Jana2020

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

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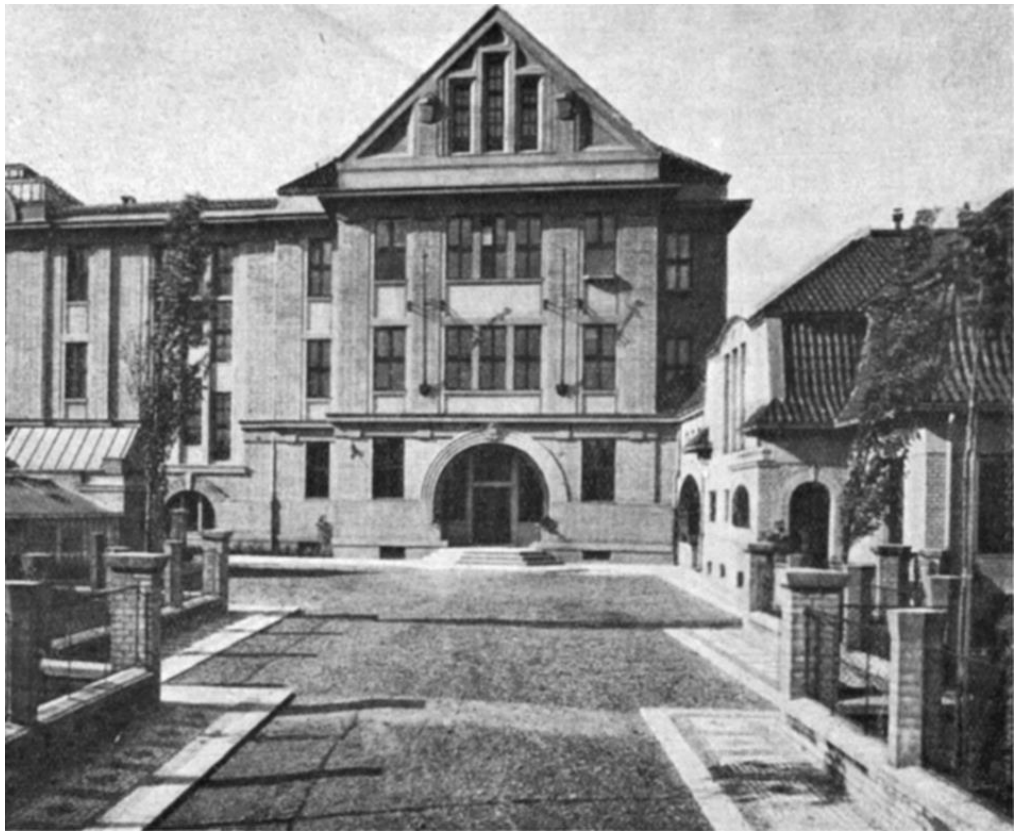

1923

2023

Since 1980…

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History

Václav Petříček

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

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

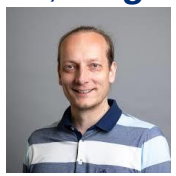
Lukáš Palatinus

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*



Jan Rohliček

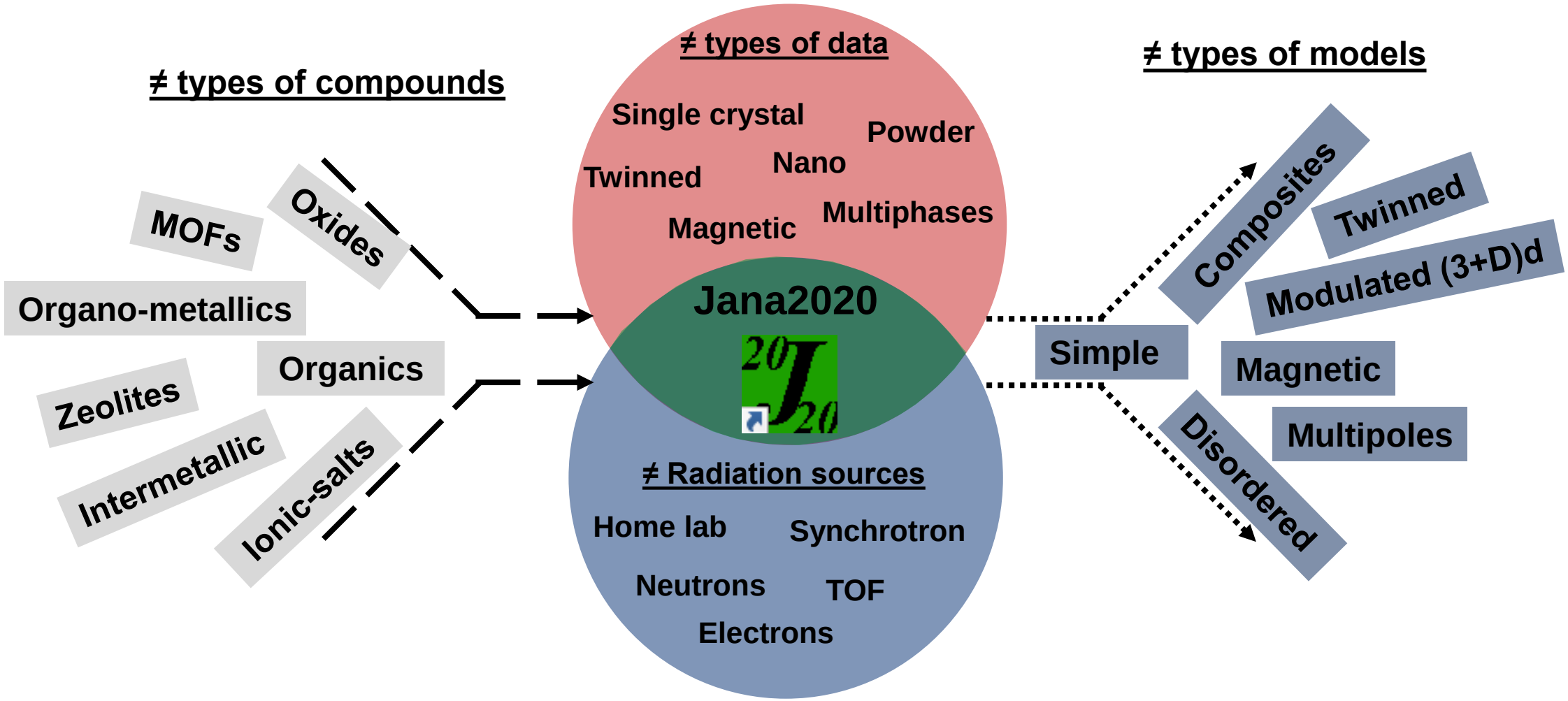
Jakub Plašil

Margarida Henriques

***2021** Jana2020*

Development of an interactive and graphical interface

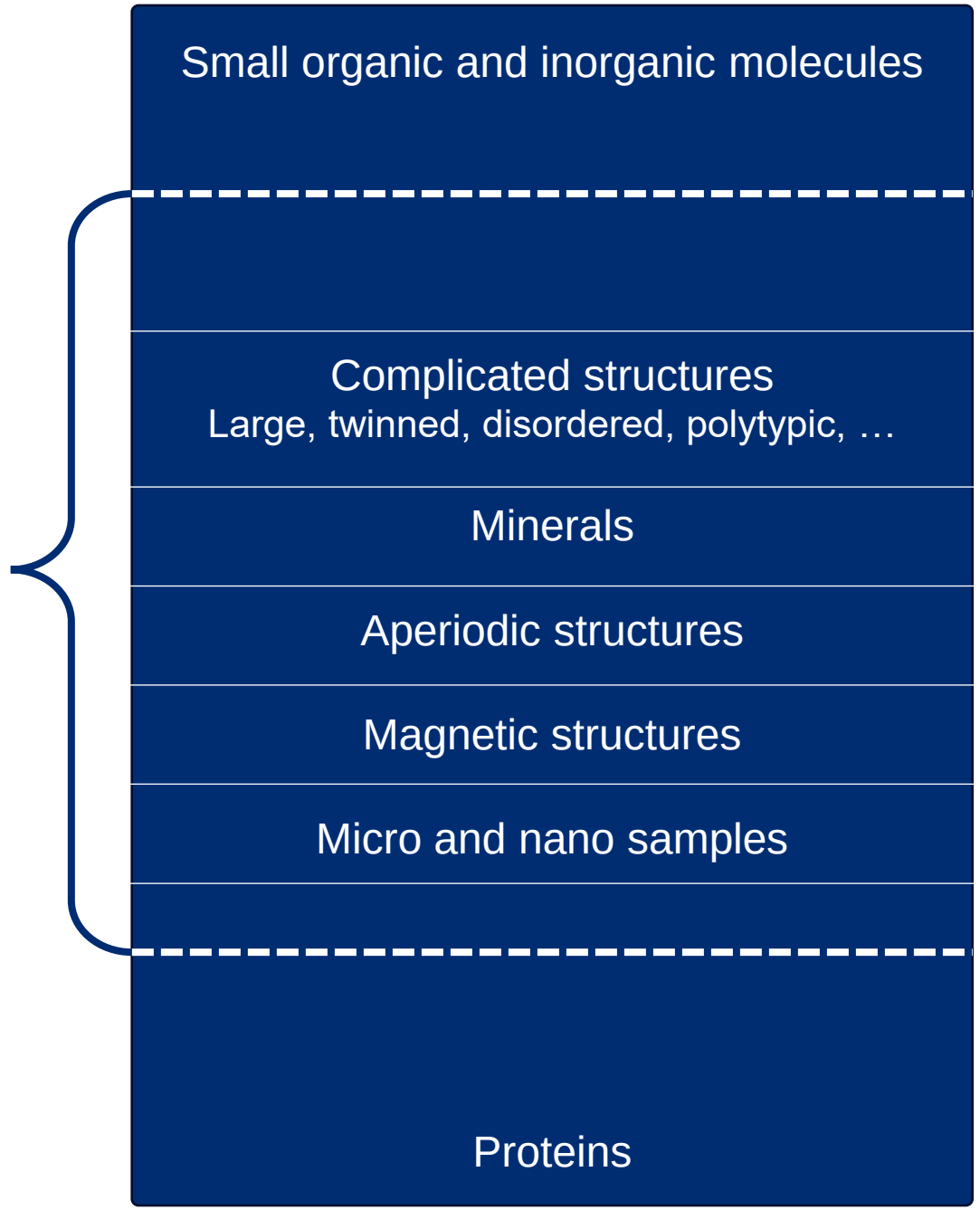
What the program offers



Topics

Basic crystallography

Advanced tools
Commensurate structures
Incommensurate structures
Composite structures
Magnetic structures



Basic crystallography

- Radiation type selection
- Symmetry determination
- External call to structure solution by Charge flipping and Direct methods
- Tools for editing structure parameters
- Fourier calculation
- Tools for adding hydrogen atoms
- Constrains and Restraints

- JanaDraw
- Graphical tools for atomic parameters, refinement commands, bond distances, angles, etc.

- Scale factor
- Atomic site coordinates and occupancies
- ADPs
- Extinction parameters

- CIF output

Advanced tools

- Transformation tools, group-subgroup relations
- Twinning (merohedric, general), treating of overlapped reflections
- Fourier methods - Fourier sections and de Wolff sections
- User equations and restrictions

- Disorder
- Split atomic positions and introduces restrictions
- Rigid body approach, local symmetry
- Anharmonic ADPs

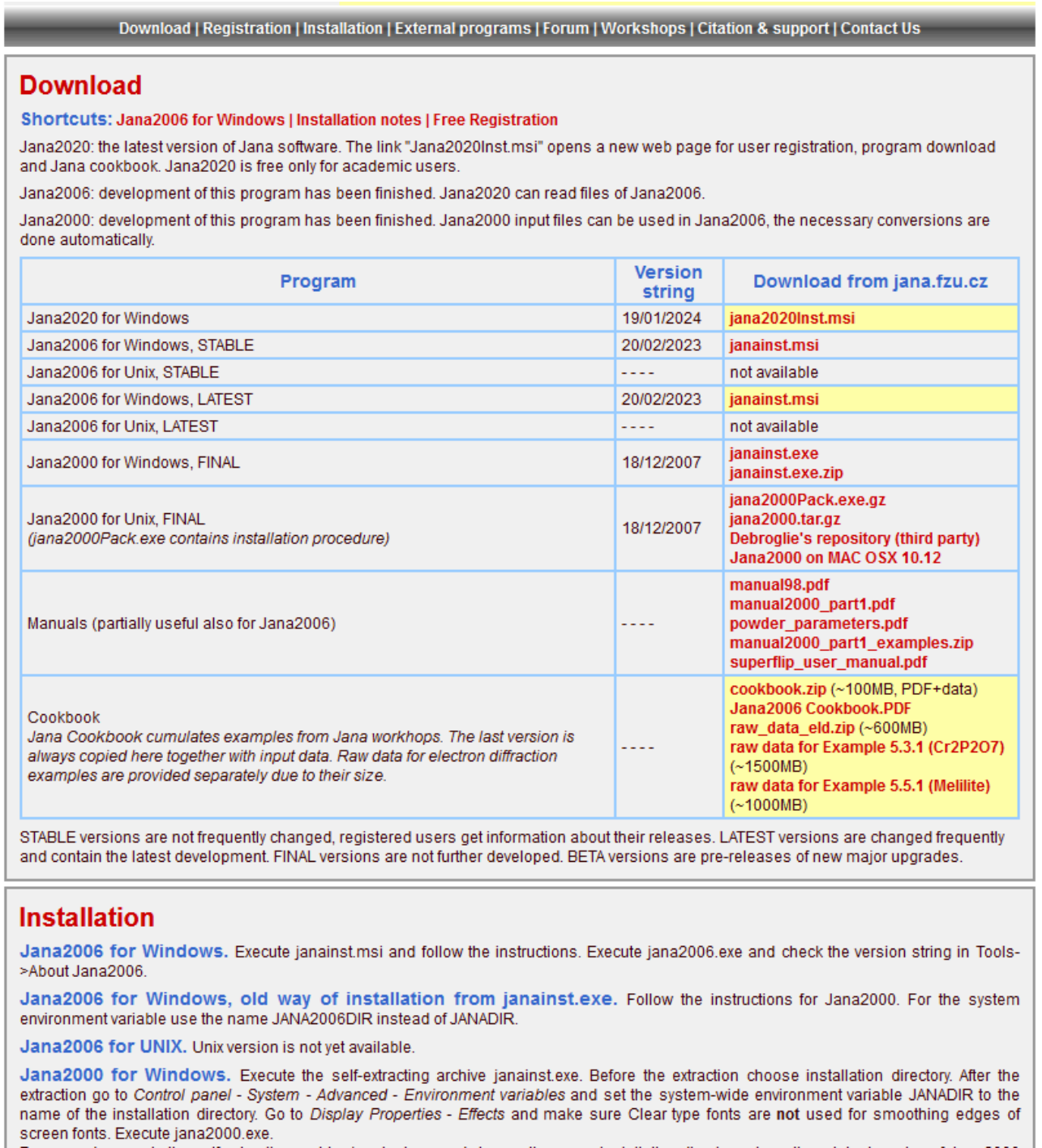
- Modulated and composite structures
- Several types of modulated functions
- Plotting of modulated parameters as a function of t
- Plotting of modulated structures
- Calculation of geometric parameters
- Visualization of the modulated structure in JanaDraw

- Multiphases for powder and single-crystal data
- Multipole refinement
- Cyclic refinement
- Fundamental approach
- Anisotropic strain broadening (generalized to satellites)

Where to get it

http://jana.fzu.cz/

Registration
Download
Installation



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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	19/01/2024	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 janainst.exe.zip
Jana2000 for Unix, FINAL *(jana2000Pack.exe contains installation procedure)*	18/12/2007	jana2000Pack.exe.gz jana2000.tar.gz Debroglie's repository (third party) Jana2000 on MAC OSX 10.12
Manuals (partially useful also for Jana2006)	----	manual98.pdf manual2000_part1.pdf powder_parameters.pdf manual2000_part1_examples.zip superflip_user_manual.pdf
Cookbook *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) Jana2006 Cookbook.PDF raw_data_eld.zip (~600MB) raw data for Example 5.3.1 (Cr2P2O7) (~1500MB) 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.

Installation

Jana2006 for Windows. Execute janainst.msi and follow the instructions. Execute jana2006.exe and check the version string in Tools->About Jana2006.

Jana2006 for Windows, old way of installation from janainst.exe. Follow the instructions for Jana2000. For the system environment variable use the name JANA2006DIR instead of JANADIR.

Jana2006 for UNIX. Unix version is not yet available.

Jana2000 for Windows. Execute the self-extracting archive janainst.exe. Before the extraction choose installation directory. After the extraction go to *Control panel - System - Advanced - Environment variables* and set the system-wide environment variable JANADIR to the name of the installation directory. Go to *Display Properties - Effects* and make sure Clear type fonts are **not** used for smoothing edges of screen fonts. Execute jana2000.exe.

Where to get it

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

Registration
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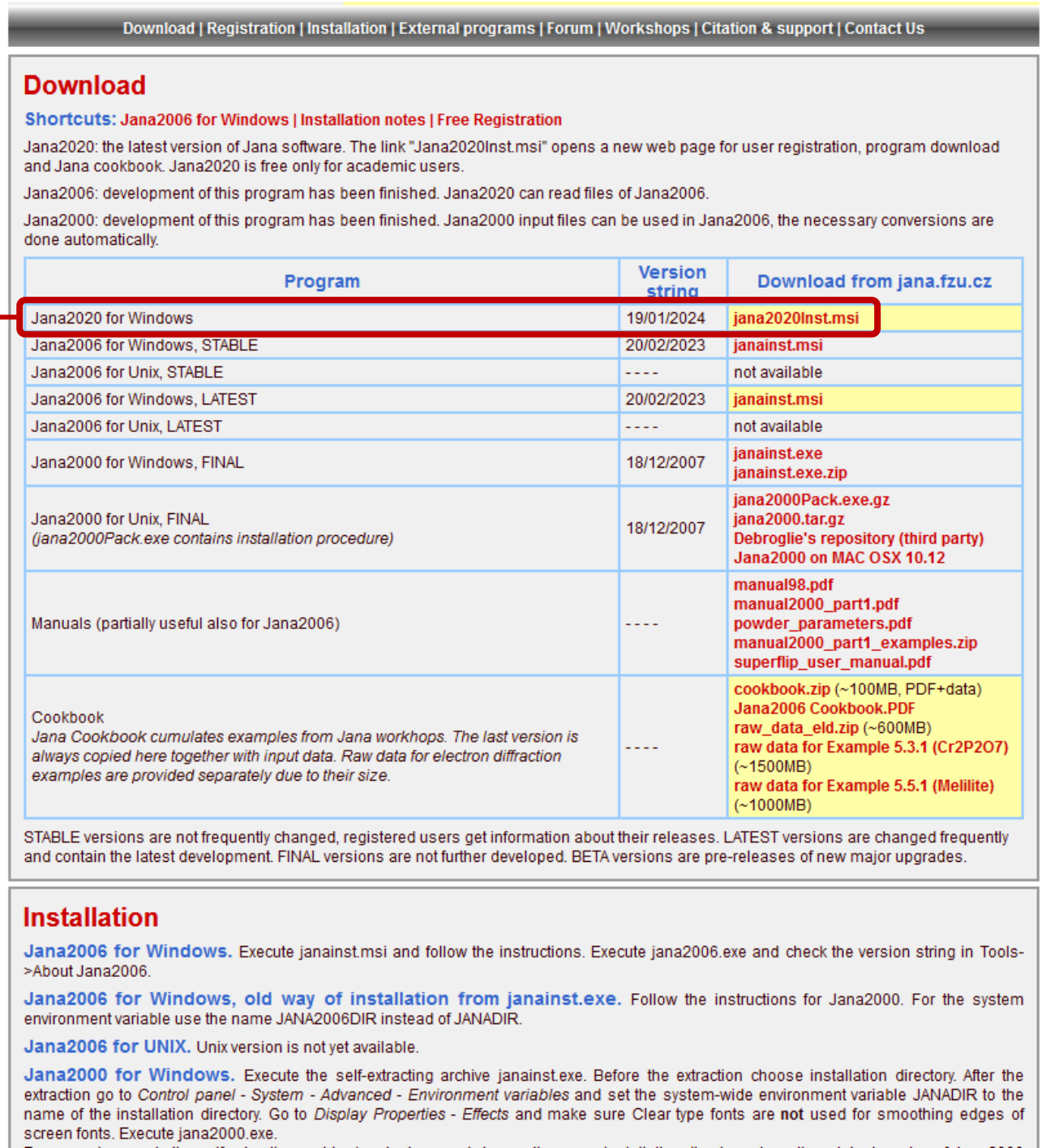
Installation



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Jana2006 for Unix, STABLE	----	not available
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Jana2006 for Unix, LATEST	----	not available
Jana2000 for Windows, FINAL	18/12/2007	janainst.exe janainst.exe.zip
Jana2000 for Unix, FINAL *(jana2000Pack.exe contains installation procedure)*	18/12/2007	jana2000Pack.exe.gz jana2000.tar.gz Debroglie's repository (third party) Jana2000 on MAC OSX 10.12
Manuals (partially useful also for Jana2006)	----	manual98.pdf manual2000_part1.pdf powder_parameters.pdf manual2000_part1_examples.zip superflip_user_manual.pdf
Cookbook *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) Jana2006 Cookbook.PDF raw_data_eld.zip (~600MB) raw data for Example 5.3.1 (Cr2P2O7) (~1500MB) raw data for Example 5.5.1 (Melilite) (~1000MB)

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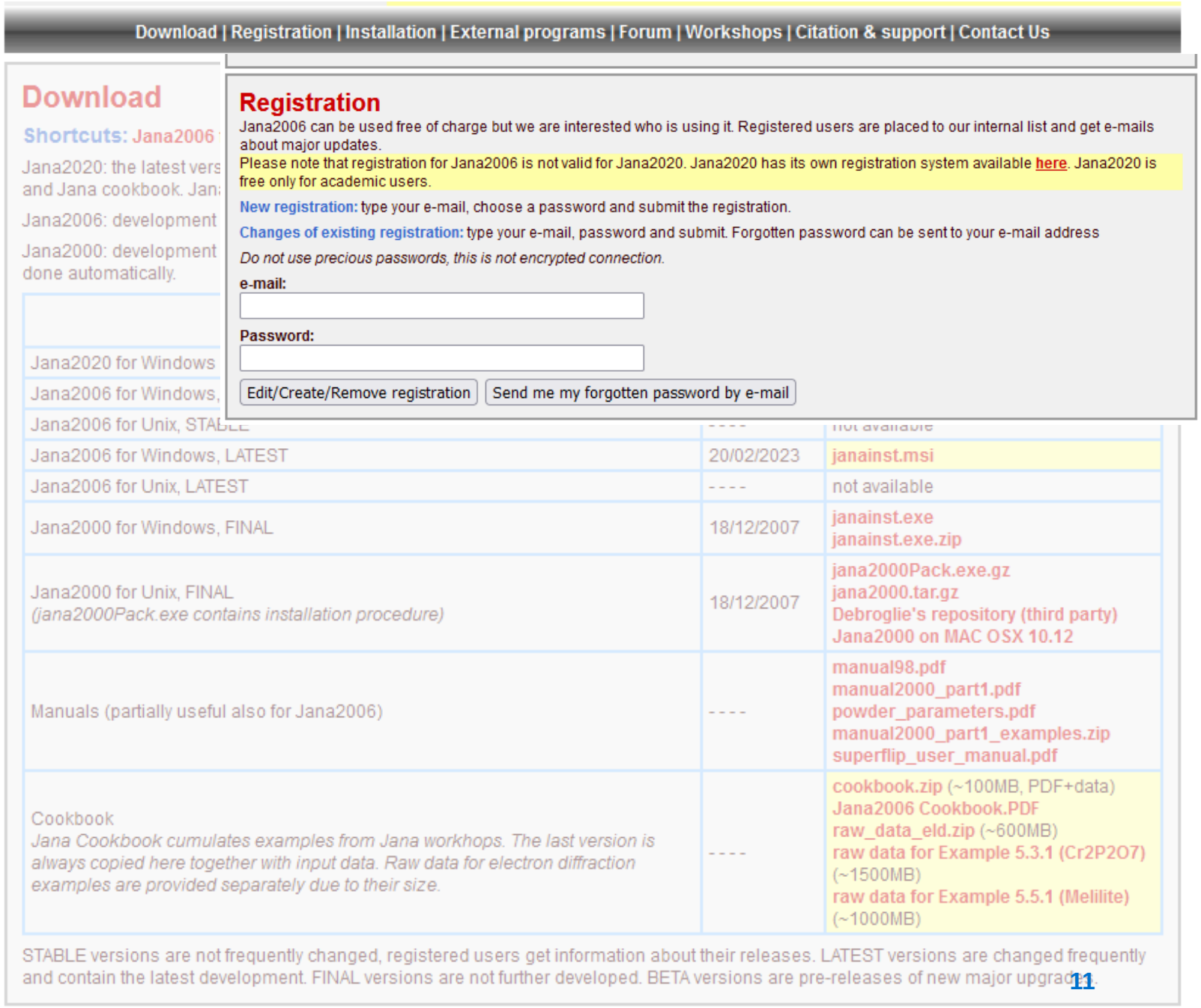
How to get it

