# Jana2020

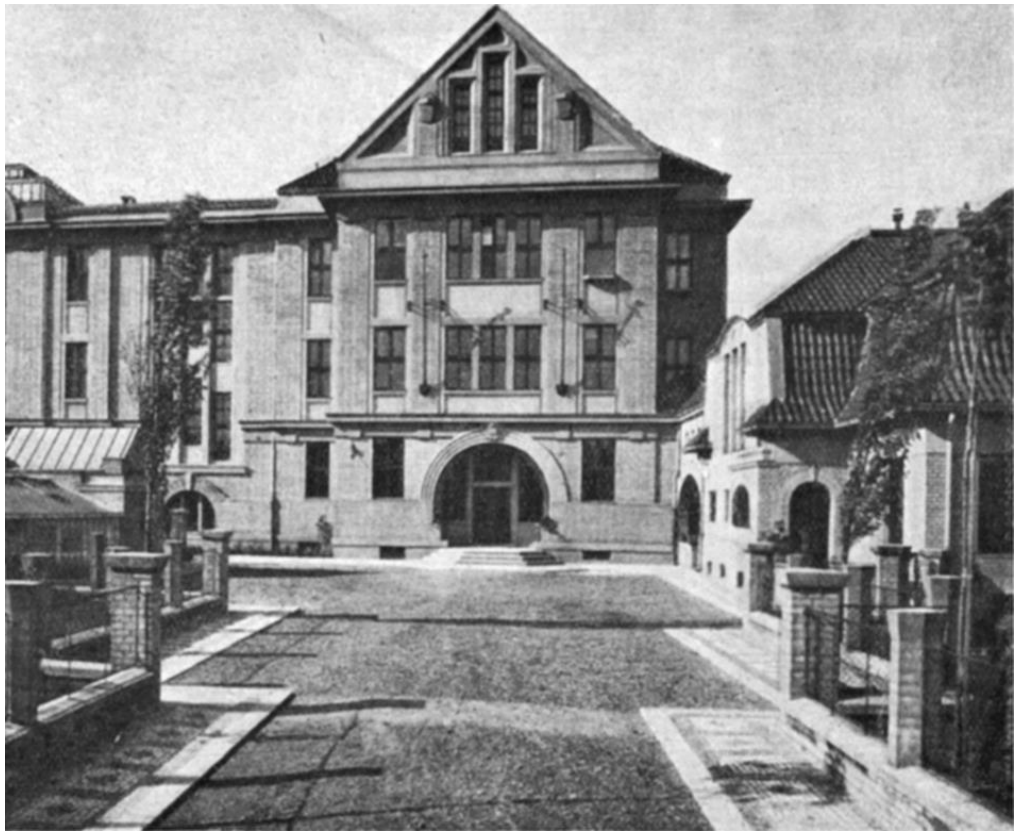
## A program for structure analysis of regular, modulated, composite, and magnetic structures

Václav Petříček, Michal Dušek, Lukáš Palatinus, Margarida Henriques

**Cinthia Antunes Corrêa**

FZU Institute of Physics of the Czech Academy of Sciences

# Institute of Physics, Prague 6, Cukrovarnická street



1923



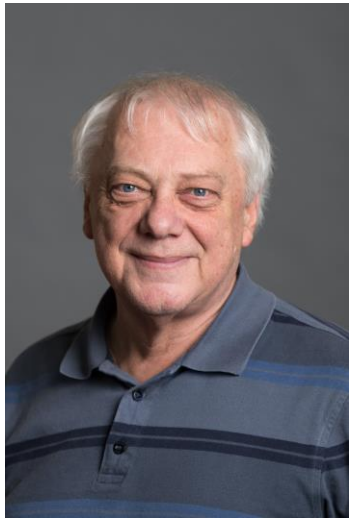
2023

# Since 1980…



FZU Institute of Physics of the Czech Academy of Sciences

# History



Václav Petříček

**1971** FZU

**1980** SDS

*Program for solution and refinement of 3d structures*

**1984** Jana

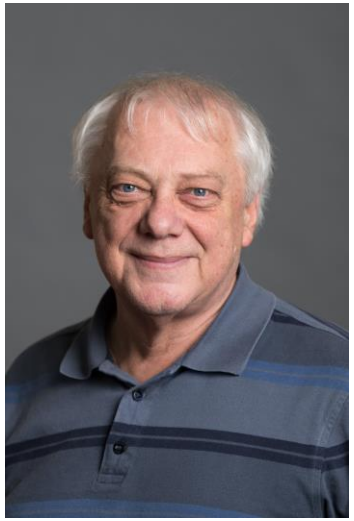
*Refinement program for modulated structures*




https://history.amercrystalassn.org/h_coppens_memoir

**Jana**- the first version developed during Vaclav's stay at Philip Coppens lab in 1984, in close collaboration with Pierre Becker - *Acta Cryst.* **A41**, 478-483 (1985).

# History



Václav Petříček

**1971** FZU

**1980** SDS

*Program for solution and refinement of 3d structures*

**1984** Jana

*Refinement program for modulated structures*

**1994** SDS94 and Jana94

*Set of programs for 3d (SDS) and modulated (Jana) structures running in text mode*

**1996** Jana96

*Modulated and 3d structures in one program. Graphical interface for DOS and UNIX X11*

Michal Dušek



**1998** Jana98

*Improved Jana96. First widely used version. Graphical interface for DOS, DOS emulation and UNIX X11*



Lukáš Palatinus

**2000** Jana2000

*Support for powder data and multiphase refinement. Graphical interface for Win32 and UNIX X11*

**2006** Jana2006

*Combination of data sources, **magnetic structures, and TOF data**. Dynamical allocation of memory. Only for Windows*

***2021** Jana2020*

*Development of an interactive and graphical interface*



Jan Rohliček



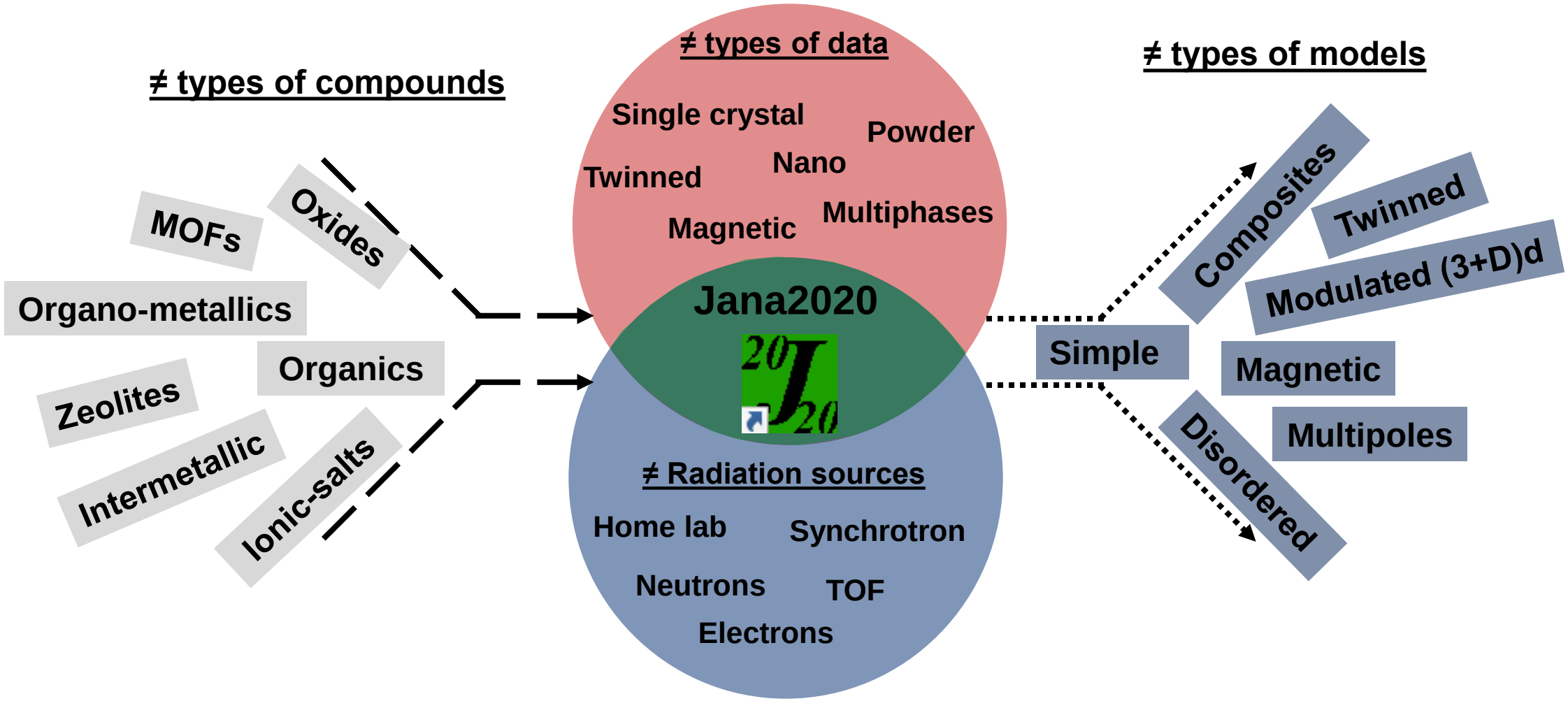
Jakub Plašil



Margarida Henriques

FZU Institute of Physics of the Czech Academy of Sciences

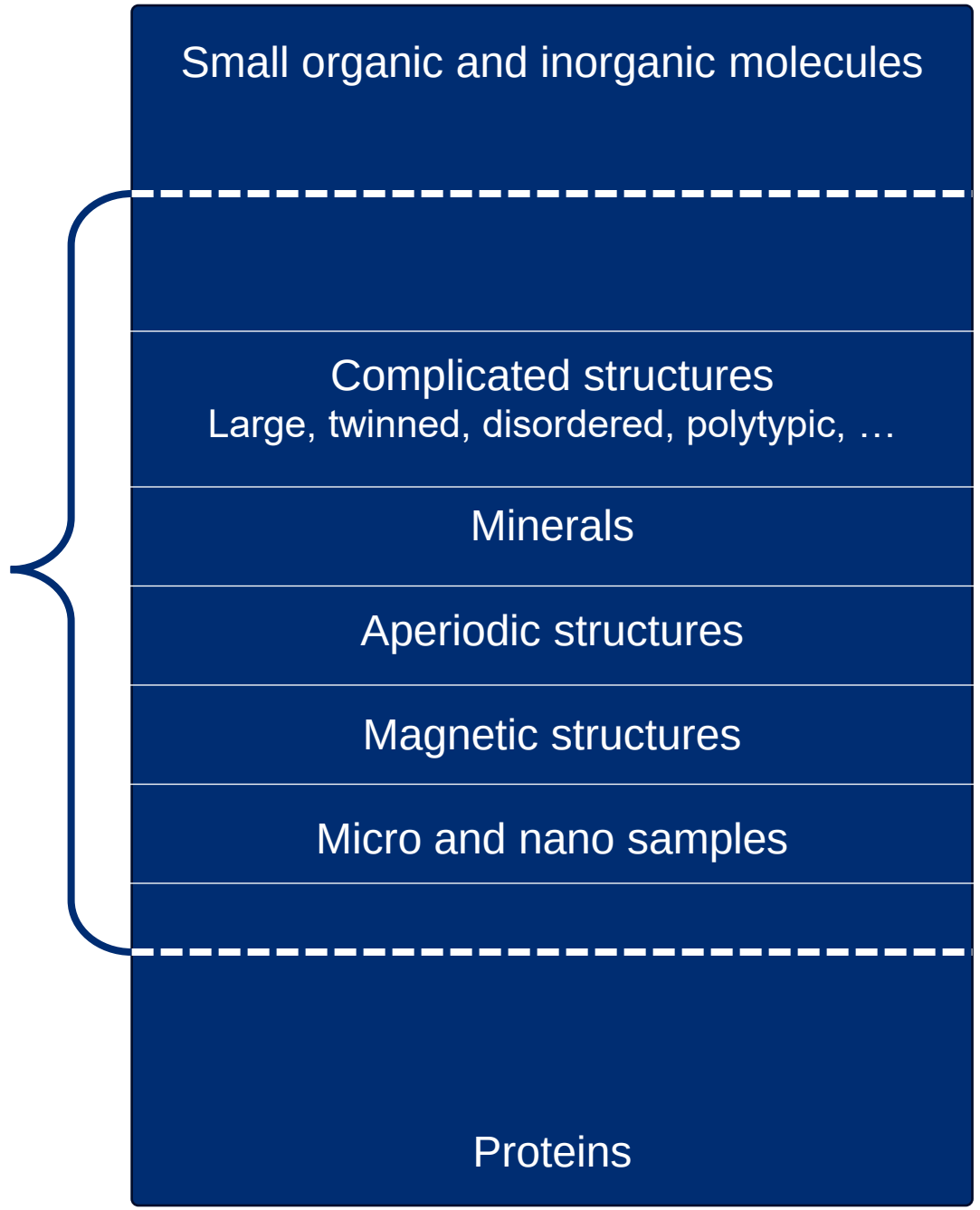
# What the program offers



# Topics

Basic crystallography

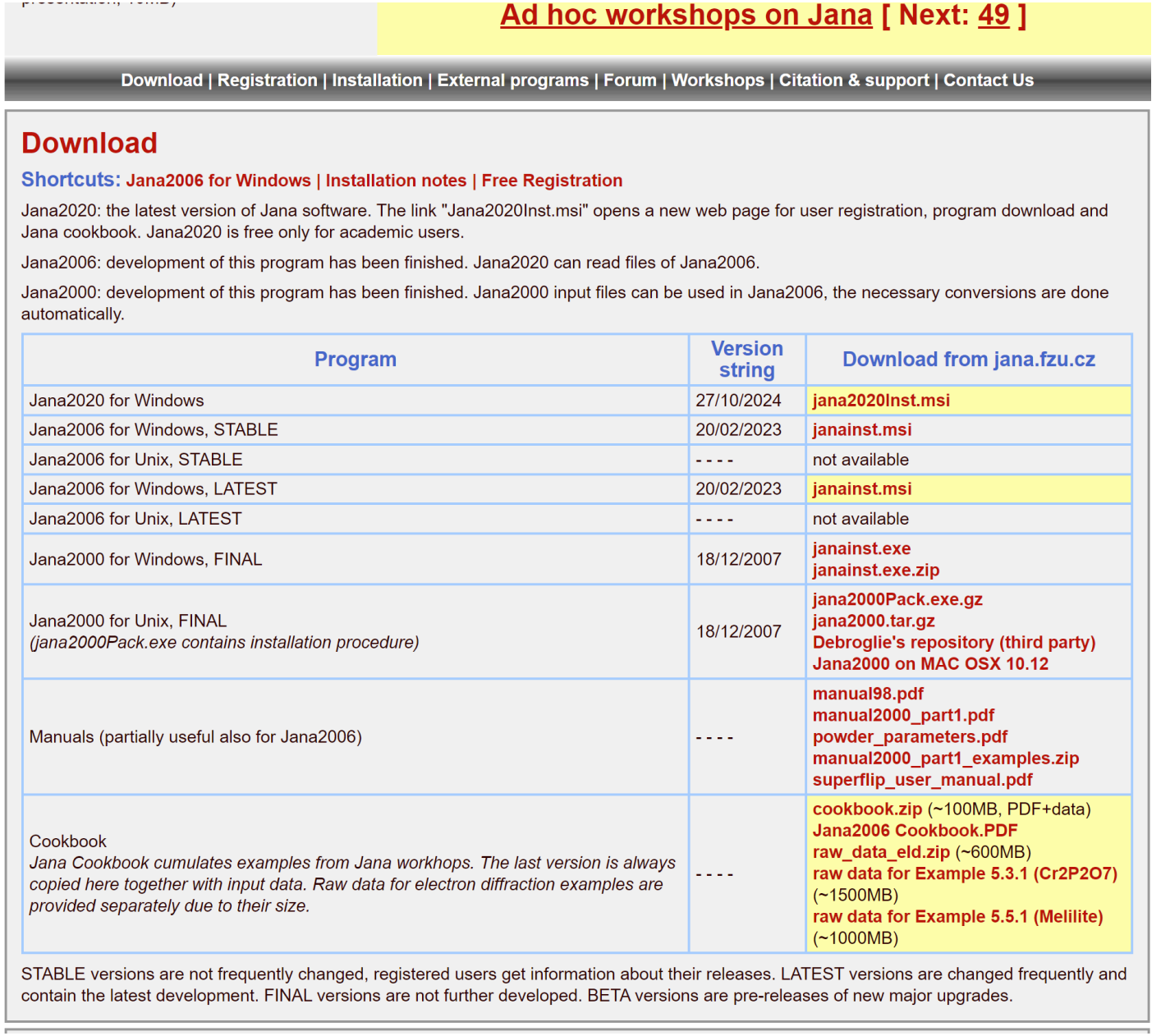
Advanced tools
Commensurate structures
Incommensurate structures
Composite structures
Magnetic structures



# Where to get it

**http://jana.fzu.cz/**

Registration
Download
Installation



Ad hoc workshops on Jana [ Next: 49 ]

Download | Registration | Installation | External programs | Forum | Workshops | Citation & support | Contact Us

## Download

**Shortcuts:** Jana2006 for Windows | Installation notes | Free Registration

Jana2020: the latest version of Jana software. The link "Jana2020Inst.msi" opens a new web page for user registration, program download and Jana cookbook. Jana2020 is free only for academic users.

Jana2006: development of this program has been finished. Jana2020 can read files of Jana2006.

Jana2000: development of this program has been finished. Jana2000 input files can be used in Jana2006, the necessary conversions are done automatically.

| Program | Version string | Download from jana.fzu.cz |
|---|---|---|
| Jana2020 for Windows | 27/10/2024 | jana2020Inst.msi |
| Jana2006 for Windows, STABLE | 20/02/2023 | janainst.msi |
| Jana2006 for Unix, STABLE | - - - - | not available |
| Jana2006 for Windows, LATEST | 20/02/2023 | janainst.msi |
| Jana2006 for Unix, LATEST | - - - - | not available |
| Jana2000 for Windows, FINAL | 18/12/2007 | janainst.exe<br>janainst.exe.zip |
| Jana2000 for Unix, FINAL<br>*(jana2000Pack.exe contains installation procedure)* | 18/12/2007 | jana2000Pack.exe.gz<br>jana2000.tar.gz<br>Debroglie's repository (third party)<br>Jana2000 on MAC OSX 10.12 |
| Manuals (partially useful also for Jana2006) | - - - - | manual98.pdf<br>manual2000_part1.pdf<br>powder_parameters.pdf<br>manual2000_part1_examples.zip<br>superflip_user_manual.pdf |
| Cookbook<br>*Jana Cookbook cumulates examples from Jana workhops. The last version is always copied here together with input data. Raw data for electron diffraction examples are provided separately due to their size.* | - - - - | cookbook.zip (~100MB, PDF+data)<br>Jana2006 Cookbook.PDF<br>raw_data_eld.zip (~600MB)<br>raw data for Example 5.3.1 (Cr2P2O7) (~1500MB)<br>raw data for Example 5.5.1 (Melilite) (~1000MB) |

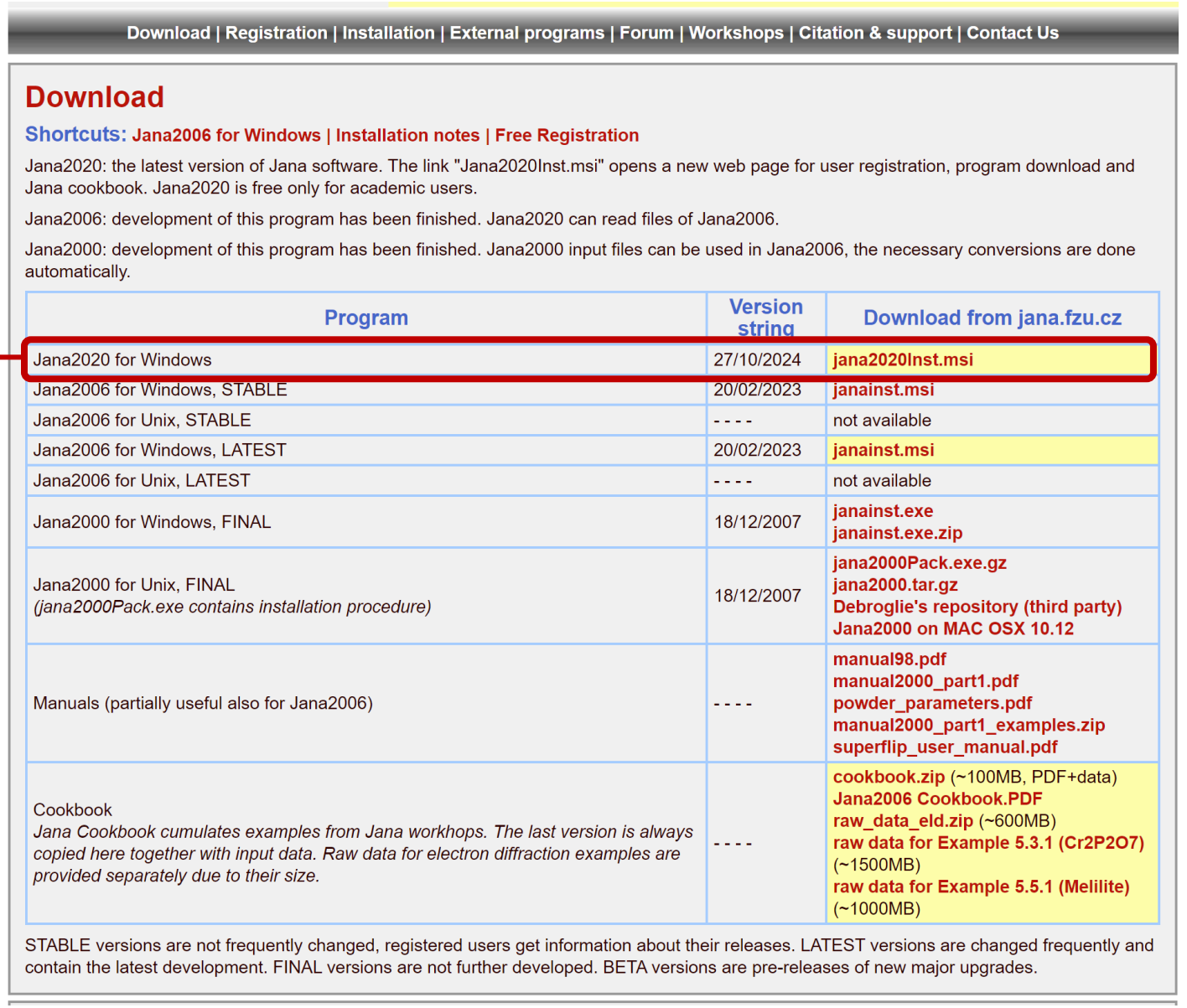
STABLE versions are not frequently changed, registered users get information about their releases. LATEST versions are changed frequently and contain the latest development. FINAL versions are not further developed. BETA versions are pre-releases of new major upgrades.

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# Where to get it

**https://jana-login.fzu.cz/jana2020**

Registration
Download
Installation



Download | Registration | Installation | External programs | Forum | Workshops | Citation & support | Contact Us

## Download

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| Program | Version string | Download from jana.fzu.cz |
|---|---|---|
| Jana2020 for Windows | 27/10/2024 | jana2020Inst.msi |
| Jana2006 for Windows, STABLE | 20/02/2023 | janainst.msi |
| Jana2006 for Unix, STABLE | - - - - | not available |
| Jana2006 for Windows, LATEST | 20/02/2023 | janainst.msi |
| Jana2006 for Unix, LATEST | - - - - | not available |
| Jana2000 for Windows, FINAL | 18/12/2007 | janainst.exe<br>janainst.exe.zip |
| Jana2000 for Unix, FINAL<br>*(jana2000Pack.exe contains installation procedure)* | 18/12/2007 | jana2000Pack.exe.gz<br>jana2000.tar.gz<br>Debroglie's repository (third party)<br>Jana2000 on MAC OSX 10.12 |
| Manuals (partially useful also for Jana2006) | - - - - | manual98.pdf<br>manual2000_part1.pdf<br>powder_parameters.pdf<br>manual2000_part1_examples.zip<br>superflip_user_manual.pdf |
| Cookbook<br>*Jana Cookbook cumulates examples from Jana workhops. The last version is always copied here together with input data. Raw data for electron diffraction examples are provided separately due to their size.* | - - - - | cookbook.zip (~100MB, PDF+data)<br>Jana2006 Cookbook.PDF<br>raw_data_eld.zip (~600MB)<br>raw data for Example 5.3.1 (Cr2P2O7) (~1500MB)<br>raw data for Example 5.5.1 (Melilite) (~1000MB) |

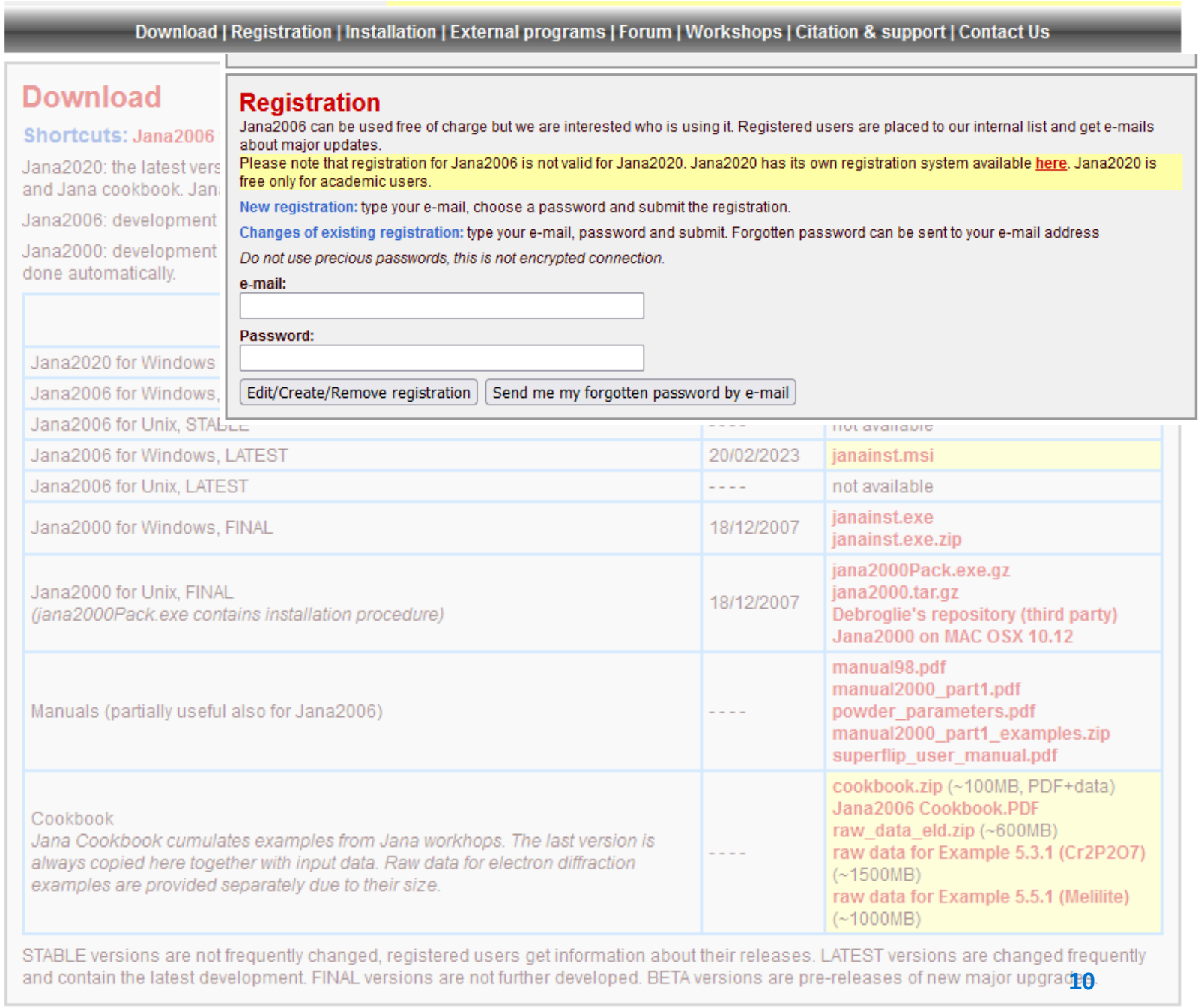
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# How to get it

**https://jana-login.fzu.cz/jana2020**

Registration



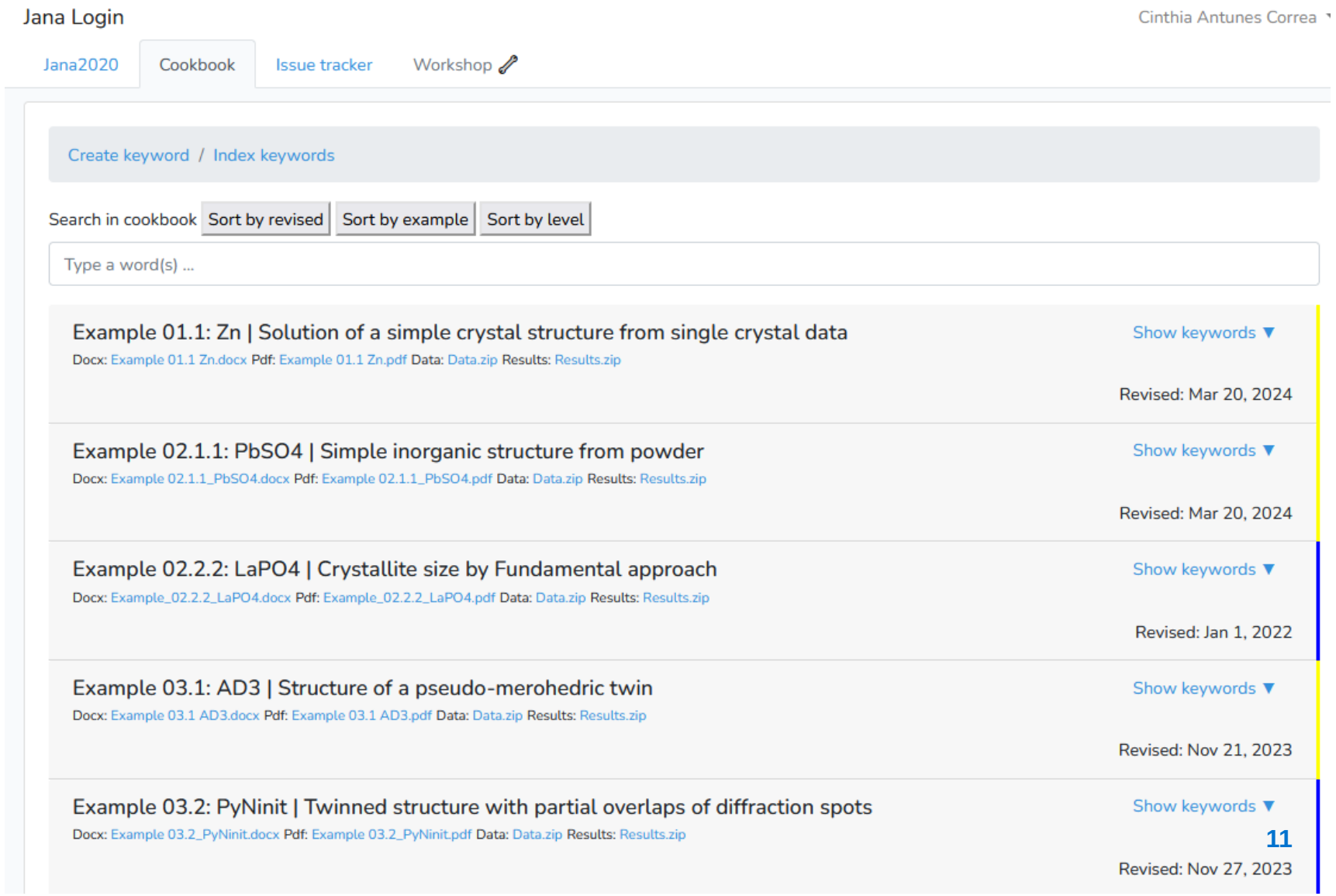

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# https://jana-login.fzu.cz/jana2020

Download

Install

Cookbook




FZU Institute of Physics of the Czech Academy of Sciences

# Where to get it

# http://jana.fzu.cz/

Workshops

## The 49th Ad Hoc Workshop on Jana Basics of Jana2020

12-13 December 2024
Institute of Physics, Cukrovarnicka 10, Prague, Czech Republic

### Program

The program is composed of four sessions. Each session starts with a lecture and continues with practical exercises. For practical exercises, the users will be provided with a cookbook, installation files and necessary data. Installation of all necessary software will be done at the beginning of the workshop. Please let us know in advance if you cannot come with a notebook.

