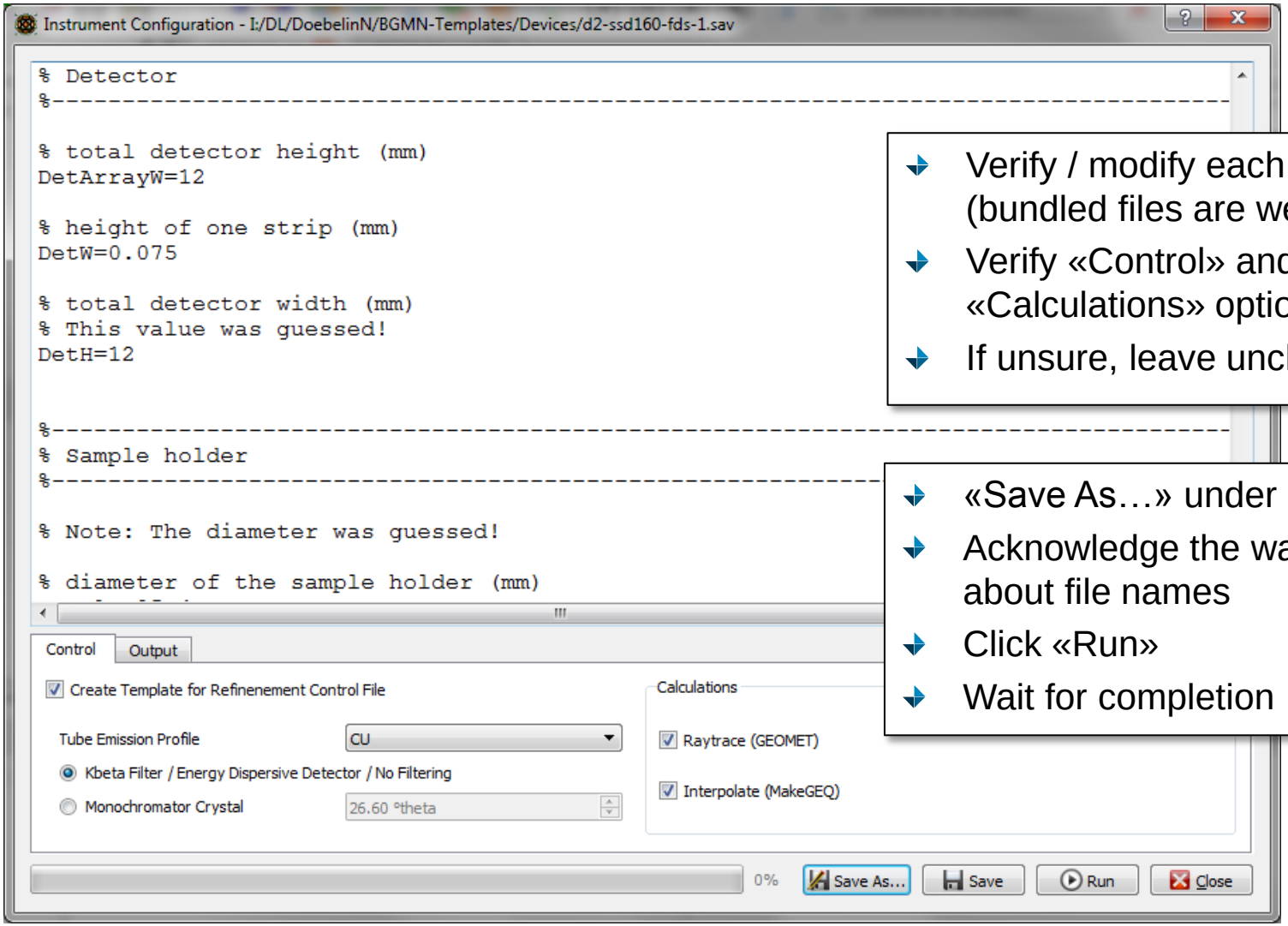
http://www.bgmn.de

Device Files



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

Device Files



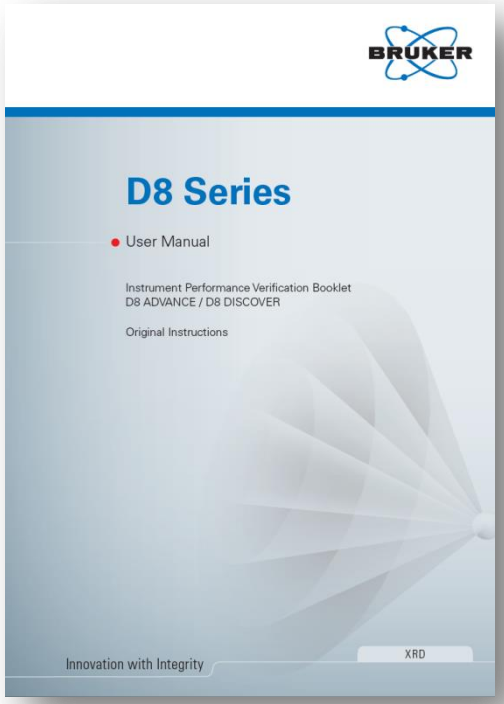
- Verify / modify each line (bundled files are well documented)