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

Registration



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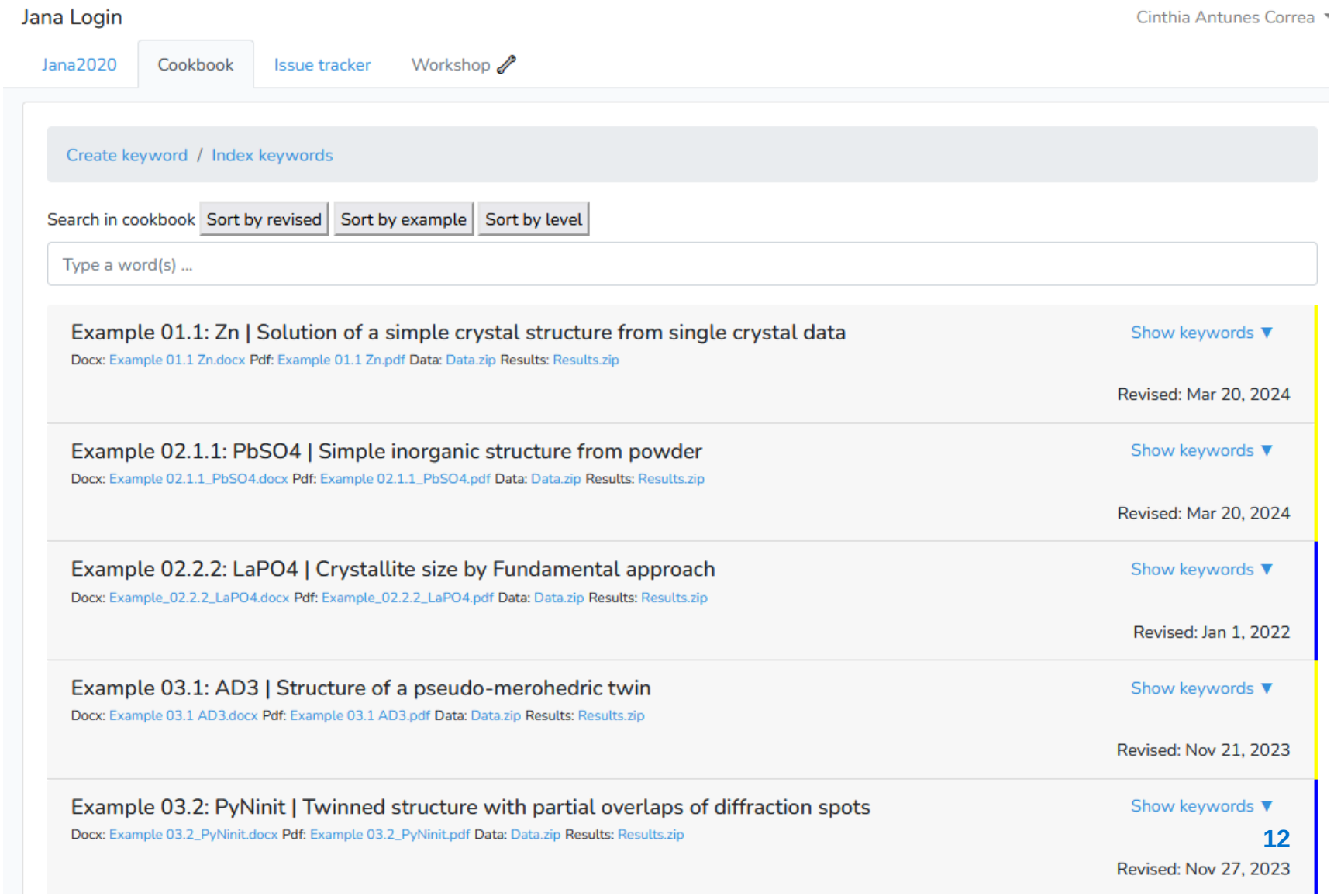
Install

Cookbook



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Where to get it

http://jana.fzu.cz/

Workshops

Institute of Physics
Department of Structure Analysis
Cukrovarnicka 10
16253 Praha 6
Czech Republic

CRYSTALLOGRAPHIC COMPUTING SYSTEM FOR STANDARD AND MODULATED STRUCTURES

Vaclav Petricek, Michal Dusek & Lukas Palatinus

Jana2006 is a crystallographic program focused to solution, refinement and interpretation of difficult, especially modulated structures. It calculates structures having up to three modulation vectors from powder as well as single crystal data measured with X-ray or neutron diffraction. The input diffraction data can be unlimitedly combined, the combination of powder neutron data with single crystal X-ray data being a typical example. The structure solution can be done using the built-in charge flipping algorithm or by calling an external direct methods program. Jana can handle multiphase structures (for both powder and single crystal data), merohedric twins as well as twins with partial overlap of diffraction spots, commensurate and composite structures. It contains powerful transformation tools for symmetry (group-subgroup relations), cell parameters and commensurate-supercell relations. Wide scale of constrains and restrains is available including a powerful rigid body approach and possibility to define a local symmetry affecting only part of the structure. The latest development of Jana concerns magnetic structures.

More about Jana2006 (PowerPoint presentation, 10MB)

News

COFUND project Physics for Future: Postdoctoral fellowships at the Institute of Physics, Prague, offer training in various disciplines including crystallography.

Jana2020 publication in Zeitschrift für Kristallographie: Please cite this article if you publish structures calculated with Jana2020.

October 18 - 20, 2023 **Jana2020 workshop**: Garching, Germany

June 18 - 23, 2023 **The 15th conference on quasicrystals**: Tel Aviv, Israel

The 26th IUCr Congress: abstract deadline 21 February 2023

August 22 - 29, 2023 **The 26th IUCr Congress**: Melbourne, Australia

June 28 - 23, 2023 **The 15th International Conference on Quasicrystals, ICQ15**: Tel Aviv, Israe

June 19 - 24, 2022 **APERIODIC2022 - 10h International Conference on Aperiodic Crystals**: Sapporo, Japan

May 23 - 27, 2022 **5th international school on aperiodic crystals**: Kutna Hora, Czechia

August 22 - 30, 2020 **The 25th IUCr Congress**: Prague, Czech Republic

IUCr 25 Highlights related to aperiodic crystallography:
Magnetic structures
Aperiodic structures
Satellite workshop on aperiodic and magnetic structures

August 20 - 21, 2020 **Workshop on Aperiodic and Magnetic Structures**: satelllite of IUCr, Prague, Czech Republic

May 31 - June 9, 2019 **Magnetic Crystallography**: Erice, Italy

March 11 - 13, 2019 Jana basic Workshop in Jena, Germany

December 10 - 13, 2018 **Jana Modulation Workshop**: La Jolla CA, USA

October 26-27, 2017 Workshop on magnetic option in Jana2006, Garching, Germany

Ad hoc workshops on Jana [Next: 47]

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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

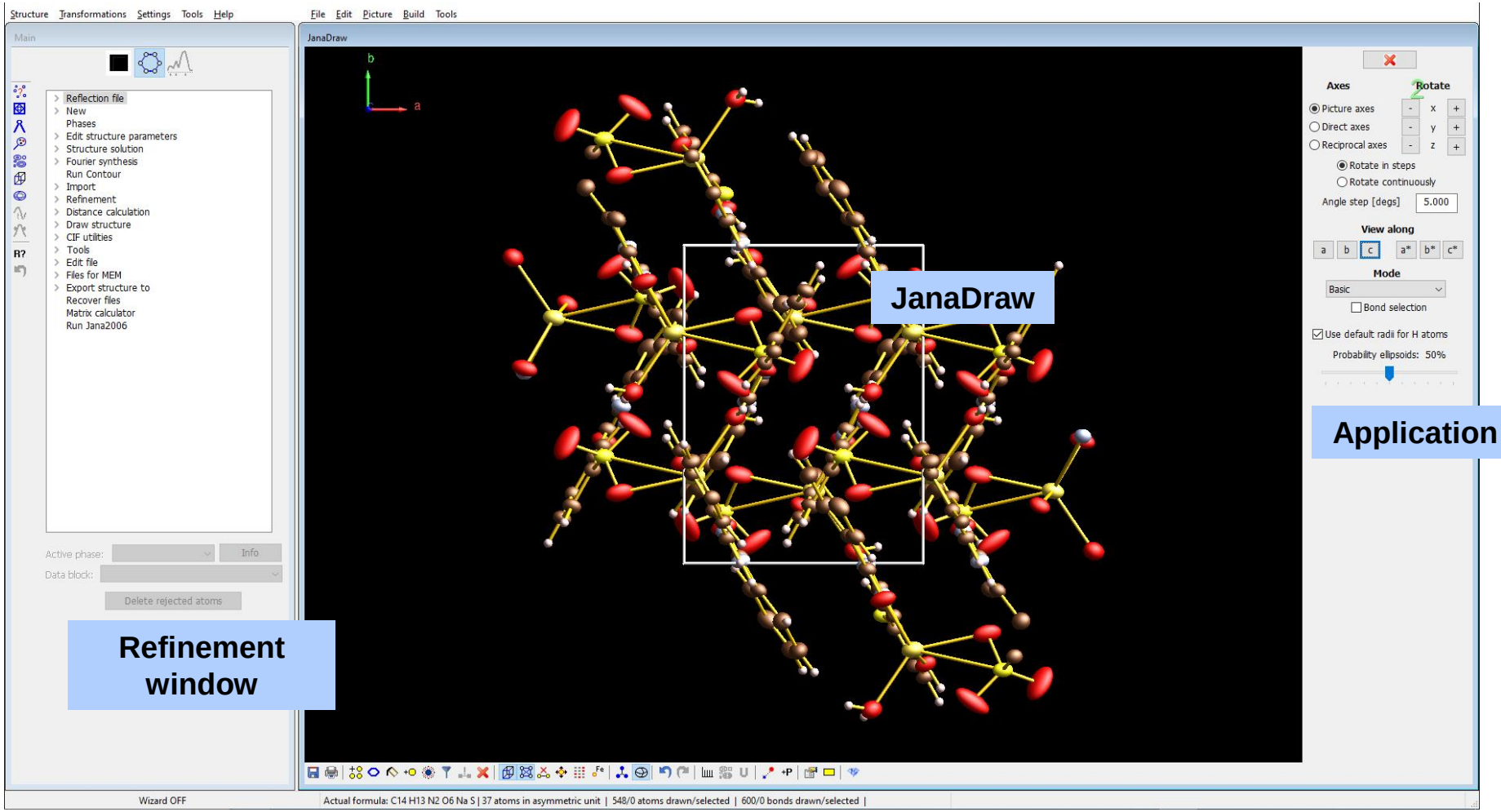
Software that can be launched in Jana2020

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

Jana2020 Interface

Left pane

Right pane



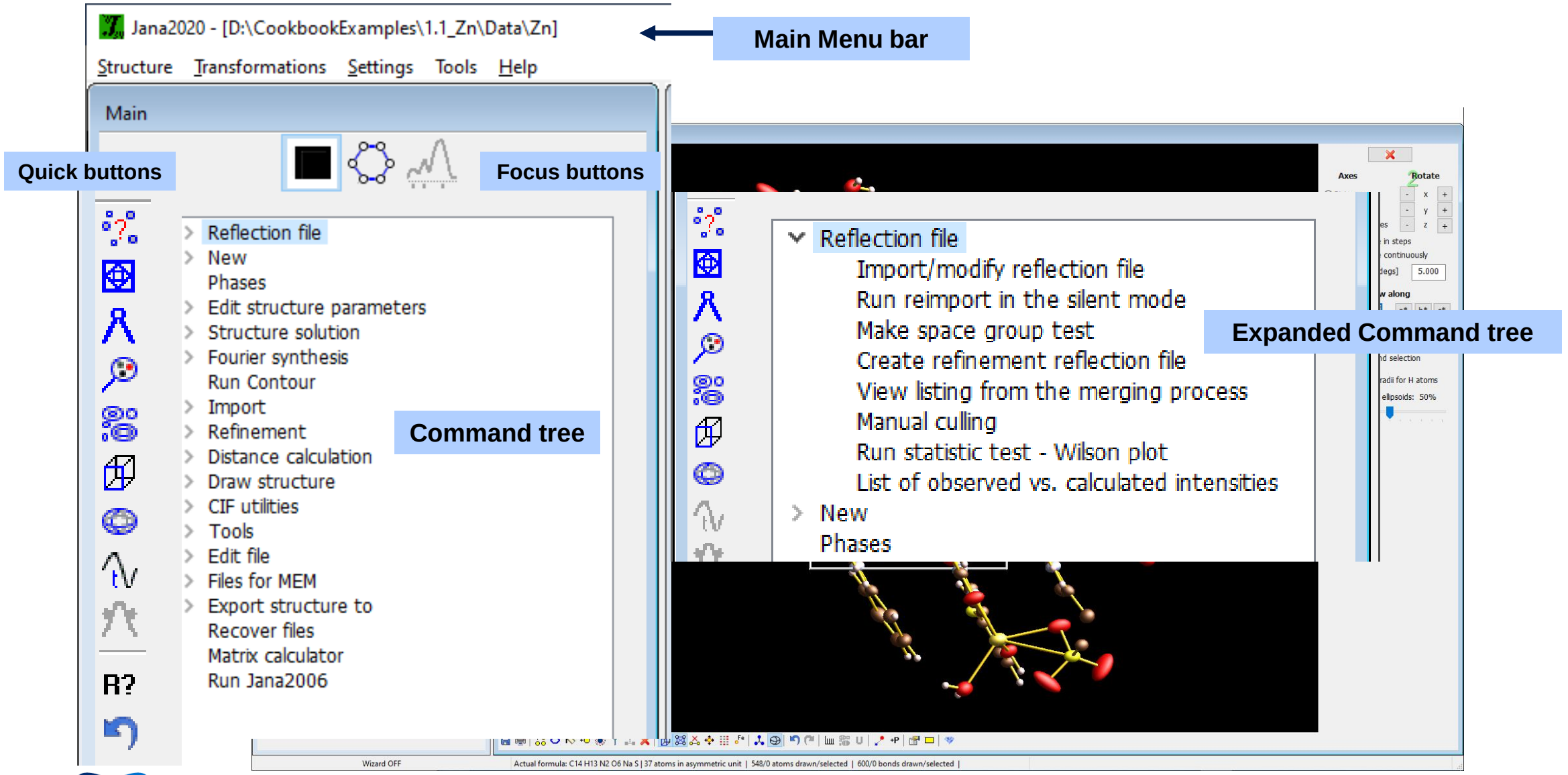
JanaDraw

Refinement window

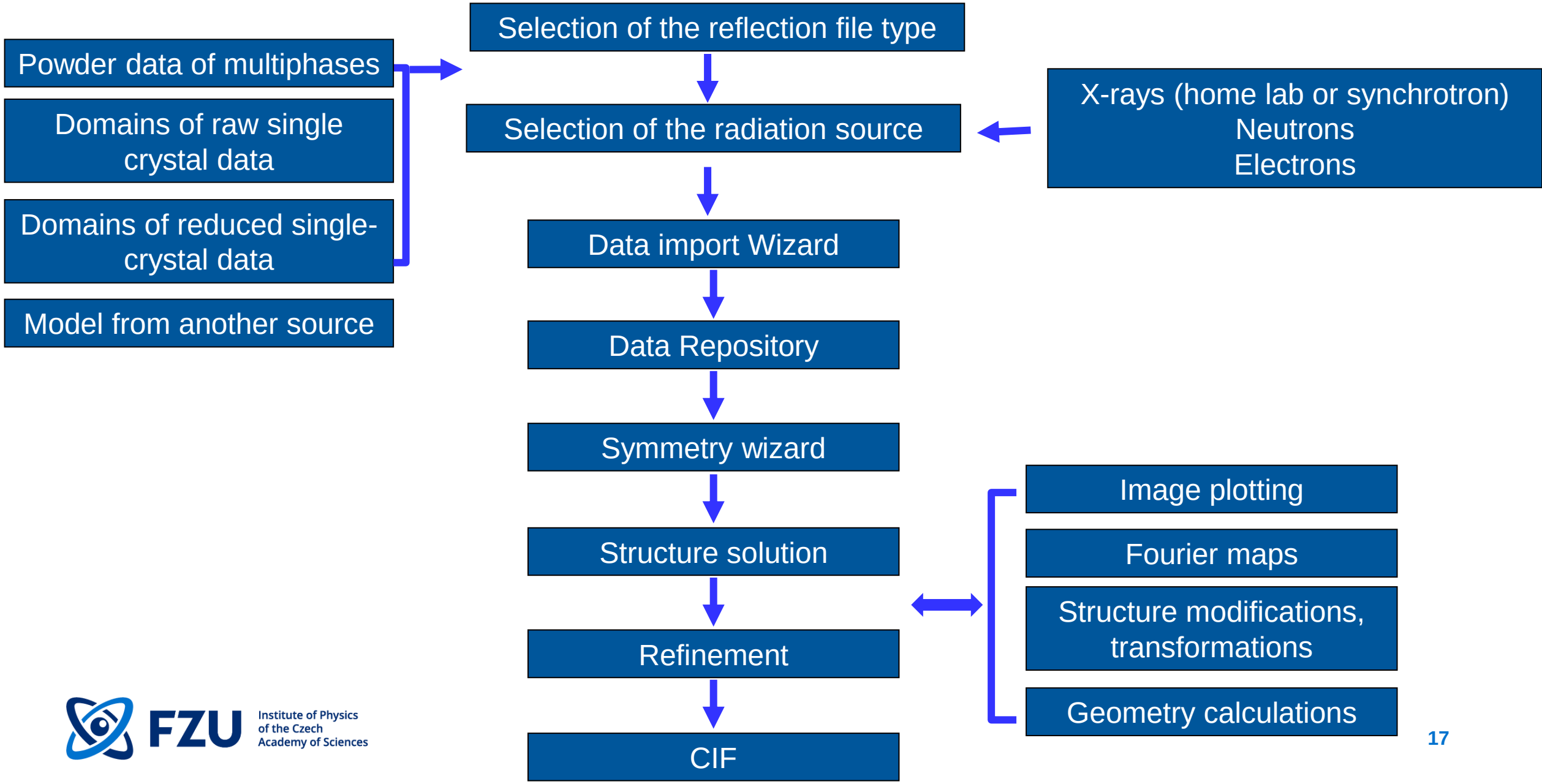
Application controls

Lower toolbar

Jana2020 Interface



Software flow scheme



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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 graphical parameters

CIF

Plotting, geometry parameters, Fourier maps

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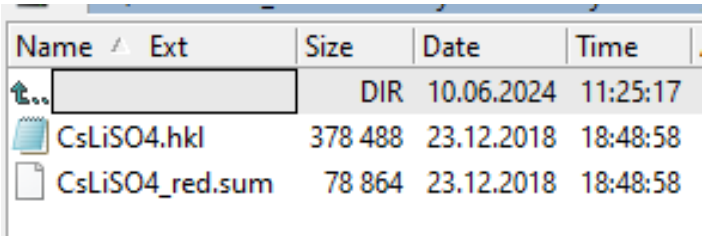
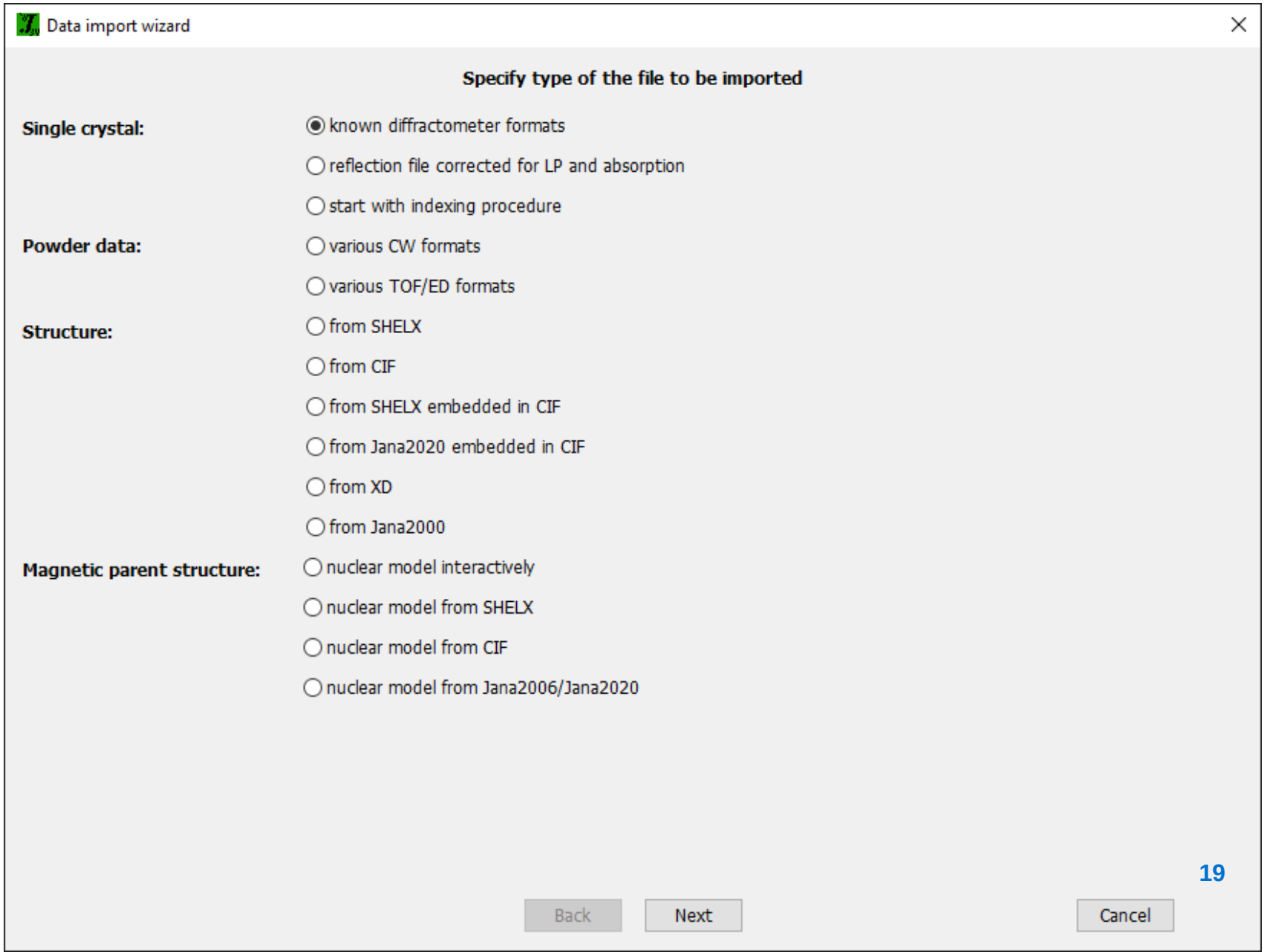
Data import wizard