**For this workshop a preliminary experience with Jana2006/Jana2020 is not needed.**

**The workshop is OFF LINE.**

Schedule of the workshop (Prague time, i.e. GMT+1):
(The schedule can be adjusted according to the wishes of the participants)

**Day 1**, 9:00-12:00, Standard structures
Lecture: Introduction to Jana2020
**Day 1**, 13:00-18:00, Powders
Lecture: Powder option in Jana2020
**Day 2**, 9:00-12:00, Twinning and disorder
Lecture: Twinning and disorder
**Day 2**, 13:00-18:00, Modulated structures
Lecture: Modulated structures and their solution in Jana2020

### Computers

**Each participant will need a laptop or PC with operating system Windows10/11, with Administration rights. The minimum screen resolution is FullHD (1920x1080 pixels).** Installation of all necessary software will be done at the beginning of the workshop.

### Workshop cookbook

Participants will be provided with the latest version of the Jana2020 Cookbook and its printed chapters related to the workshop examples. The Cookbook cumulates detailed instructions for all examples presented so far in some of Jana2020 workshops.

### Participants

| | |
|---|---|
| 1 | Zhansaule Bagindyk, Kazakhstan |
| 2 | Rakhat Agassultanov, Kazakhstan |
| 3 | Maksat Karlykan, Kazakhstan |
| 4 | Jamil Flores Gonzales, Czechia |

### Connection to on line workshop

No online connection

### Organizers

The workshop is organized by Department of structure analysis at the Institute of Physics and Special interest group on aperiodic crystals at ECA.

### Transportation

*Institute of Physics has two buildings 15 km apart! Make sure you are travelling to proper building at Cukrovarnicka street 10, Prague 6.*

**Taxi:** We recommend using **AAA taxi**. Yellow cars are located in front of the Vaclav Havel airport terminals.

**Public transport:** Connections can be found at the **DPP web page**. The target stations Sibeliova or Vozovna Stresovice are within 150 m from the institute.

### Acommodation

For accomodation, we recommend several hotels withing walking distance to the institute:

**Hotel U Sladku**
**Hotel Pyramida**
**Hotel Marketa**

### Lunches and coffee breaks

Lunches in the Institute's canteen and coffee breaks are paid for by the Department of Structure Analysis. Lunches must be ordered in advance, participants will be contacted before the seminar.

### Fees

There are no registration fees for Jana workshops. Consequently, no financial support can be provided.

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# Software distributed with Jana2020

- Superflip – structure solution by charge flipping
- Dyngo – reflection intensities from the dynamical theory of diffraction
- Marching cube - isosurfaces

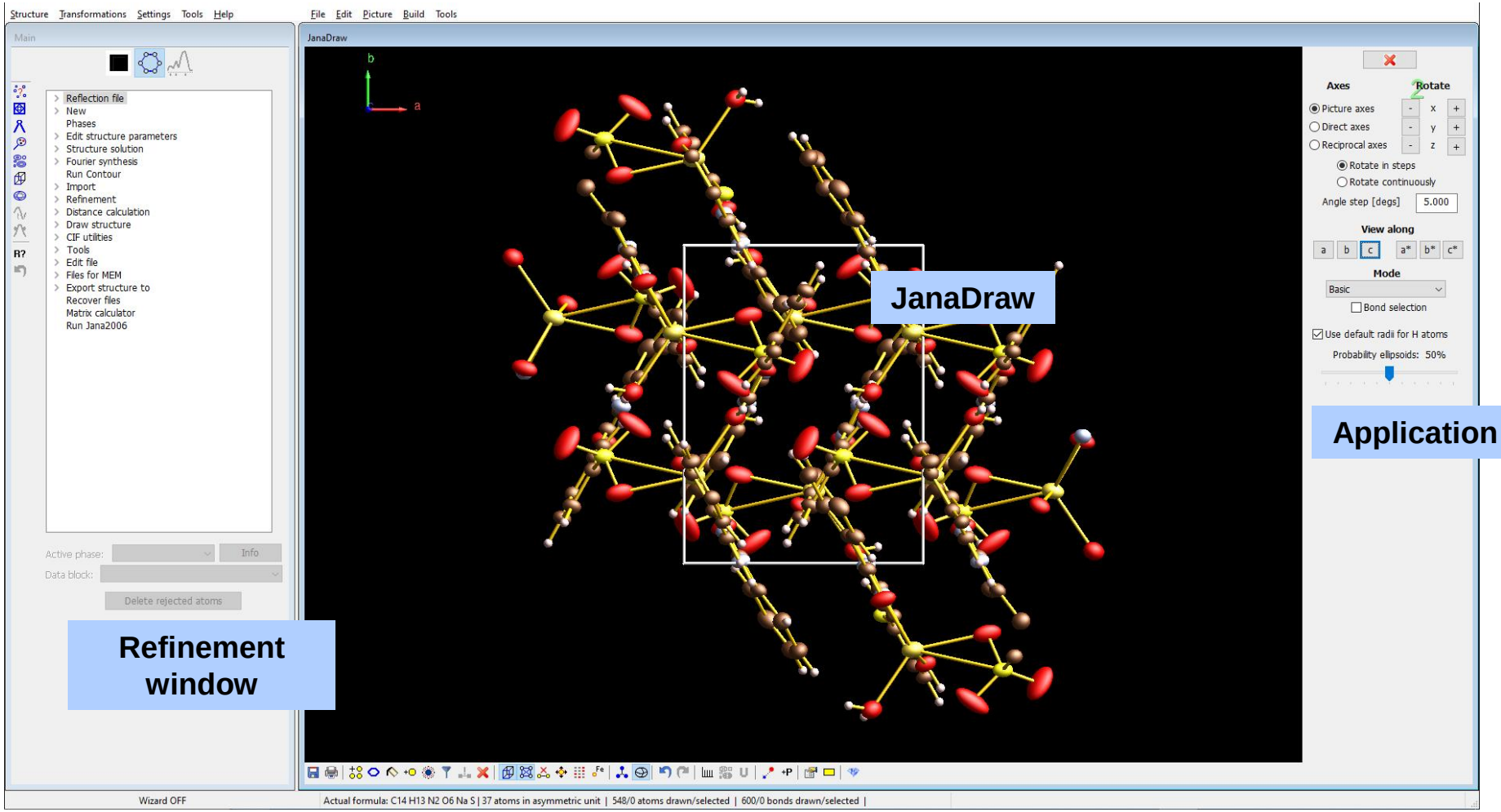
# Software that can be launched from Jana2020

- Plotting programs (Diamond, Mercury, Vesta …. )
- Structure solution programs (SHELXT, SIRWARE)
- Bilbao crystallographic server
- ISODISTORT

# Jana2020 Interface

Left pane

Right pane



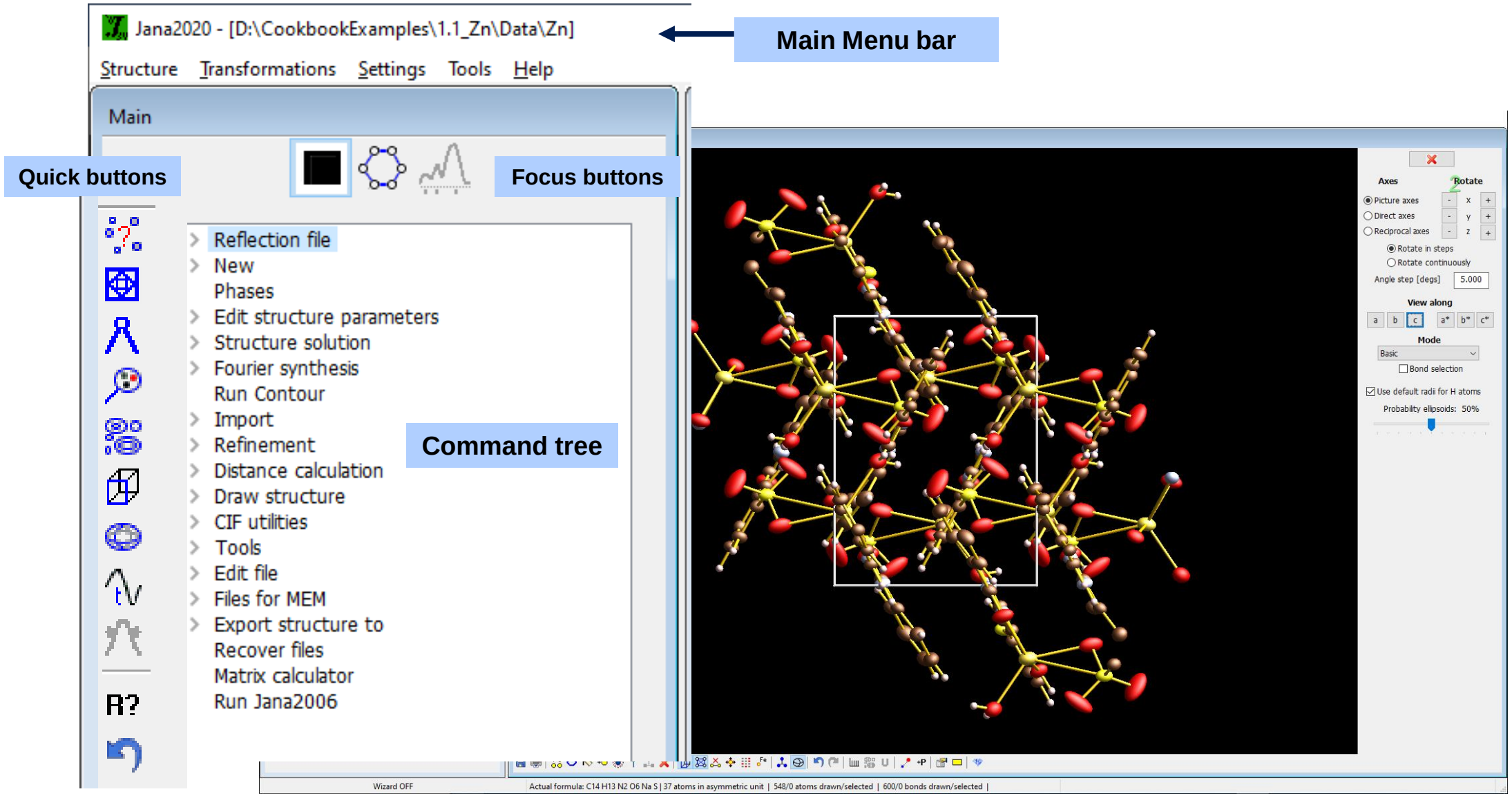

JanaDraw

Refinement window

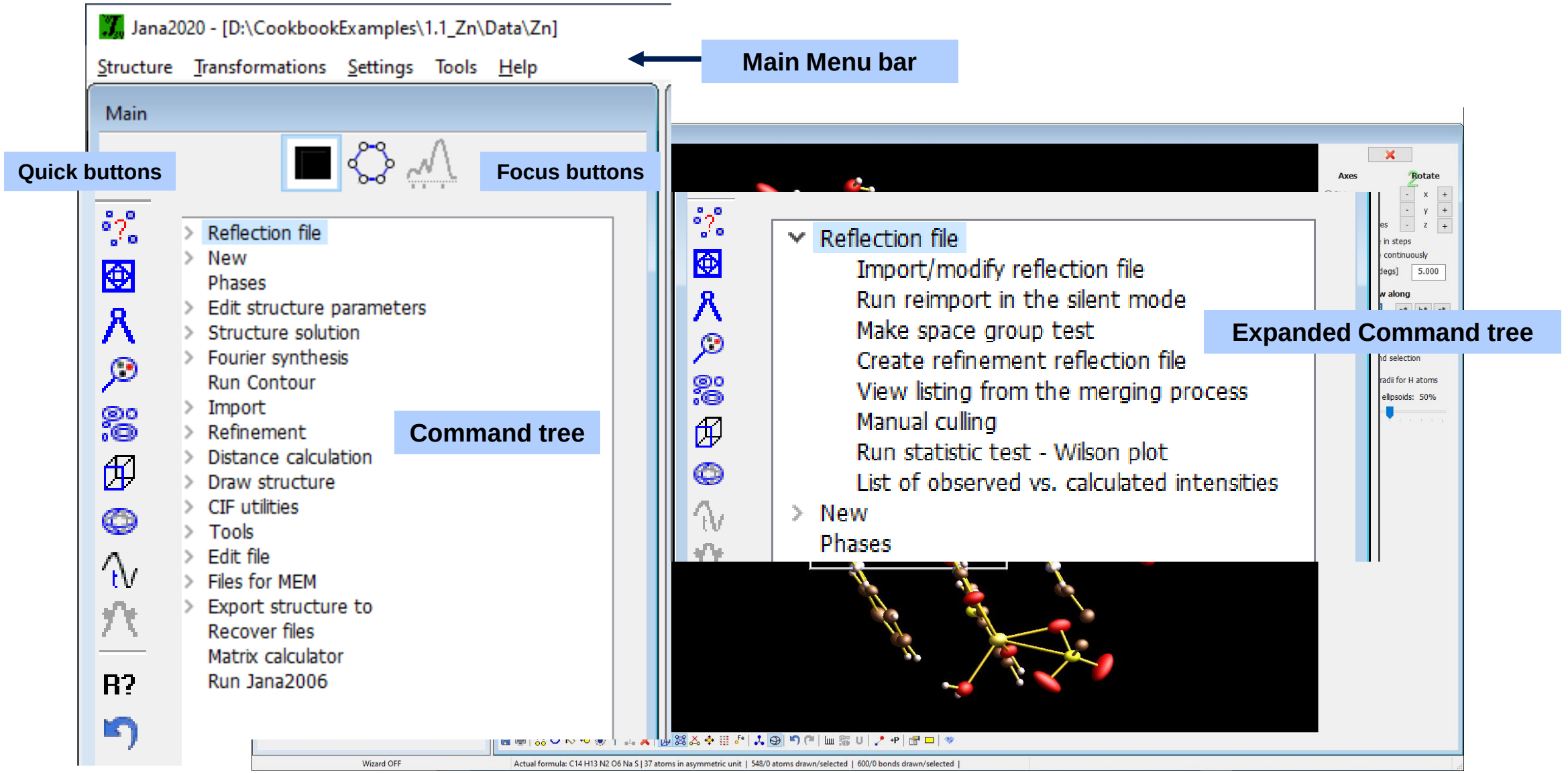
Application controls

Lower toolbar

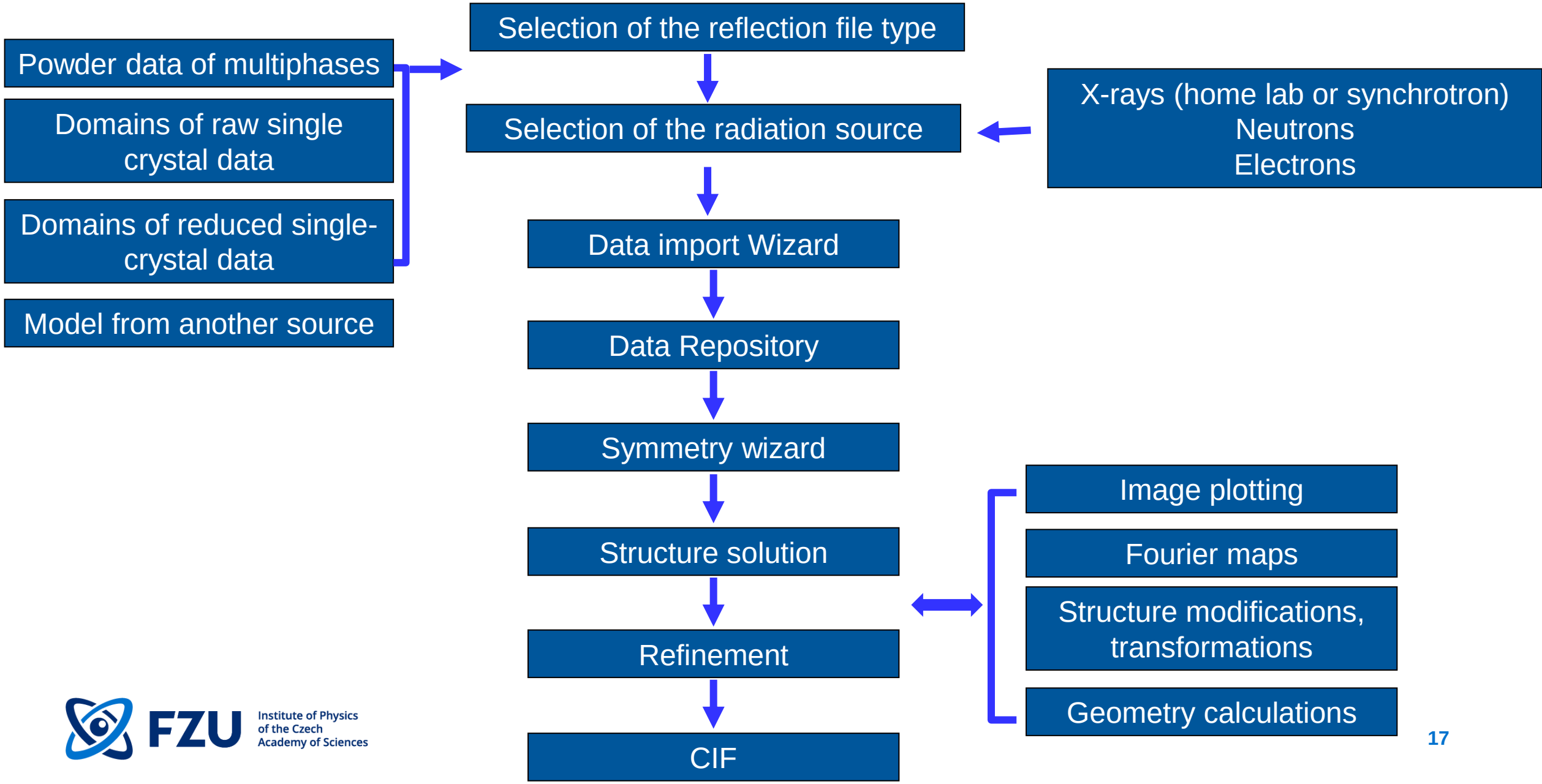
# Jana2020 Interface



# Jana2020 Interface



# Software flow scheme



# Software flow scheme and files created

*Reading of one or more data sets*

Data import Wizard

**M50** – basic crystal information, form factors, program options
**M95** – data repository

*Determining symmetry, merging symmetry equivalent reflections, absorption correction*
*Refinement of powder profile parameters*

Symmetry wizard

**M90 –** refinement reflection file

*Solution by Superflip or by calling external programs*

Structure solution

**M40 –** structure model
**M41 –** powder profile parameters

*JanaDraw*

Refinement

**Jdhst –** graphical parameters

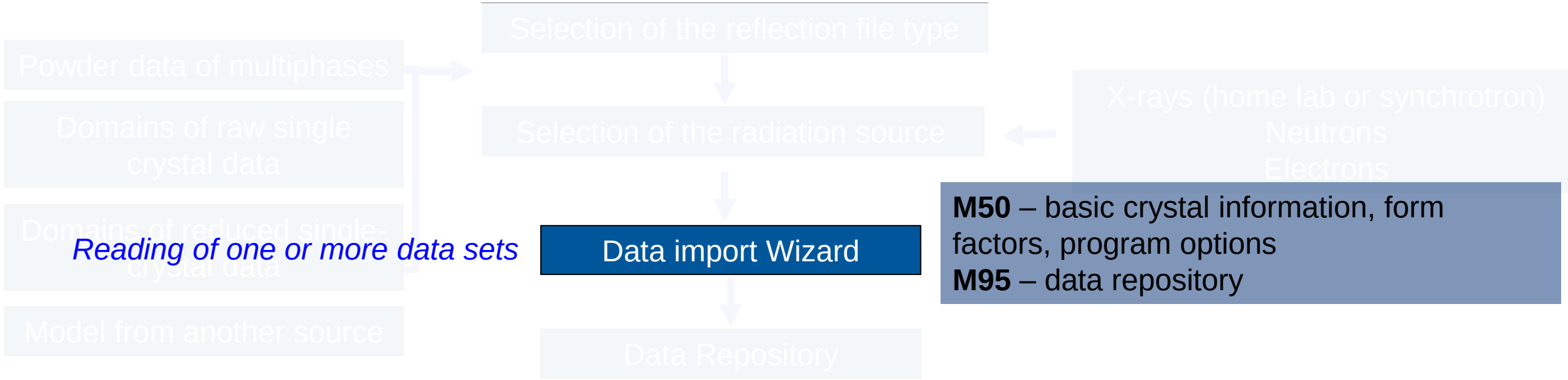
**ref** – refinement parameters

CIF

Plotting, geometry parameters, Fourier maps

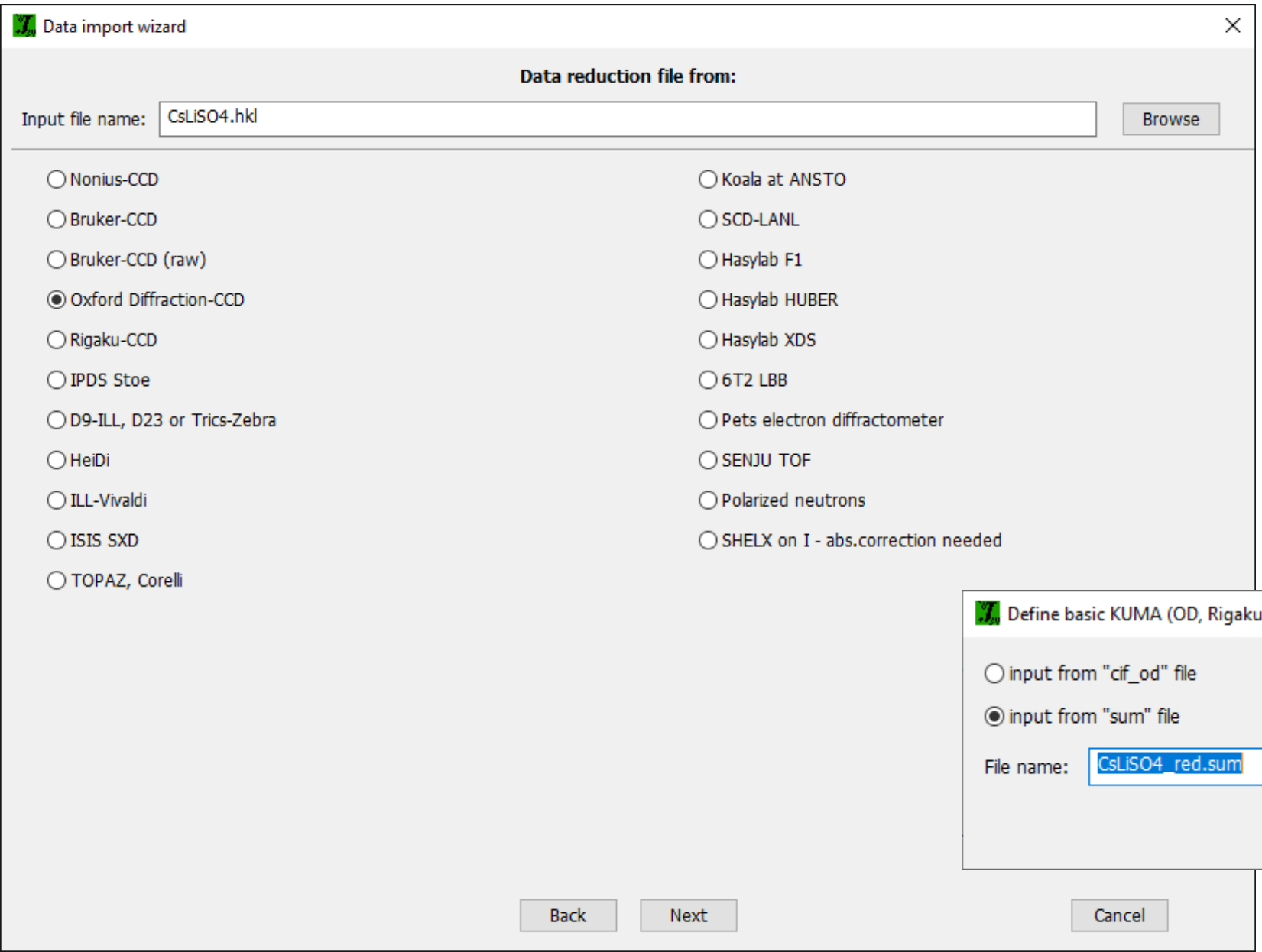
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# Software flow scheme and files created



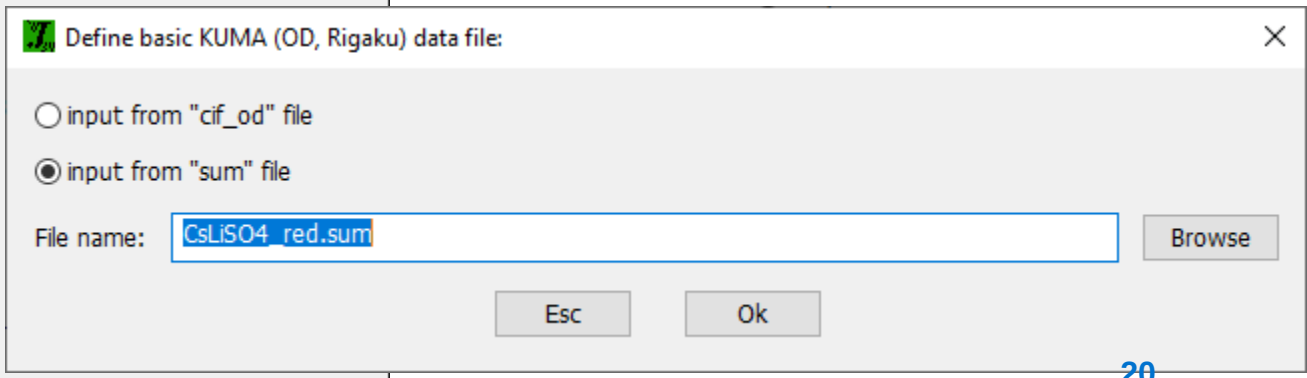
# Data import wizard

**Input data: single crystal, powder, TOF**

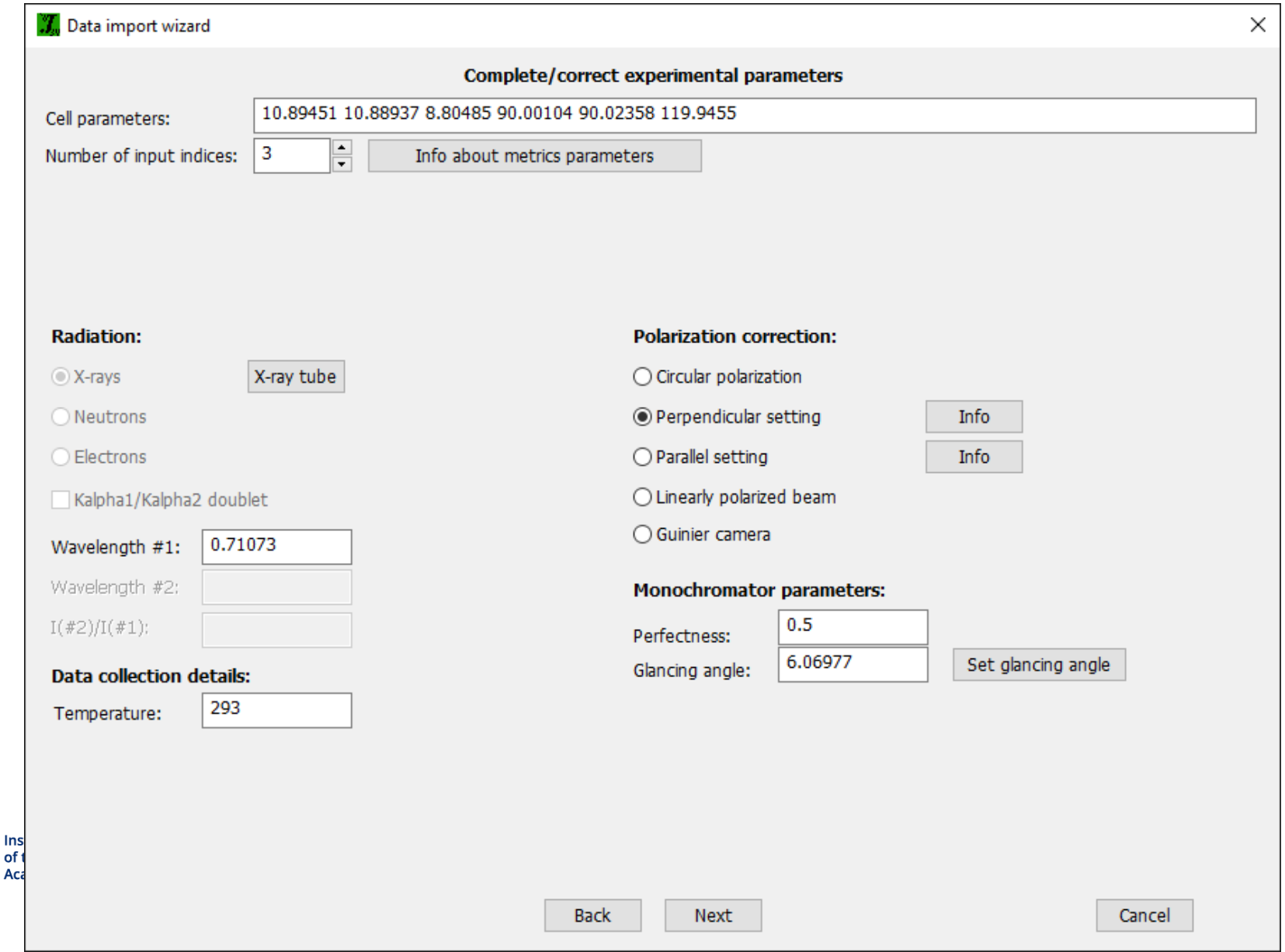



- **Conventional lab XRD**
- **Synchrotron sources**
- **Neutron sources**
- **Electron diffraction (kinematical and dynamic approaches)**