- Verify «Control» and «Calculations» options
- If unsure, leave unchanged

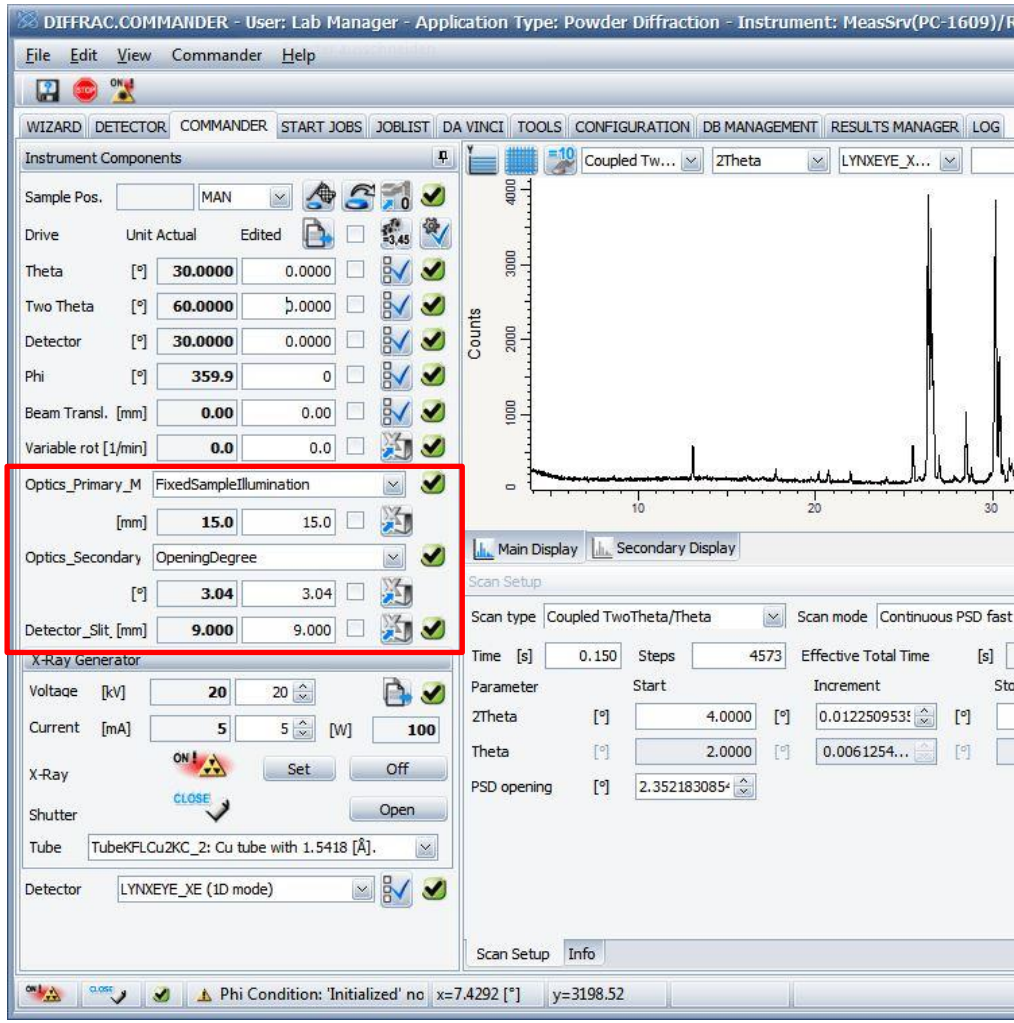
- «Save As…» under a new name
- Acknowledge the warning message about file names
- Click «Run»
- Wait for completion

Device Files

Get instrument parameters from:

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

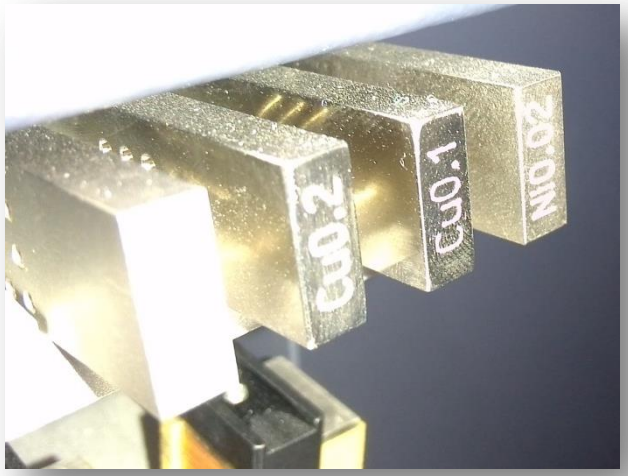


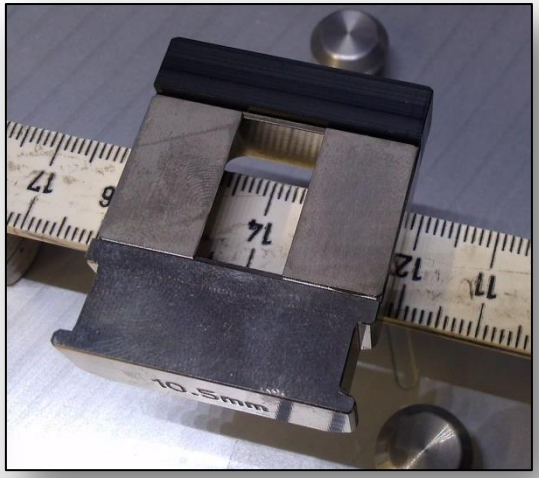


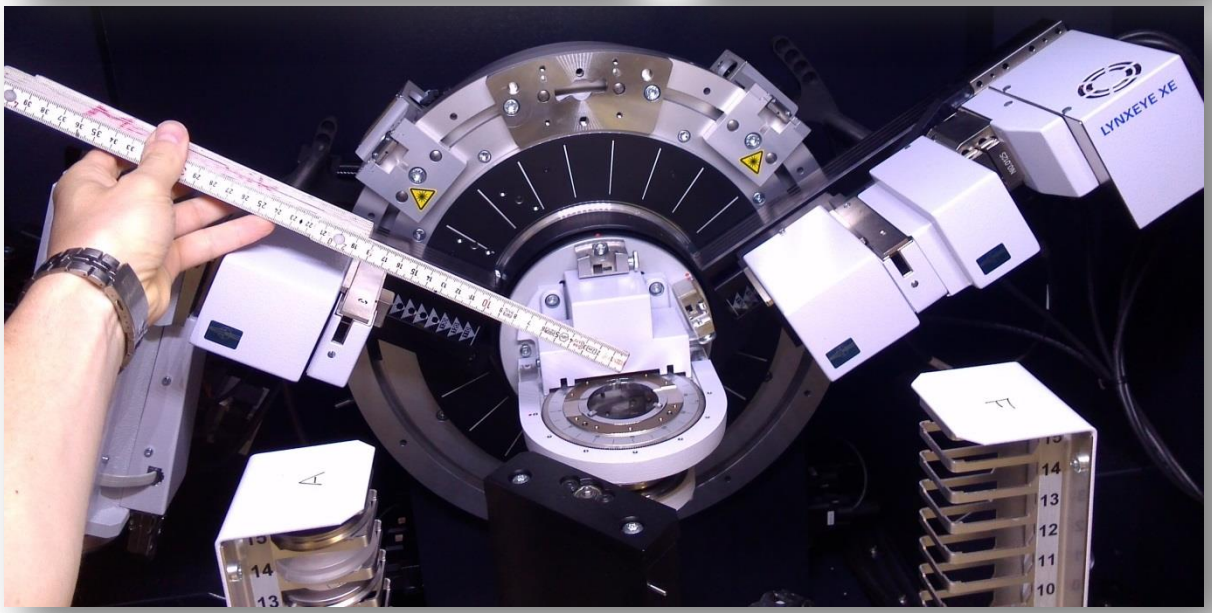
Device Files

…

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







Tutorial on http://profex.doebelin.org

PROFEX

OPEN SOURCE XRD AND RIETVELD REFINEMENT

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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.