Name	Ext	Size	Date	Time
..		DIR	10.06.2024	11:25:17
CsLiSO4.hkl		378 488	23.12.2018	18:48:58
CsLiSO4_red.sum		78 864	23.12.2018	18:48:58



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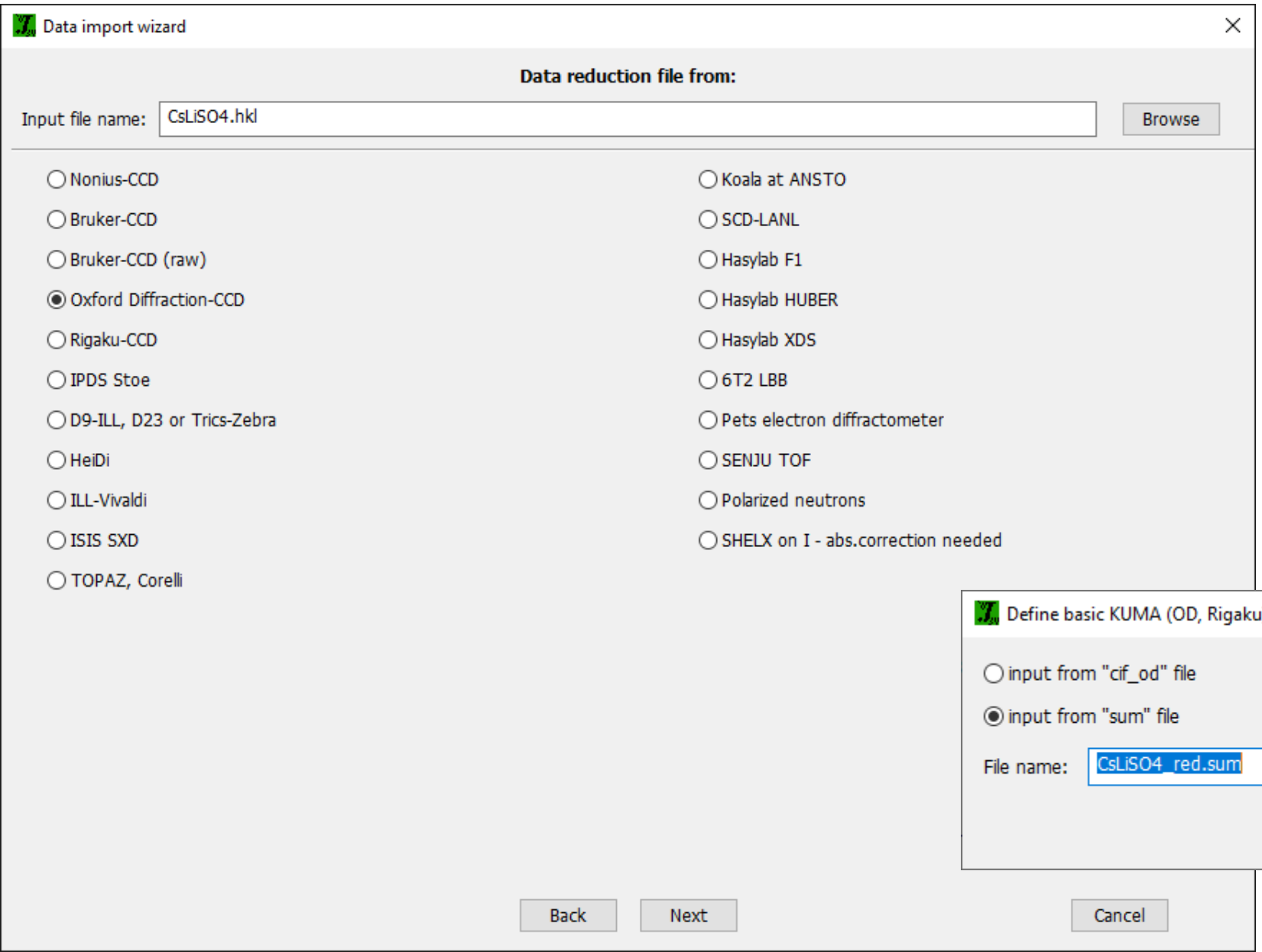
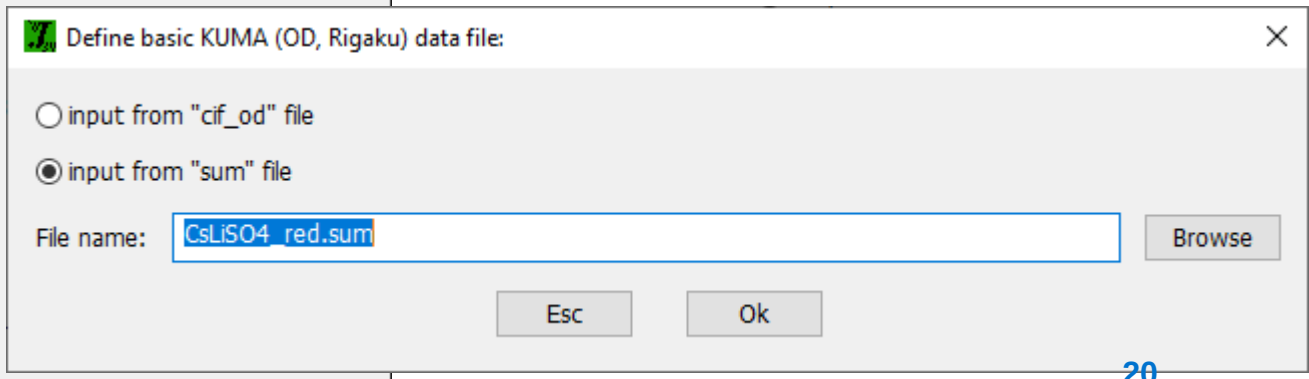
Data import wizard

Input data: single crystal, powder, TOF

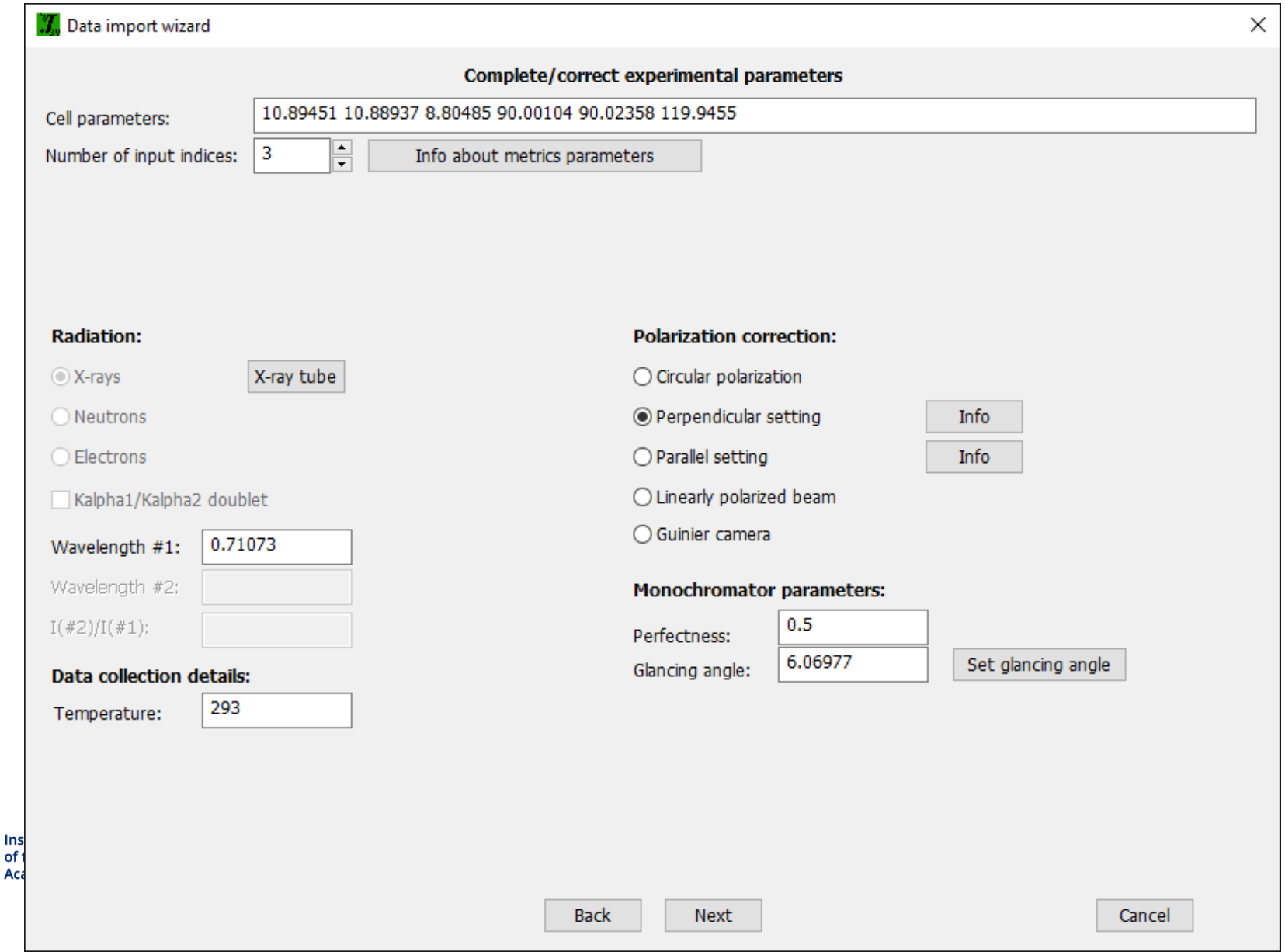


- **Conventional lab XRD**
- **Synchrotron sources**
- **Neutron sources**
- **Electron diffraction (kinematical and dynamic approaches)**

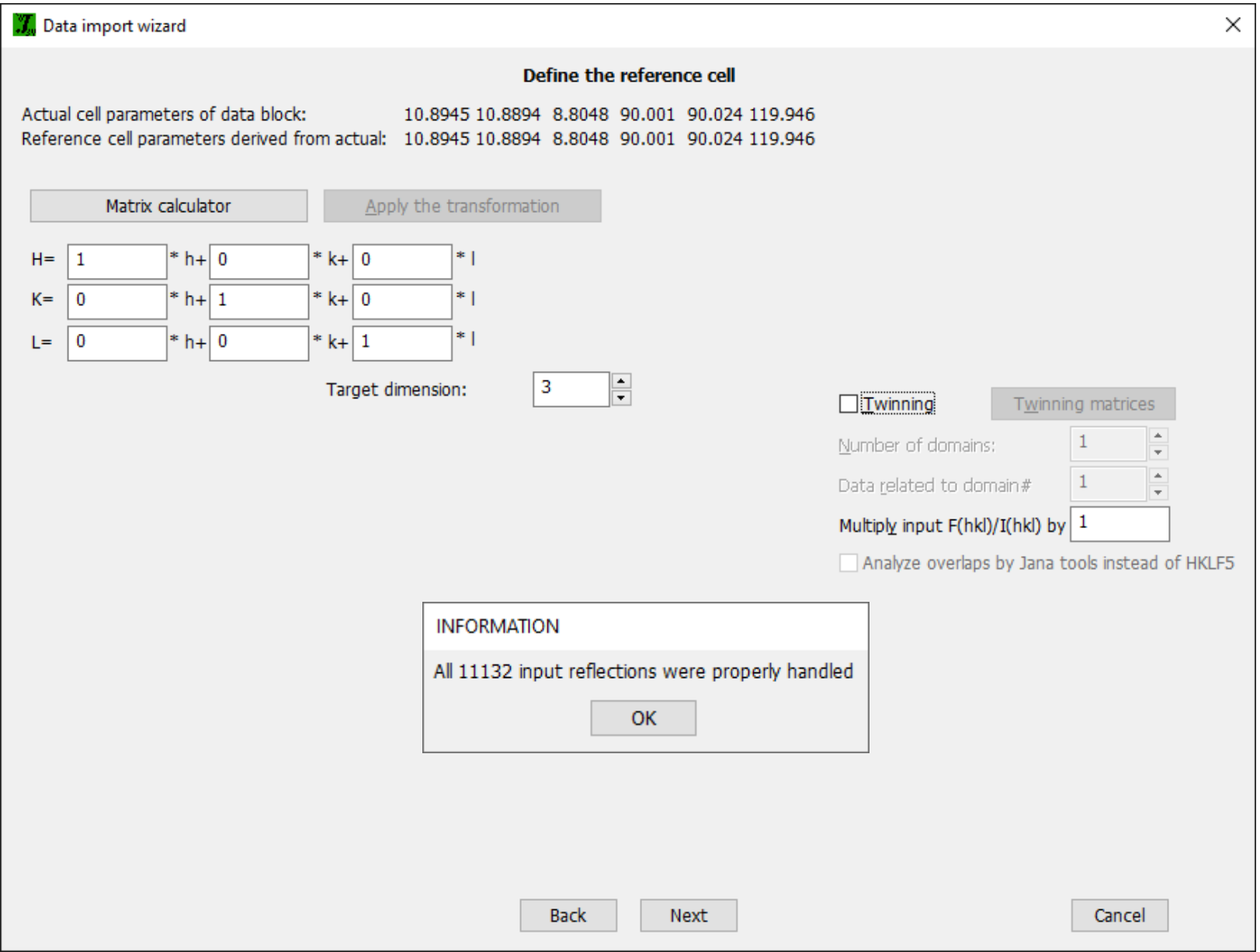
Data from different sources can be combined during refinements.

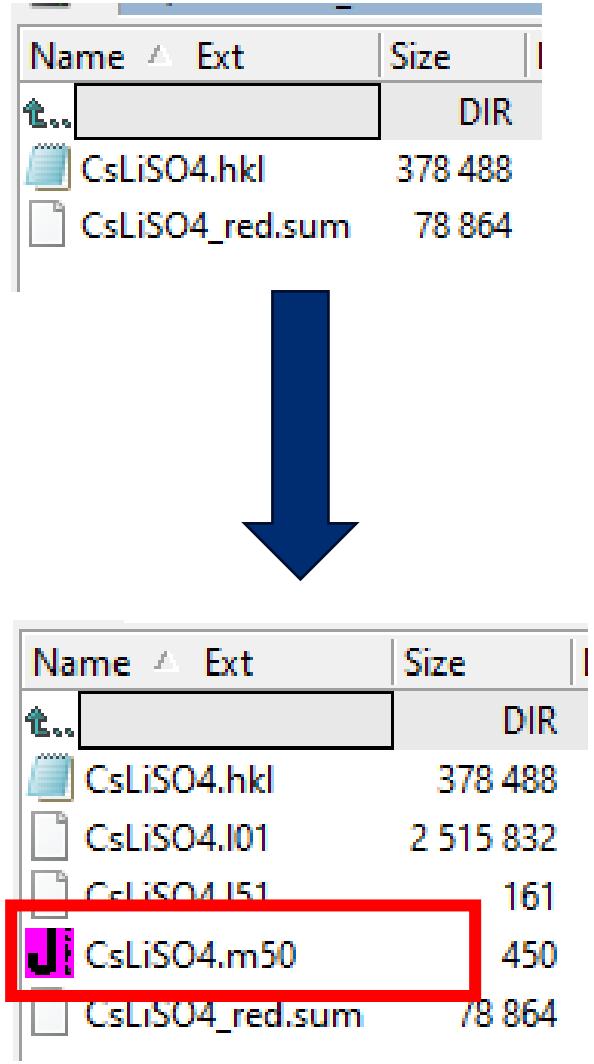


Data import wizard



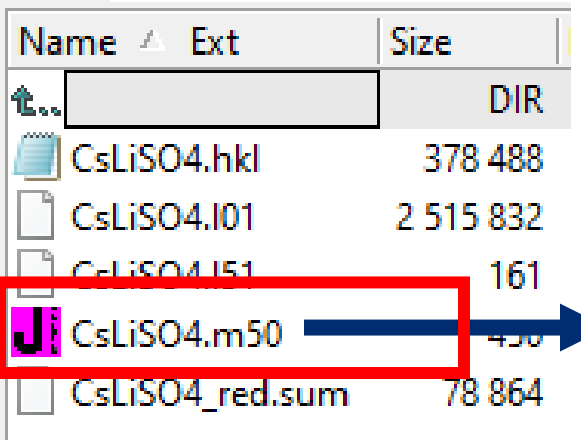
Data import wizard





Data import wizard

M50 – basic crystal information, form factors, program options

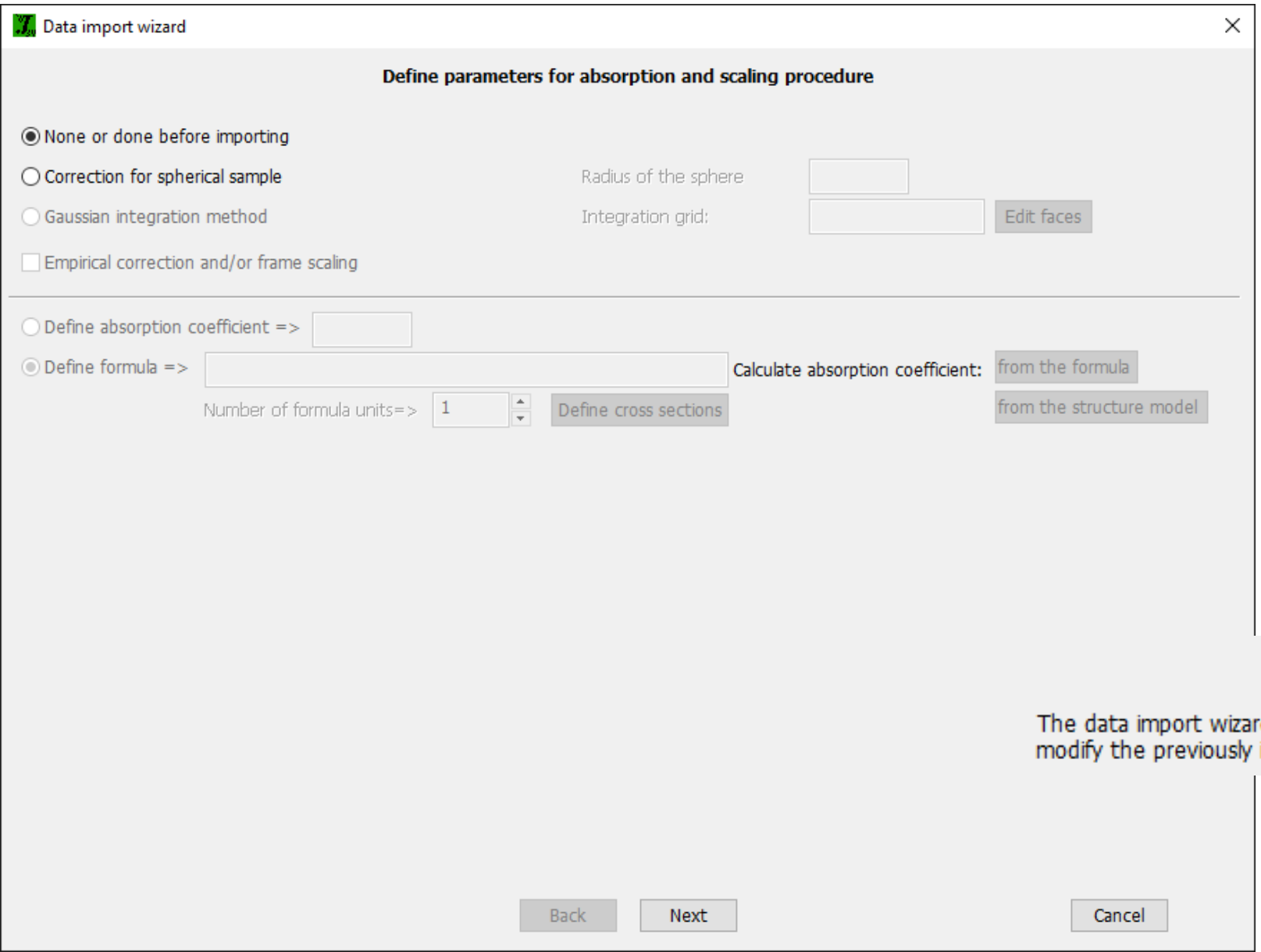


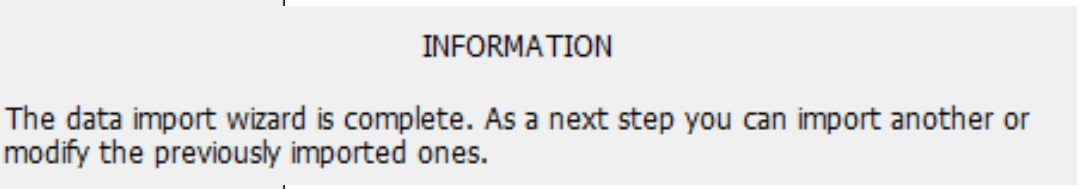
D:\Conferences_Trips_Seminars\2024.06.22_Workshop_Knoxville-US_American Physical Society Meeting\Examples\3.3.1_CsLiSO4_flow\Data\CsLiSO4.m50