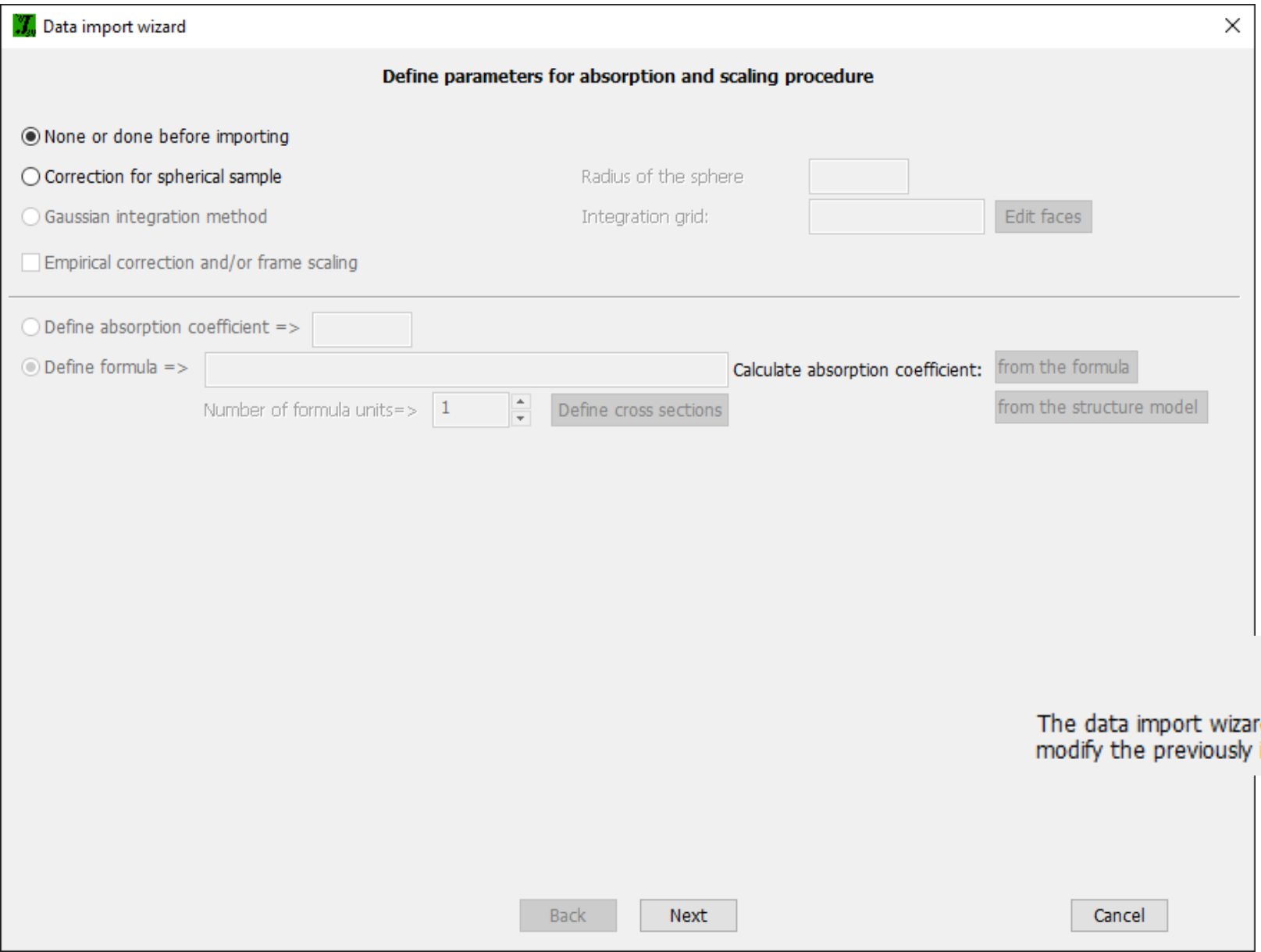
**Data from different sources can be combined during refinements.**

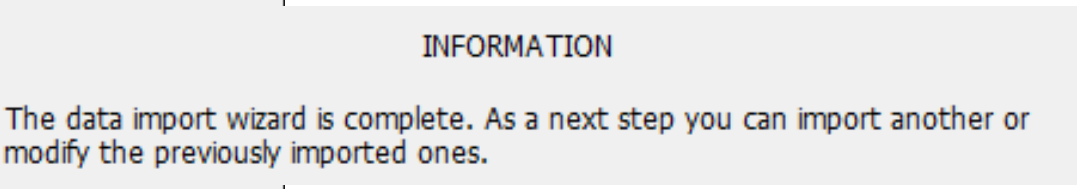


# Data import wizard

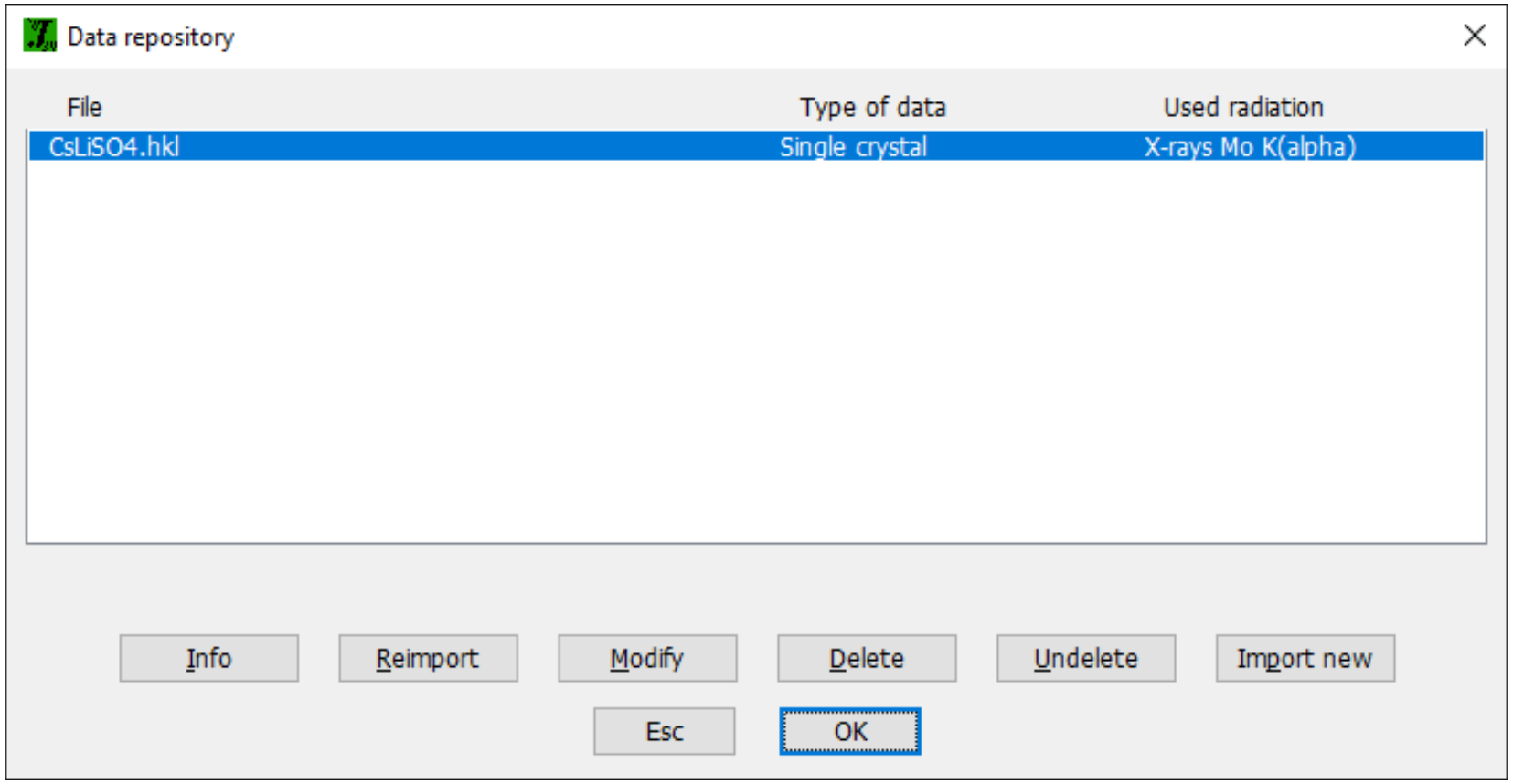


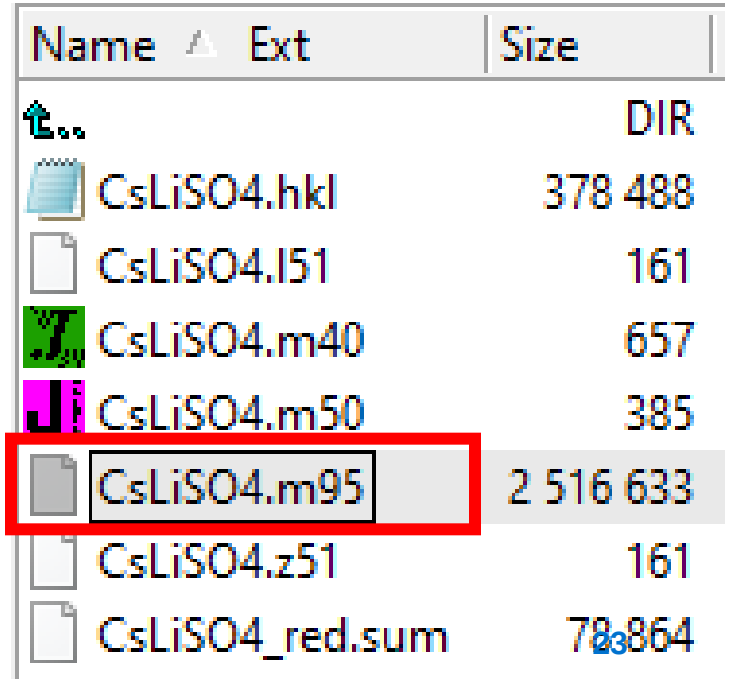
# Data import wizard



# Data import wizard




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# Software flow scheme and files created

Selection of the reflection file type

Powder data of multiphases

Domains of raw single crystal data

Selection of the radiation source

X-rays (home lab or synchrotron)
Neutrons
Electrons

Model from another source

*Determining symmetry, merging symmetry equivalent reflections, absorption correction*
*Refinement of powder profile parameters*

Symmetry wizard

**M90** refinement reflection file

Image plotting

# Symmetry wizard

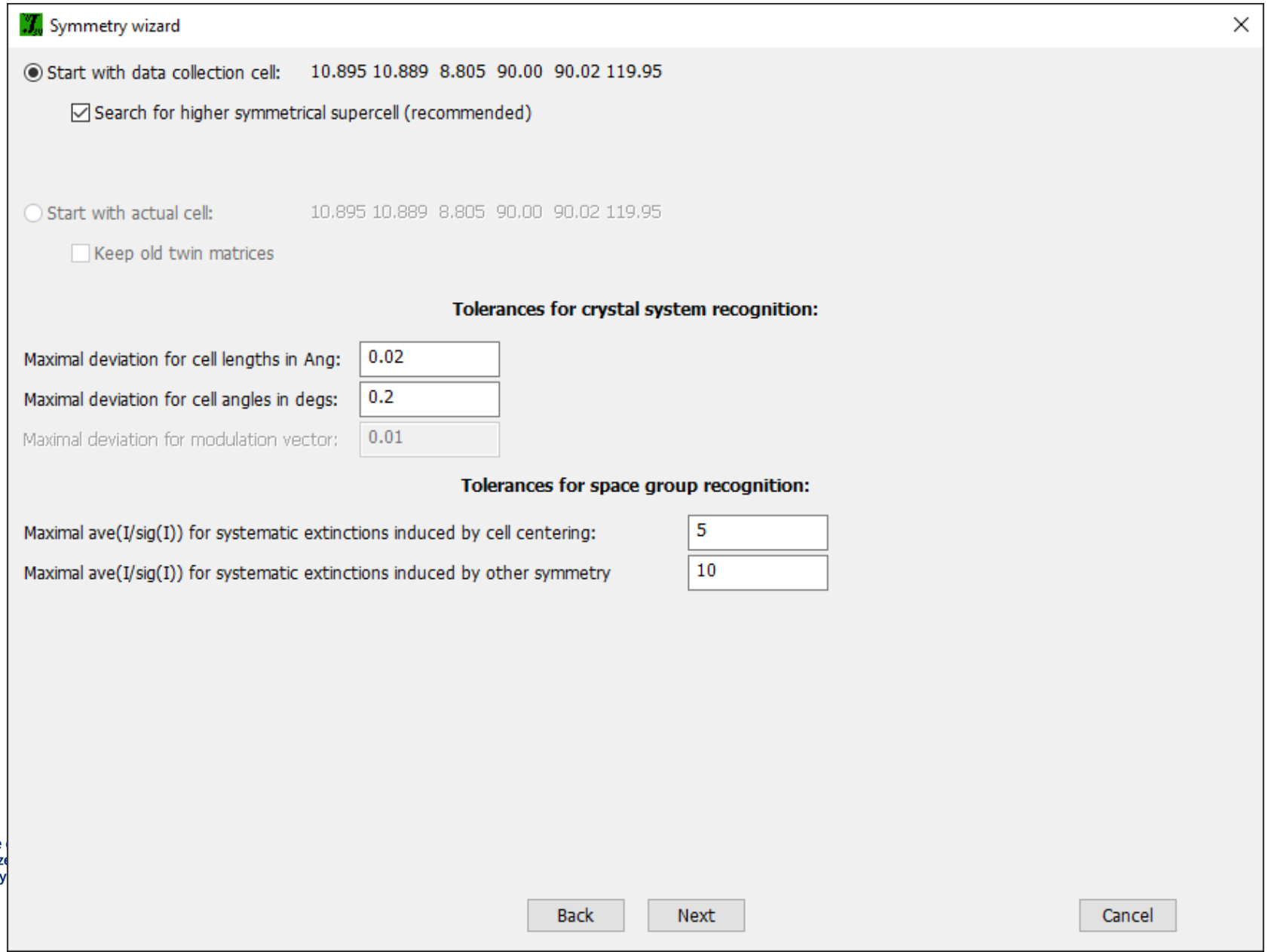
*Determining symmetry, merging symmetry equivalent reflections, absorption correction*
*Refinement of powder profile parameters*

- Superspace approach is implemented for (3+d) with  d=1,2,3 modulated systems
- It accepts any (reasonable) setting of space groups, including non-standard centering vectors
- Systematic extinctions are derived analytically
- It supports an interactive transformation to lower symmetry
- Local symmetry can be applied to individual atoms and also to (rigid body) groups
- All symmetry restrictions of structural parameters are derived analytically from symmetry operations and the actual position of the atom (magnetic and structural modulations)

# Symmetry wizard

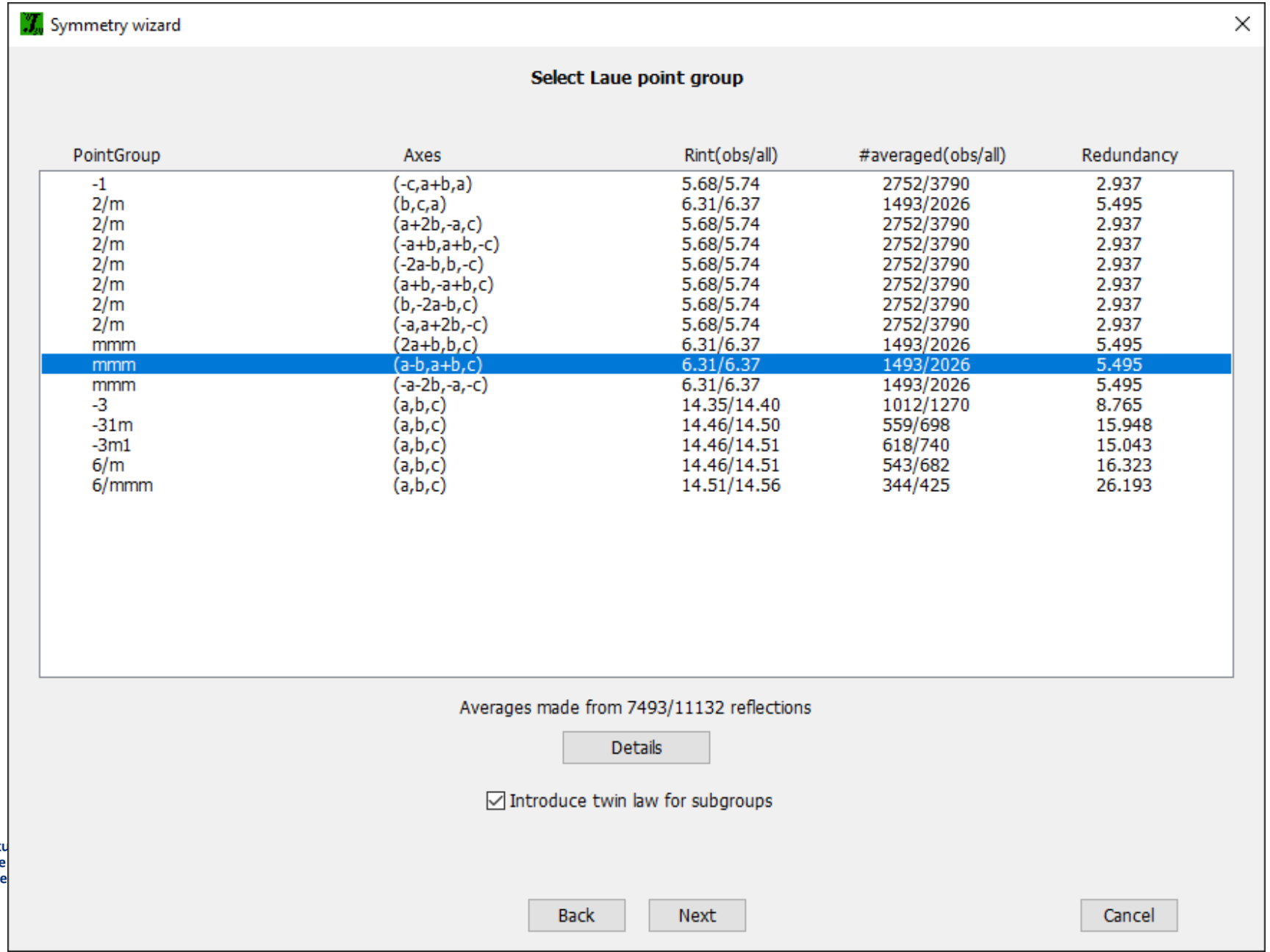


# Symmetry wizard



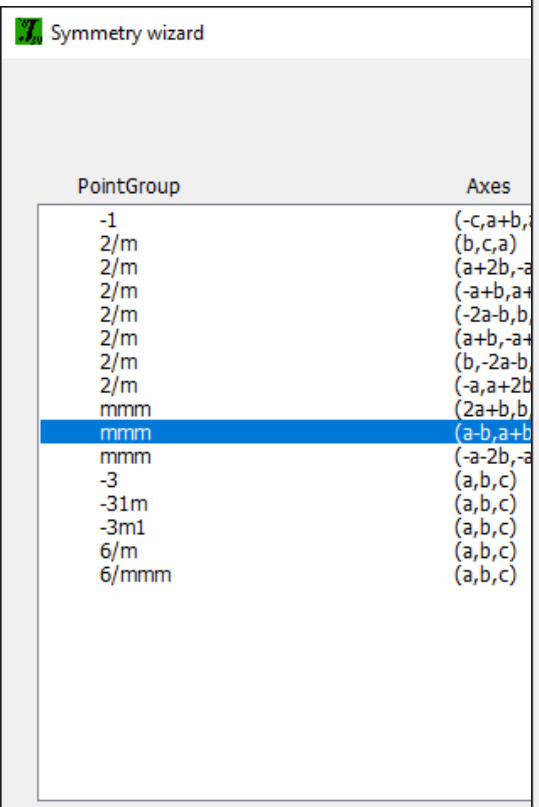

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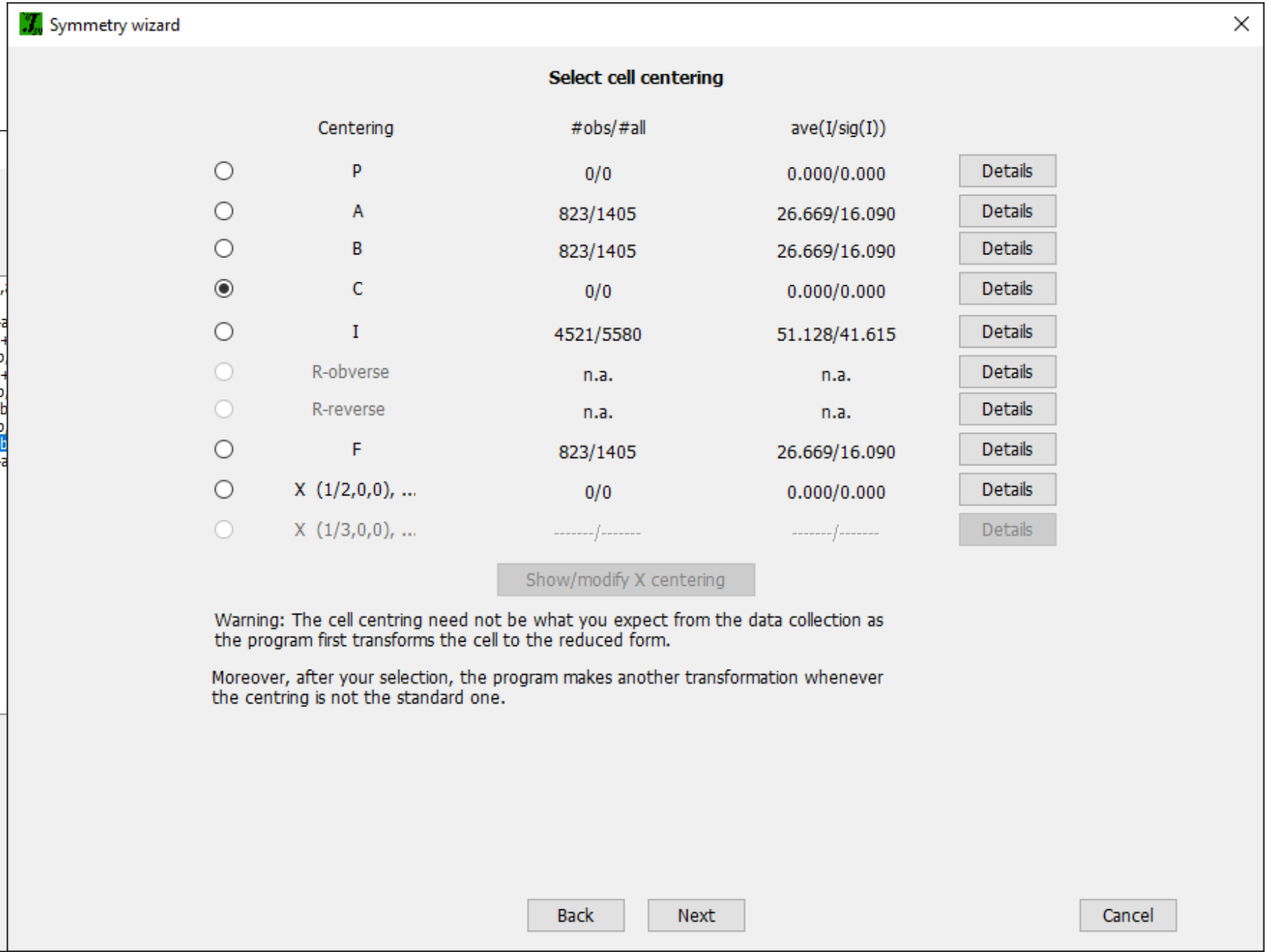
# Symmetry wizard



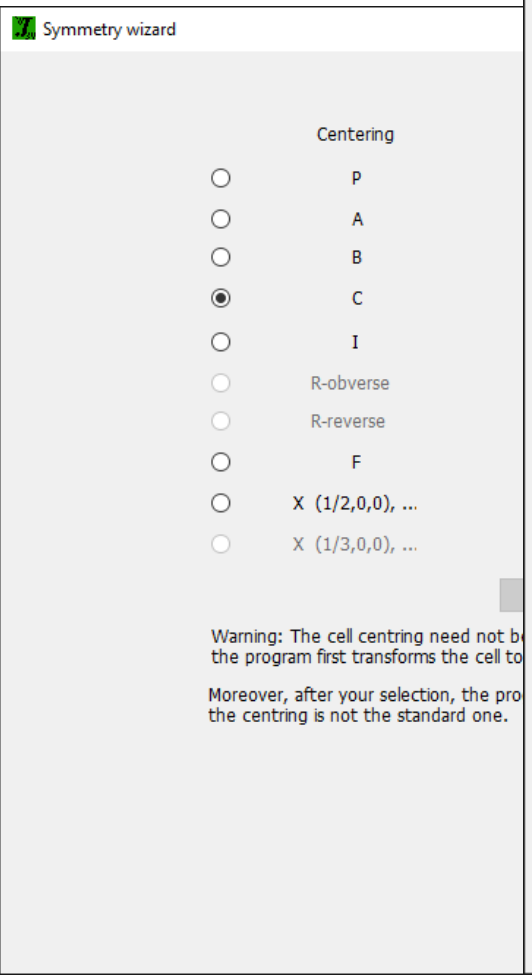

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# Symmetry wizard



# Symmetry wizard




Symmetry wizard

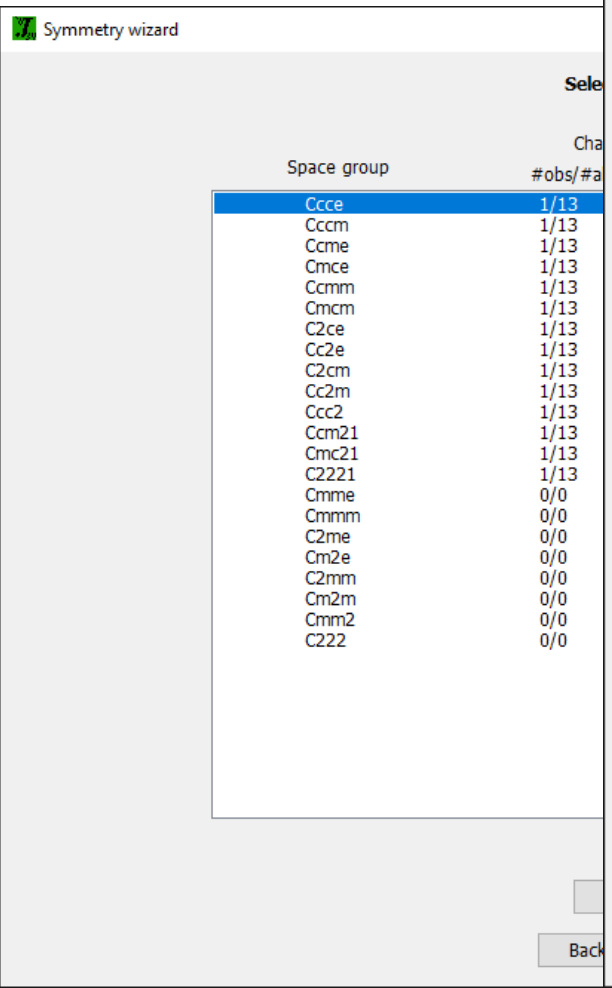
**Select space group**

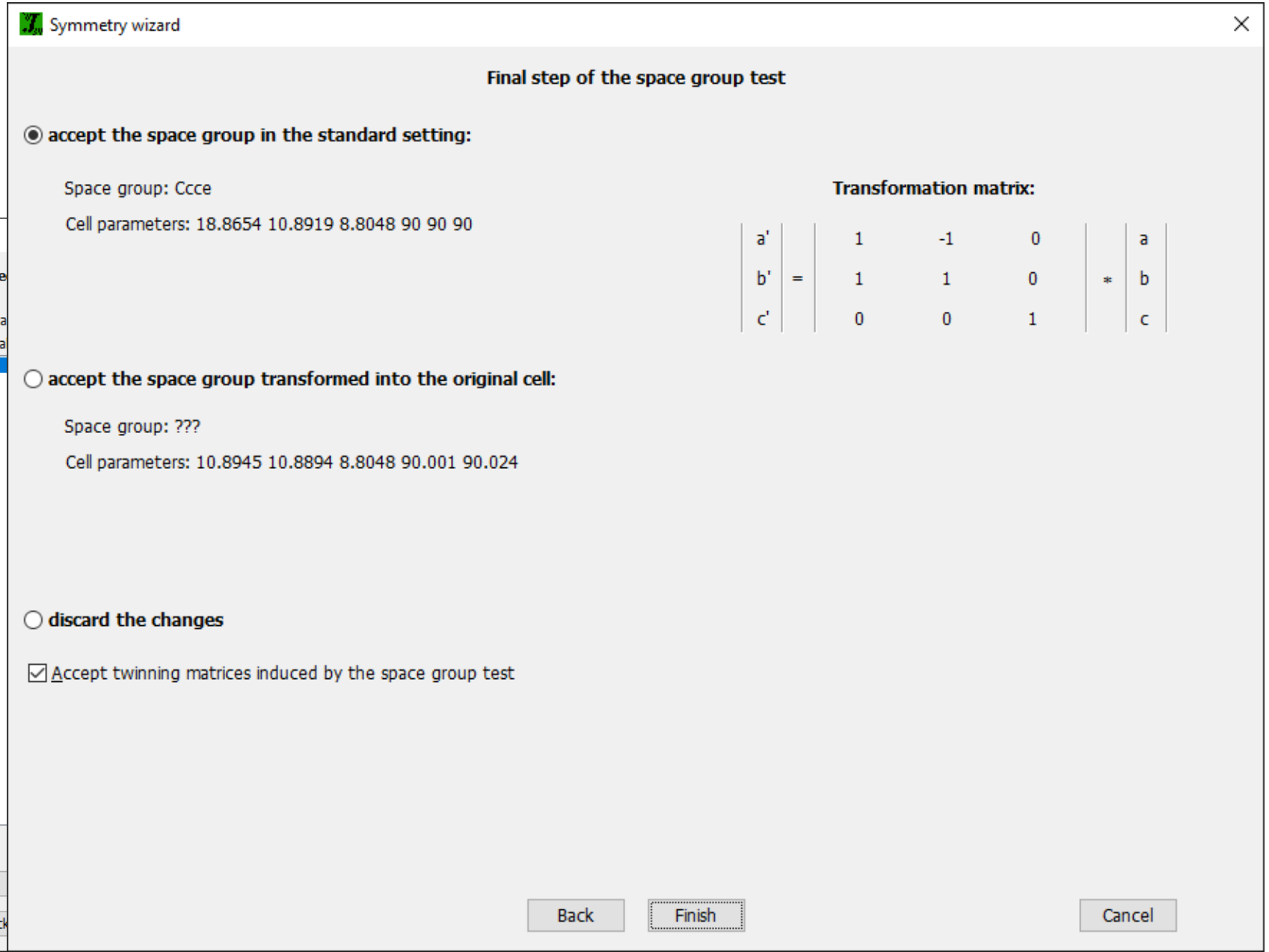
| Space group | Characteristics for systematically absent reflections | | |
|---|---|---|---|
| | #obs/#all | ave(I/sig(I)) | Figure of merit |
| Ccce | 1/13 | 4.308/1.108 | 0.17532 |
| Cccm | 1/13 | 4.308/1.108 | 0.17532 |
| Ccme | 1/13 | 4.308/1.108 | 0.17532 |
| Cmce | 1/13 | 4.308/1.108 | 0.17532 |
| Ccmm | 1/13 | 4.308/1.108 | 0.17532 |
| Cmcm | 1/13 | 4.308/1.108 | 0.17532 |
| C2ce | 1/13 | 4.308/1.108 | 0.17532 |
| Cc2e | 1/13 | 4.308/1.108 | 0.17532 |
| C2cm | 1/13 | 4.308/1.108 | 0.17532 |
| Cc2m | 1/13 | 4.308/1.108 | 0.17532 |
| Ccc2 | 1/13 | 4.308/1.108 | 0.17532 |
| Ccm21 | 1/13 | 4.308/1.108 | 0.17532 |
| Cmc21 | 1/13 | 4.308/1.108 | 0.17532 |
| C2221 | 1/13 | 4.308/1.108 | 0.17532 |
| Cmme | 0/0 | --------/-------- | 1.00000 |
| Cmmm | 0/0 | --------/-------- | 1.00000 |
| C2me | 0/0 | --------/-------- | 1.00000 |
| Cm2e | 0/0 | --------/-------- | 1.00000 |
| C2mm | 0/0 | --------/-------- | 1.00000 |
| Cm2m | 0/0 | --------/-------- | 1.00000 |
| Cmm2 | 0/0 | --------/-------- | 1.00000 |
| C222 | 0/0 | --------/-------- | 1.00000 |