File Edit Search View Convert Options Help

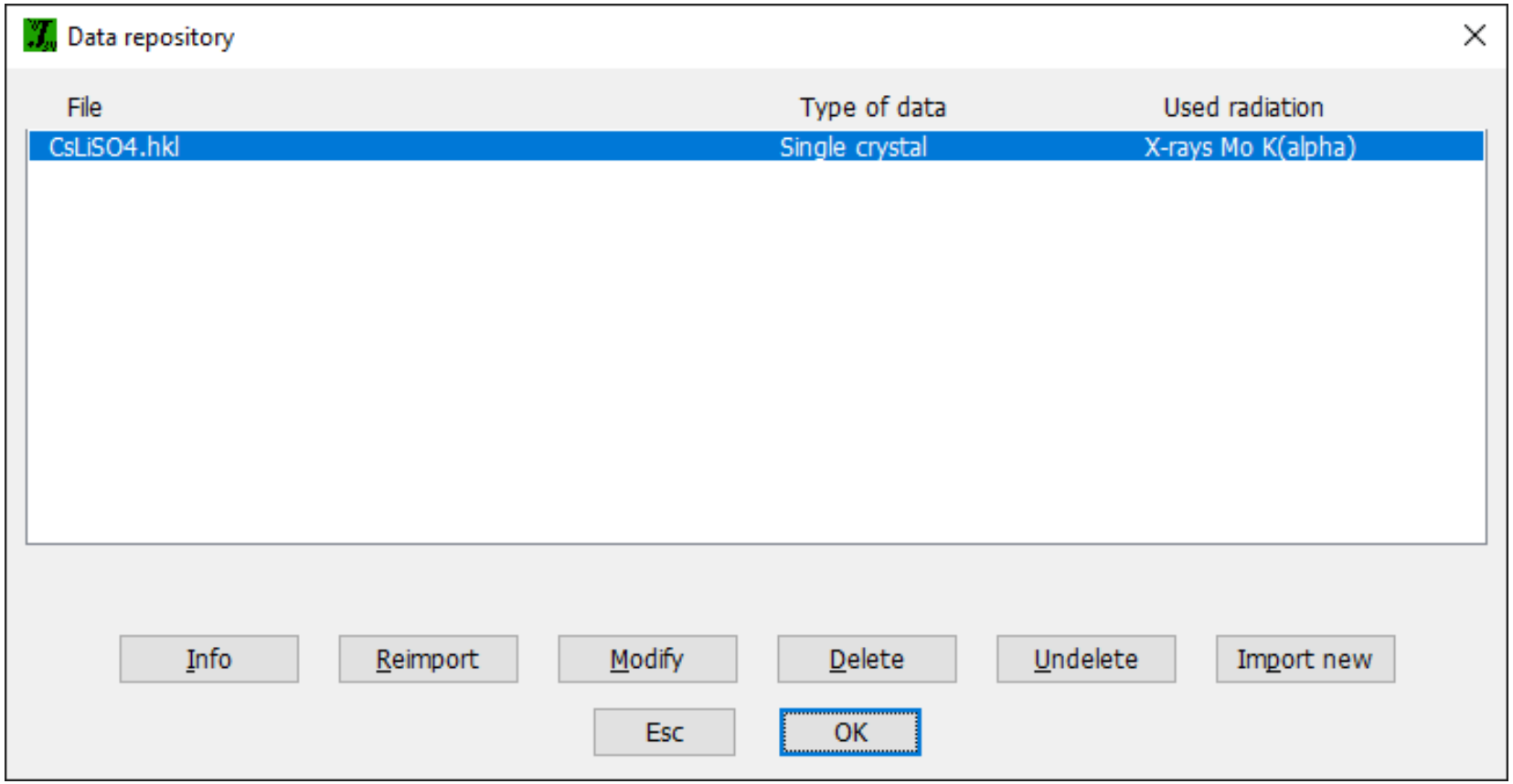
```
Version Jana2020
title
cell 10.89451 10.88937 8.80485 90.001 90.0236 119.9455
esdcell 0.00058 0.00058 0.00041 0.0041 0.0041 0.0056
spgroup P1 1 1
lattice P
symmetry x y z
unitsnumb 0
lambda 0.71073 radtype 1 lpfactor 1
monangle 6.0823 perfmono 0
roundmethod 1 autrefkeys 1
end
**********************************************************************
refine
end refine
fourier
end fourier
dist
end dist
contour
end contour
```

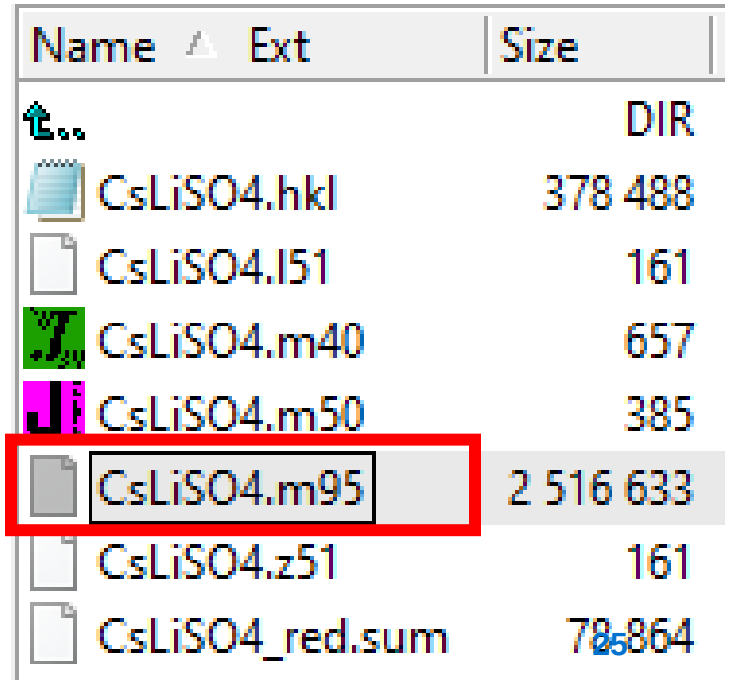
Data import wizard





Data import wizard





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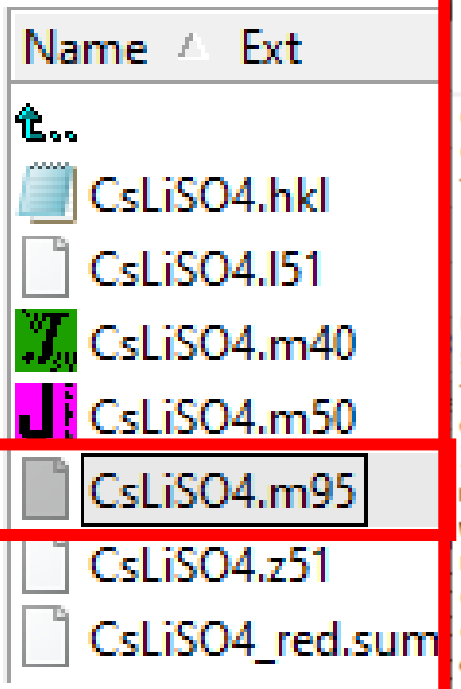
Data import wizard

M95 – data repository



D:\Conferences_Trips_Seminars\2024.06.22_Workshop_Knoxville-US_American Physical Society Meeting\Examples\3.3.1_CsLiSO4_flow\Data\CsLiSO4.m95 - Viewer

File Edit Search View Convert Options Help

```
commcell 10.89451 10.88937 8.80485 90.001 90.0236 119.9455
commcellesd 0.00058 0.00058 0.00041 0.0041 0.0041 0.0056
trcell
    1.000000    0.000000    0.000000
    0.000000    1.000000    0.000000
    0.000000    0.000000    1.000000
refblock Block1
sourcefile CsLiSO4.hkl
filedate 23/12/2018 filetime 18:48:58
difcode 3 correspond 1 corrlp -1 corrabs 0 hklf5 0 useexpcorr 1
lambda 0.71073 radtype 1 polarization 1 datcolltemp 293
monangle 6.06977 perfmono 0.5
wshelxa -999 wshelxb -999
nref 11132 ndim95 3 nlines 22264 scmax 1 scale 1
cell 10.89451 10.88937 8.80485 90.001 90.0236 119.9455
cellesd 0.00058 0.00058 0.00041 0.0041 0.0041 0.0056
ormat
    0.072049   -0.022105    0.042122
   -0.046074   -0.092350   -0.055744
    0.062511    0.047060   -0.089540
end
Data Block1
       1 -13   3  -1   0.00   0.00  26.47  26.47   0.413907E+04   0.112029E+03     0.010   1   1   0
   0.100000E+01   0.100000E+01  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000       1   1.00000   1.00000
       2 -13   3   0   0.00   0.00  26.35  26.35   0.111946E+02   0.838333E+02     0.020   1   1   0
   0.100000E+01   0.100000E+01  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000       1   1.00000   1.00000
       3 -13   3   1   0.00   0.00  26.47  26.47   0.421077E+04   0.113997E+03     0.030   1   1   0
   0.100000E+01   0.100000E+01  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000       1   1.00000   1.00000
       4 -13   4  -2   0.00   0.00  26.21  26.21   0.323159E+02   0.767376E+02     0.040   1   1   0
   0.100000E+01   0.100000E+01  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000       1   1.00000   1.00000
       5 -13   4  -1   0.00   0.00  25.86  25.86   0.142616E+04   0.773008E+02     0.050   1   1   0
   0.100000E+01   0.100000E+01  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000       1   1.00000   1.00000
```

FZU

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

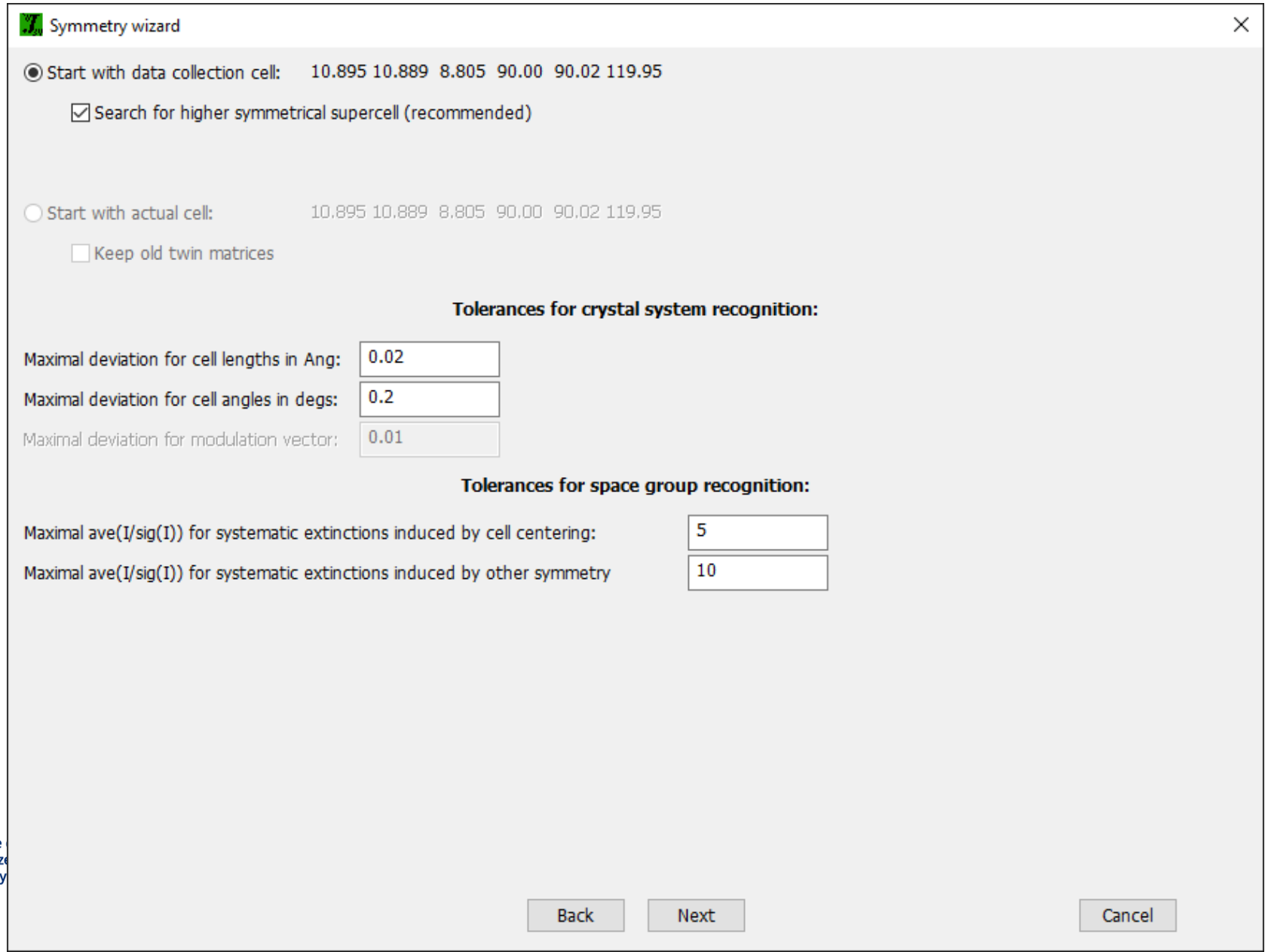
Symmetry wizard

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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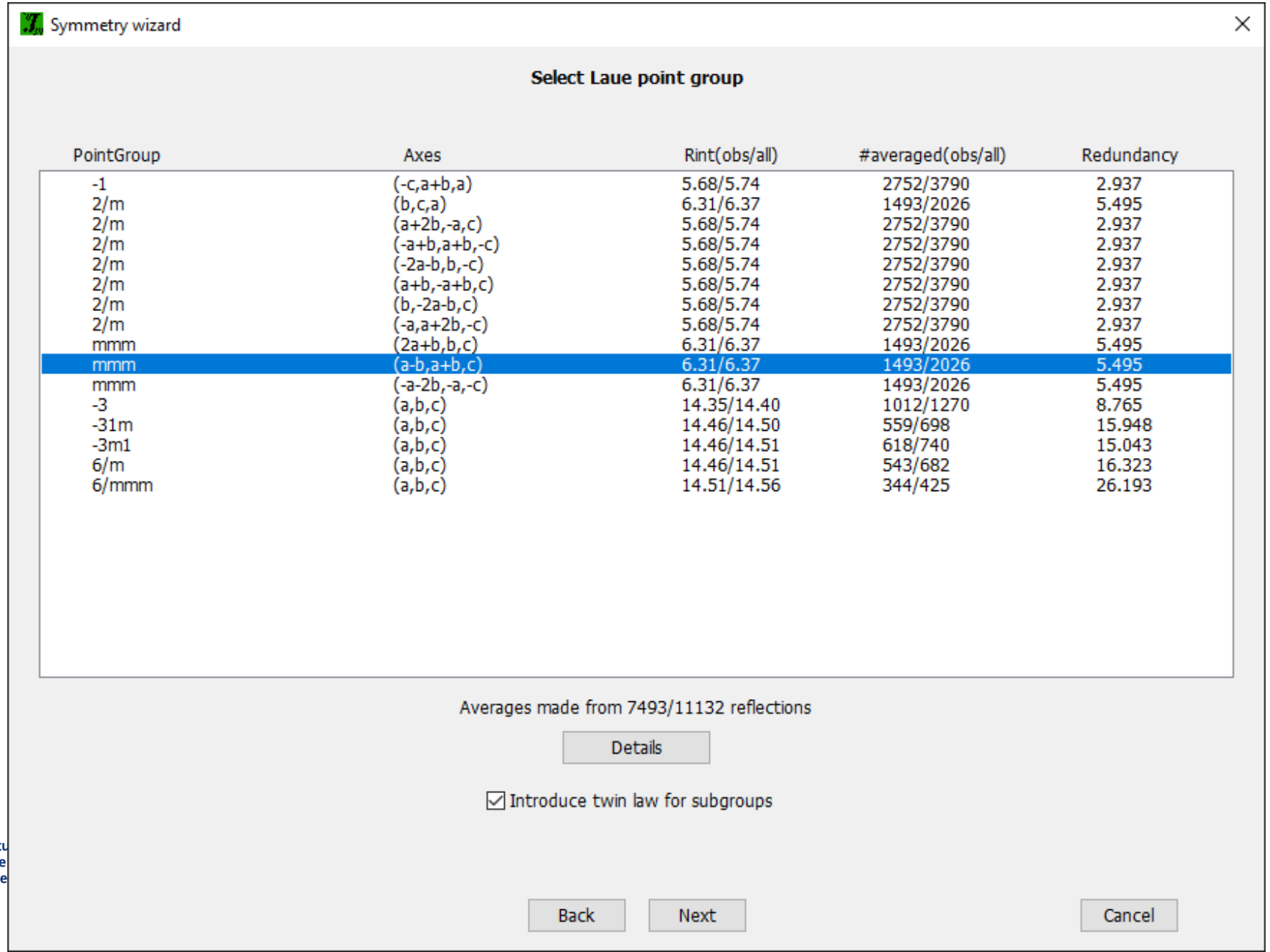
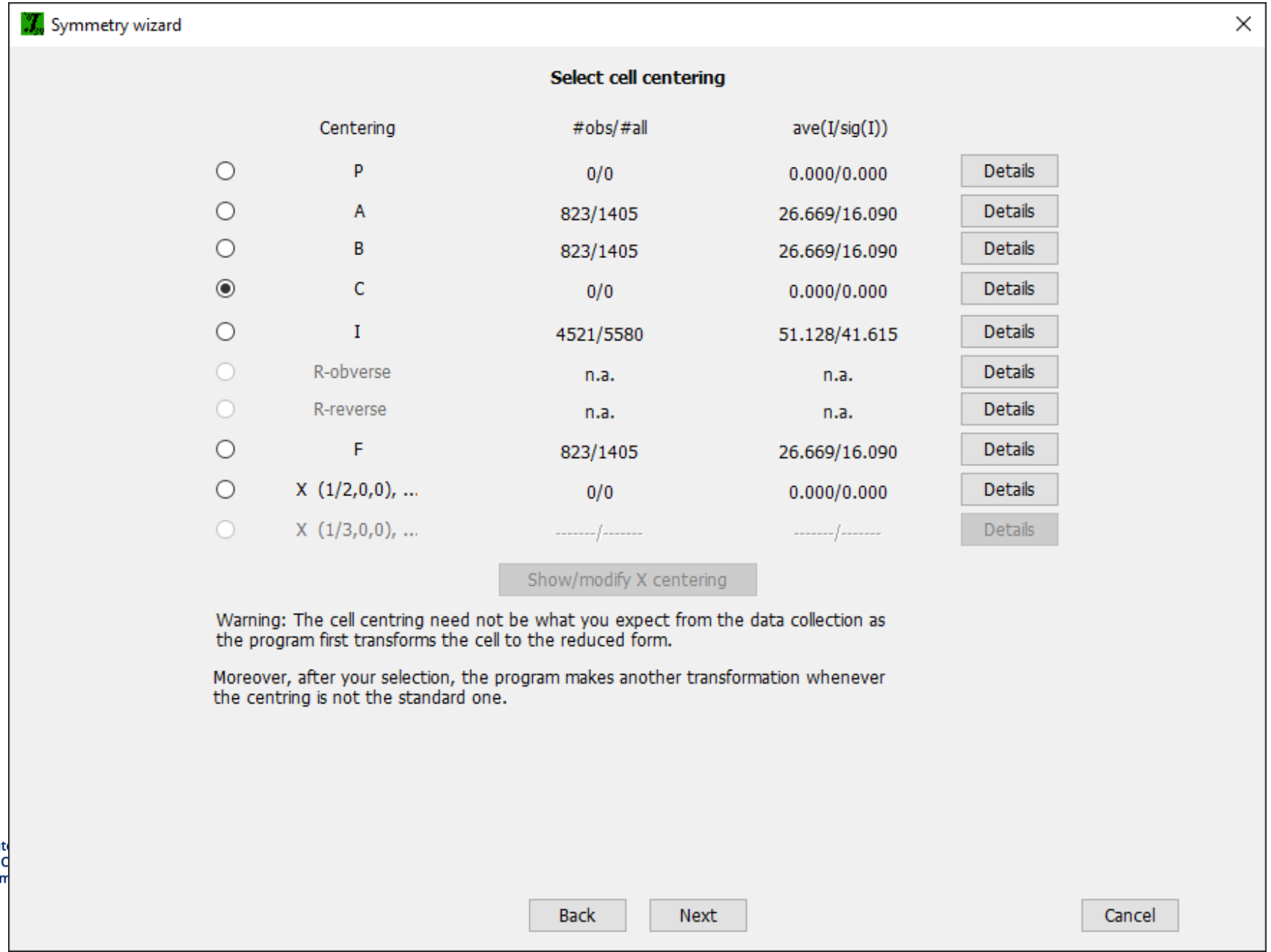
Symmetry wizard



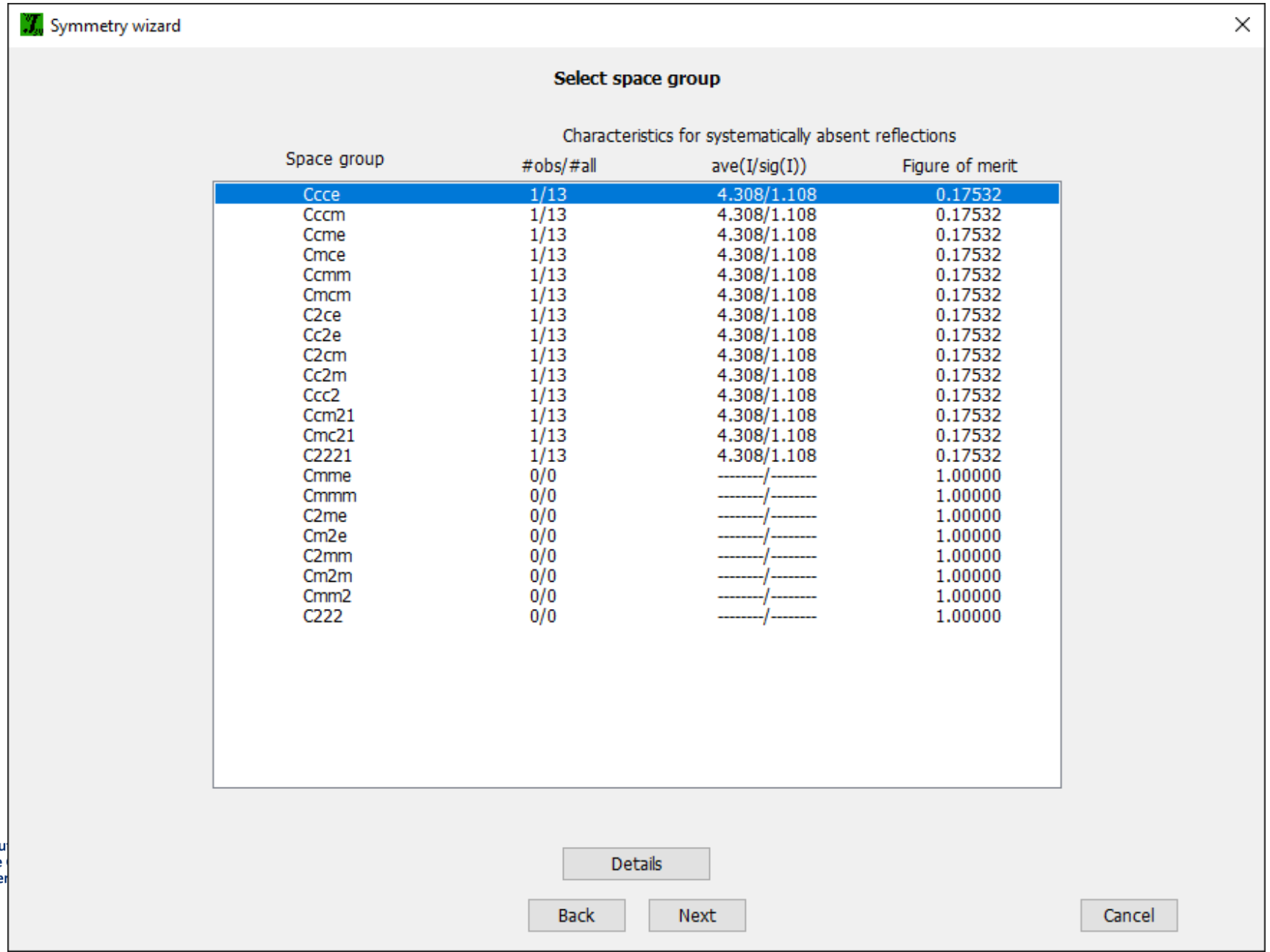
FZU Institu of the Acade

Symmetry wizard

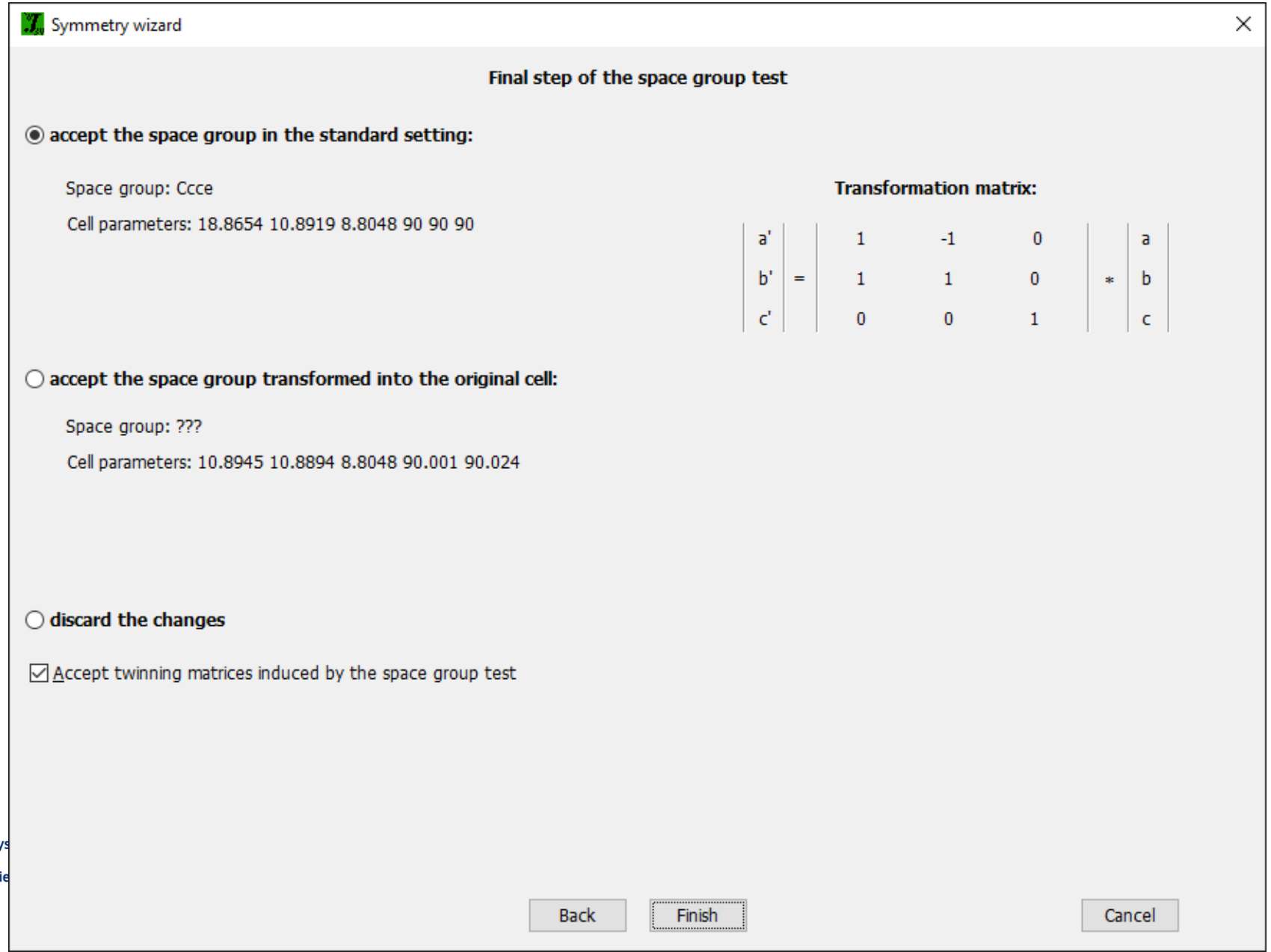


FZU Institute of the C Academ

Symmetry wizard

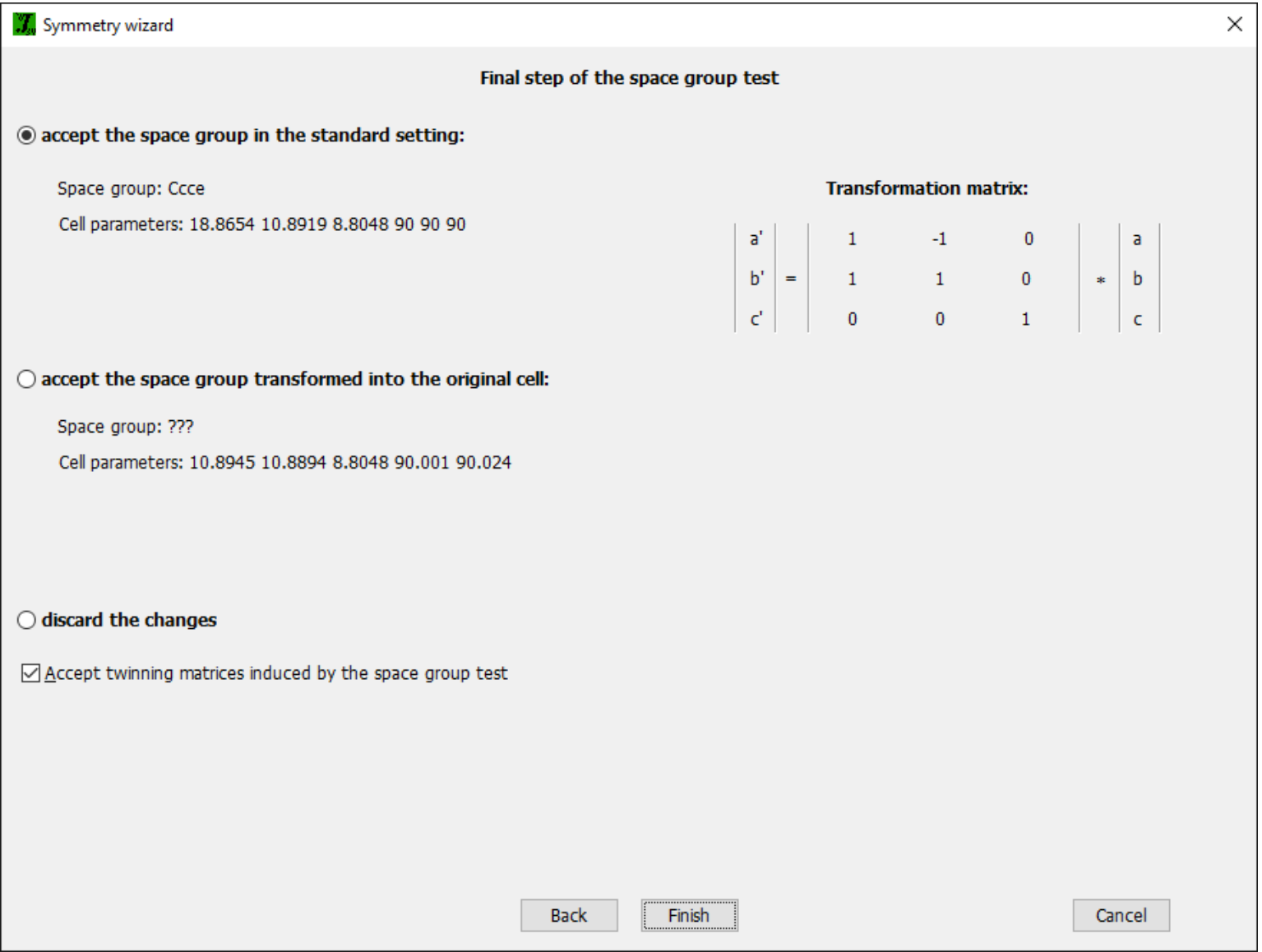


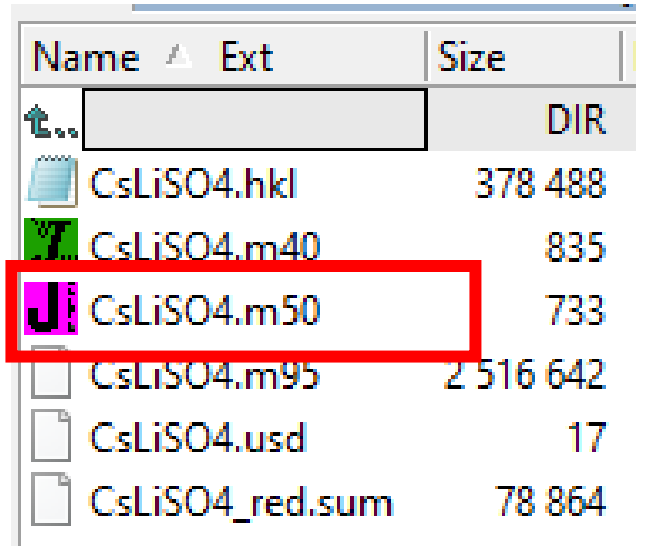
Symmetry wizard



FZU Institute of Phys of the Czech Academy of Scie

Symmetry wizard





Symmetry wizard

M50 – basic crystal information, form factors, program options

D:\Conferences_Trips_Seminars\2024.06.22_Workshop_Knoxville-US_American Physical Society Meeting\Examples\3.3.1_CsLiSO4_flow\Data\CsLiSO4.m50

File Edit Search View Convert Options Help

```
Version Jana2020
title
cell 10.89451 10.88937 8.80485 90.001 90.0236 119.9455
esdcell 0.00058 0.00058 0.00041 0.0041 0.0041 0.0056
spgroup P1 1 1
lattice P
symmetry x y z
unitsnumb 0
lambda 0.71073 radtype 1 lpfactor
monangle 6.0823 perfmono 0
roundmethod 1 autrefkeys 1
end
**********
refine
end refine
fourier
end fourier
dist
end dist
contour
end contour
```

D:\Conferences_Trips_Seminars\2024.06.22_Workshop_Knoxville-US_American Physical Society Meeting\Examples\3.3.1_CsLiSO4_flow\Data\CsLiSO4.m50

File Edit Search View Convert Options Help

```
Version Jana2020
title
cell 18.86539 10.89194 8.80485 90 90 90
esdcell 0.00063 0.00109 0.00041 0 0 0
spgroup Ccce 68 3
lattice C
symmetry x y z
symmetry -x -y z
symmetry -x y -z
symmetry x -y -z
symmetry -x -y+1/2 -z+1/2
symmetry x y+1/2 -z+1/2
symmetry x -y+1/2 z+1/2
symmetry -x y+1/2 z+1/2
unitsnumb 16
twin 3
     0.5000    -0.5000     0.0000
     1.5000     0.5000     0.0000
     0.0000     0.0000     1.0000
    -0.5000    -0.5000     0.0000
     1.5000    -0.5000     0.0000
     0.0000     0.0000     1.0000
roundmethod 1 autrefkeys 1
end
**********
refine
end refine
fourier
end fourier
dist
end dist
contour
end contour
```

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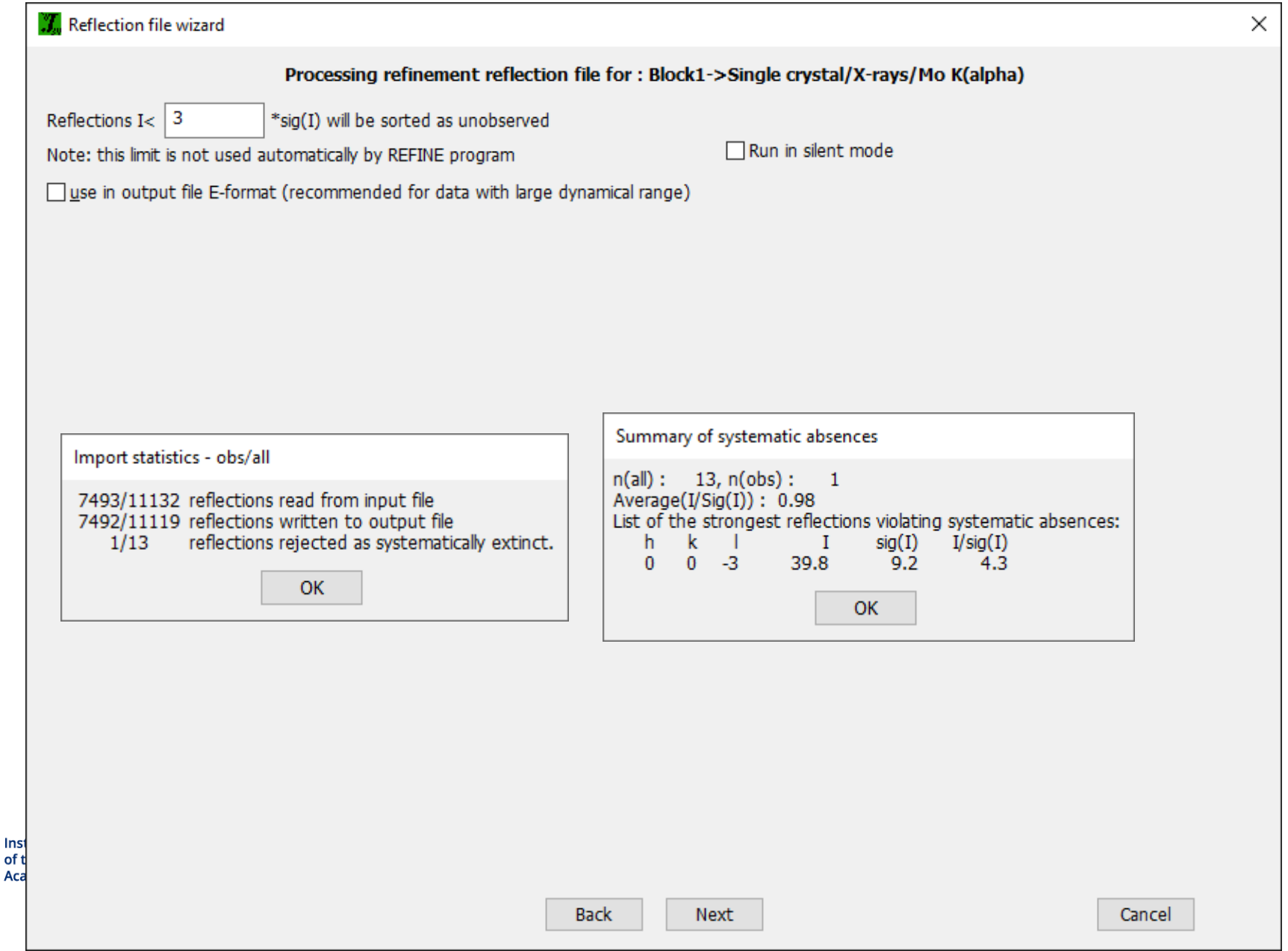
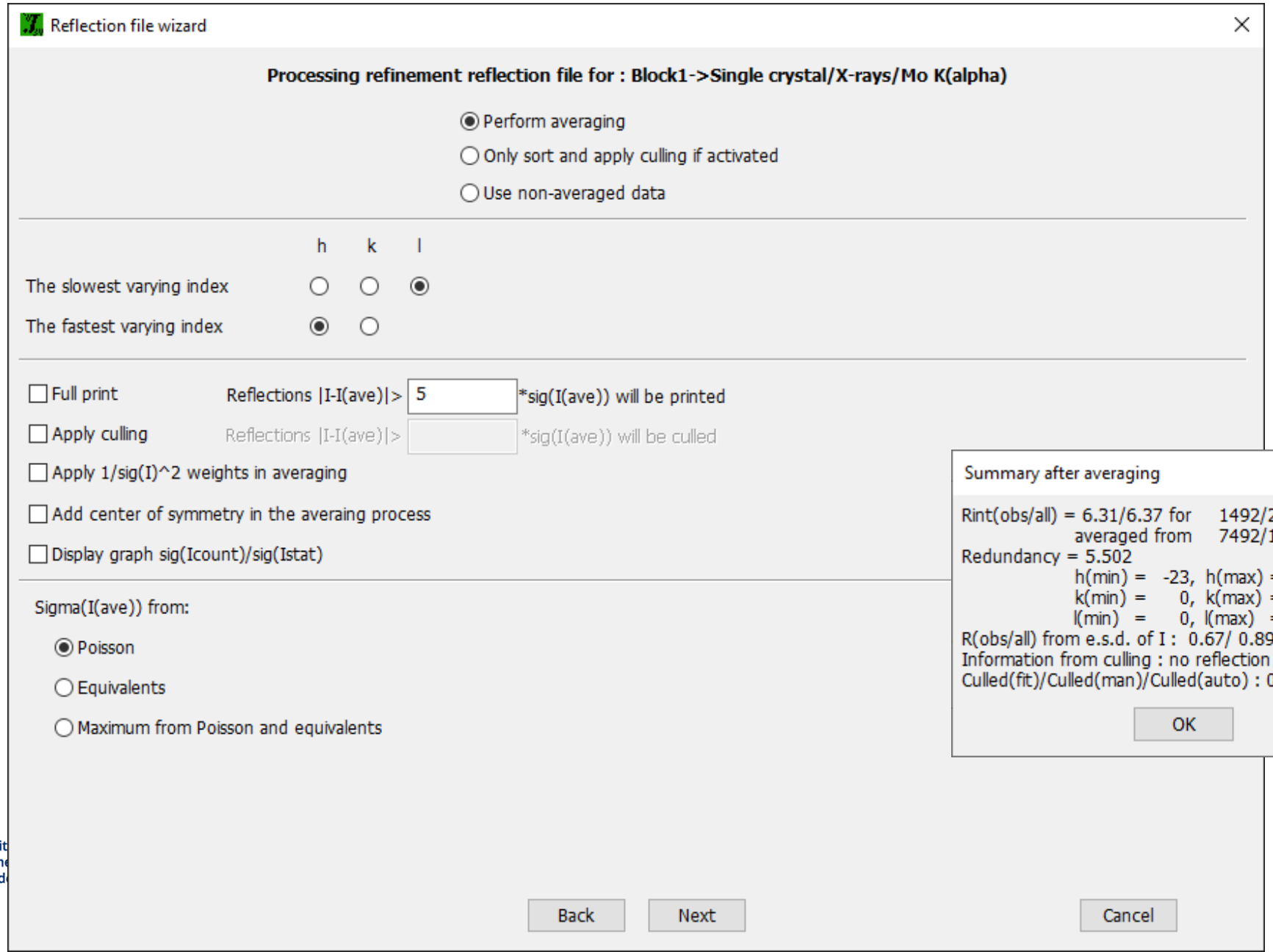
Reflection file wizard



Reflection file wizard



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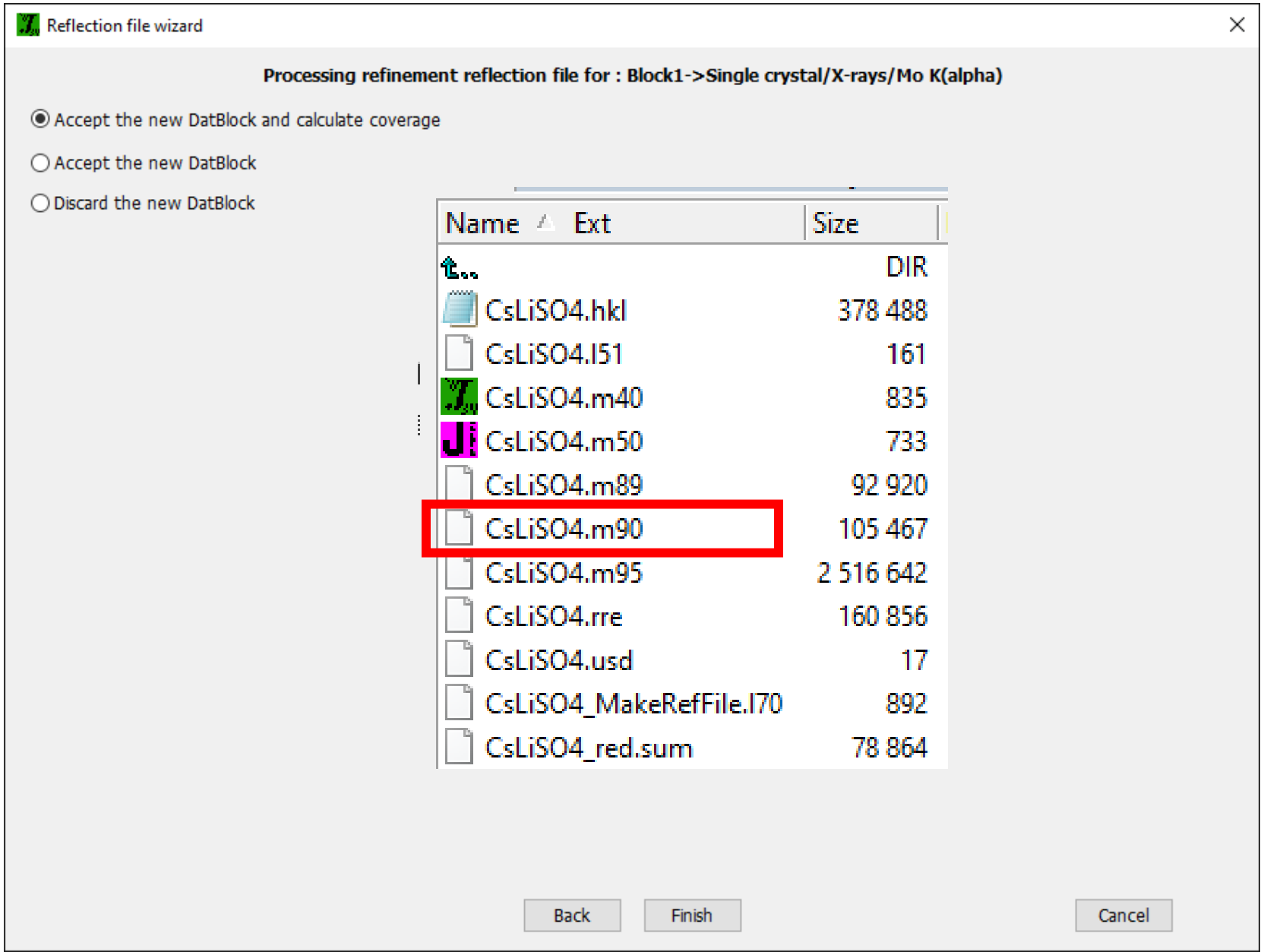
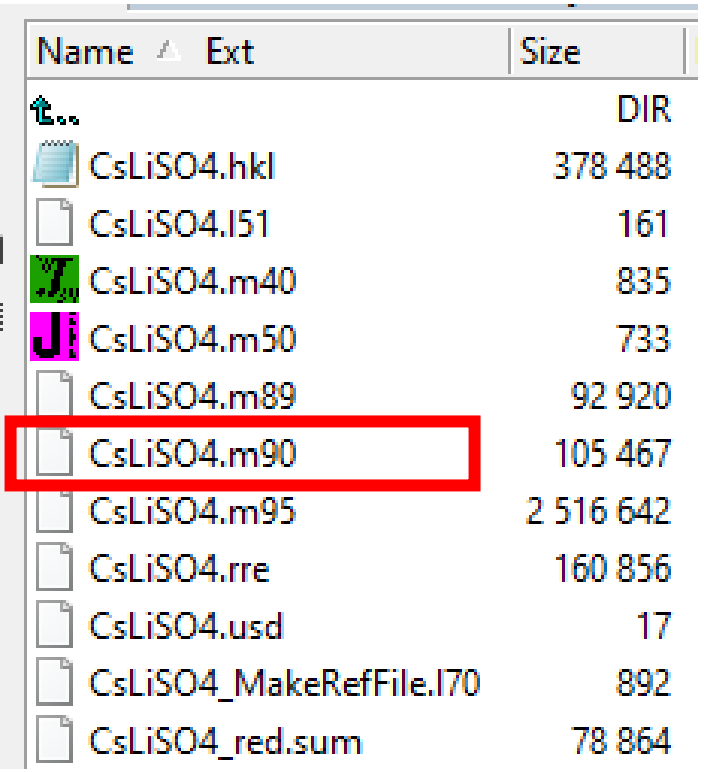
Reflection file wizard



FZU

Reflection file wizard

M90 refinement reflection file



D:\Conferences_Trips_Seminars\2024.06.22_Workshop_Knoxville-US_American Physical Society Meeting\Examp