Details

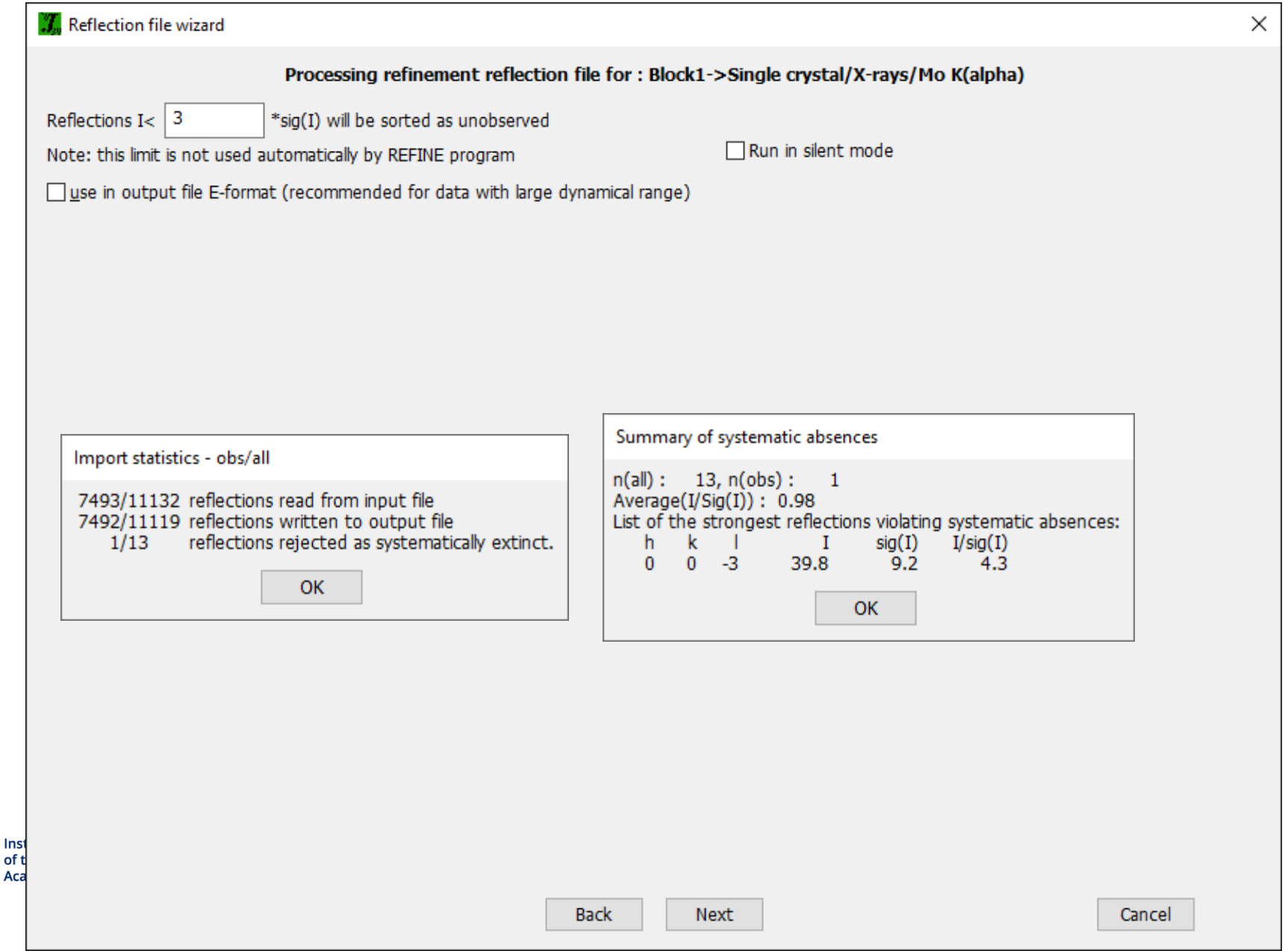
Back Next Cancel

# Symmetry wizard

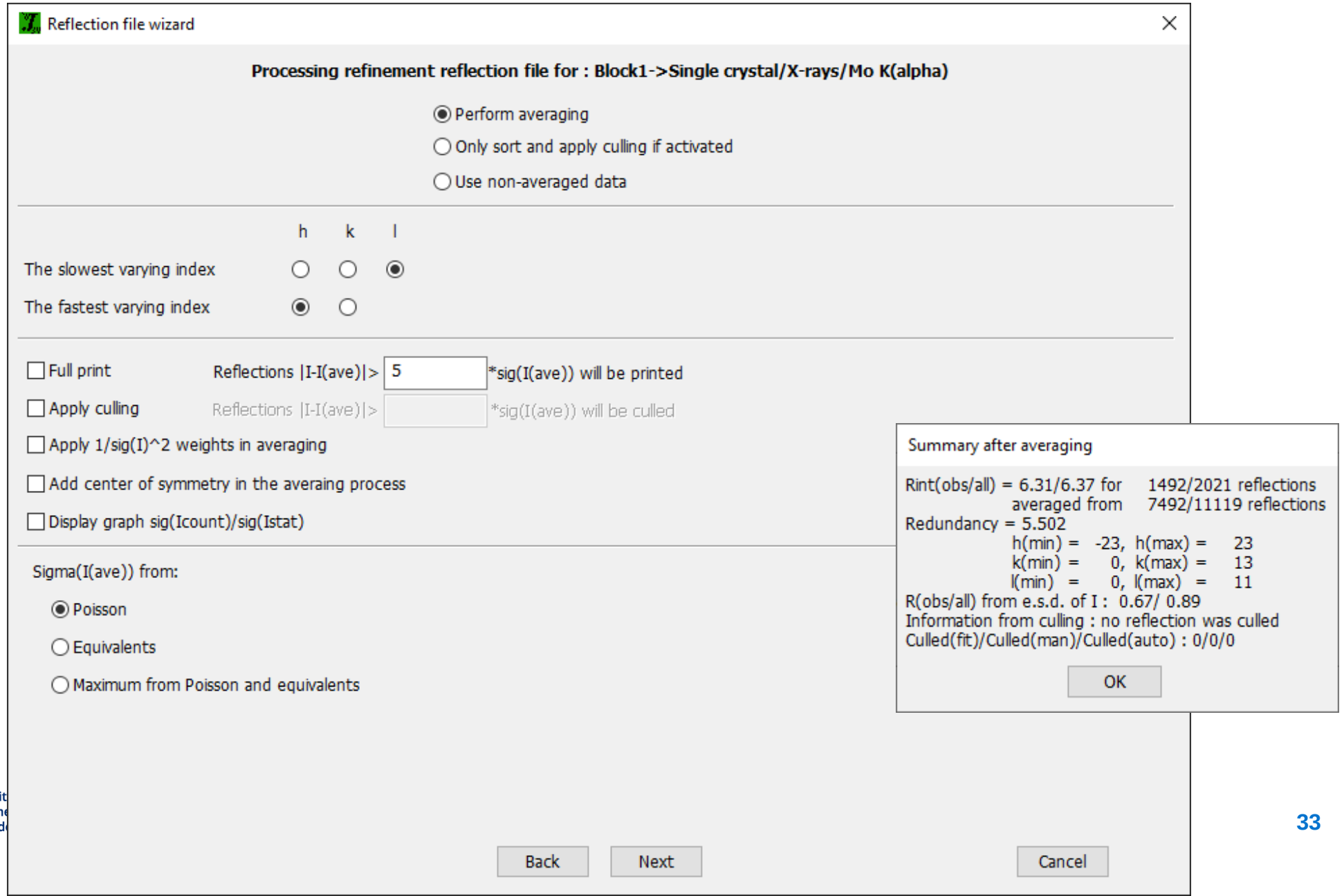


# Reflection file wizard

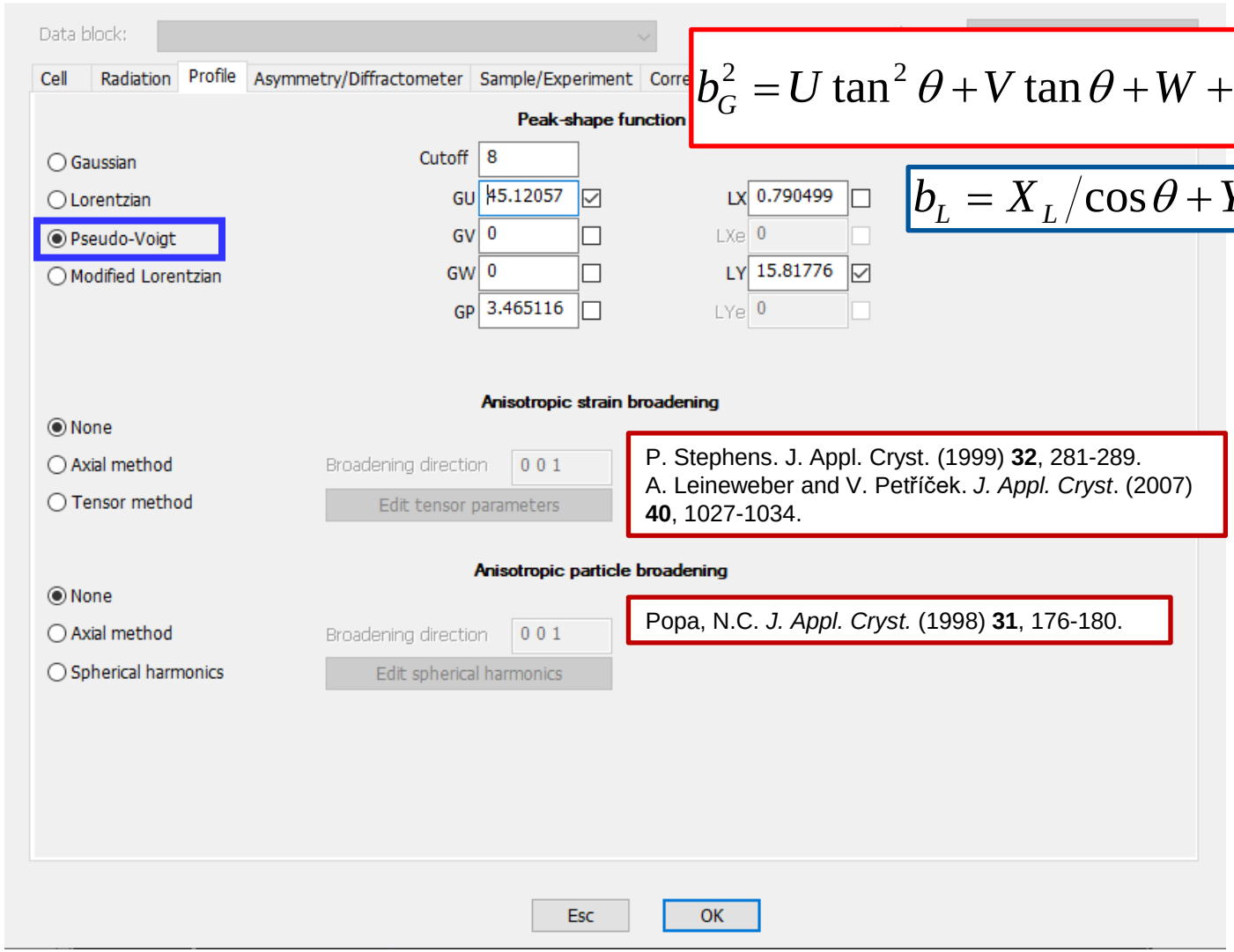


# Reflection file wizard



# Powder

$$pV(H,x) = \eta L(H,x) + (1-\eta)G(H,x)$$

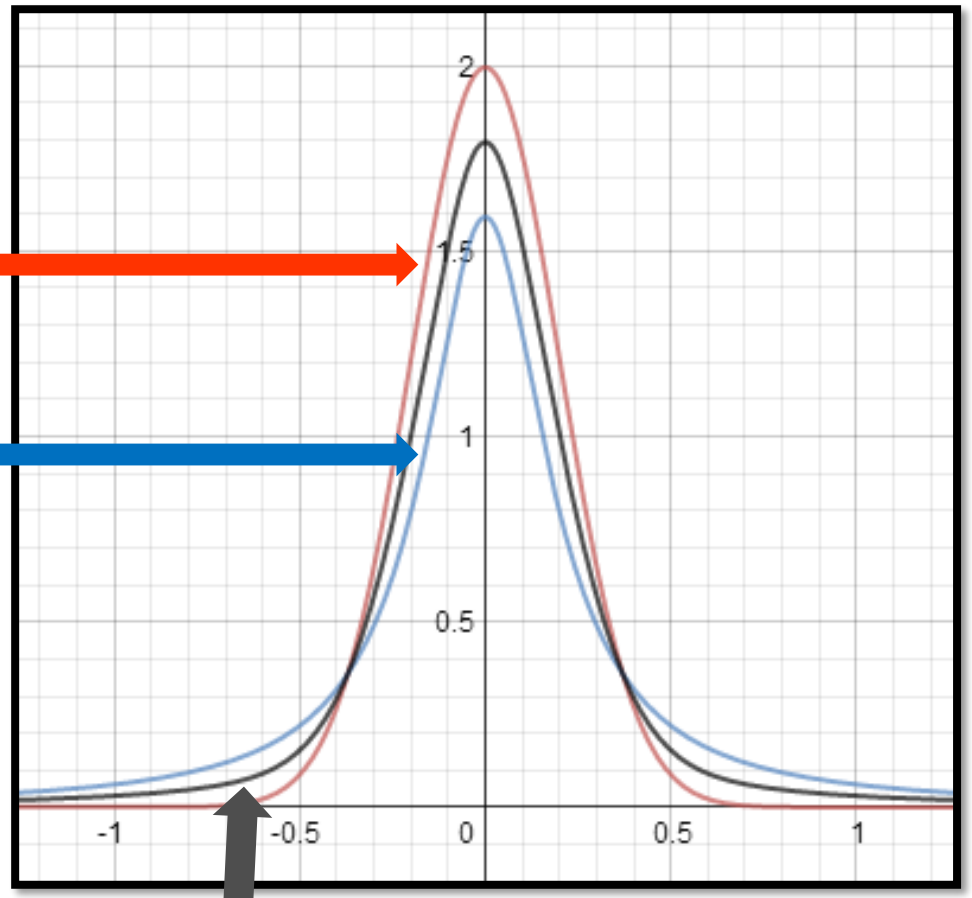



$$b_G^2 = U\tan^2\theta + V\tan\theta + W + \frac{P}{\cos^2\theta}$$

$$b_L = X_L/\cos\theta + Y_L\tan\theta$$

P. Stephens. J. Appl. Cryst. (1999) **32**, 281-289.
A. Leineweber and V. Petříček. *J. Appl. Cryst*. (2007) **40**, 1027-1034.

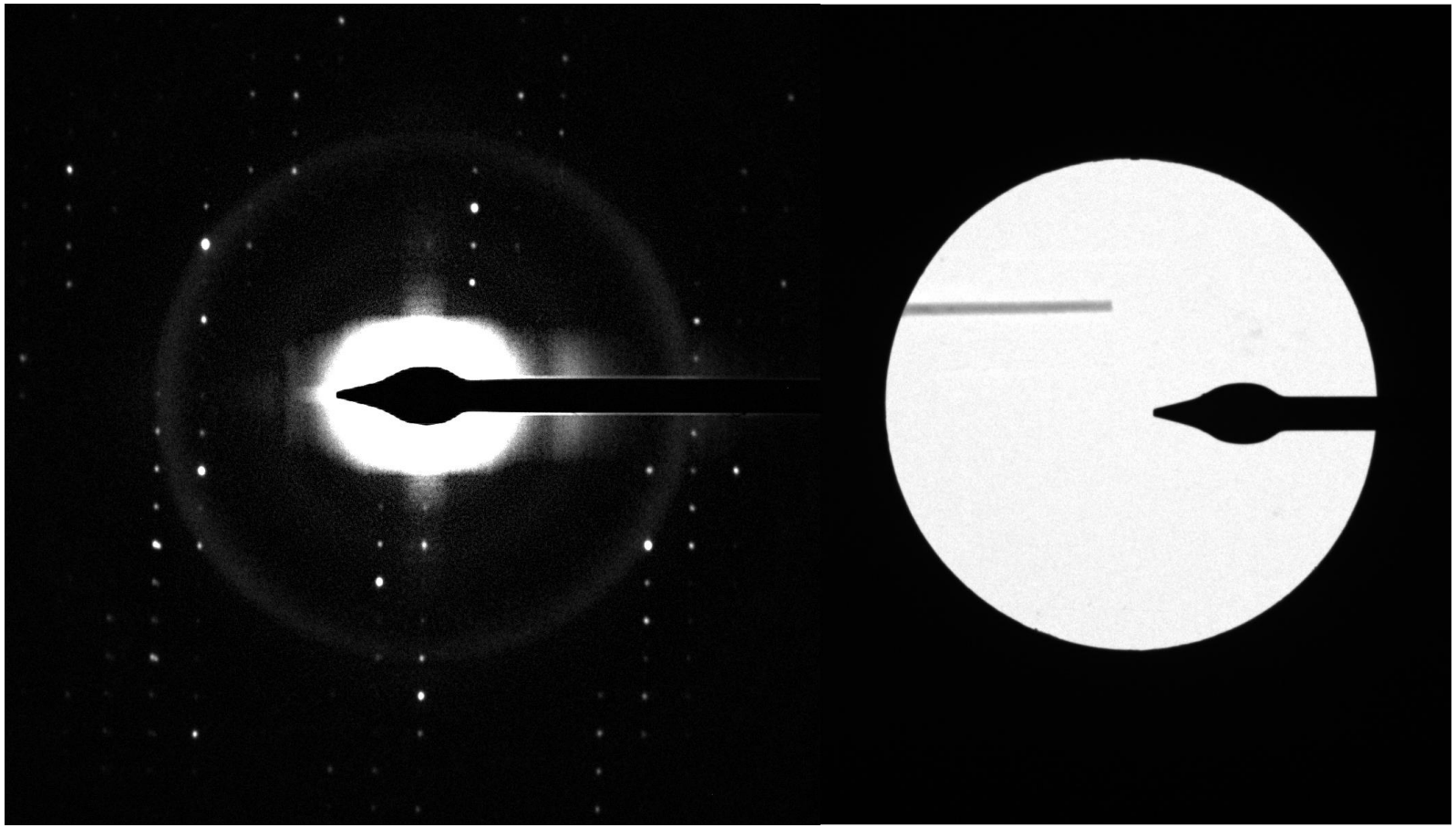
Popa, N.C. *J. Appl. Cryst.* (1998) **31**, 176-180.




$$pV(H,x) = \eta L(H,x) + (1-\eta)G(H,x)$$

# Electron diffraction

Jana2020 communicates with DYNGO, which calculates intensities of reflections using the dynamic diffraction theory. If the dynamical diffraction theory is used, the accuracy of the result approaches that of single crystal X-ray diffraction.



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L. Palatinus, C. A. Corrêa et al. **Acta Crystallographica B71**, 740-751 (2015).
L. Palatinus, V. Petříček, C. A. Corrêa. ***Acta Crystallographica* A71**, 235-244 (2015).
L. Palatinus et al. **Science 355** (6321), 166-169 (2017).

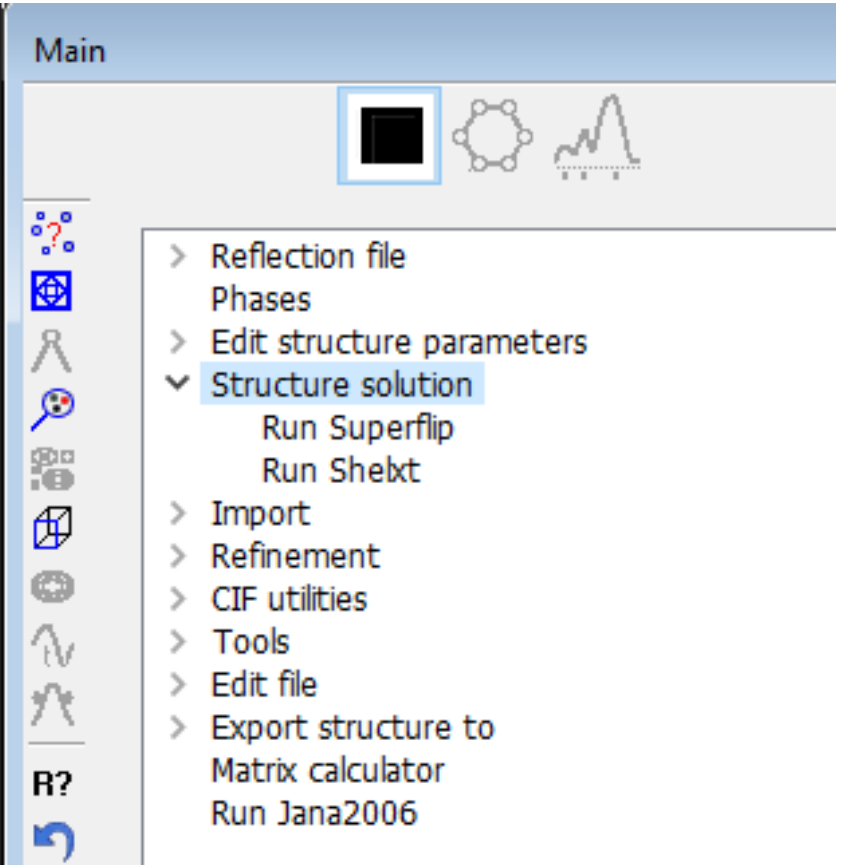
# Structure solution

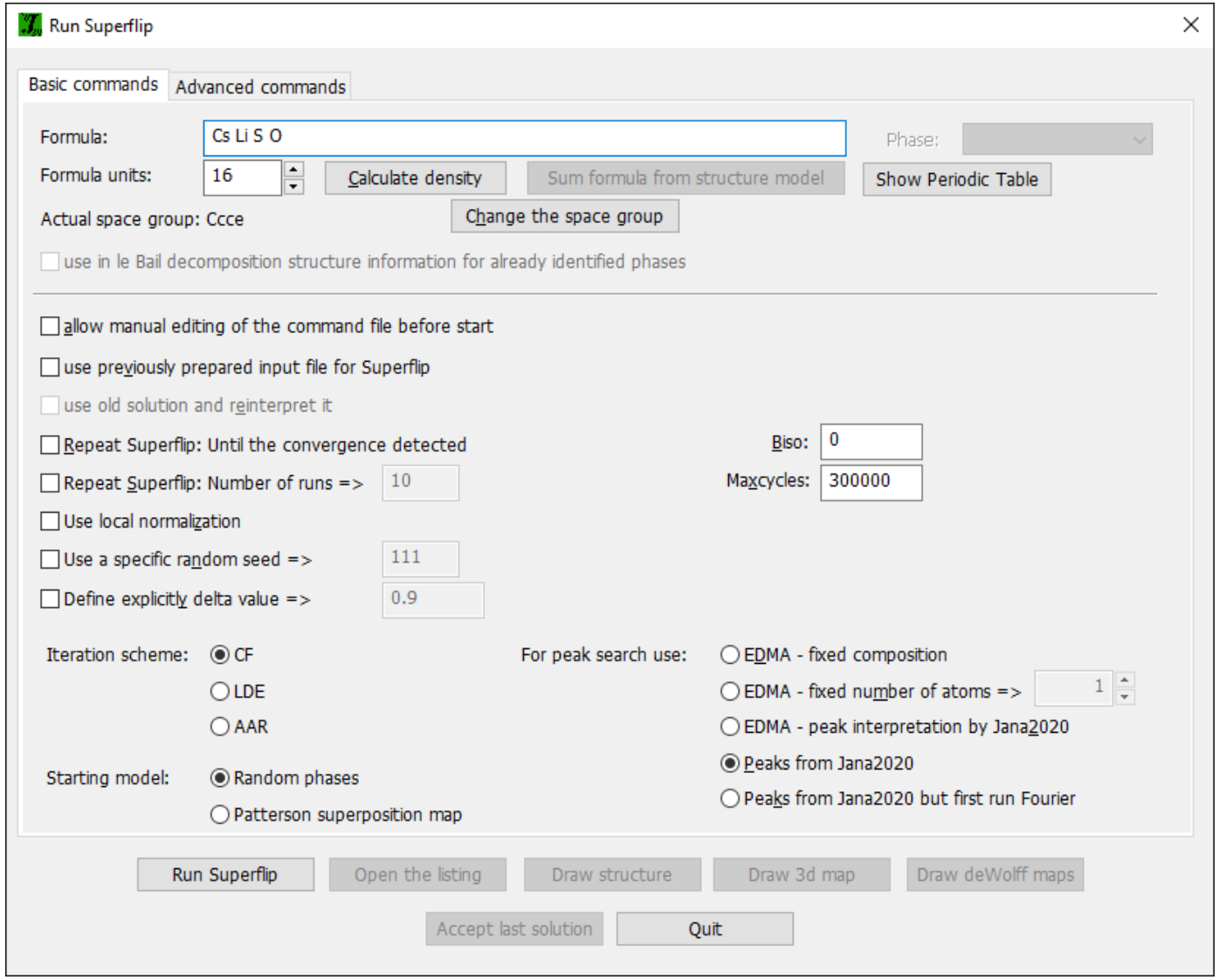
*Solution by Superflip or by calling external programs*

Structure solution

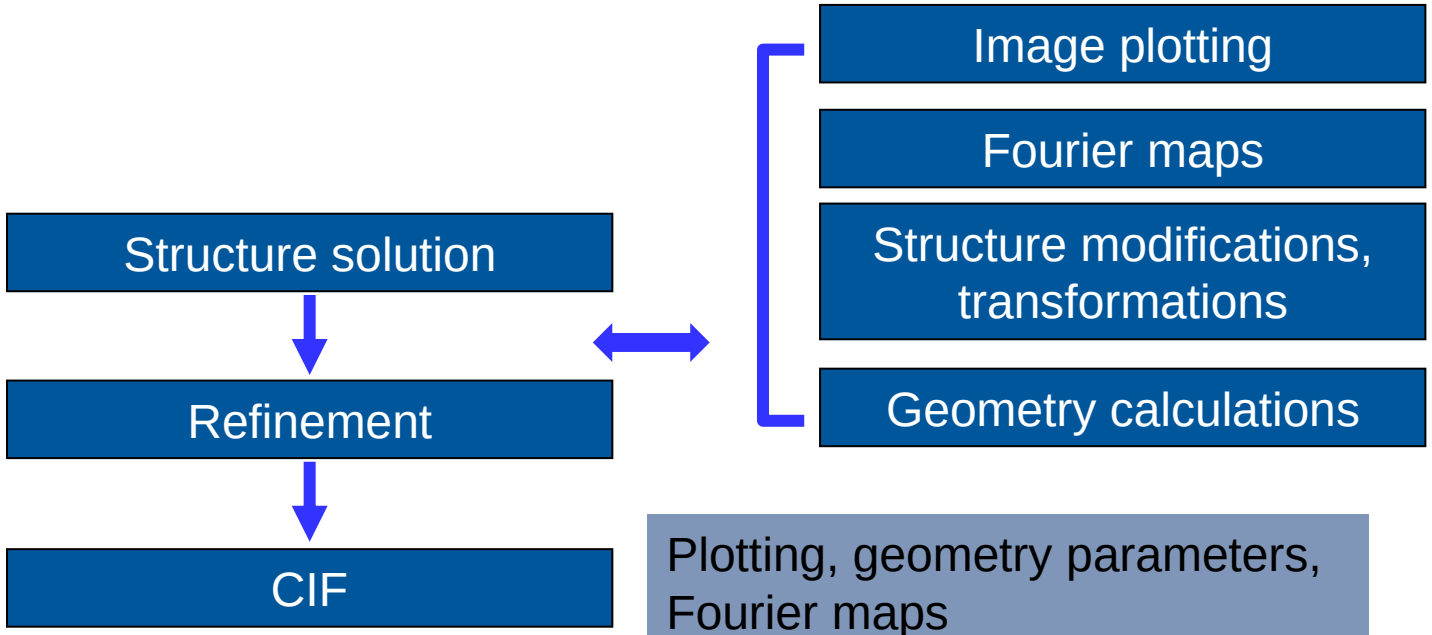
**M40** structure model
**M41** powder profile parameters

# Structure solution



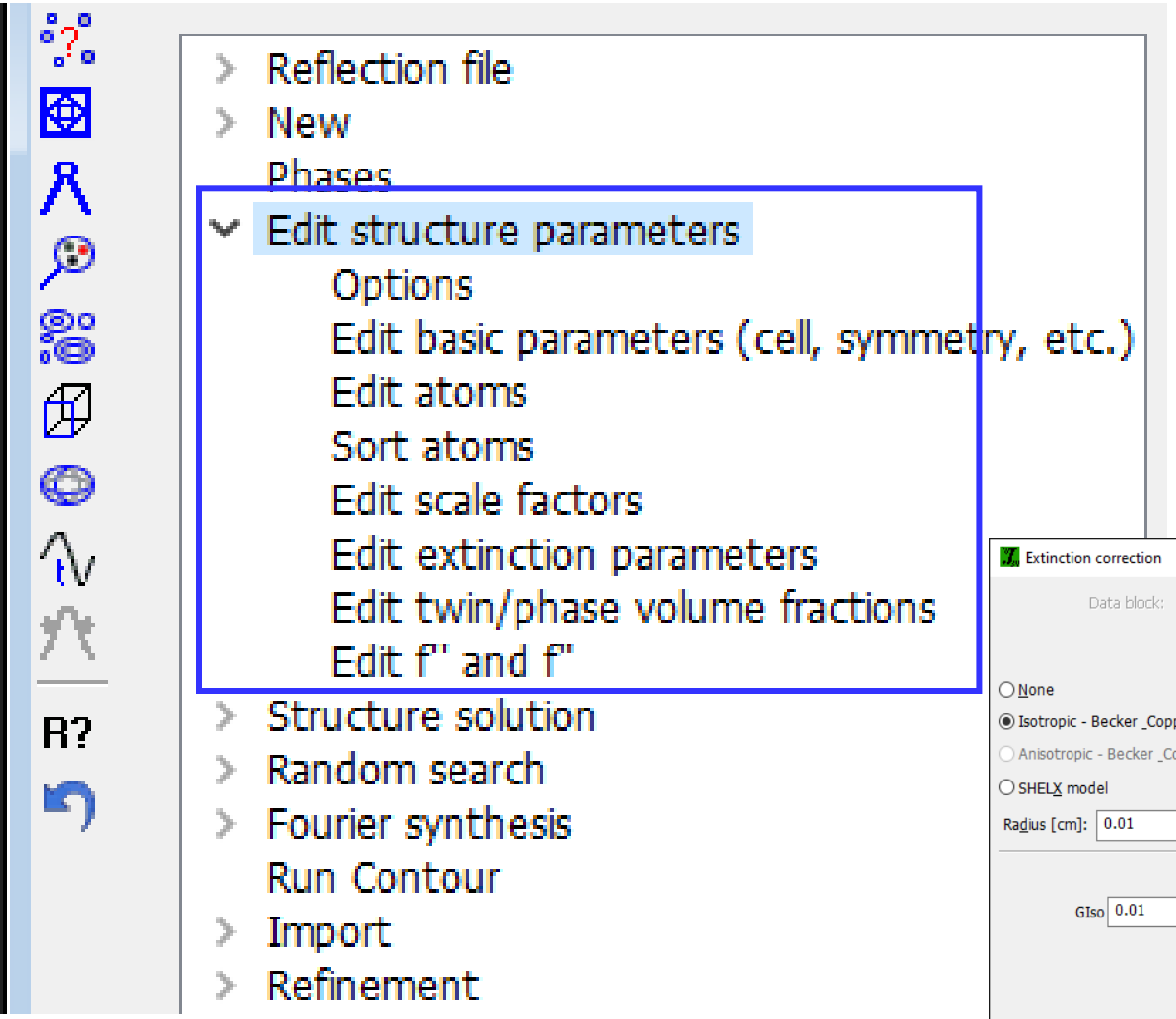



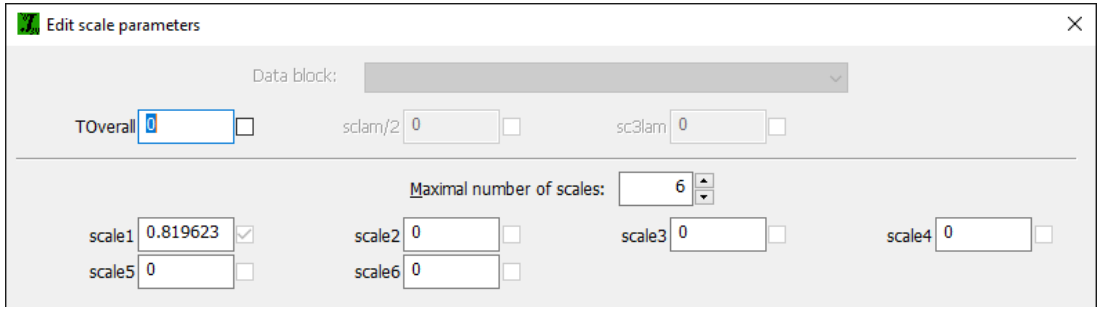
# Software flow scheme and files created

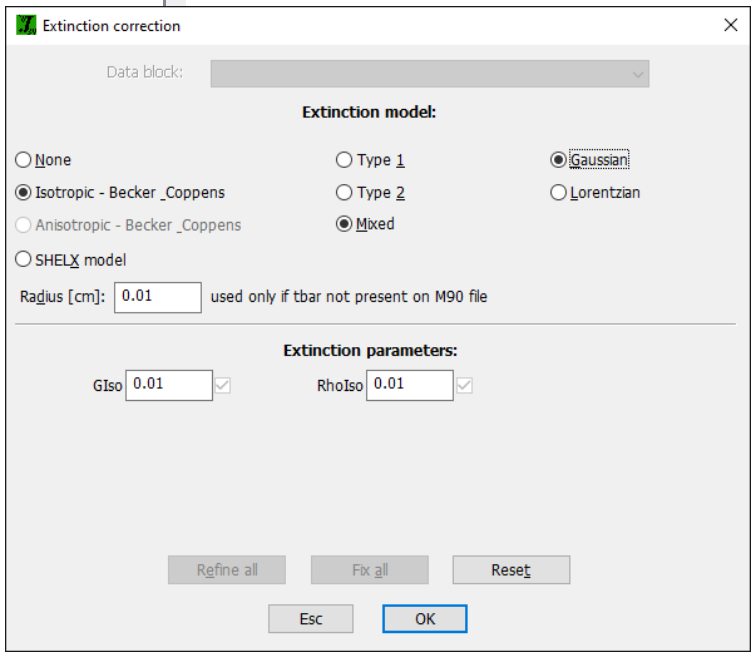


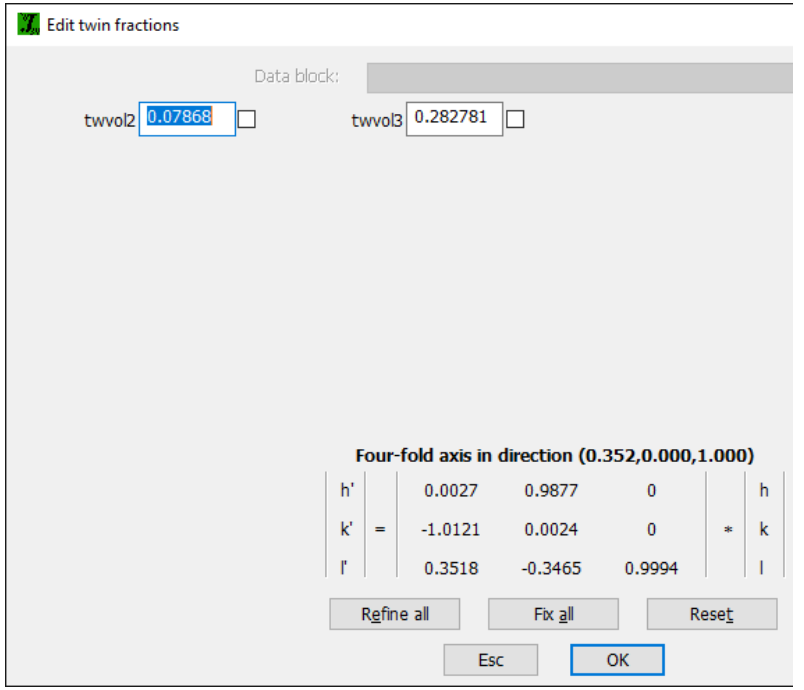
# Refinement

Each refinable parameter of a structure model has a refinement key and an individual name



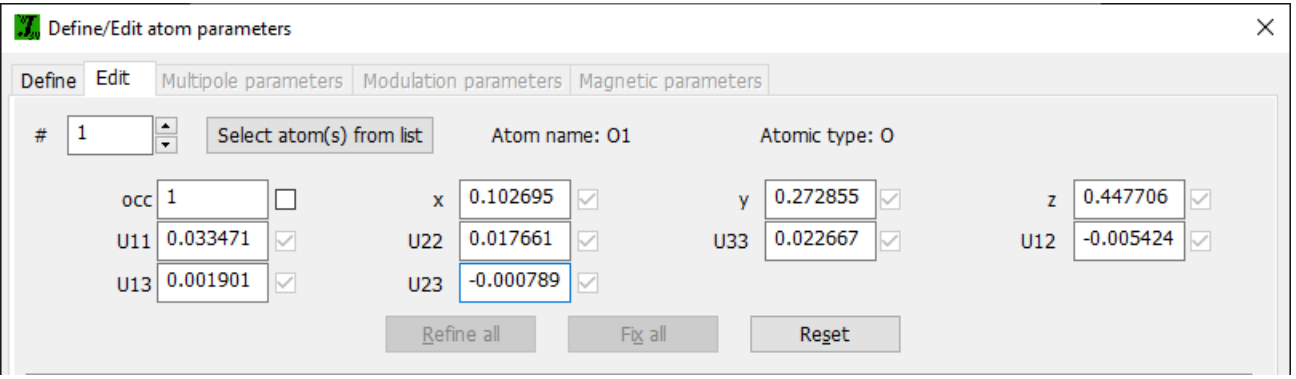



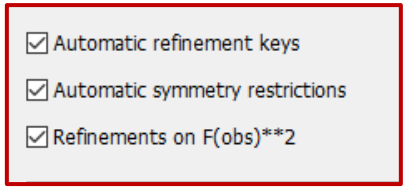



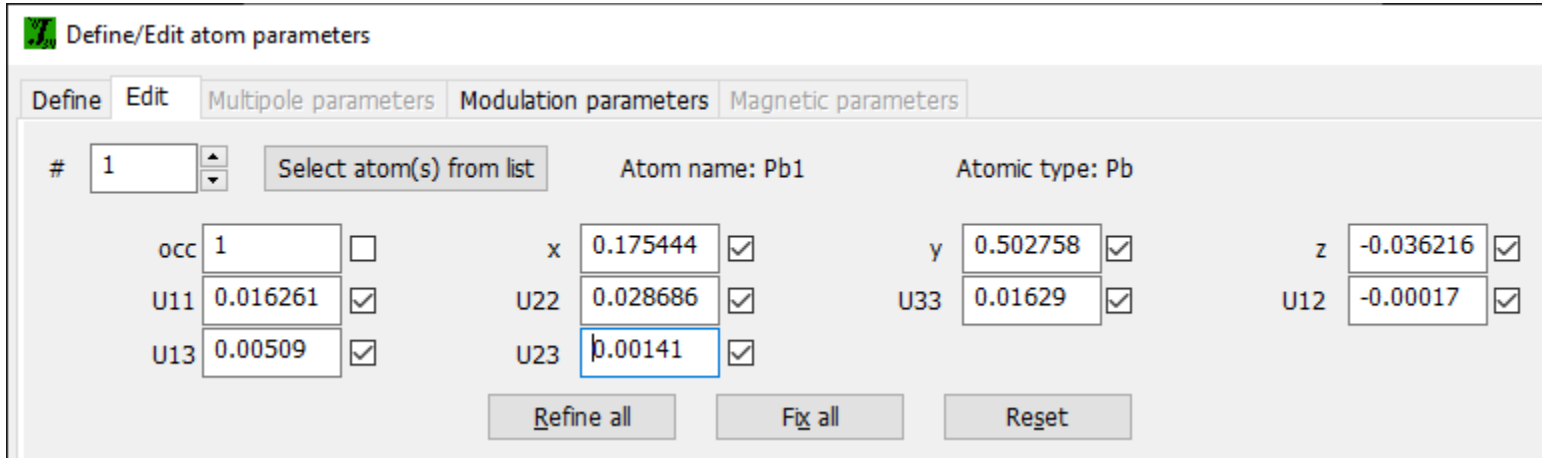

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# Refinement

Refinement keys that are automatically set up to be refined, are blocked for the user.

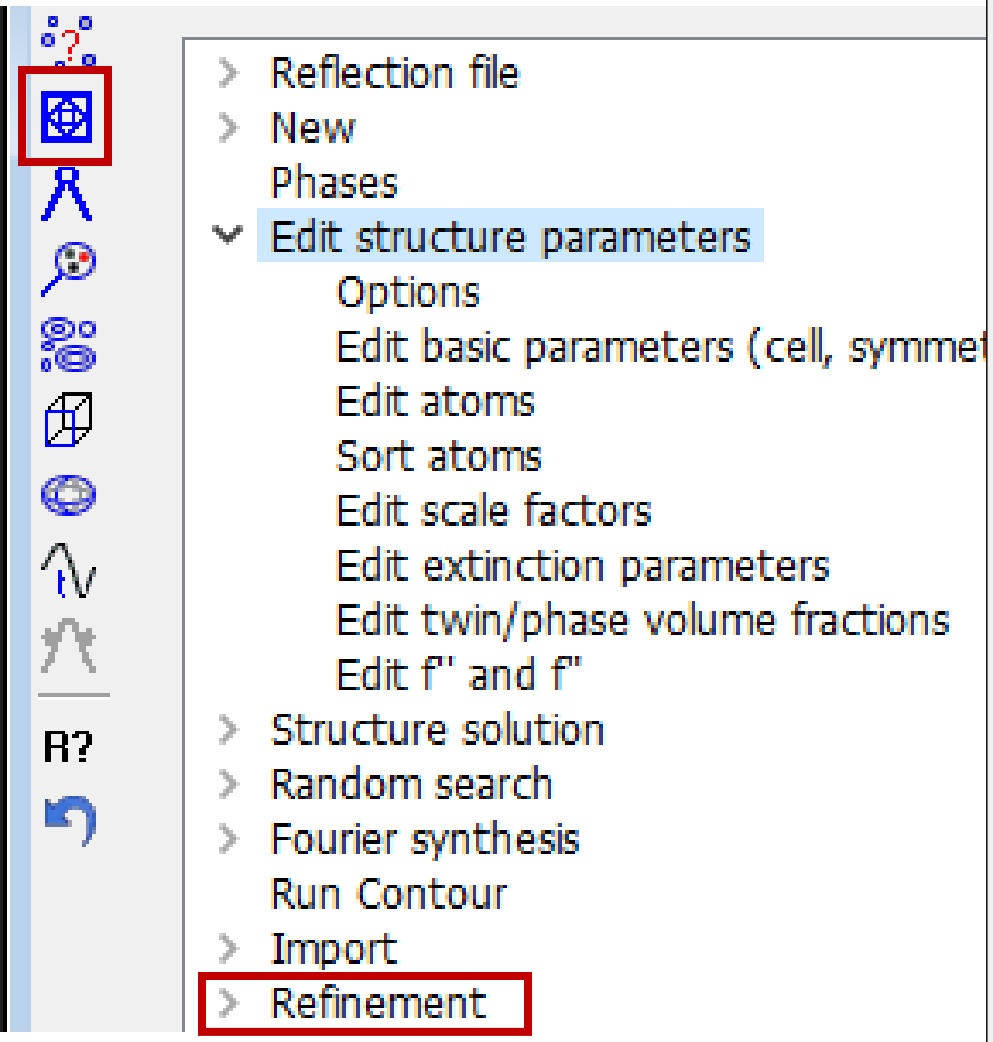


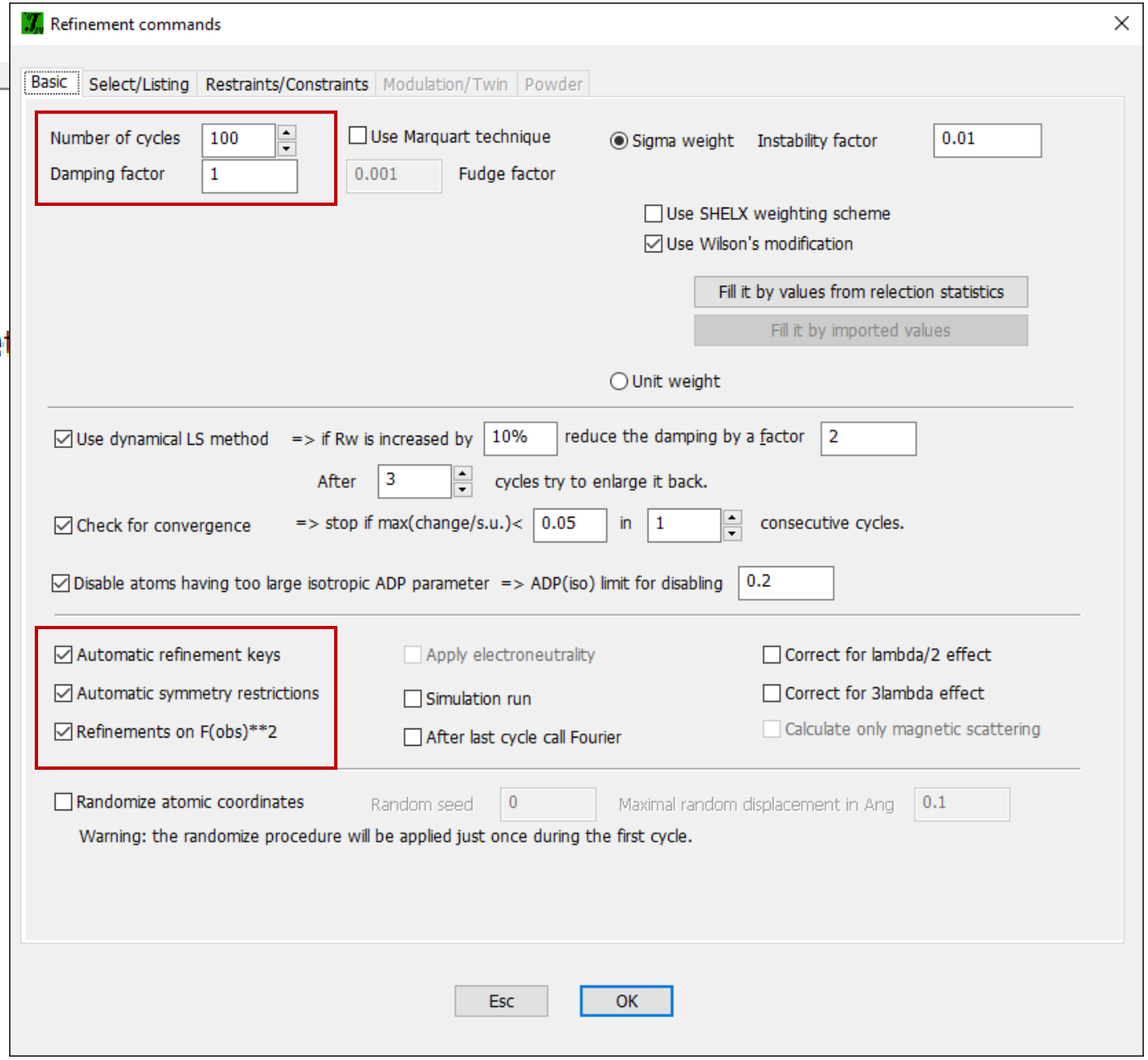




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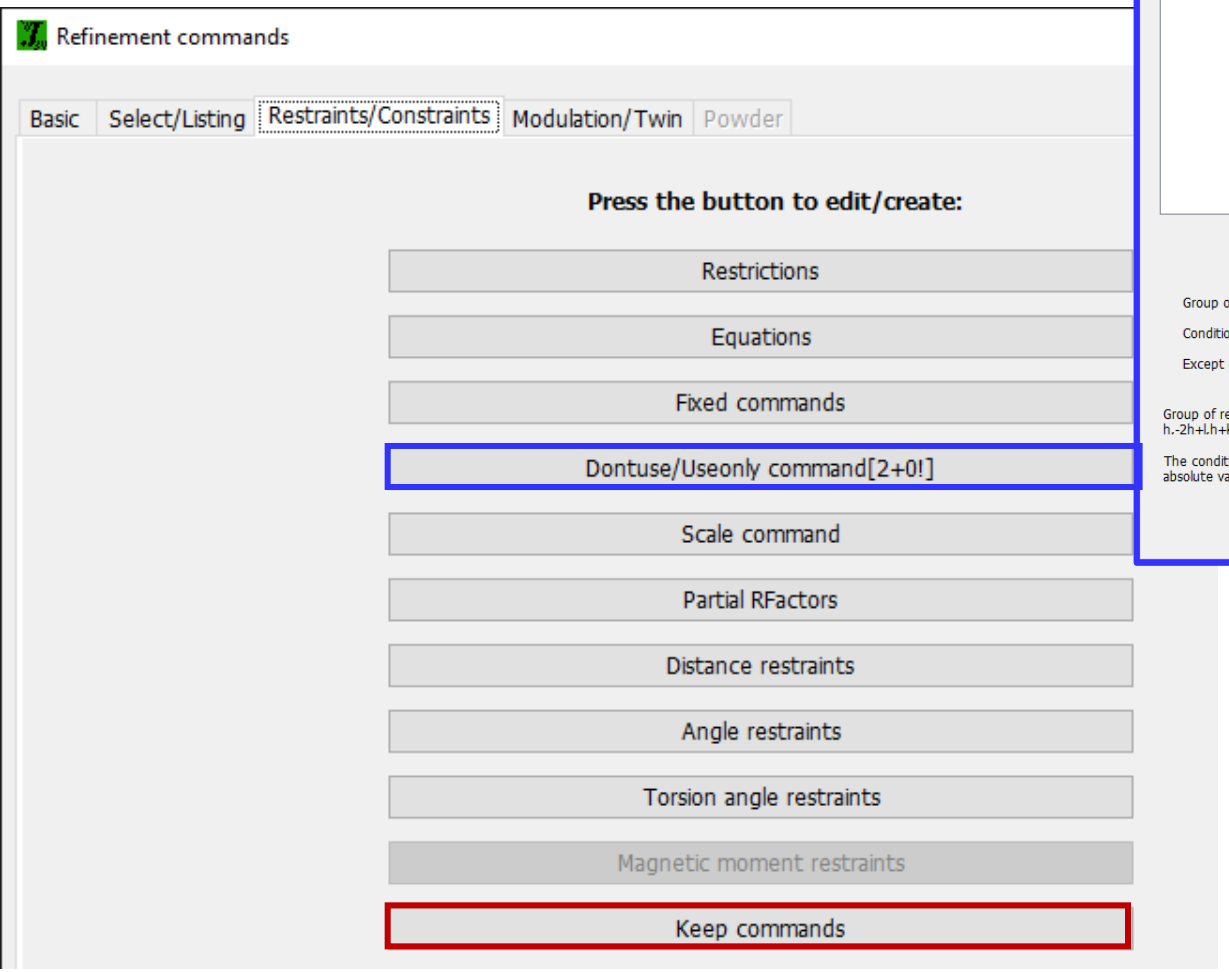
# Refinement

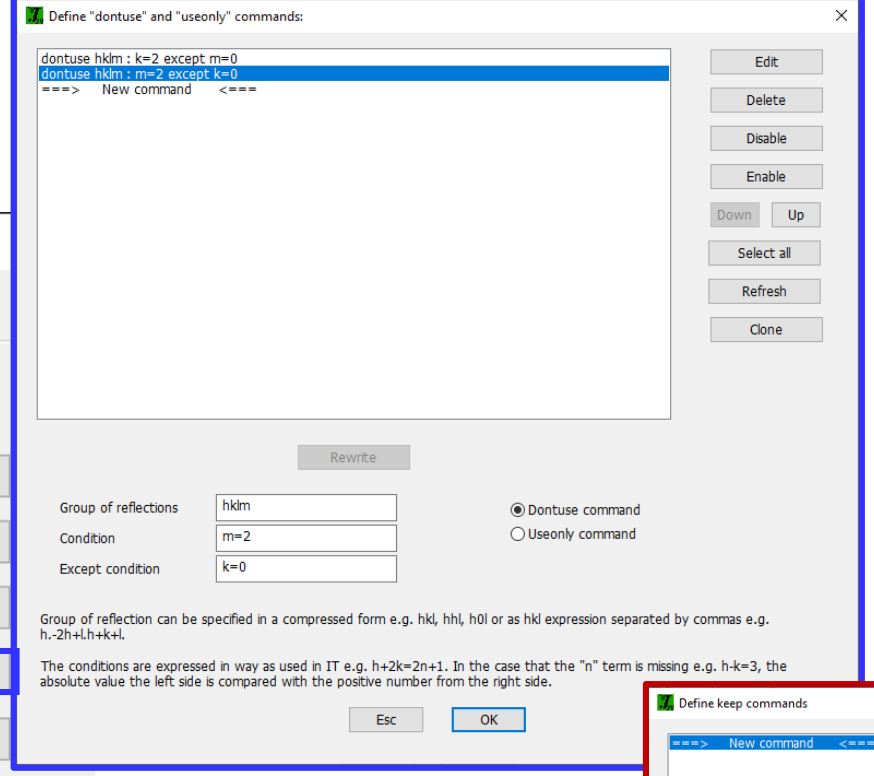


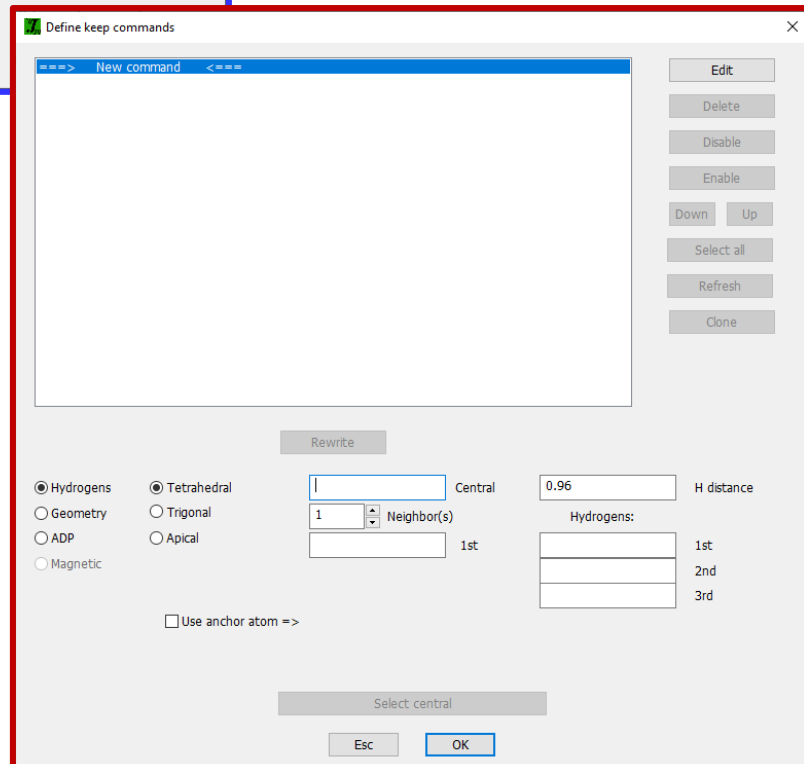




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# Refinement




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# Advanced tools – Constraints, restraints, user equations

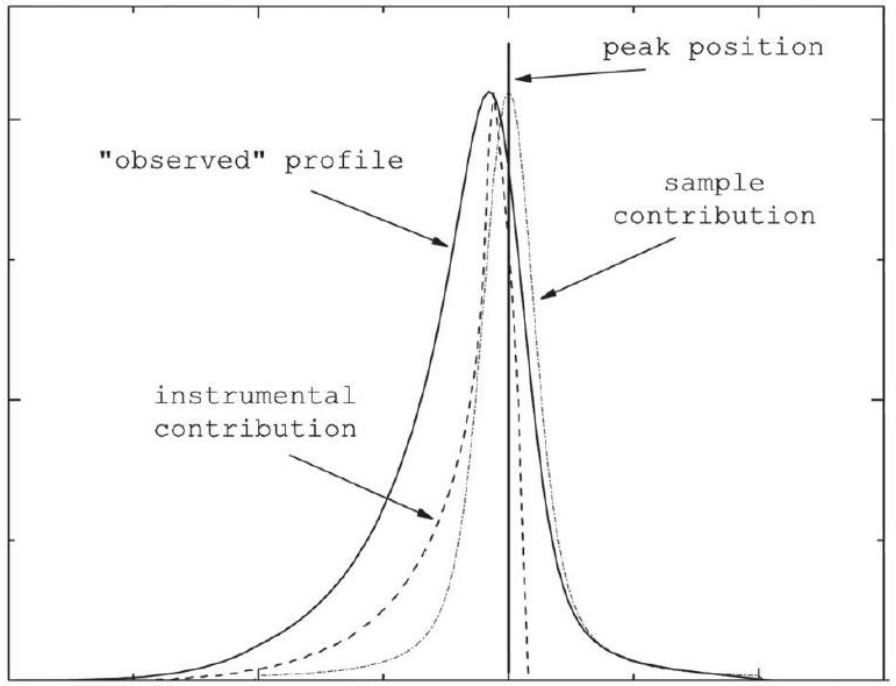
```
  restric C39a 2 C39b
  restric C9a 2 C9b
. . . .
  equation : x[c8x]=x[c8]
  equation : y[c8x]=y[c8]
  equation : z[c8x]=z[c8]
  equation : x[n3x]=x[n3]
  equation : y[n3x]=y[n3]
  equation : z[n3x]=z[n3]
. . . .
  equation : aimol[mol1#2]=1-aimol[mol1#1]
  equation : aimol[mol2#2]=1-aimol[mol2#1]
  equation : aimol[mol4#2]=1-aimol[mol4#1]
  equation : aimol[mol5#2]=1-aimol[mol5#1]
  equation : aimol[mol6#2]=1-aimol[mol6#1]
. . . .
  keep hydro triang C3 2 1 C2 C4 0.96 H1c3
  keep ADP riding C3 1.2 H1c3
  keep hydro tetrahed C13 1 3 C8x 0.96 H1c13 H2c13 H3c13
  keep ADP riding C13 1.2 H1c13 H2c13 H3c13
```

# Advanced tools – Fundamental approach

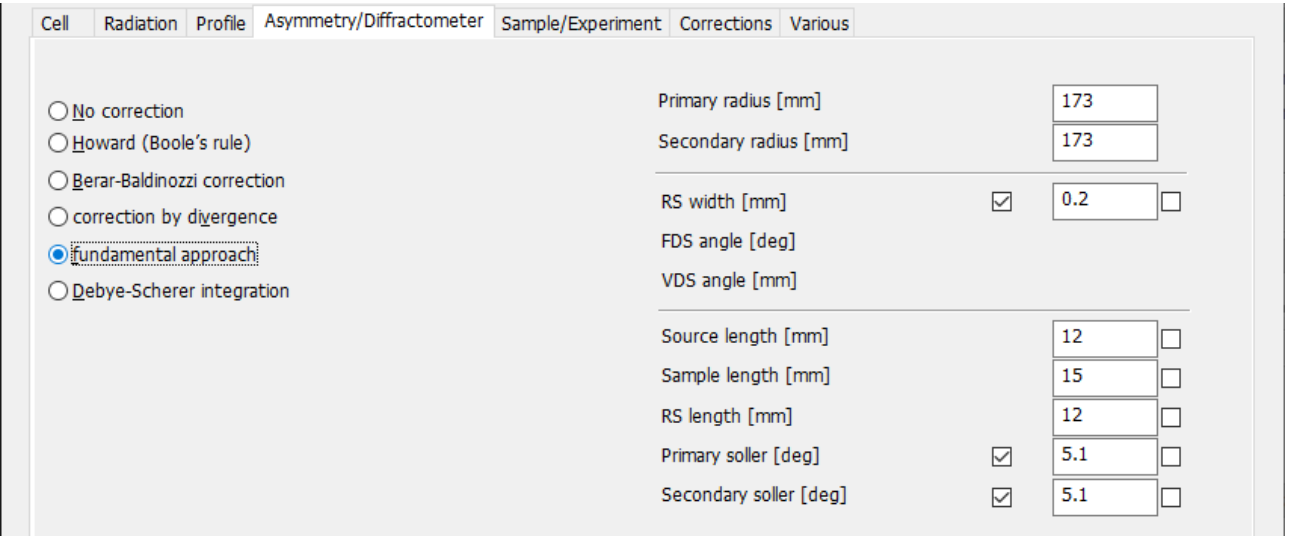
Final profile — Sample contribution — Instrumental contribution