File Edit Search View Convert Options Help

```
eformat91 0
datblock Block1
nref 2021 obslim 3 sctom90 1 norefitems 1 diffscales 1 dataave 1 scalelim 10 hklf5 0
wshelxa -999 wshelxb -999
indslowest 3 indfastest 1 addcentrsymm 0 sigimethod 1 multave 1
flimprint 5 flimcull -1 avesigwt 0 unstab 0.043818
radtype 1 dattype 1
lambda 0.71073 lpfactor 1 monangle 6.06977 perfmono 0.5
datcolltemp 293
end
Data Block1
   4   0   0  42819.3     99.6   1   0   1  0.0000
   6   0   0     46.7      6.1   1   0   1  0.0000
   8   0   0  71549.6    106.0   1   0   1  0.0000
  10   0   0     -2.5      7.3   1   0   1  0.0000
  12   0   0  44463.9    122.3   1   0   1  0.0000
  14   0   0      4.6     13.8   1   0   1  0.0000
  16   0   0   6353.1     55.6   1   0   1  0.0000
  18   0   0     12.0     21.7   1   0   1  0.0000
  20   0   0   4864.1     56.7   1   0   1  0.0000
  22   0   0     -2.1     31.8   1   0   1  0.0000
 -22   2   0   4473.8     58.8   1   0   1  0.0000
 -20   2   0      6.6     26.4   1   0   1  0.0000
 -18   2   0   9837.9     75.2   1   0   1  0.0000
 -16   2   0     -1.4     19.3   1   0   1  0.0000
 -14   2   0   4830.5     46.3   1   0   1  0.0000
 -12   2   0      1.3     12.7   1   0   1  0.0000
```

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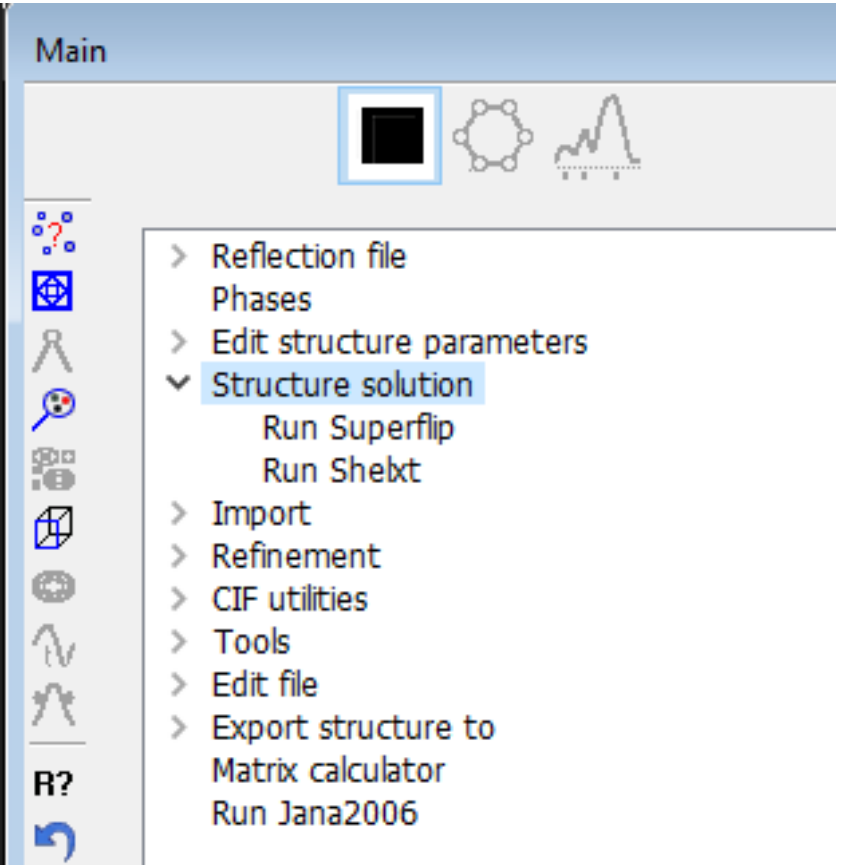
Structure solution

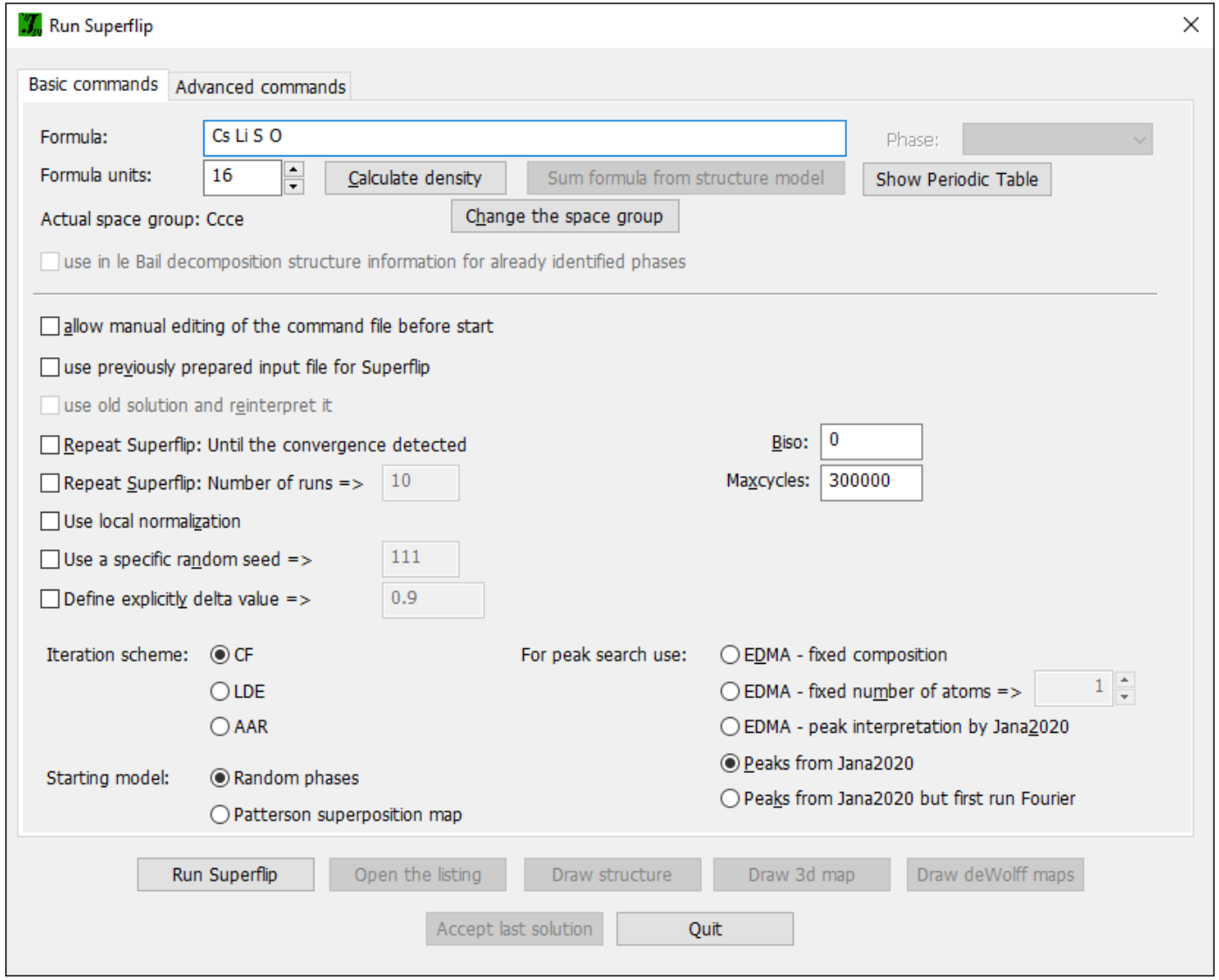
Solution by Superflip or by calling external programs

Structure solution

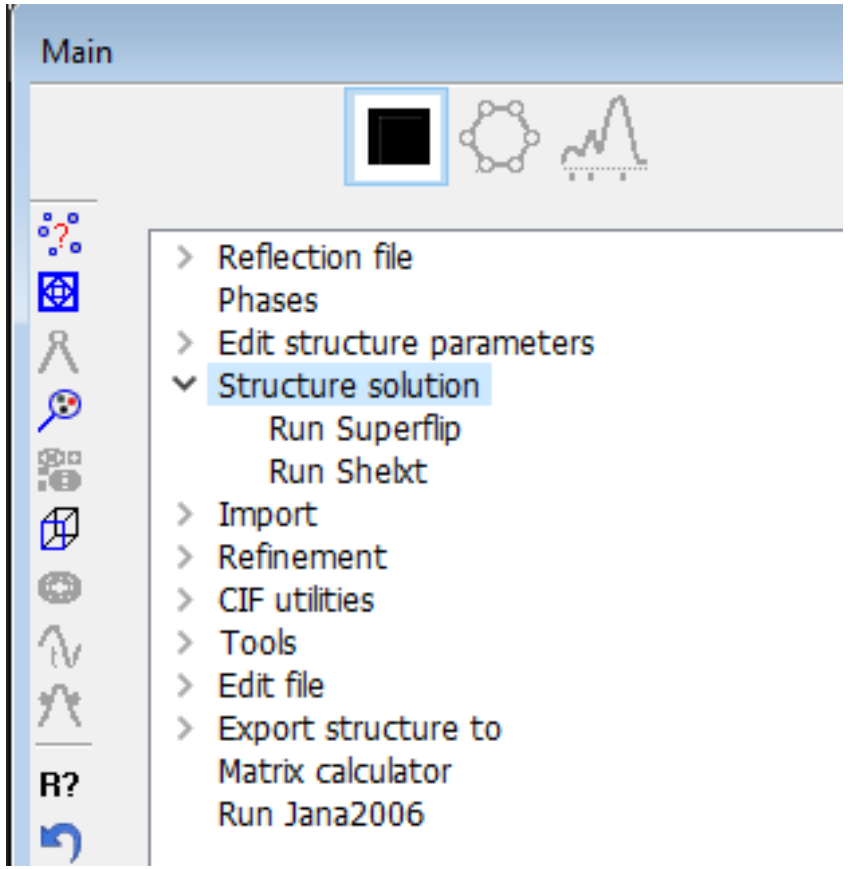
M40 structure model
M41 powder profile parameters

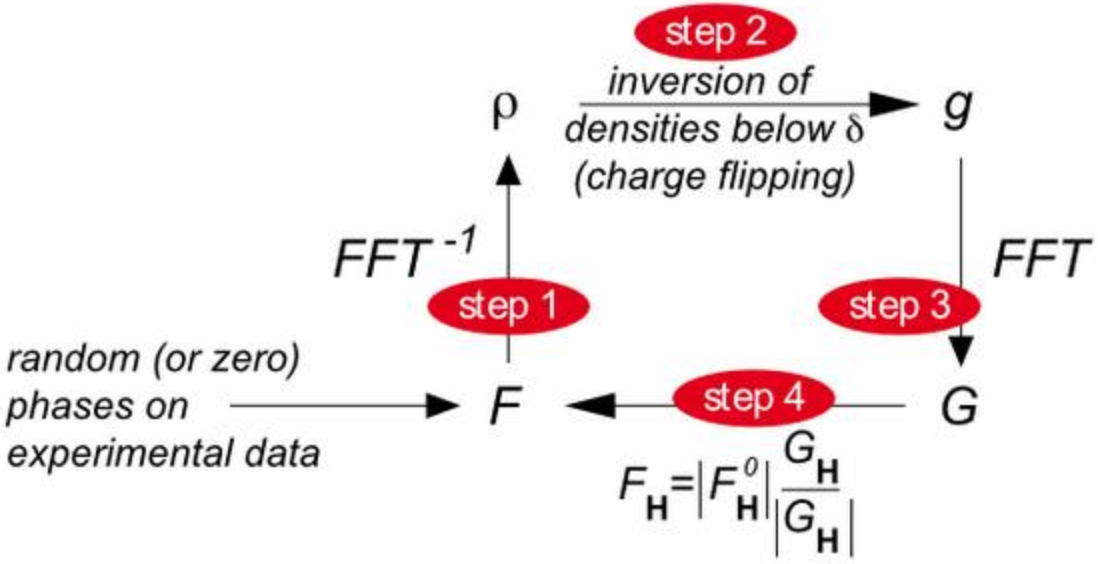
Structure solution





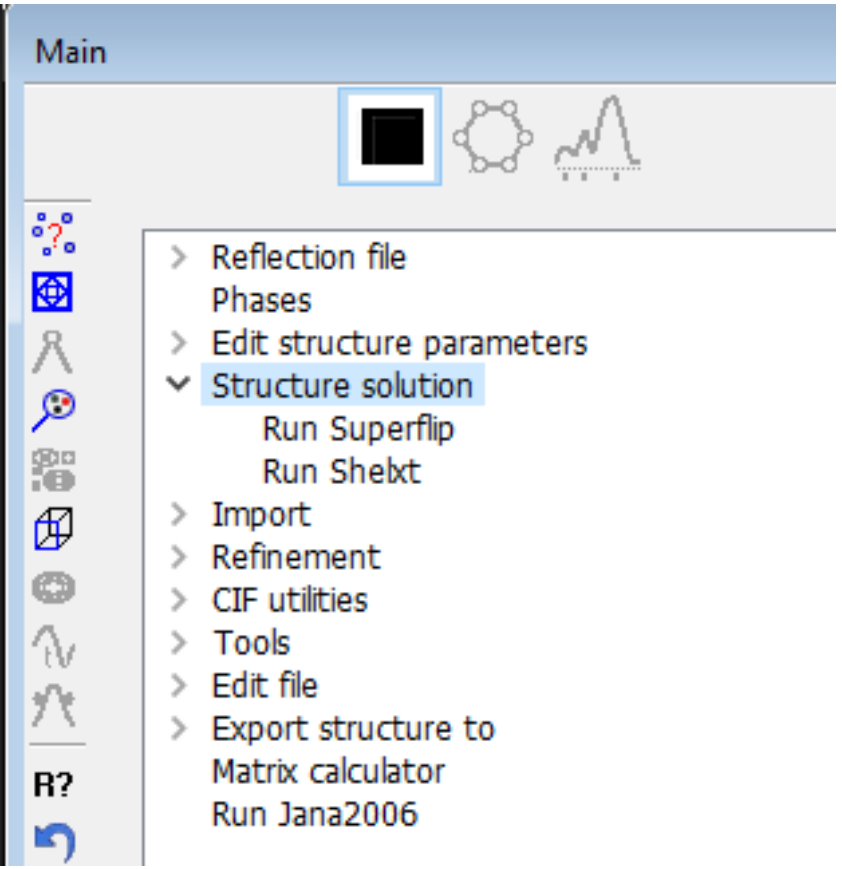
Structure solution

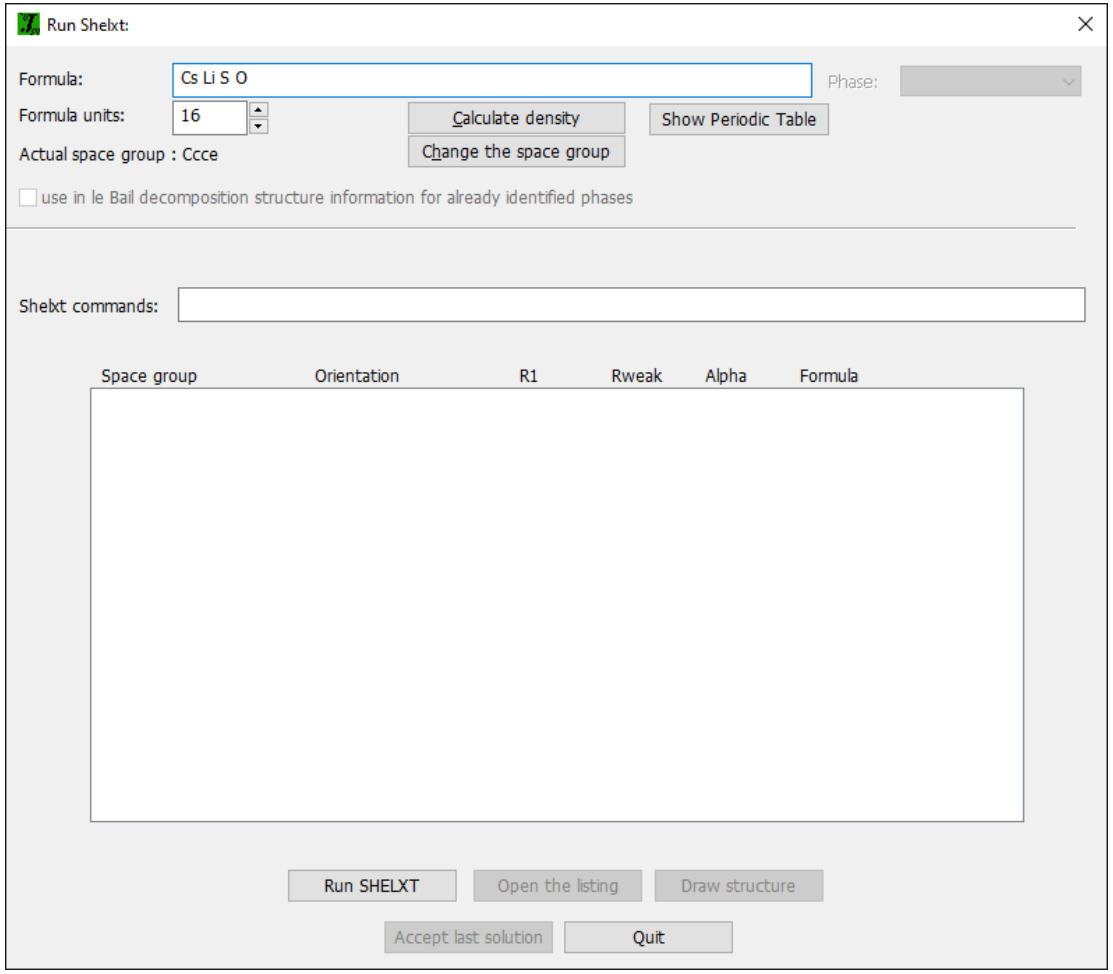




https://www.epfl.ch/schools/sb/research/iphys/teaching/crystallography/charge-flipping/

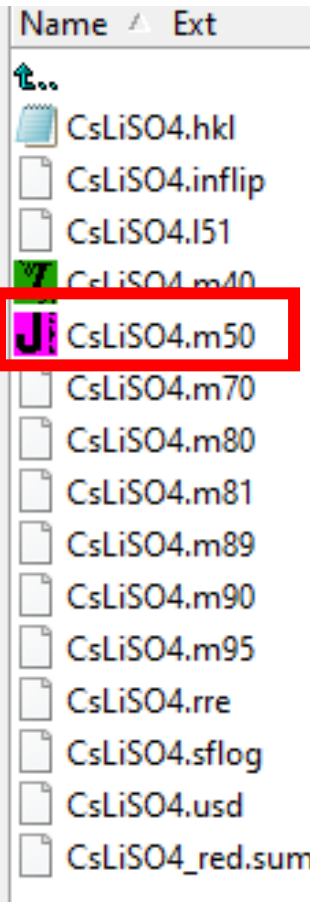
Structure solution





Structure solution

M50 – basic crystal information, form factors, program options



D:\Conferences_Trips_Seminars\2024.06.22_Workshop_

File Edit Search View Convert Options Help

```
Version Jana2020
title
cell 18.86539 10.89194 8.80485 90 90 90
esdcell 0.00063 0.00109 0.00041 0 0 0
spgroup Ccce 68 3
lattice C
symmetry x y z
symmetry -x -y z
symmetry -x y -z
symmetry x -y -z
symmetry -x -y+1/2 -z+1/2
symmetry x y+1/2 -z+1/2
symmetry x -y+1/2 z+1/2
symmetry -x y+1/2 z+1/2
unitsnumb 16
twin 3
     0.5000    -0.5000     0.0000
     1.5000     0.5000     0.0000
     0.0000     0.0000     1.0000
    -0.5000    -0.5000     0.0000
     1.5000    -0.5000     0.0000
     0.0000     0.0000     1.0000
roundmethod 1 autrefkeys 1
end
**********************************************
refine
end refine
fourier
end fourier
dist
end dist
contour
end contour
```

D:\Conferences_Trips_Seminars\2024.06.22_Workshop_Kn

File Edit Search View Convert Options Help

```
Version Jana2020
title
cell 18.86539 10.89194 8.80485 90 90 90
esdcell 0.00063 0.00109 0.00041 0 0 0
spgroup Ccmm 63 3
lattice C
symmetry x y z
symmetry -x -y z+1/2
symmetry -x y -z
symmetry x -y -z+1/2
symmetry -x -y -z
symmetry x y -z+1/2
symmetry x -y z
symmetry -x y z+1/2
unitsnumb 16
atlist Cs Li S O4
formtab -62
atom Cs atradius 2.72 color 14254185
atom Li atradius 1.57 color 134224116
atom S atradius 1.04 color 255250000
atom O atradius 0.74 color 254003000
twin 3
     0.5000    -0.5000     0.0000
     1.5000     0.5000     0.0000
     0.0000     0.0000     1.0000
    -0.5000    -0.5000     0.0000
     1.5000    -0.5000     0.0000
     0.0000     0.0000     1.0000
roundmethod 1 autrefkeys 1
end
**********************************************
refine
end refine
fourier
end fourier
dist
end dist
contour
end contour
```

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Structure so

M40 structure model

Number of atoms and molecules in the 1st composite part

Number of atoms and molecules in the 2st composite part

Name	Ext	Size
..		DIR
CsLiSO4.hkl		378 488
CsLiSO4.inflip		112 989
CsLiSO4.l51		161
CsLiSO4.m40		19 500
CsLiSO4.m50		902
CsLiSO4.m70		815
CsLiSO4.m80		185 484
CsLiSO4.m81		1 152 000
CsLiSO4.m89		92 920
CsLiSO4.m90		105 467
CsLiSO4.m95		2 516 642
CsLiSO4.rre		164 492
CsLiSO4.sflog		11 286
CsLiSO4.usd		17
CsLiSO4_red.sum		78 864

D:\Conferences_Trips_Seminars\2024.06.22_Workshop_Knoxville-US_American Physical Society M

File Edit Search View Convert Options Help

```
   19    0    0    1    0
1.000000 0.000000 0.000000 0.000000 0.333333 0.333333
0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
Cs1       1  1     0.500000 0.742000 0.267000 0.750000
 0.037995 0.000000 0.000000 0.000000 0.000000 0.000000      0000000000
Cs2       1  1     0.250000 0.514000 0.500000 0.750000
 0.037995 0.000000 0.000000 0.000000 0.000000 0.000000      0000000000
Cs3       1  1     0.250000 1.005000 0.500000 0.750000
 0.037995 0.000000 0.000000 0.000000 0.000000 0.000000      0000000000
O1        4  1     0.500000 0.582000 0.251000 0.250000
 0.037995 0.000000 0.000000 0.000000 0.000000 0.000000      0000000000
O2        4  1     0.500000 0.667000 0.500000 0.454000
 0.037995 0.000000 0.000000 0.000000 0.000000 0.000000      0000000000
O3        4  1     1.000000 0.583000 0.249000 0.445000
 0.037995 0.000000 0.000000 0.000000 0.000000 0.000000      0000000000
O4        4  1     0.500000 0.832000 0.500000 0.448000
                                                           0000000000
                                                           0000000000
Li1       2  1     0.500000 0.751000 0.500000 0.500000
 0.037995 0.000000 0.000000 0.000000 0.000000 0.000000      0000000000
                                                           0000000000
 0.037995 0.000000 0.000000 0.000000 0.000000 0.000000      0000000000
Li3       2  1     1.000000 0.875000 0.378000 0.497000
 0.037995 0.000000 0.000000 0.000000 0.000000 0.000000      0000000000
```

Header numbers
Scale parameters
Extinction parameters

atomic type
occupancy
atomic position
atomic name
ADPs

Refinement
1 – yes
0 – no

```
-------------------------   s.u. block   ------------------------------------
 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
 0.000000 0.000000 0.000000
 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
Cs1                0.000000 0.000000 0.000000 0.000000
 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
Cs2                0.000000 0.000000 0.000000 0.000000
```