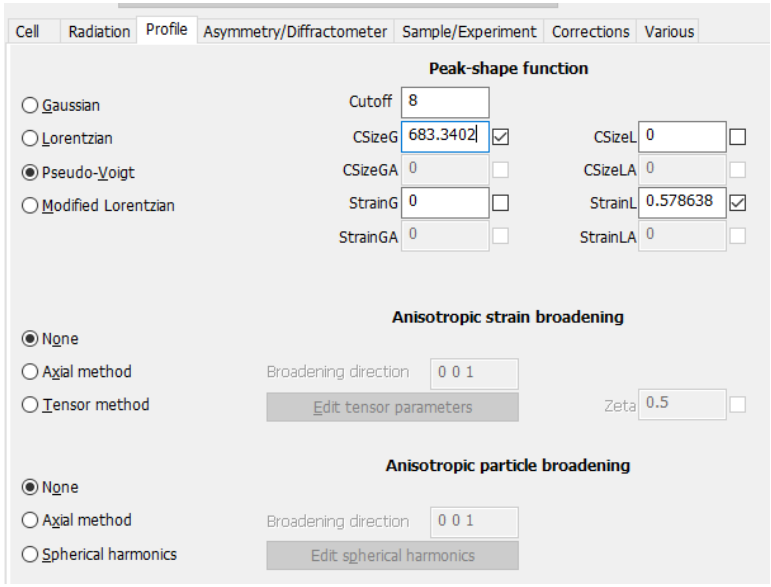
$$H(2\theta) = F(2\theta) \otimes G(2\theta)$$

crystalline size and stress — optics sample holder detector source

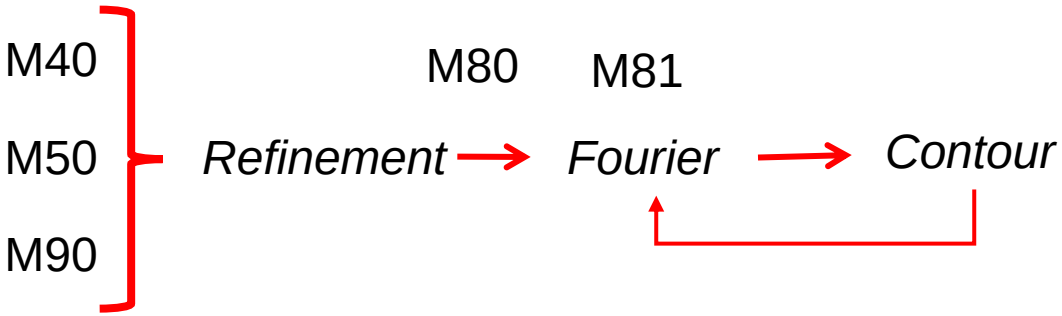


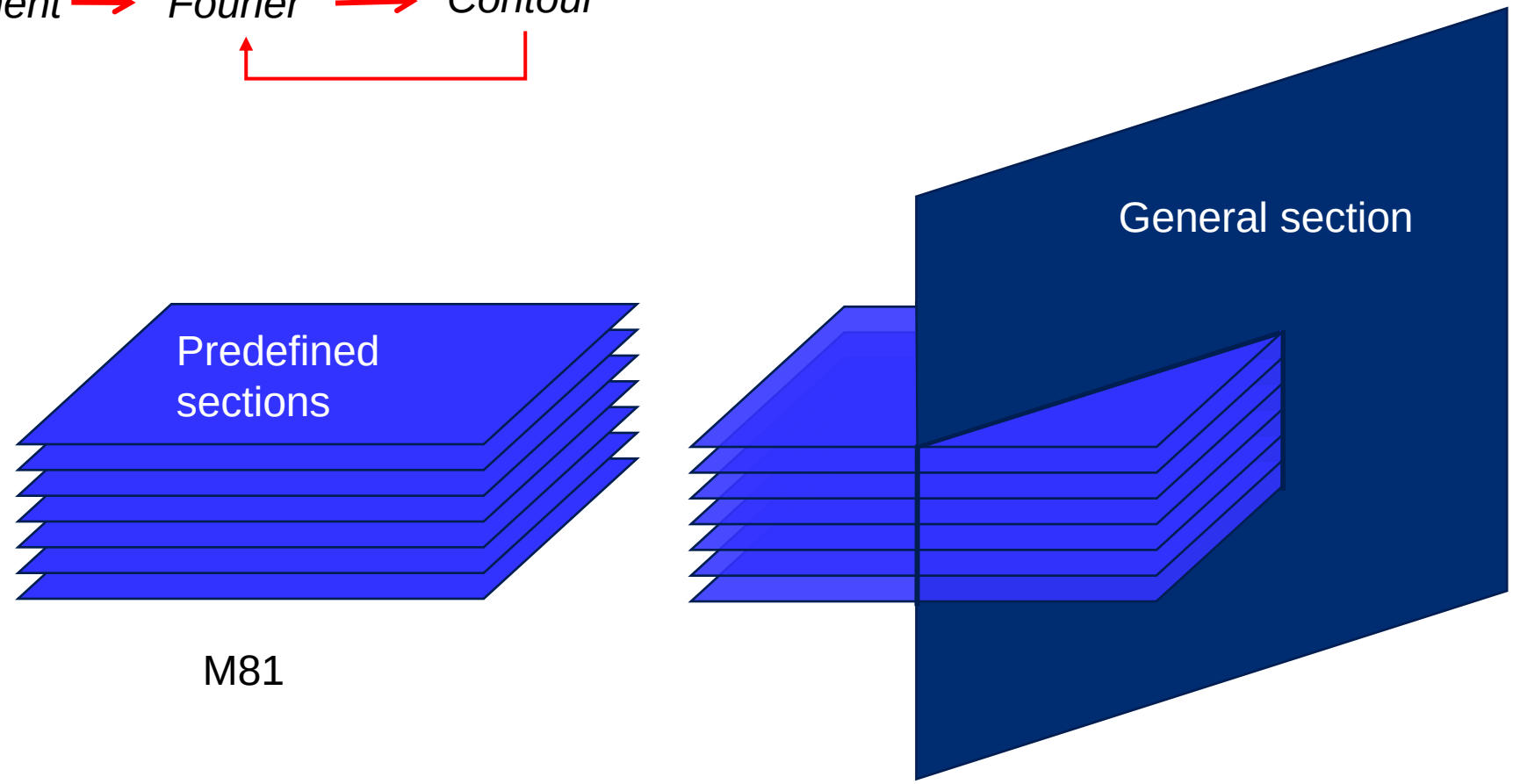

R.W.Cheary and A.A.Coelho. **J.Appl.Cryst. 31,** 851-861 (1998).



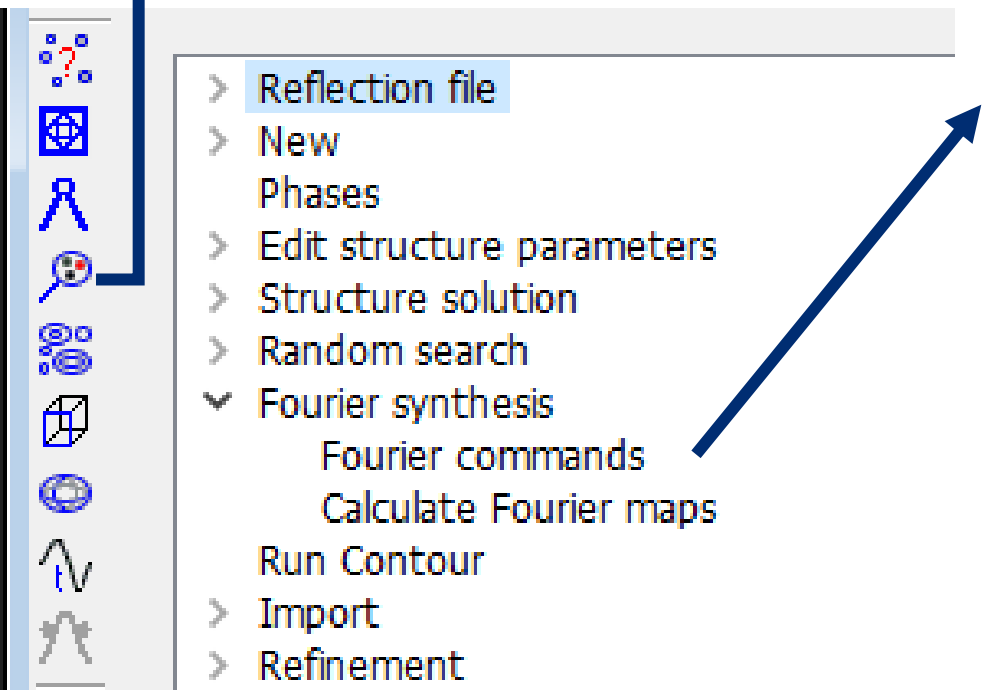
# Fourier maps

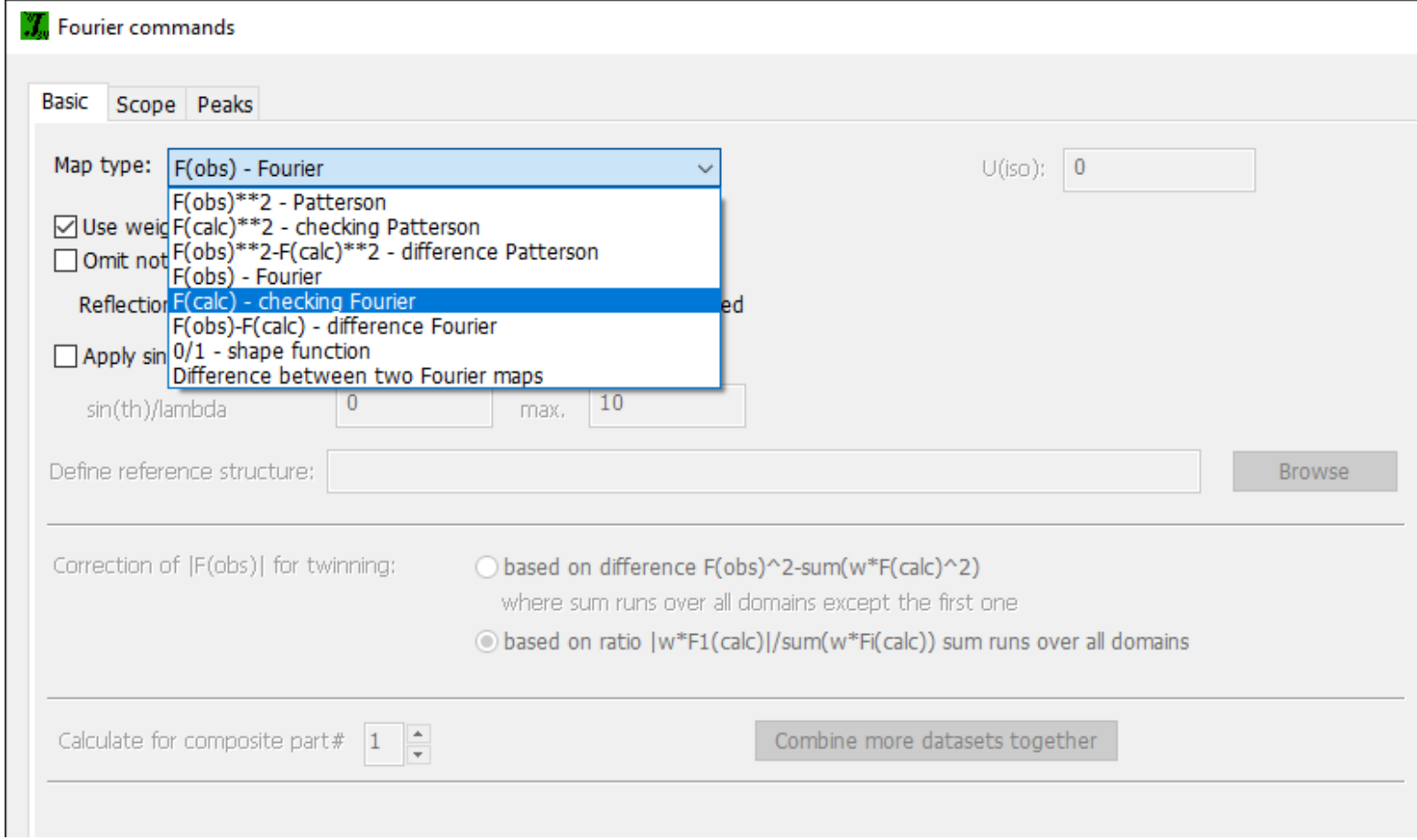



Contour can plot a predefined section, or it can calculate and plot general sections. For arbitrary general sections, the predefined section must cover at least asymmetric unit of the elementary cell.

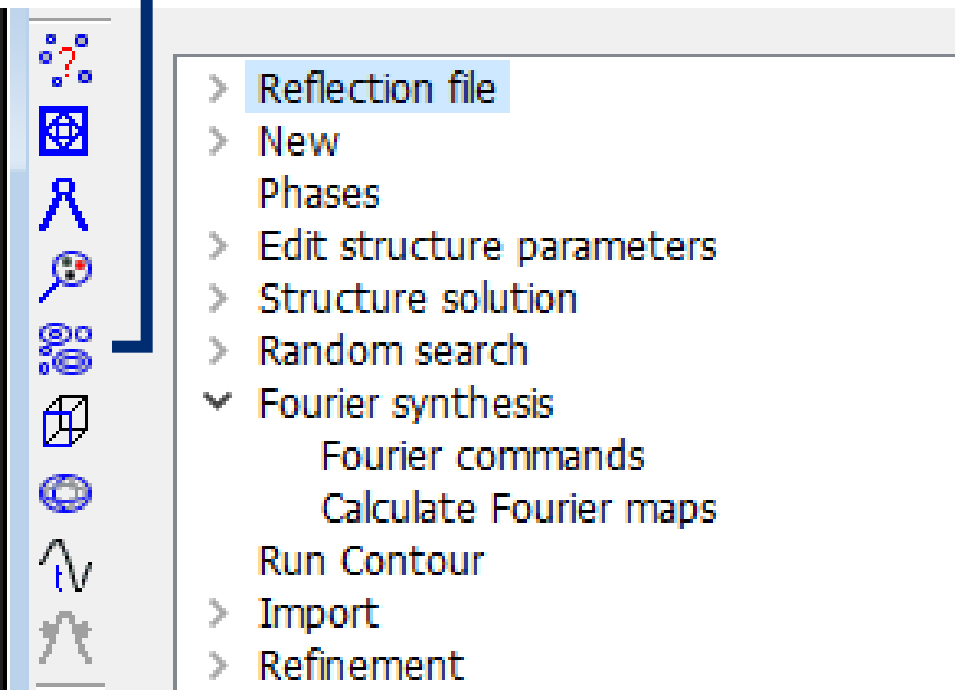
# Fourier maps

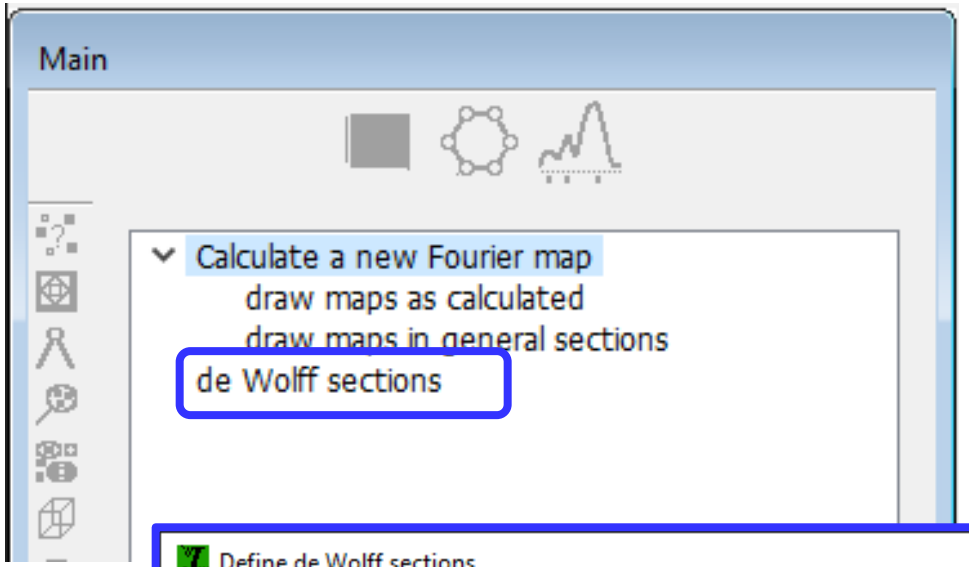


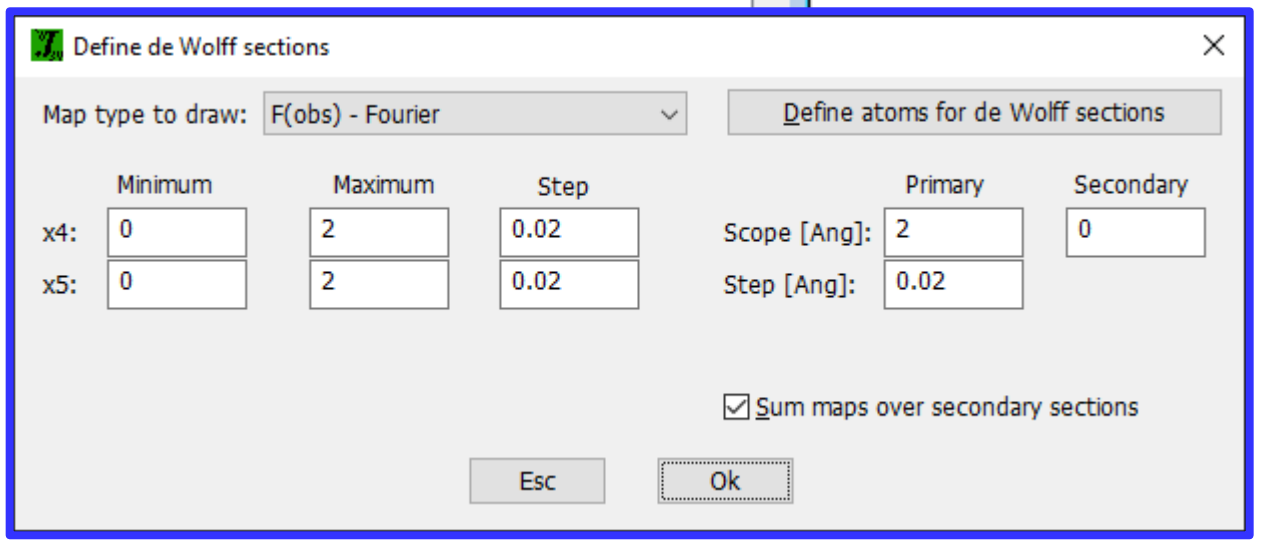




Contour can plot a predefined section, or it can calculate and plot general sections. For arbitrary general sections the predefined section must cover at least asymmetric unit of the elementary cell.

# Fourier maps



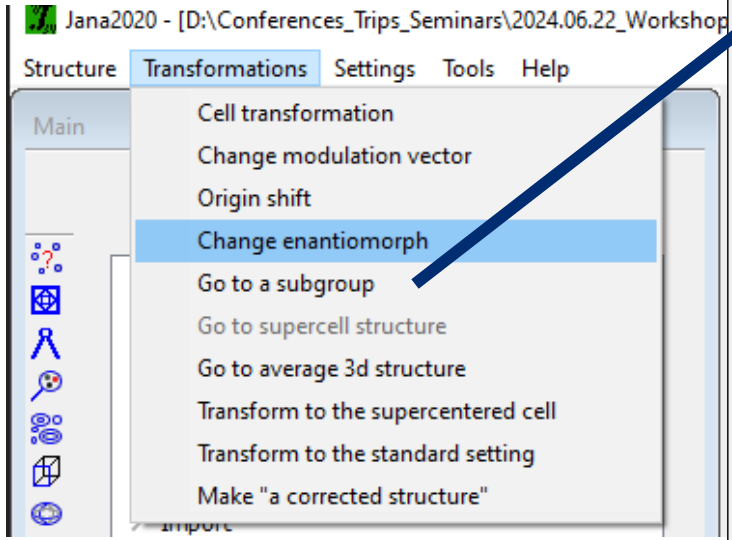



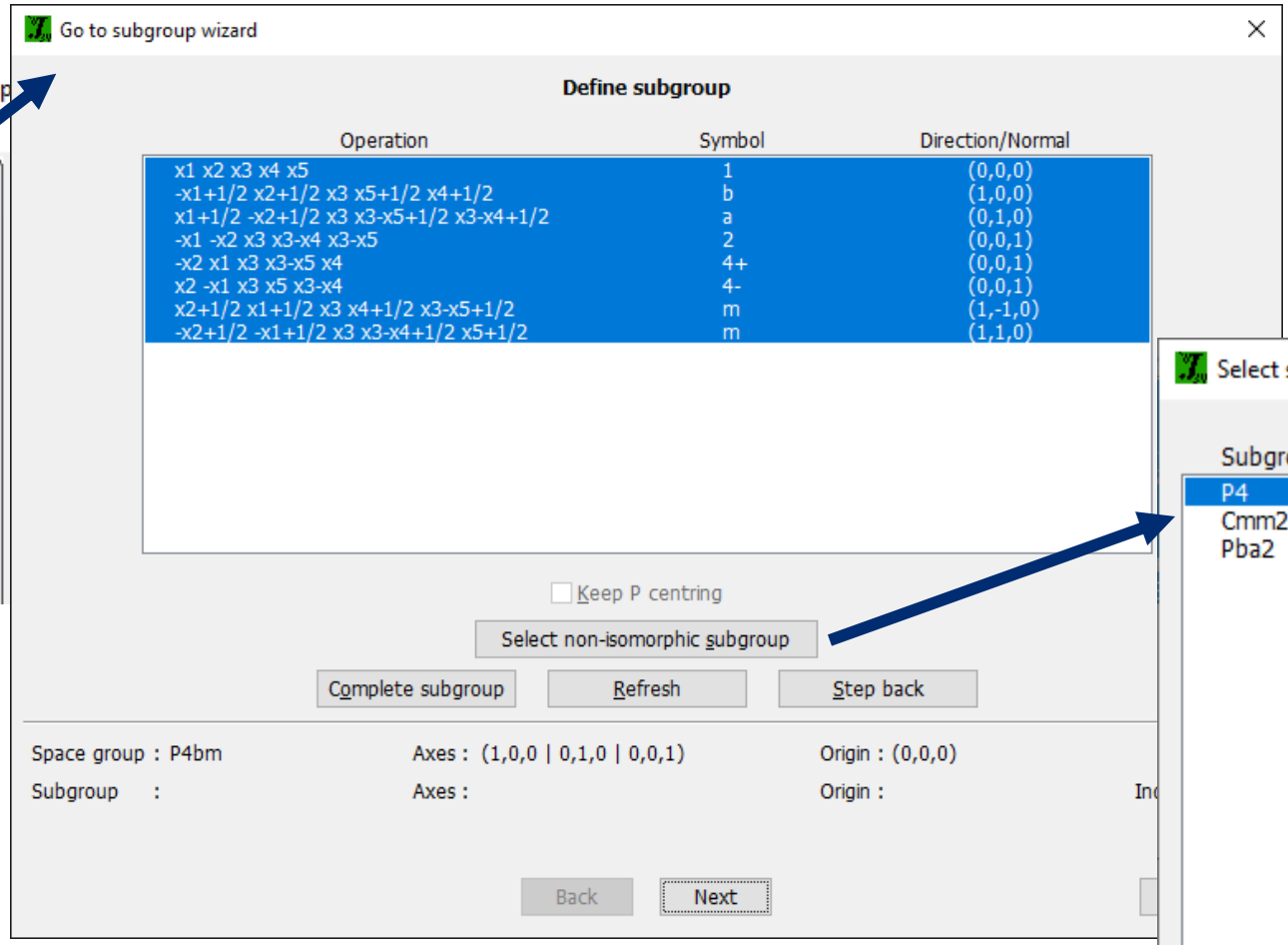



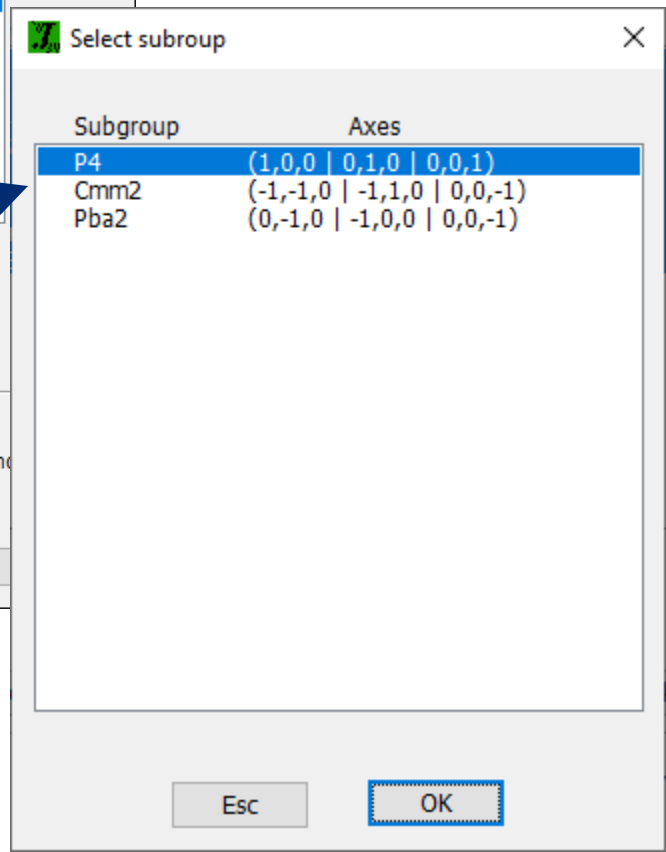



P.M.de Wolff, Acta Cryst. (1974). A30, 777-785

# Advanced tools – Group-subgroup transformation

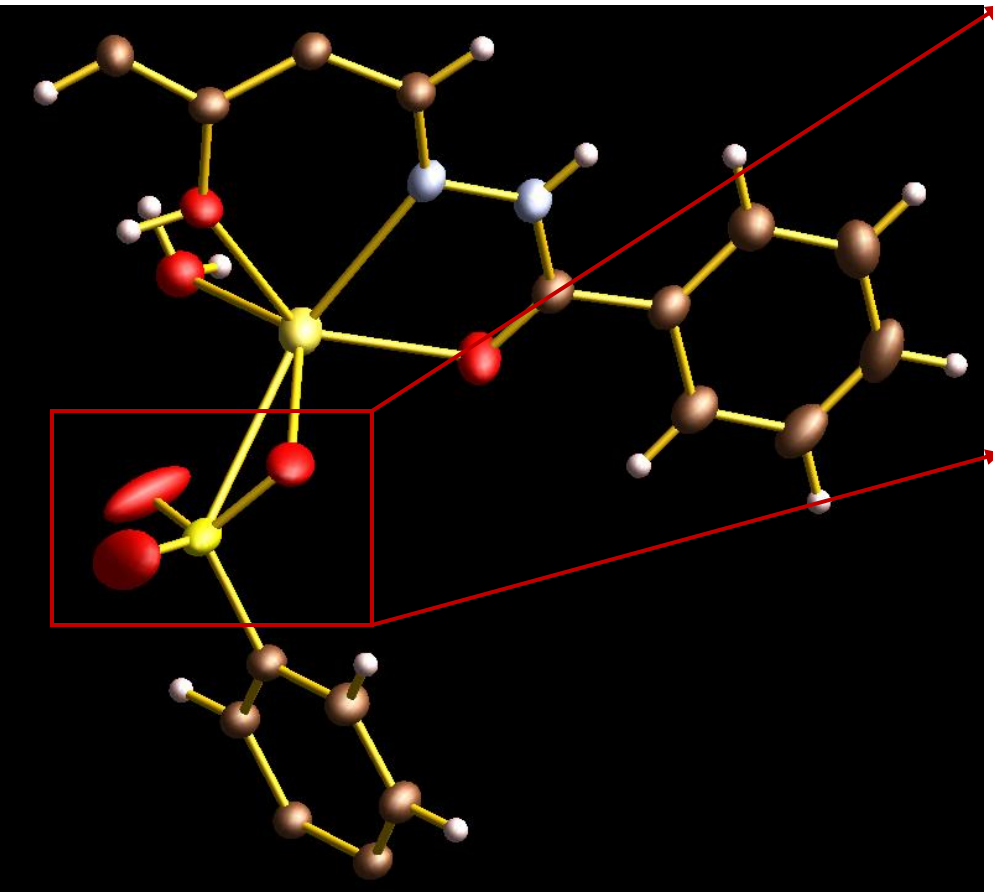


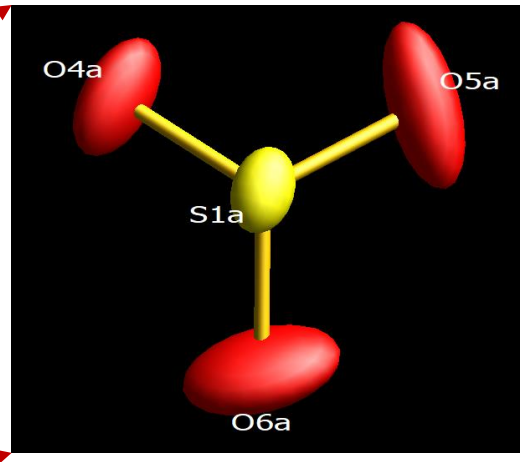




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# Advanced tools – Disorder, atom split, rigid body

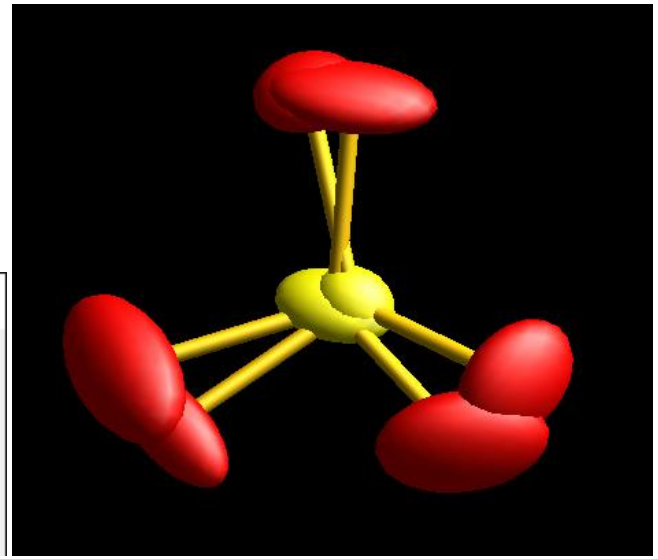





Information from refinement:

RFactors overview

R factors : [3094=2820+274/230], Damping factor: 1.0000
GOF(obs)= 2.83 GOF(all)= 2.75
R(obs)= 4.11 wR2(obs)= 13.93 R(all)= 4.42 wR2(all)= 14.20
Last wR2(all): 14.20
Maximum change/s.u. : 0.0339 for x[H2O2]



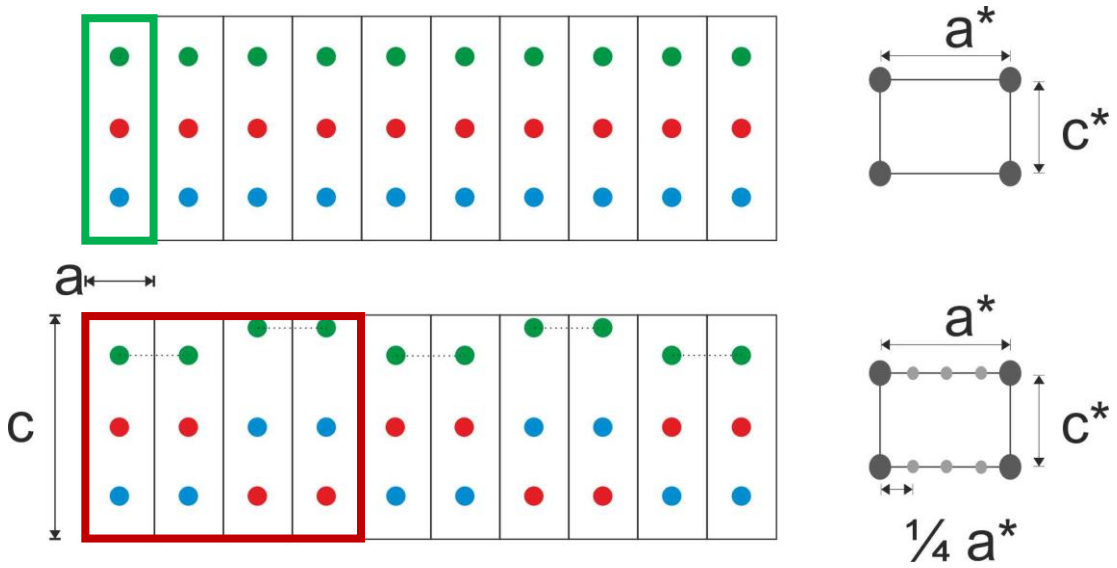
Information from refinement:

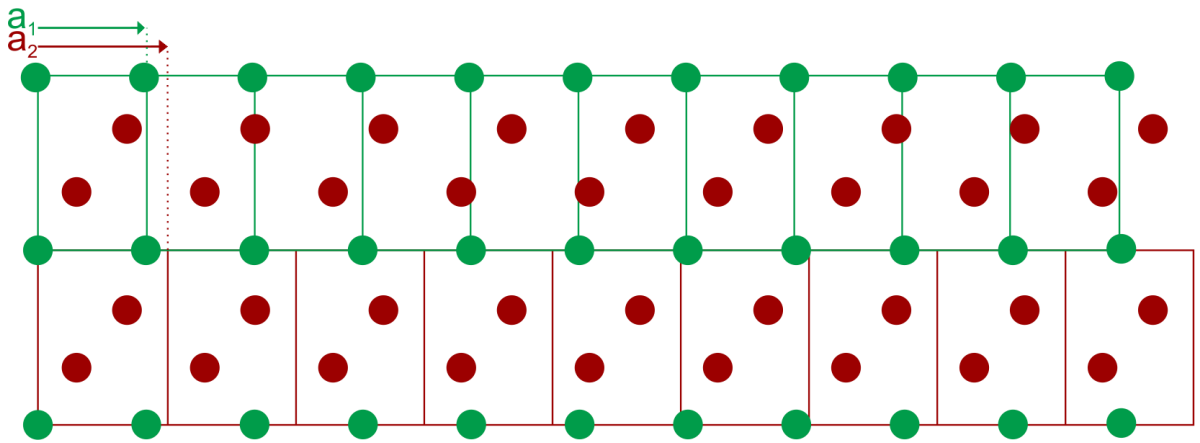
RFactors overview

R factors : [3094=2818+276/259], Damping factor: 1.0000
GOF(obs)= 2.18 GOF(all)= 2.12
R(obs)= 3.24 wR2(obs)= 10.50 R(all)= 3.52 wR2(all)= 10.73
Last wR2(all): 10.73 10.73 10.73 10.73 10.73 10.73 10.73 10.73
Maximum change/s.u. : 0.0459 for ztrans[molec#2]

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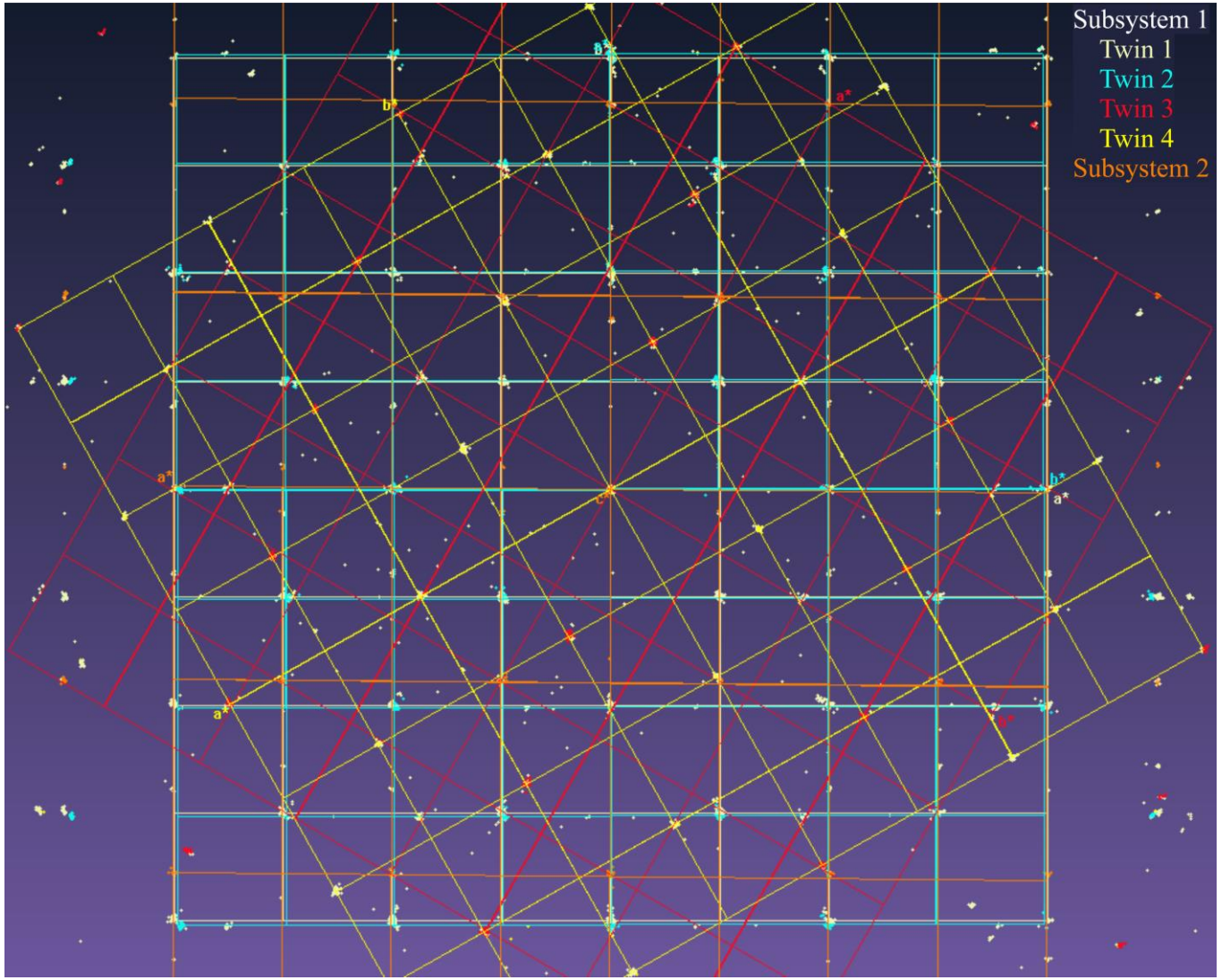
# Advanced tools – composites

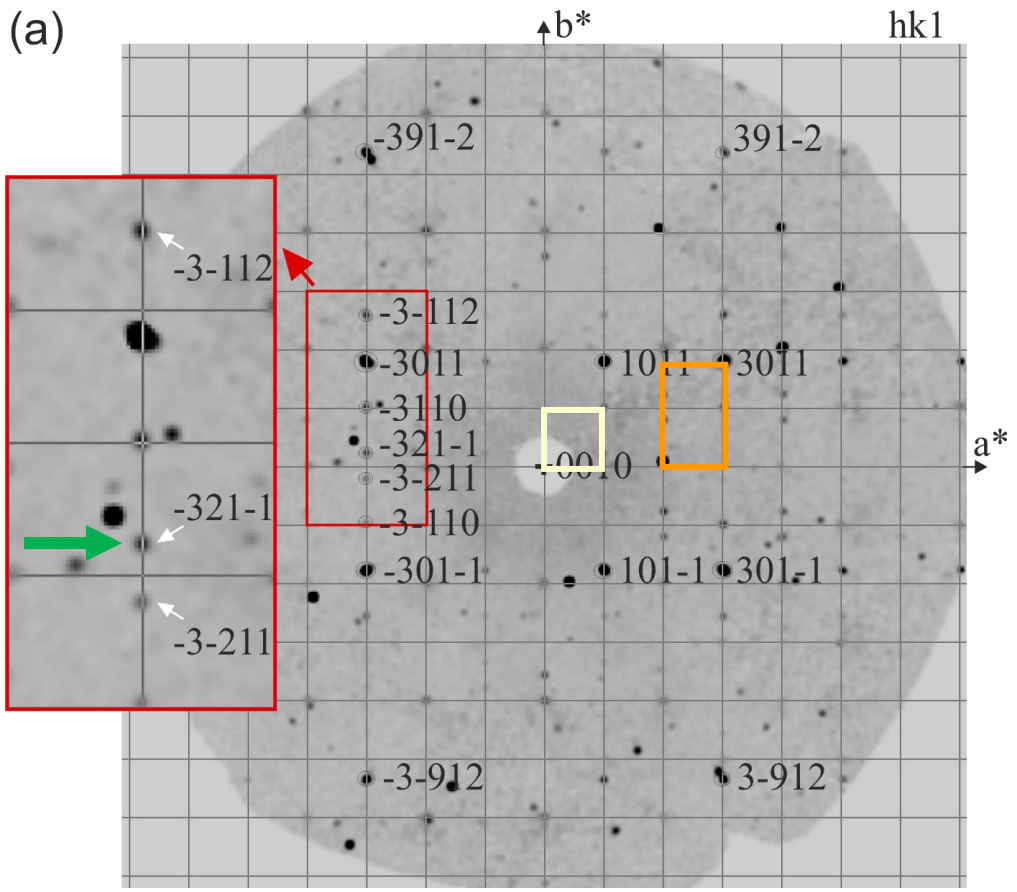


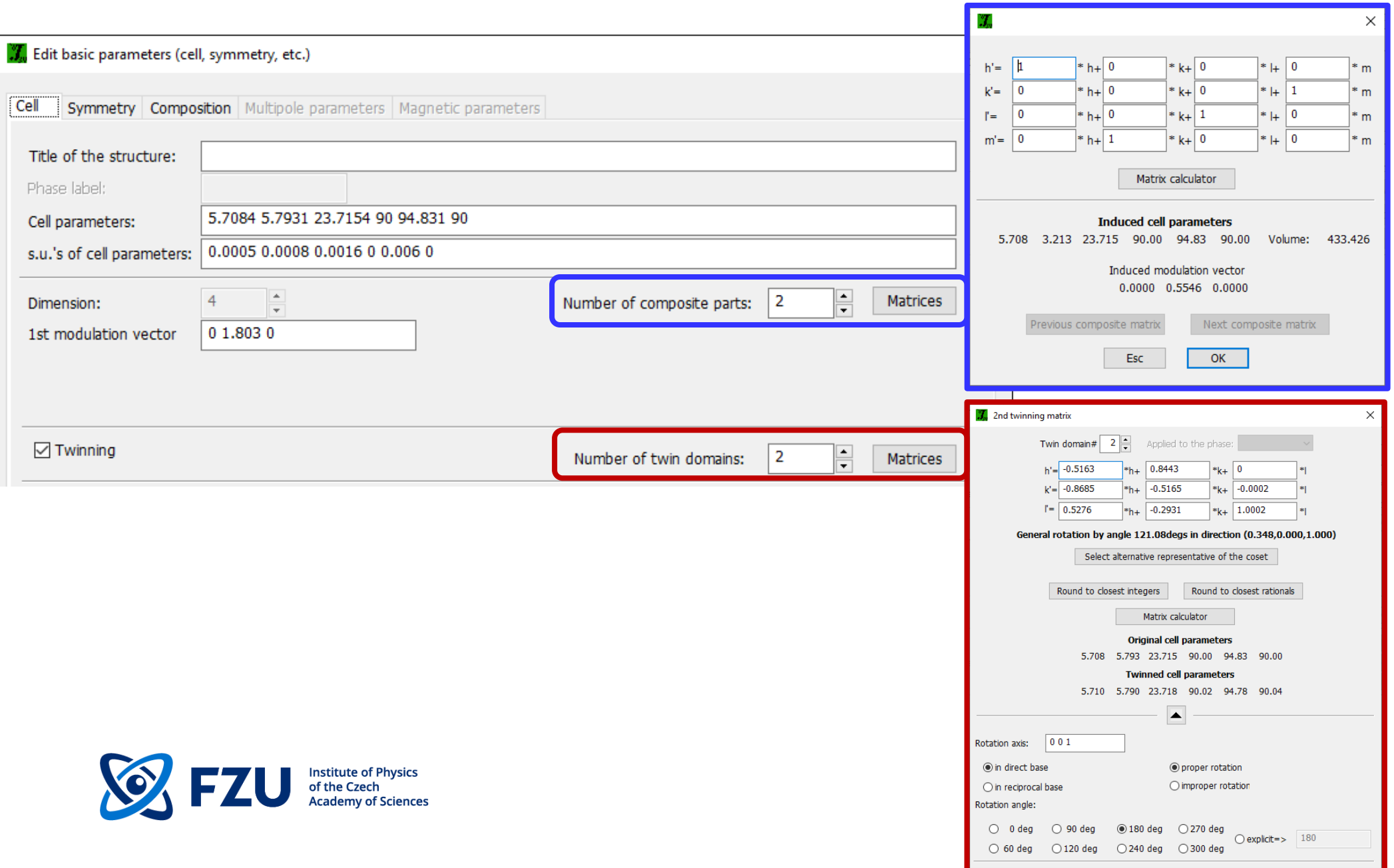

We can find two coexisting lattices, which cannot be described by a simple common supercell -> incommensurate composites

# Advanced tools – Twins, composites



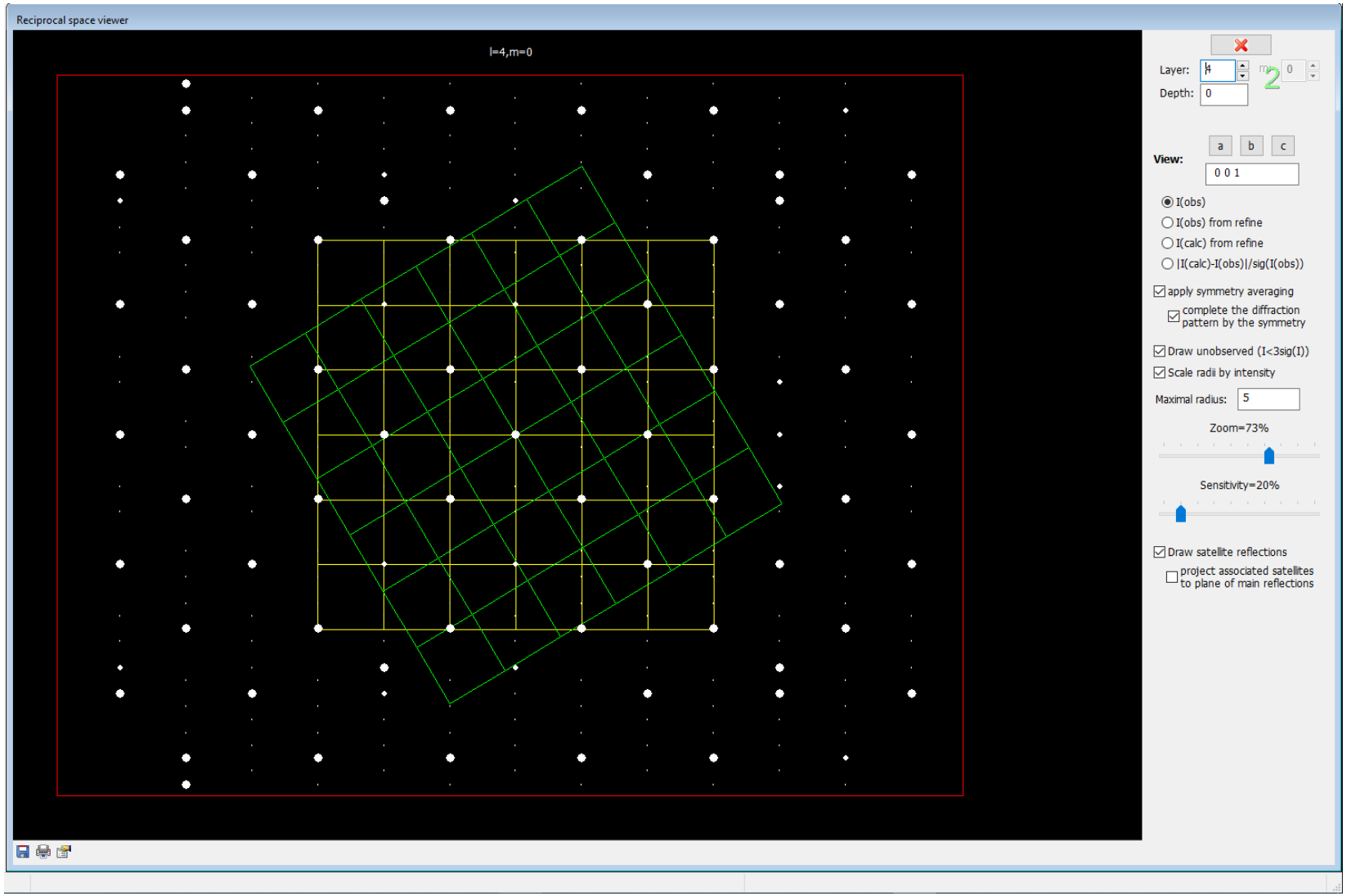
# Advanced tools – Twins, composites




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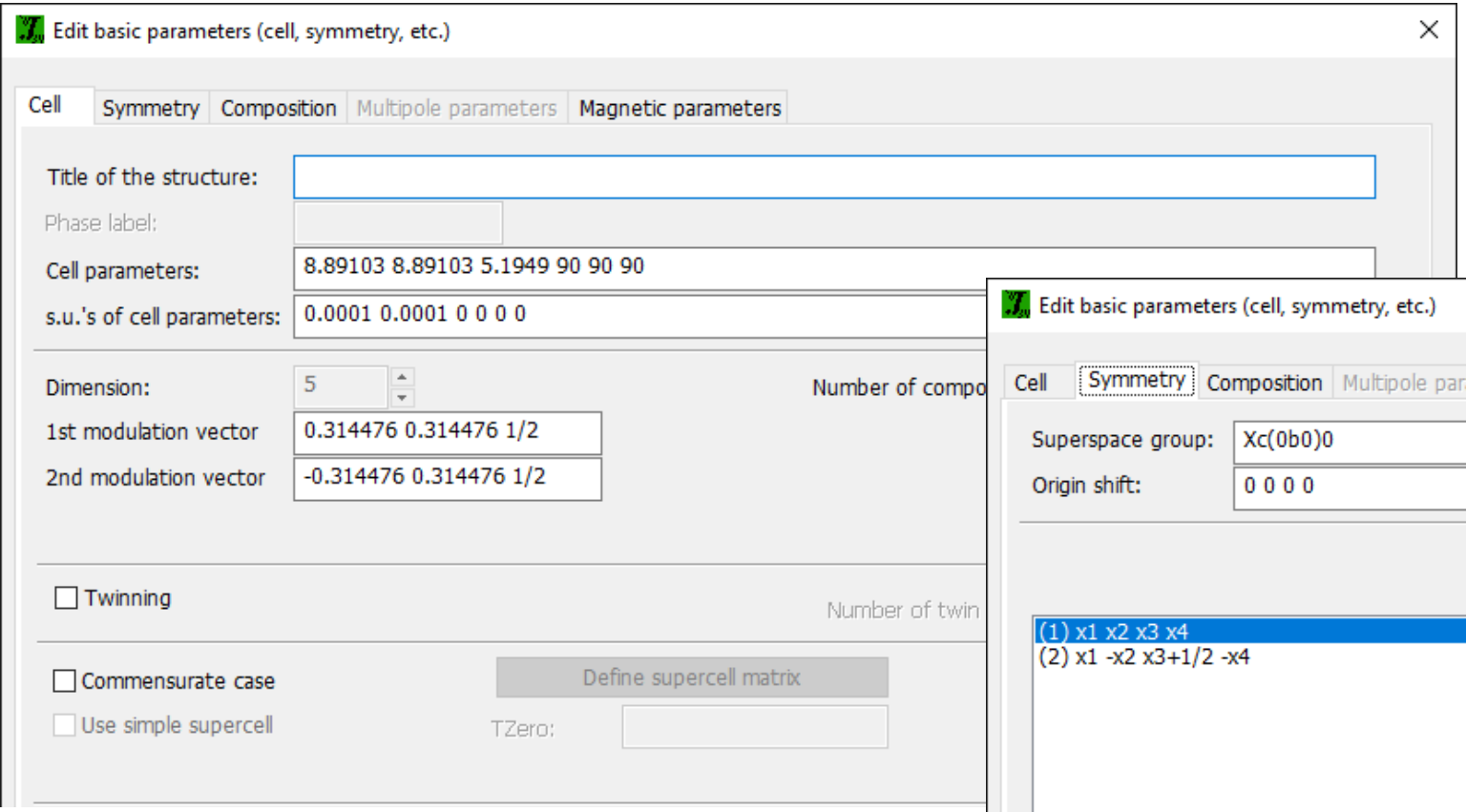
# Advanced tools – Twins, composites

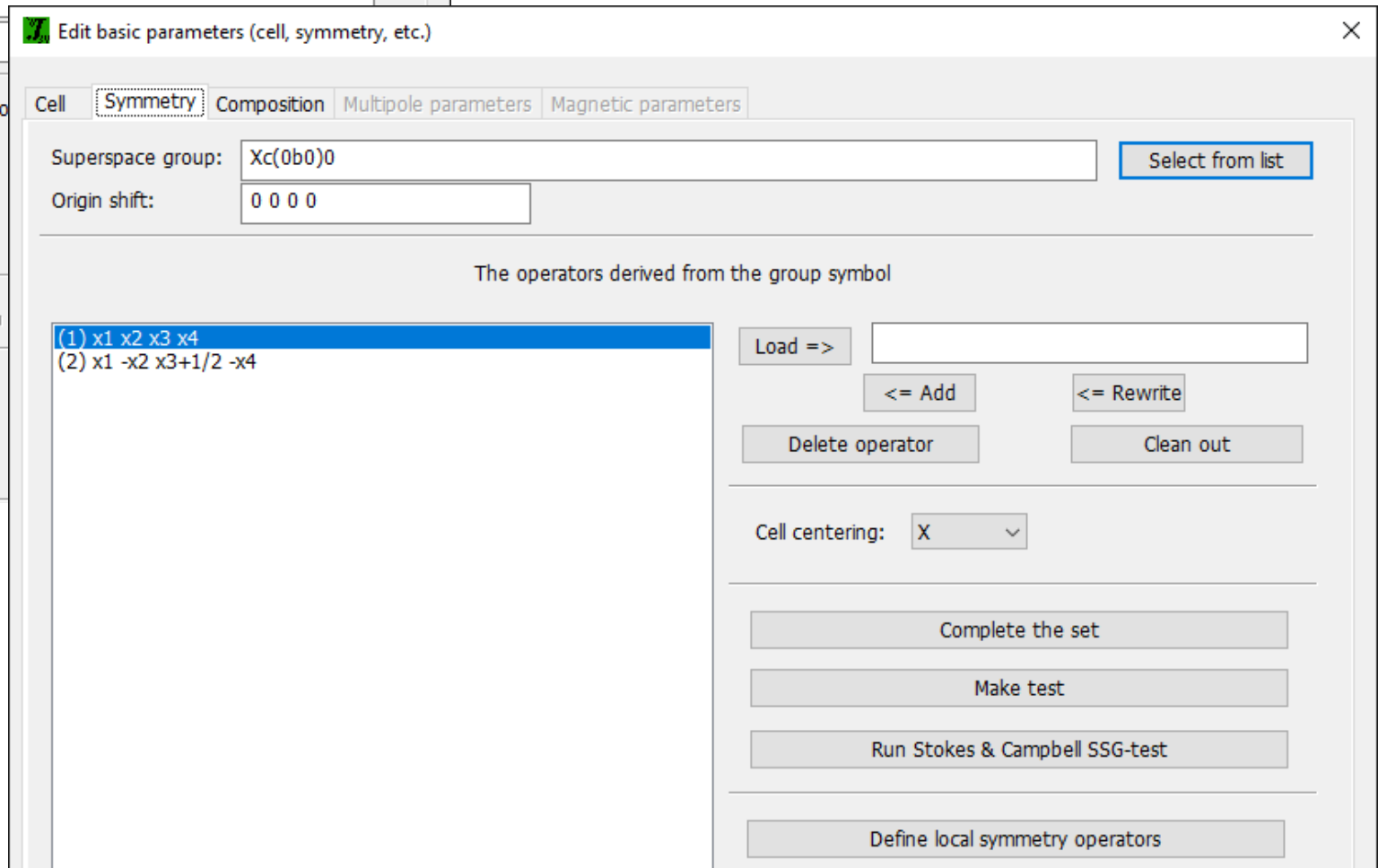
- Reflection file
- New
- Phases
- Edit structure parameters
- Structure solution
- Random search
- Fourier synthesis
- Run Contour
- Import
- Refinement
- Distance calculation
- Draw structure
- Grapht
- CIF utilities
- Tools
  - Search for possible twinning
  - Run reciprocal space viewer
  - Draw 2d displacements
  - Make tables for publication
  - Generate DCRED file for CrysAlis
- Edit file
- Files for MEM
- Recover files
- Matrix calculator
- Run Jana2006




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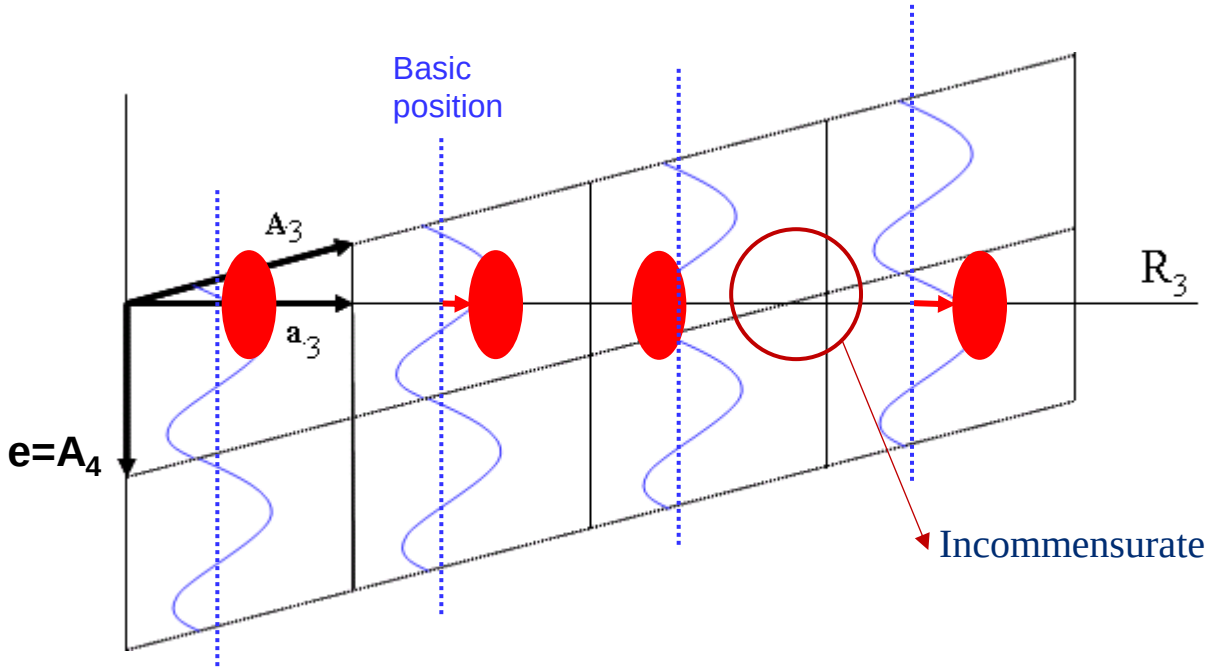
# Advanced tools – modulated structures




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# Modulated structures




p -> site occupancy, position, ADP parameters

$$p(x_4) = p_0 + \sum_n \left(p_{s,n} sin2\pi n x_4 + p_{c,n} cos2\pi n x_4\right)$$

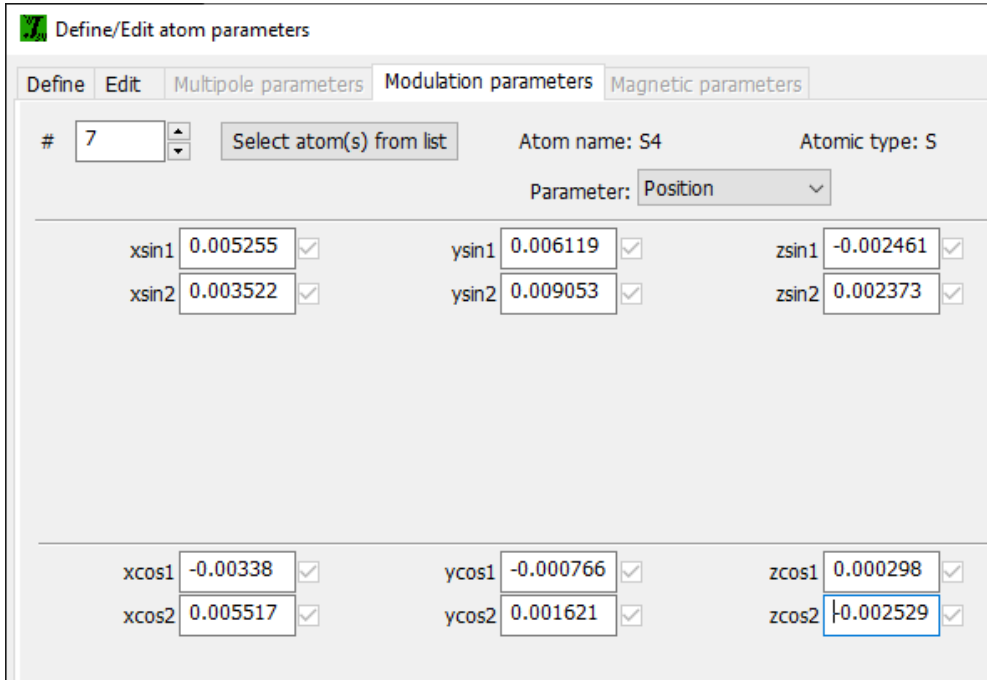
Any periodic function can be written as a Fourier series. The Fourier amplitudes define the modulation functions of the atom.

## Harmonic modulation from arbitrary displacements

The position r of an atom is the sum of the basic structure position and the modulation function u.

$$\mathbf{r} = \bar{\mathbf{r}} + \mathbf{u}$$

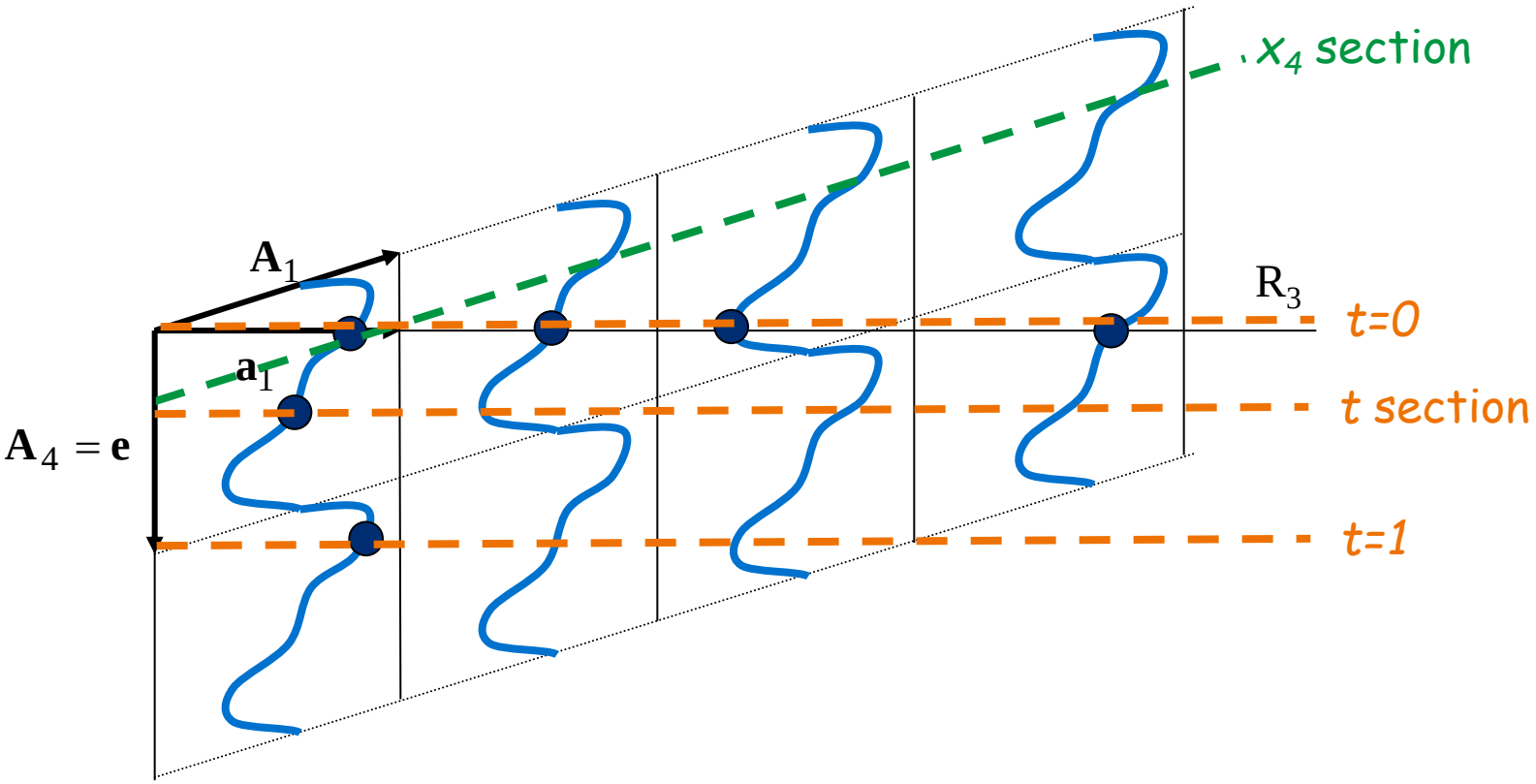
$$\mathbf{u}(\bar{x}_4) = \sum_{n=1}^{m} \mathbf{A}_{s,n} \sin(2\pi n \bar{x}_4) + \sum_{n=1}^{m} \mathbf{A}_{c,n} \cos(2\pi n \bar{x}_4)$$




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# Modulated structures

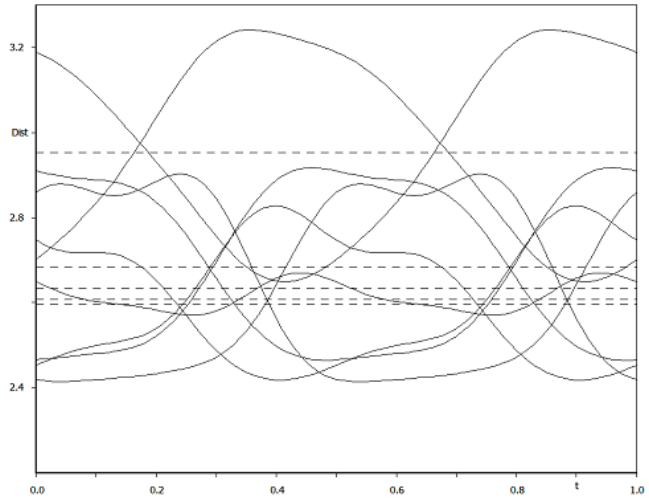
## Modulation parameters as function of t




$$x_4 = t + \bar{\mathbf{r}} \cdot \mathbf{q}$$

The parameter t is a real number describing the initial phase of the wave.

Grapht

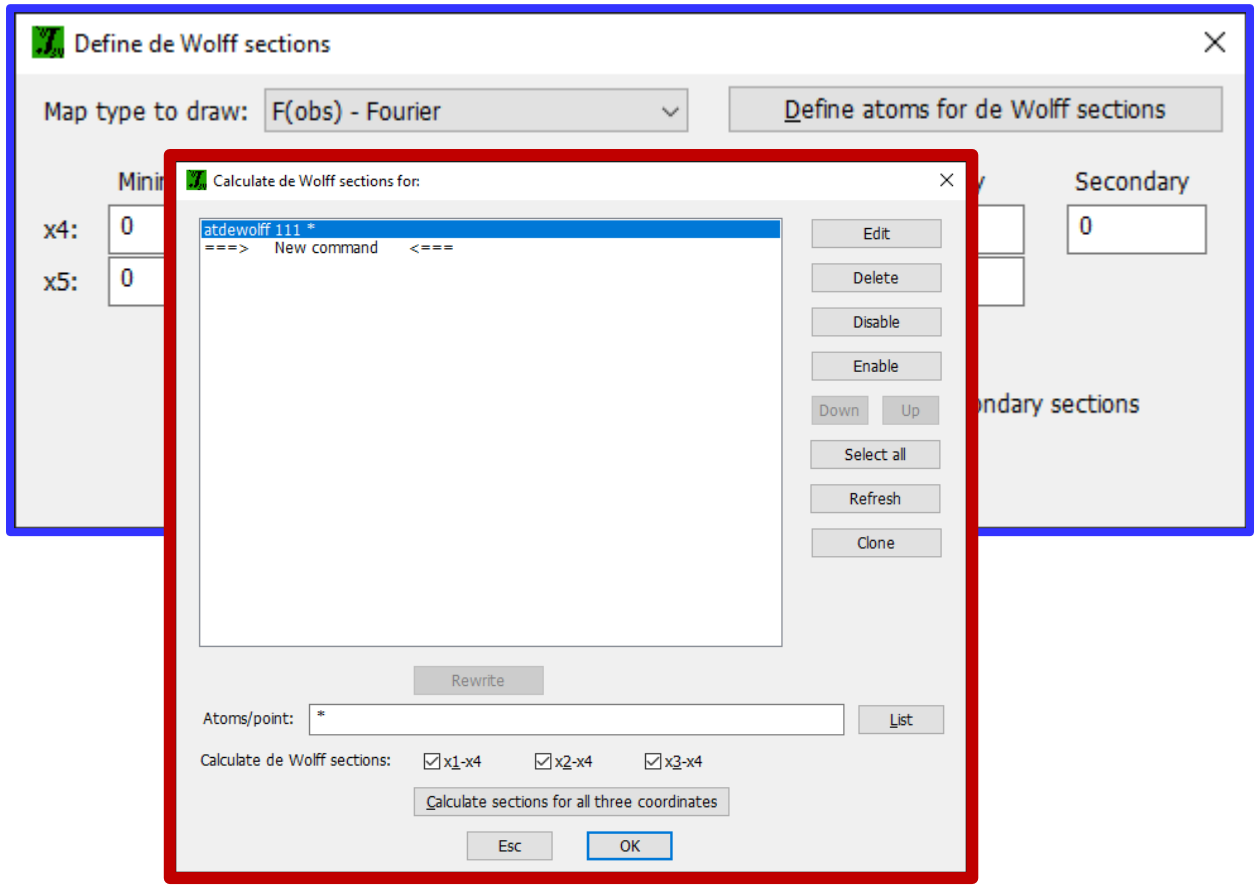


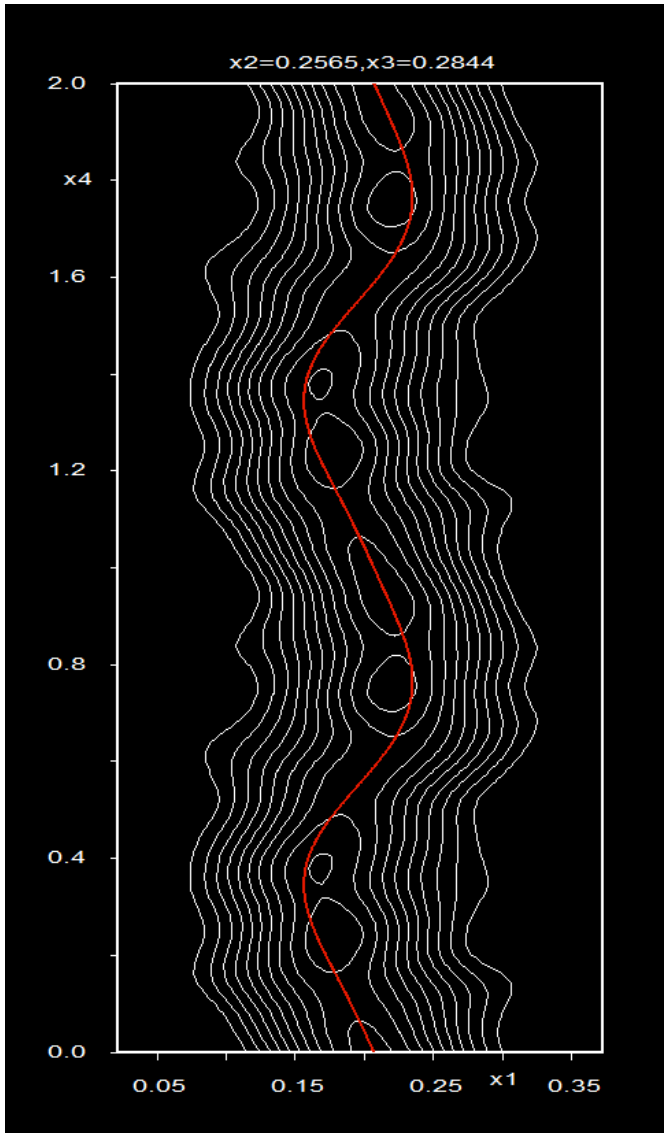

distance Na-O1

Cookbook example 5.2

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# Advanced tools – Fourier sections



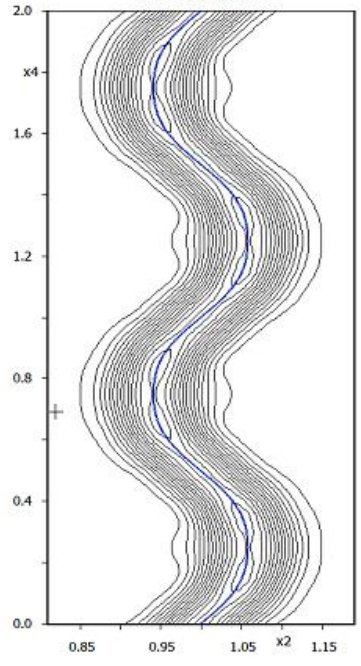

**Checking results in Fourier:**

**$A_i$-$A_4$ Fourier sections**

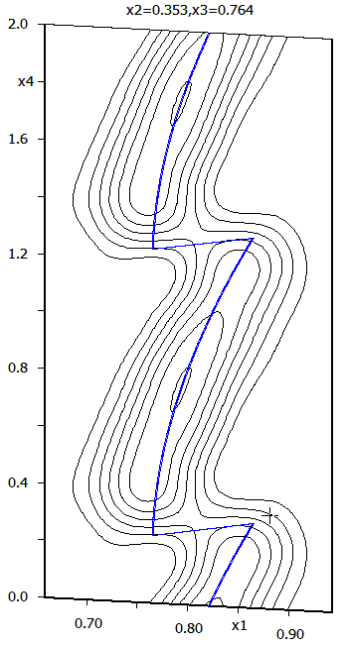
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# Modulated structures - Special modulation functions

## Displacive modulation

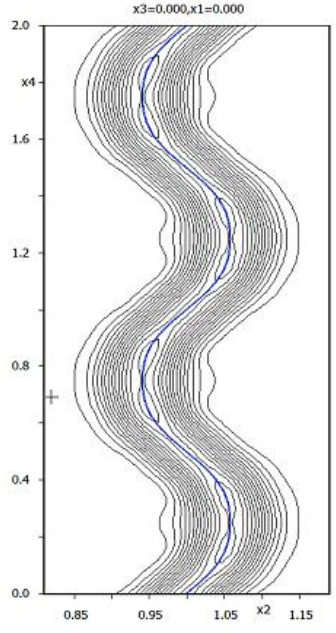



harmonic

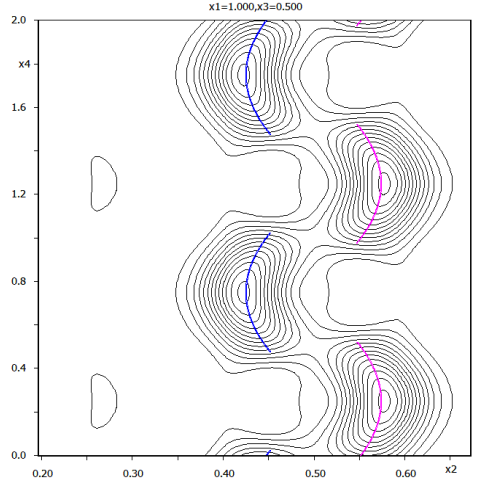



Saw-tooth

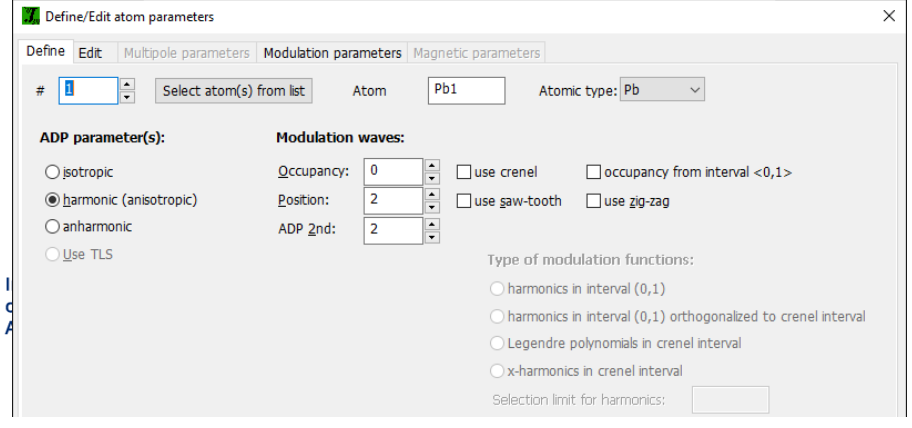
## Occupational modulation

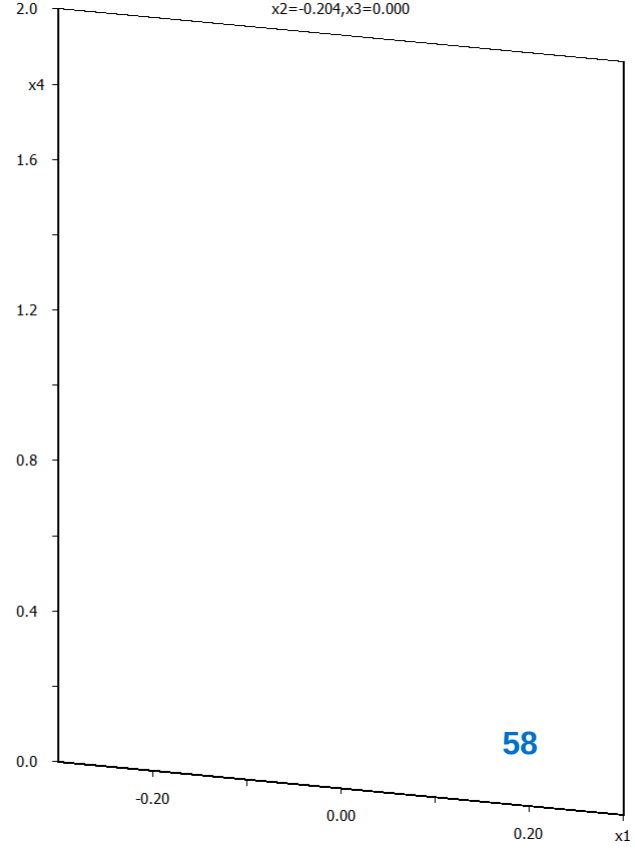



harmonic

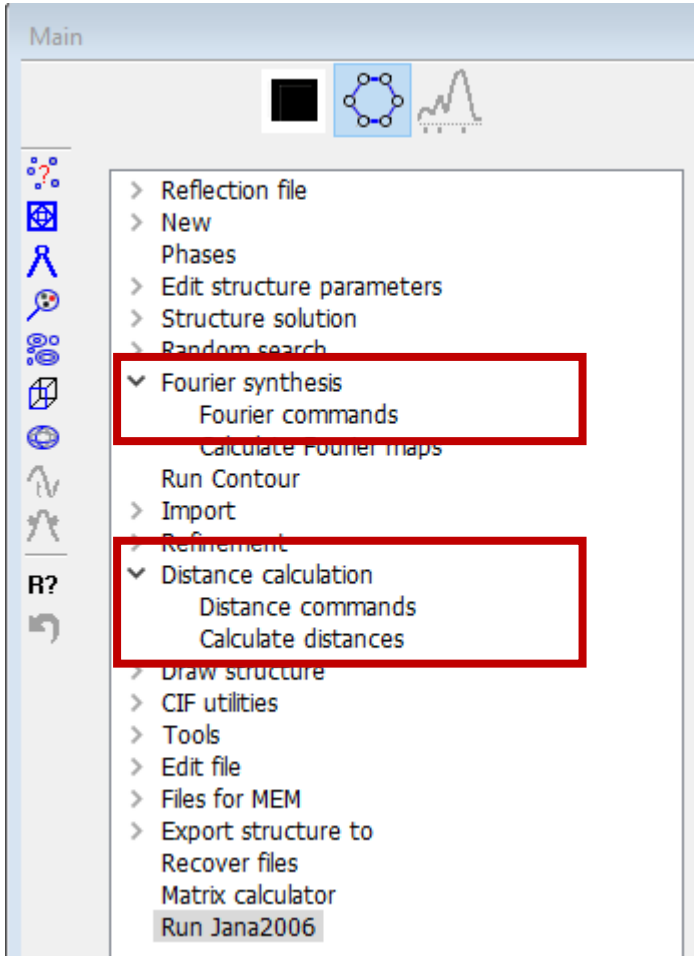


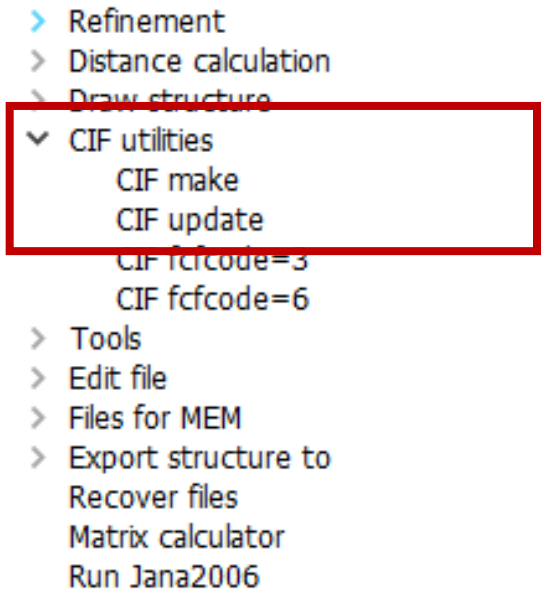

Crenel

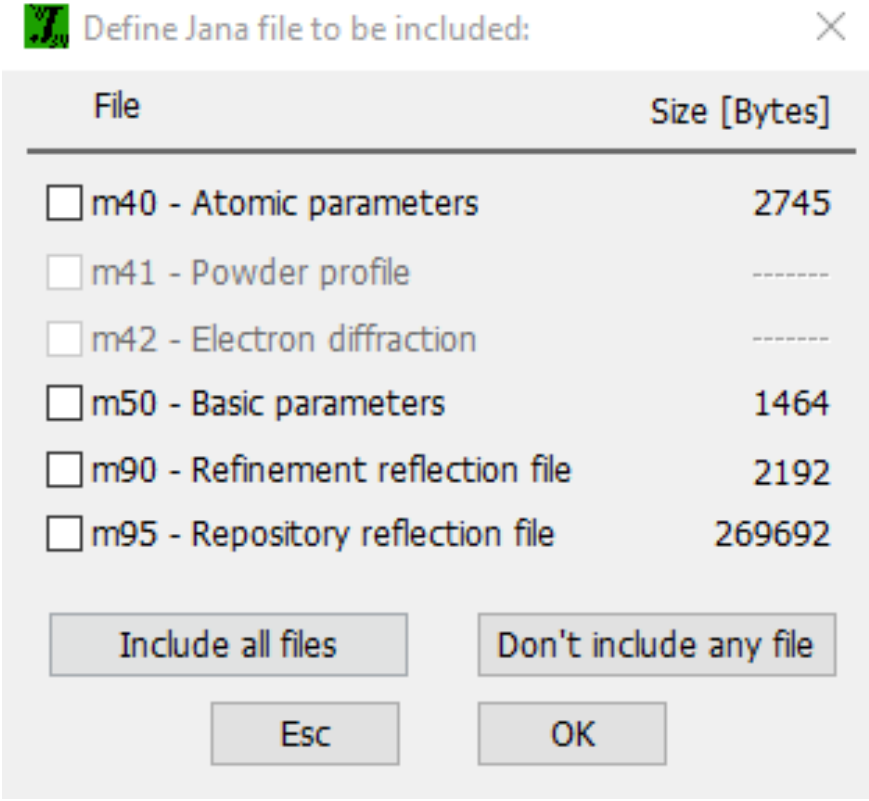


# Results - CIF



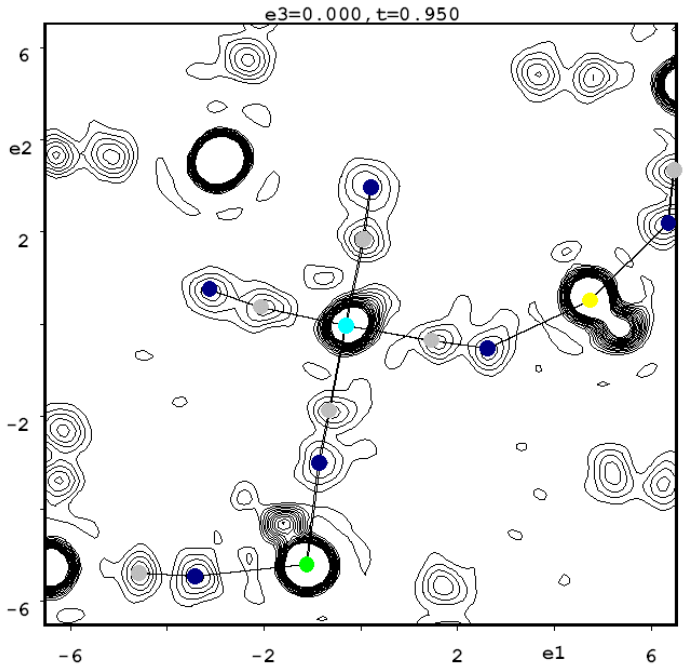




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bilbao crystallographic server

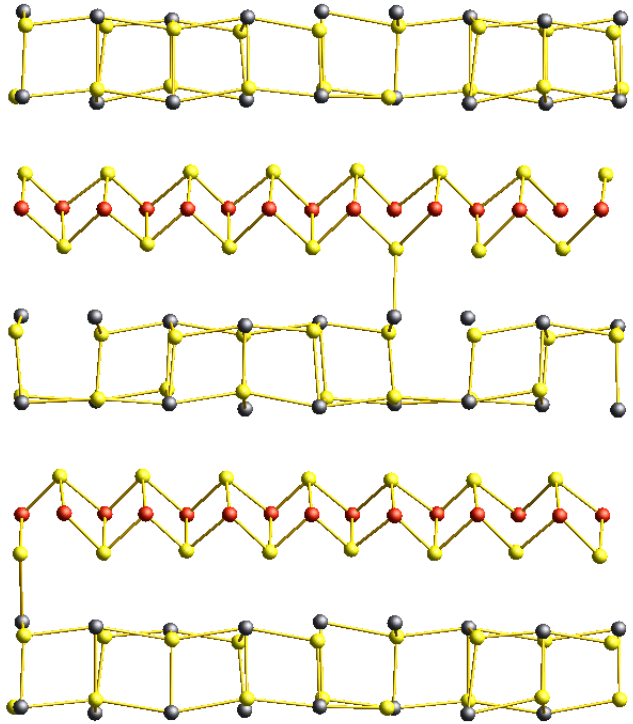
# Results presentation

## Fourier maps as a movie




## JanaDraw movie



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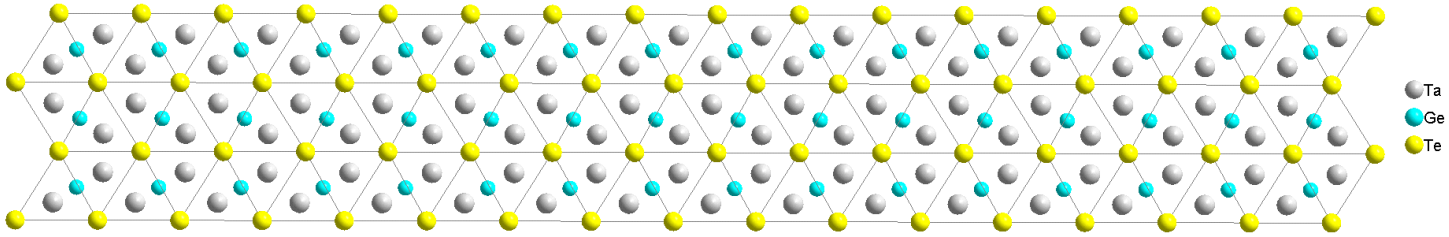
# Results presentation

The modulation curves and corresponding density maps play a crucial role during the solution and refinement process. But the final presentation should be made in the 3d real space. Several cells and more different sections are to be presented to see various configurations in the modulated crystal:

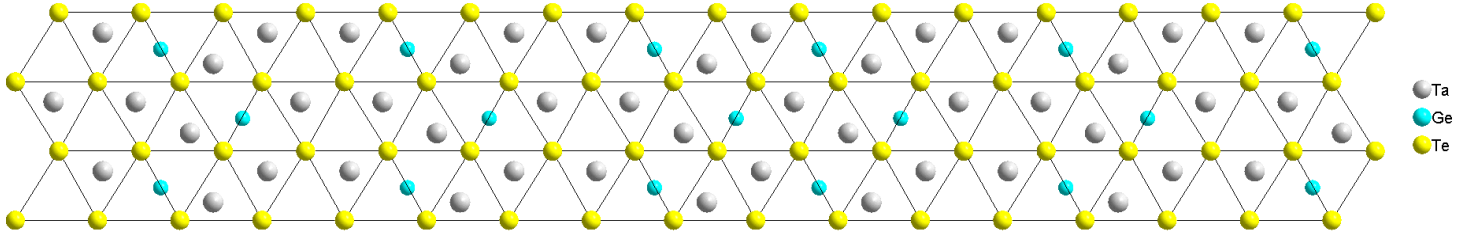
The same example as for the crenel function - $TaGe_{0.354}Te$

F. Boucher, M.Evain & V. Petříček, (1996). *Acta Cryst.*, B**52**, 100

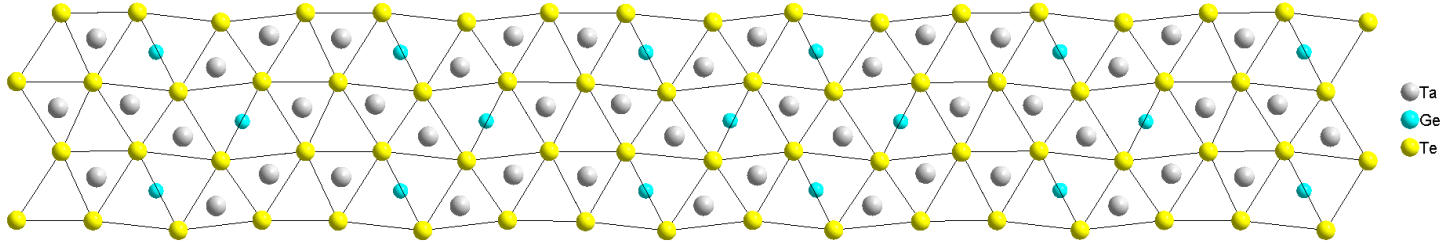
Average structure




Only occupational modulation




Final result




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# Conclusions

- A simple structure can be solved in 5 min
- The JanaDraw helps to analyze the structure
- Jana2020 has several advanced tools for complex structures
- Works up to (3+3)d including composite structures, modulation of occupancies, positions, ADPs up to 6$^{th}$ order of anharmonicity
- Site symmetry restrictions are derived analytically from symmetry operations
- (3+3) Fourier maps
- It can handle merohedric, reticular, and pseudo-merohedric twinning
- It can combine data from different sources – x-ray, electrons, and neutron; powder, and single crystal data
- Magnetic structures

- Hands-on workshops

- If you need help:

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Morgane Poupon: poupon@fzu.cz
Václav Petříček: petricek@fzu.cz
Michal Dušek: dusek@fzu.cz



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# Thank you for your attention!