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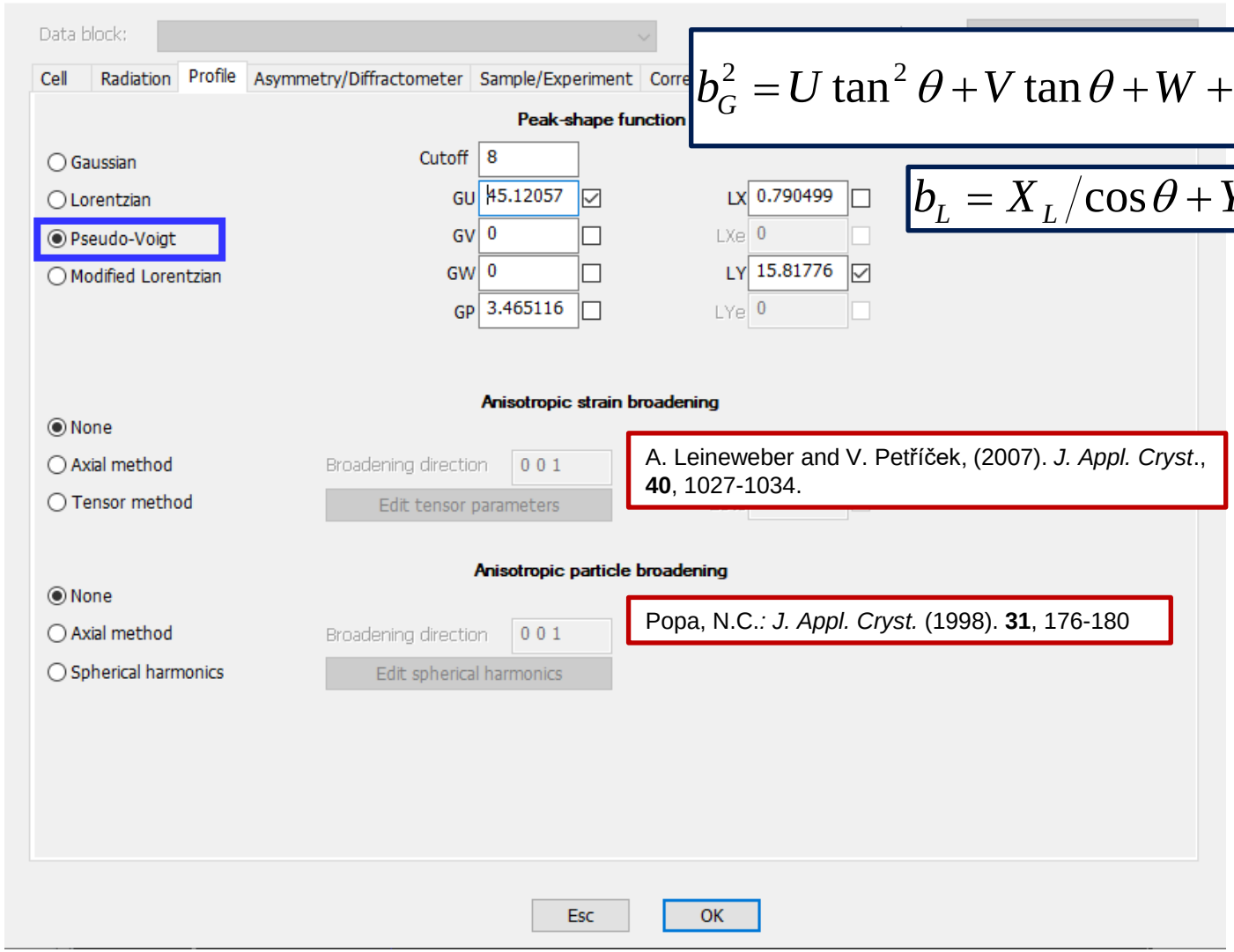
Powder

M41 powder profile parameters

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



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

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

A. Leineweber and V. Petříček, (2007). *J. Appl. Cryst.*, **40**, 1027-1034.

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

```
File  Edit  Search  View  Convert  Options  Help
usecutoff 0 cutoffmn 0.5 cutoffmx 200
usecutoffsat 0 cutoffsatmn 0.5 cutoffsatmx 200
bckgtype 1 bckgnum 20 manbckg 0 useeach 1 wtlebail 1 uklebail 0 asymm 1 usehs 0
rough 0 illum 2 focusBB 1
ksycos 0
proffun 3 splitprof 0 strain 2 partbroad 0 cutoff 20
skipfrdl 0
satfrmod 1 nomixedsat 0
end
!*********************************************************************************
# Shift parameters - zero, sycos, sysin
 13.50416 0.000000 0.000000                                    100
# Background parameters
 138.5775-199.4433 184.1889-110.4183 46.04121-12.55705         111111
 19.30088-22.02500 13.72963-21.31904 21.01167-9.540096         111111
-5.994739 12.71424 3.461570-6.105811 5.838707-6.732096         111111
-3.507062 2.129189                                             11
# Asymmetry parameters
 0.316905                                                      0
# Cell parameters - a,b,c,alpha,beta,gamma
 2.931795 2.931795 2.931795 90.00000 90.00000 90.00000         100000
# Modulation vector(s)
 0.387806 0.000000 0.000000                                    100
 0.000000 0.387806 0.000000                                    000
 0.000000 0.000000 0.387806                                    000
# Gaussian parameters - U,V,W,P
 7.848618-69.60195 25.91316-0.000000                           0000
# Lorentzian parameters - LX,LXe,LY,LYe
 7.236400 0.000000 5.087200 0.000000 3.461450                  00000
# Strain parameters
-0.092791 0.000000-0.000000 0.032307-0.000000 0.032307         000000
-0.000000 0.000000-0.000000-0.000000-0.092791-0.000000         000000
 0.032307-0.000000-0.092791 1.886114-0.232410 0.029169         000000
!---------------------------   s.u. block   ---------------------------------
# Shift parameters - zero, sycos, sysin
 0.043674 0.000000 0.000000
# Background parameters
 0.183179 0.373787 0.476198 0.570372 0.647194 0.708068
 0.739880 0.768320 0.803722 0.817608 0.864349 0.905523
 0.976577 1.052613 1.099470 1.152462 1.176762 1.168416
 1.148237 0.969566
# Asymmetry parameters
 0.000000
# Cell parameters - a,b,c,alpha,beta,gamma
 0.000023 0.000023 0.000023 0.000000 0.000000 0.000000
# Modulation vector(s)
 0.000089 0.000000 0.000000
 0.000000 0.000089 0.000000
 0.000000 0.000000 0.000089
# Gaussian parameters - U,V,W,P
 0.000000 0.000000 0.000000 0.000000
# Lorentzian parameters - LX,LXe,LY,LYe
 0.000000 0.000000 0.000000 0.000000 0.000000
# Strain parameters
 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
```

Powder profile parameters

Profile functions:

Gaussian:

$$G(b_G, x) = \frac{1}{\sqrt{2\pi b_G}} \exp\left(-x^2 / 2b_G^2\right)$$

$$b_G^2 = \frac{H_G^2}{8 \ln 2}$$

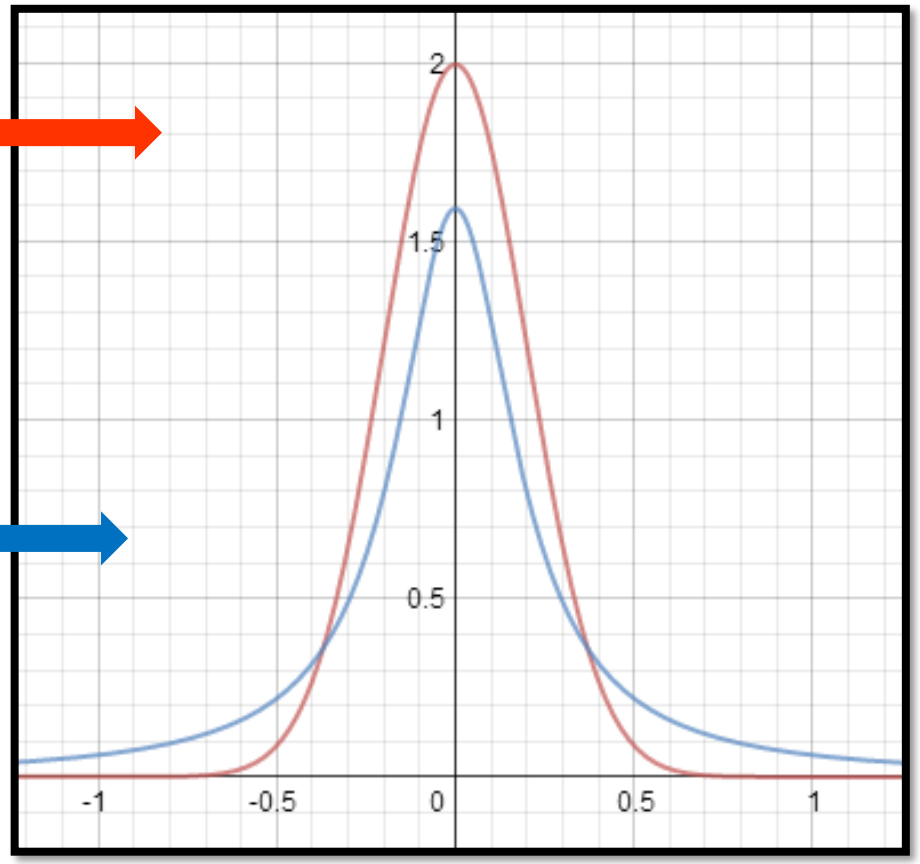
Where H_G is Full-Width at Half-Maximum

Lorentzian:

$$L(b_L, x) = \frac{2}{\pi b_L} \frac{1}{1 + (2x/b_L)^2}$$

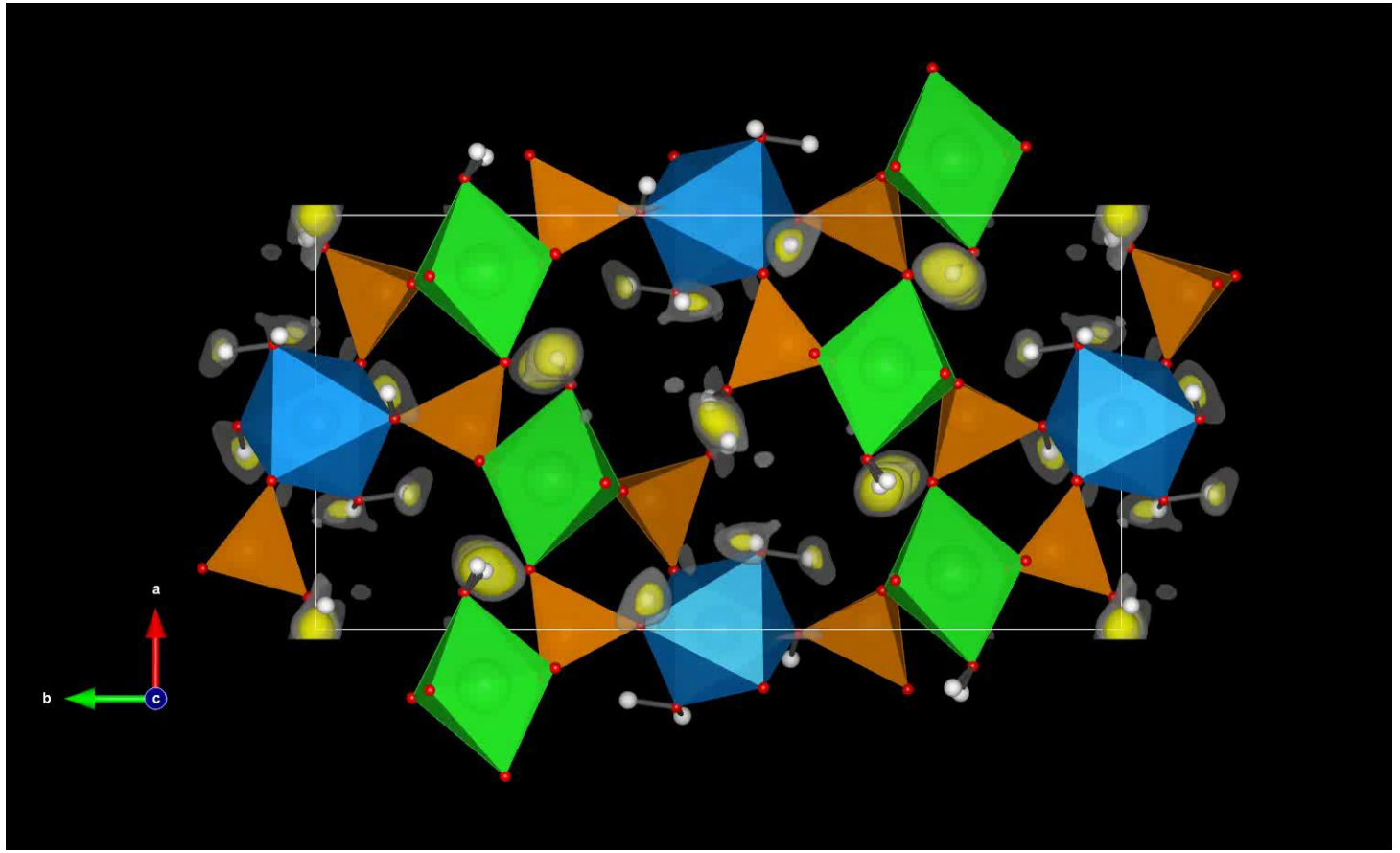
$$b_L = H_L$$

Where H_L is Full-Width at Half-Maximum



Electron diffraction

If the dynamical diffraction theory is used, the accuracy of the result approaches that of single crystal X-ray diffraction. Jana2020 communicates with DYNGO (by Lukas Palatinus). DYNGO calculated intensities of reflections and their derivatives using the dynamic diffraction theory



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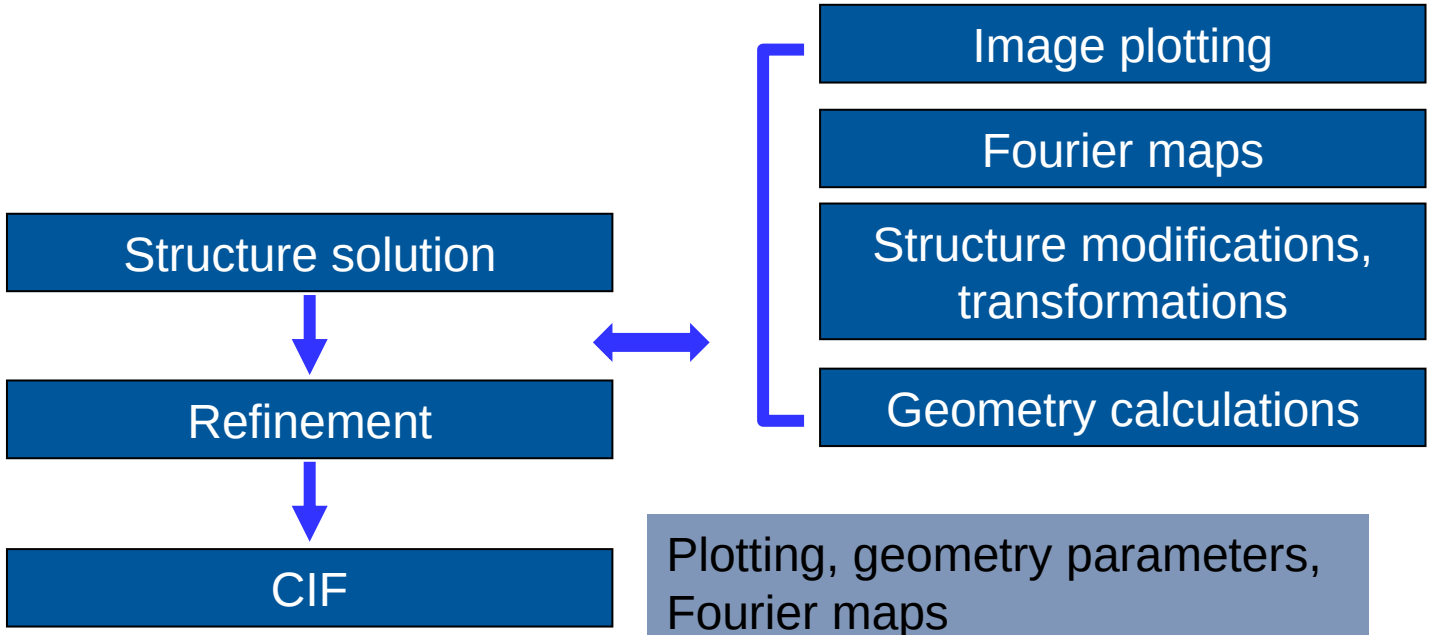
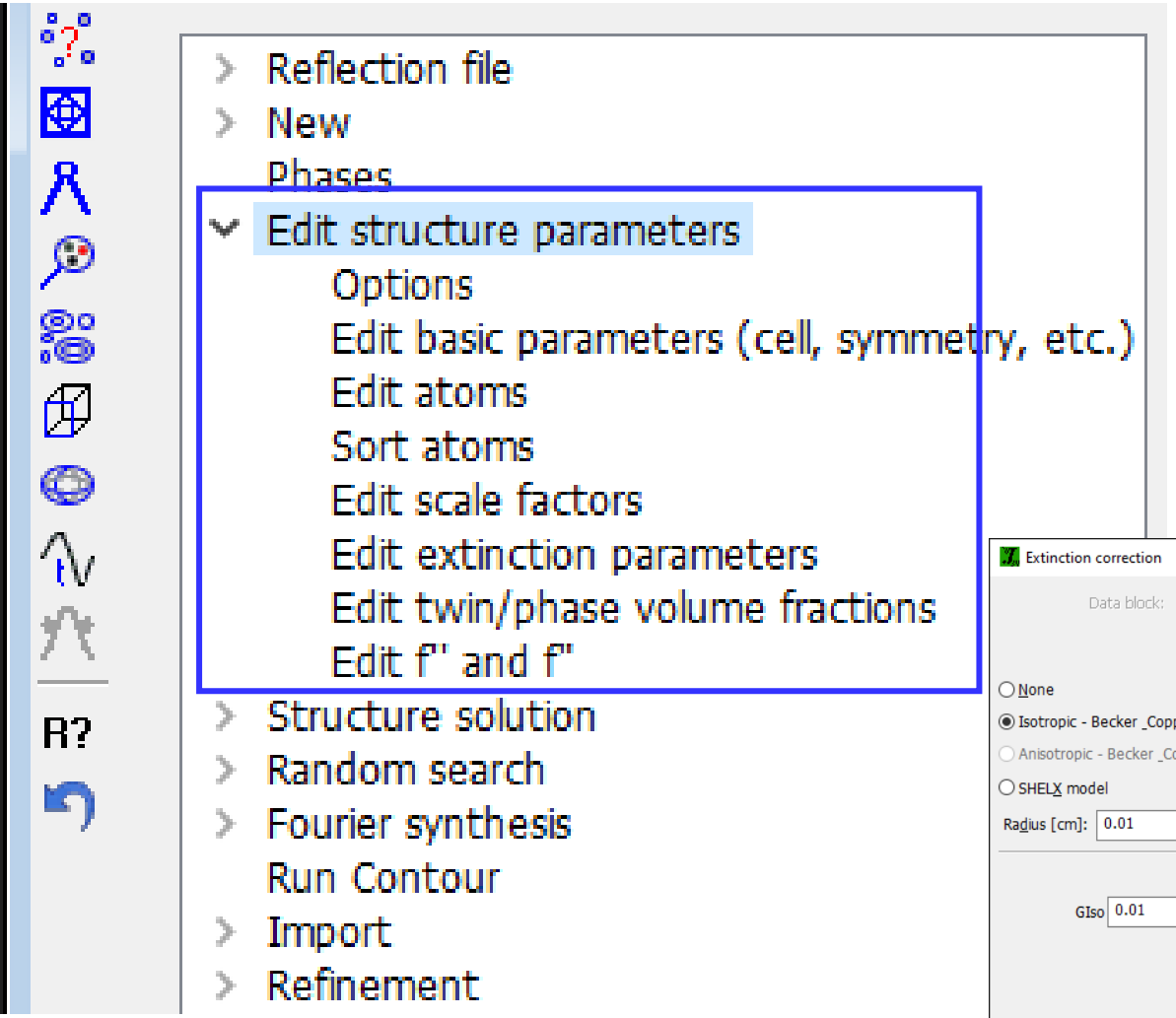
L. Palatinus, C. A. Corrêa et al. **Acta Crystallographica B71**, 740-751 (2015).
L. Palatinus, V. Petříček, C. A. Corrêa. ***Acta Crystallographica* A71**, 235-244 (2015).
L. Palatinus et al. **Science 355** (6321), 166-169 (2017).

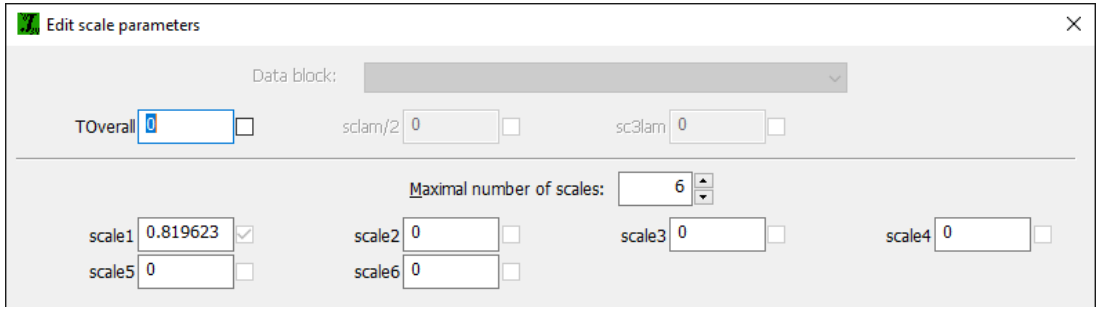
Software flow scheme and files created

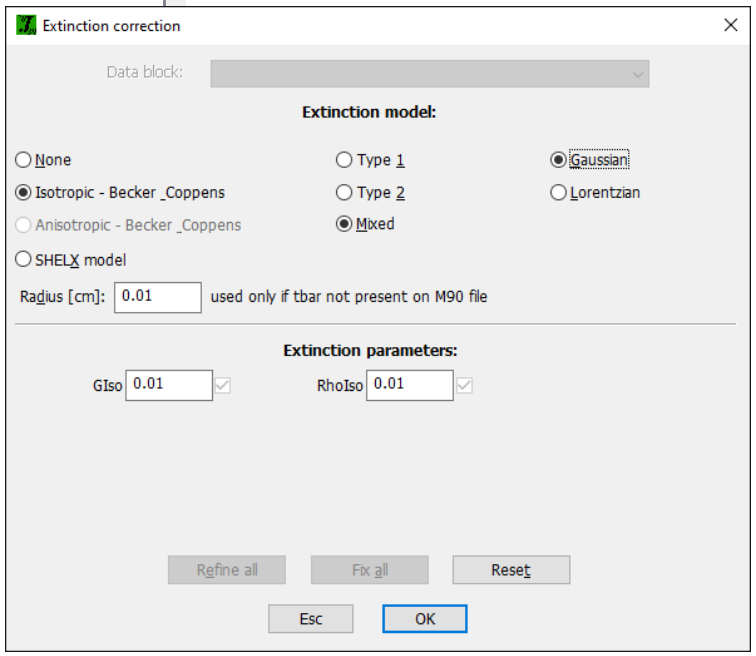


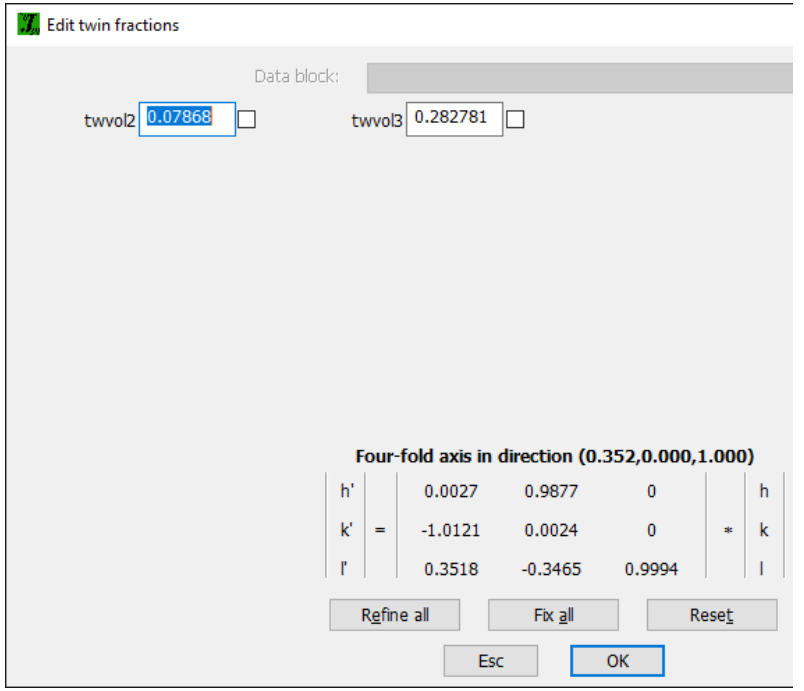
Refinement

Each refinable parameter of a structure model has a refinement key.









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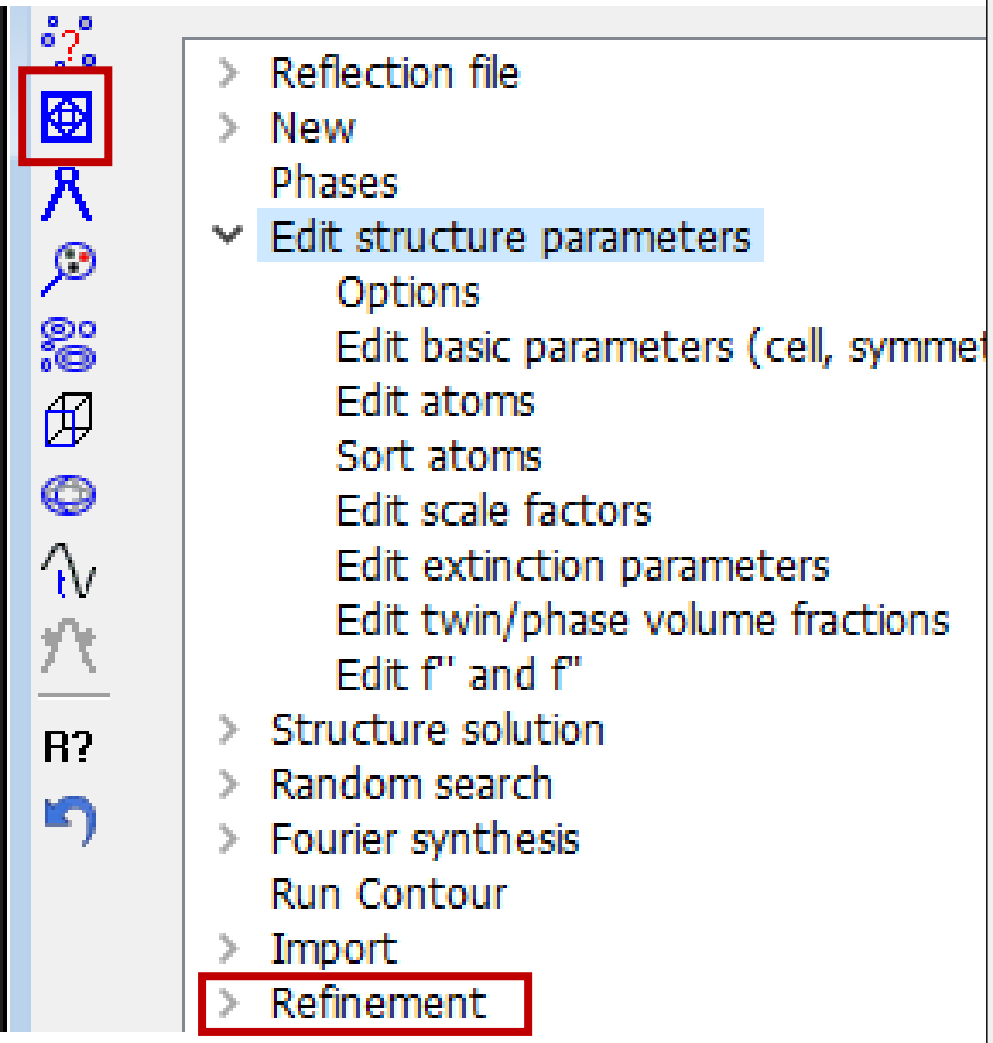
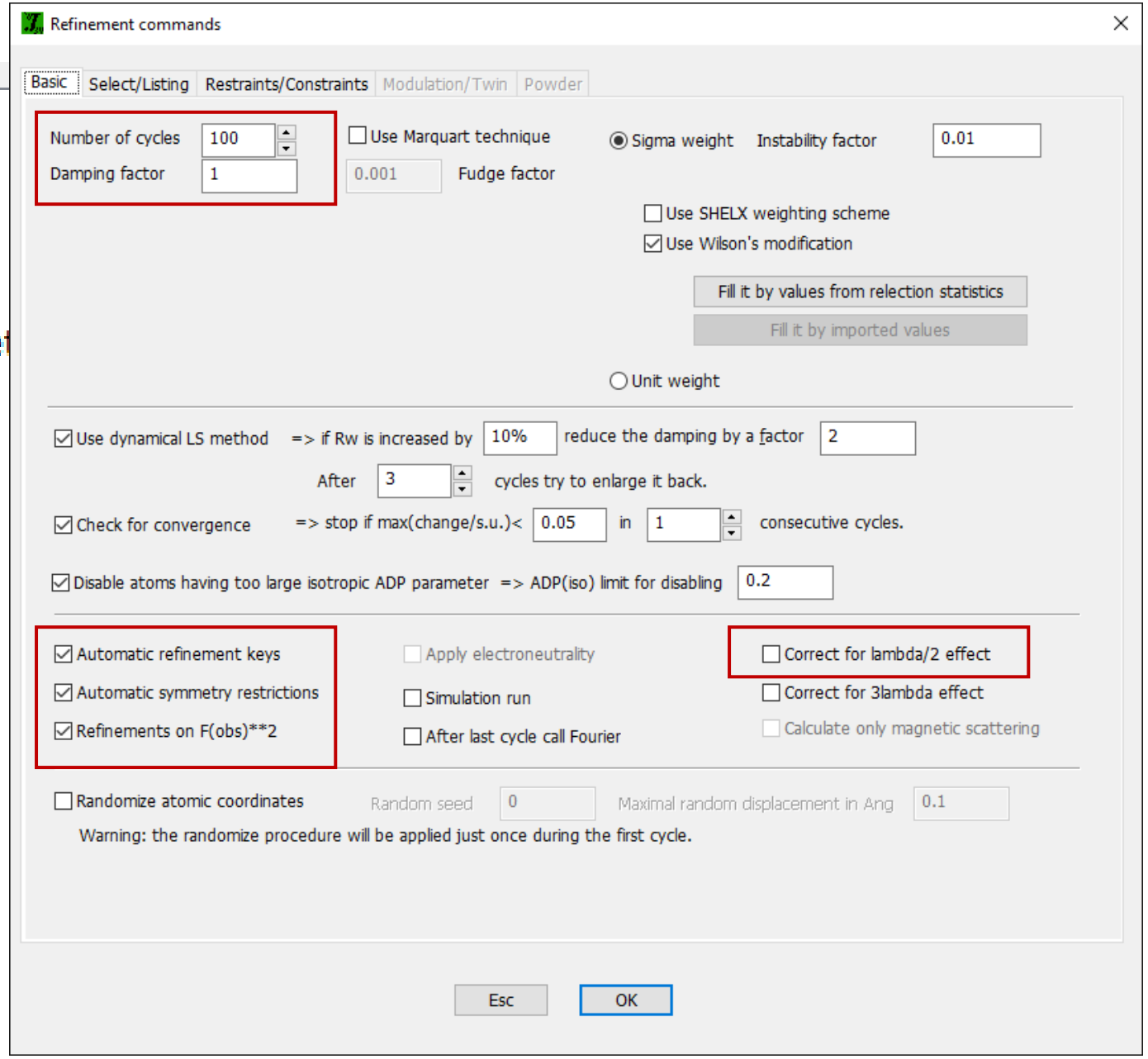
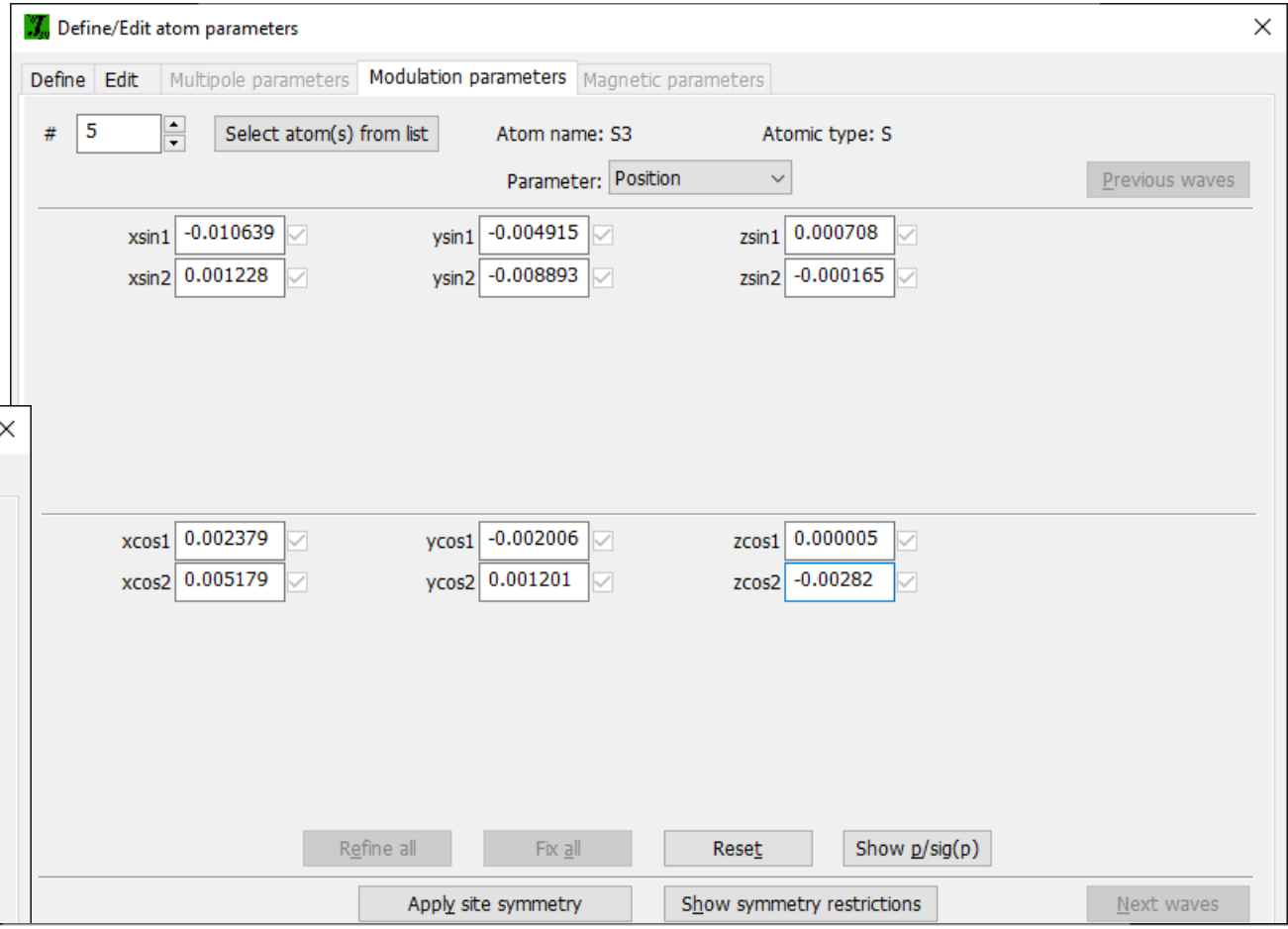
Refinement

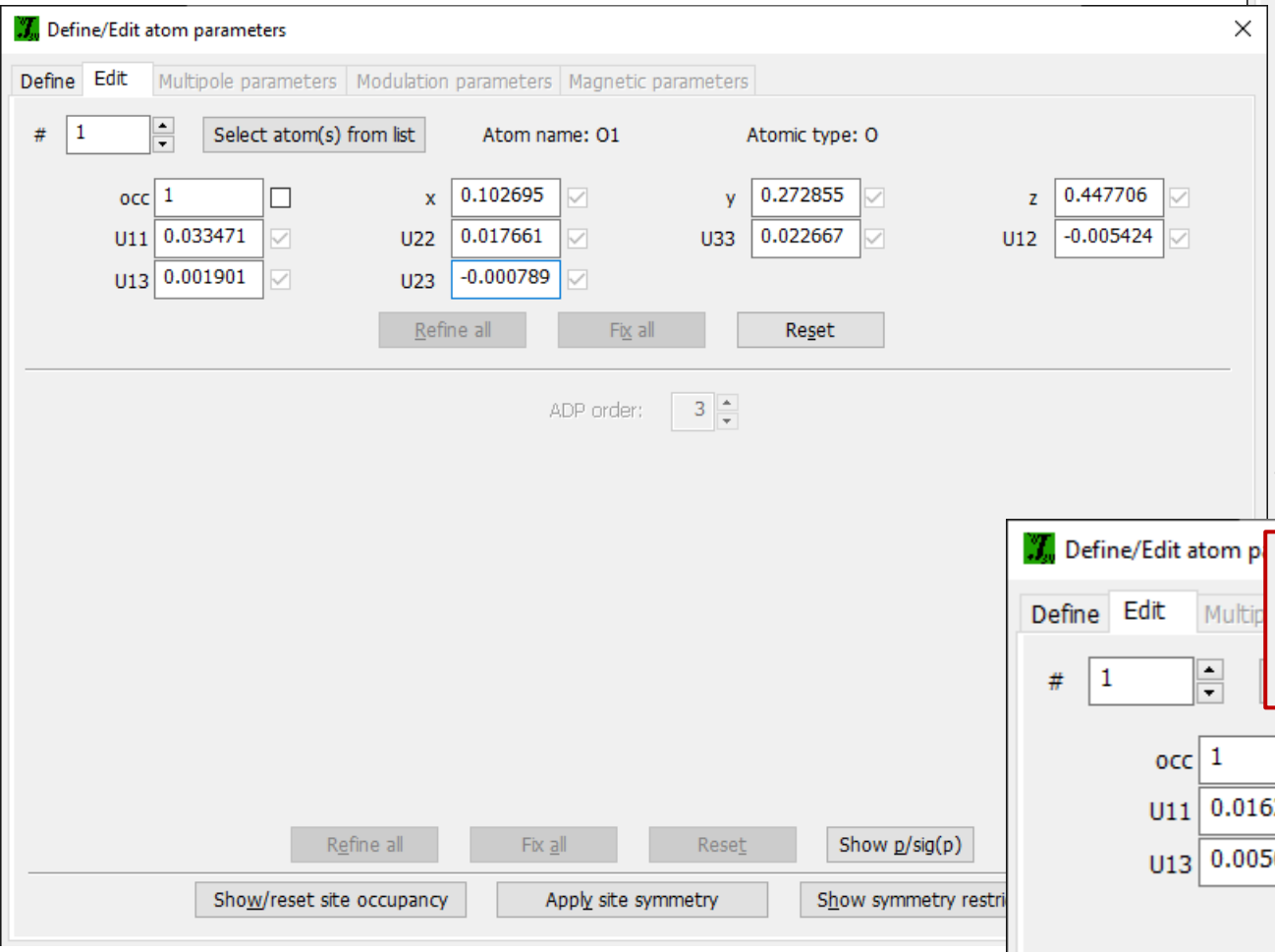

Reflection file
New
Phases
Edit structure parameters
Options
Edit basic parameters (cell, symmet
Edit atoms
Sort atoms
Edit scale factors
Edit extinction parameters
Edit twin/phase volume fractions
Edit f' and f"
Structure solution
Random search
Fourier synthesis
Run Contour
Import
Refinement

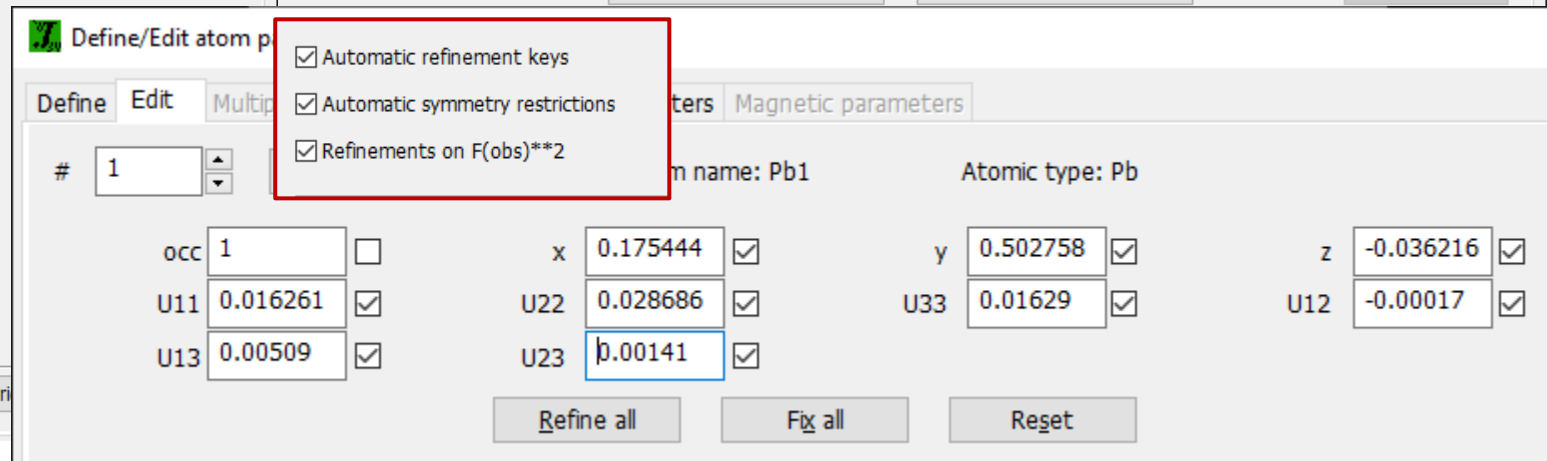

Refinement commands
Basic
Select/Listing
Restraints/Constraints
Modulation/Twin
Powder
Number of cycles 100
Damping factor 1
Use Marquart technique
0.001 Fudge factor
Sigma weight
Instability factor 0.01
Use SHELX weighting scheme
Use Wilson's modification
Fill it by values from relection statistics
Fill it by imported values
Unit weight
Use dynamical LS method => if Rw is increased by 10% reduce the damping by a factor 2
After 3 cycles try to enlarge it back.
Check for convergence => stop if max(change/s.u.)< 0.05 in 1 consecutive cycles.
Disable atoms having too large isotropic ADP parameter => ADP(iso) limit for disabling 0.2
Automatic refinement keys
Automatic symmetry restrictions
Refinements on F(obs)**2
Apply electroneutrality
Simulation run
After last cycle call Fourier
Correct for lambda/2 effect
Correct for 3lambda effect
Calculate only magnetic scattering
Randomize atomic coordinates
Random seed 0
Maximal random displacement in Ang 0.1
Warning: the randomize procedure will be applied just once during the first cycle.
Esc
OK

Refinement

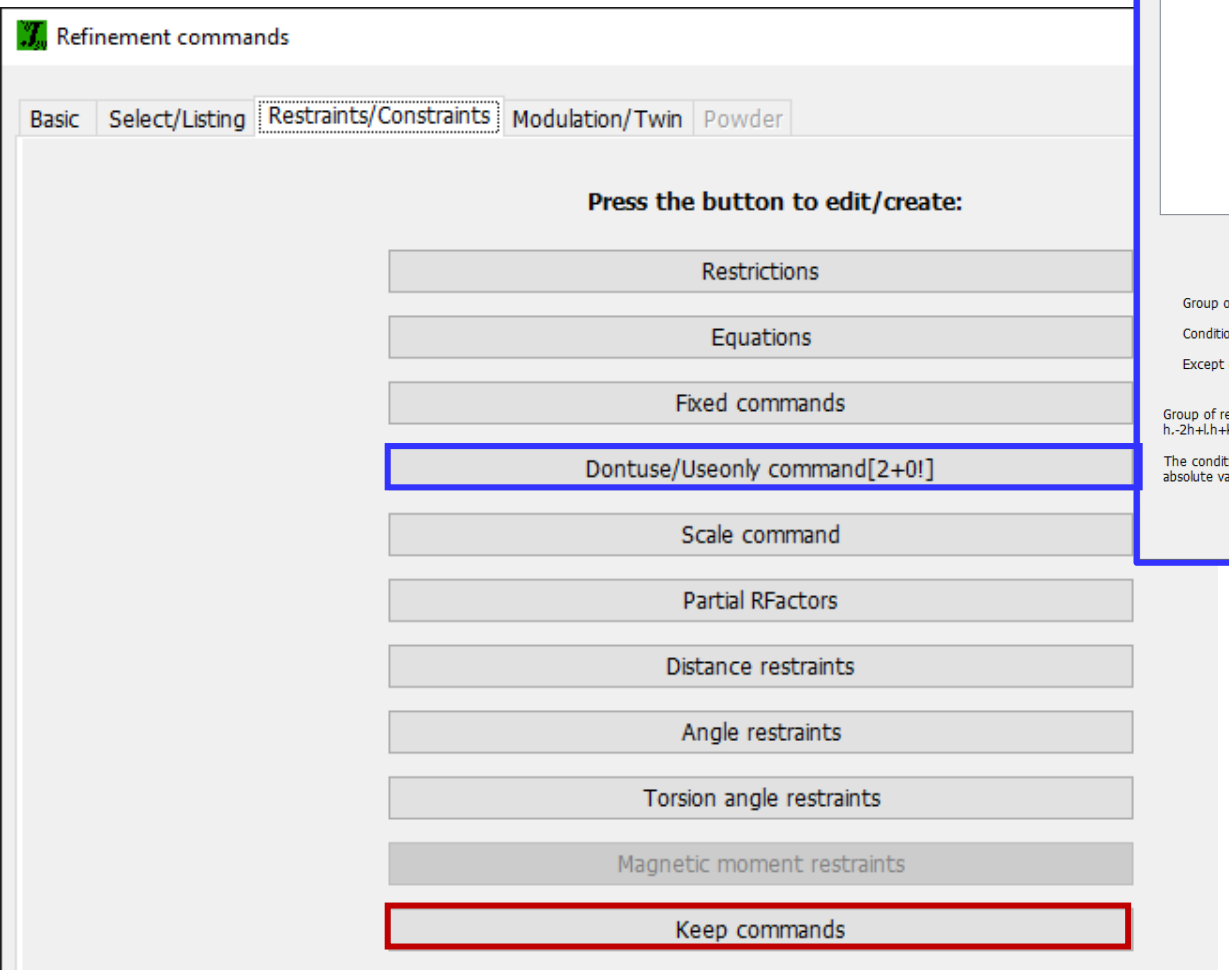
Refinement keys that are automatically set up to be refined, are blocked for the user.

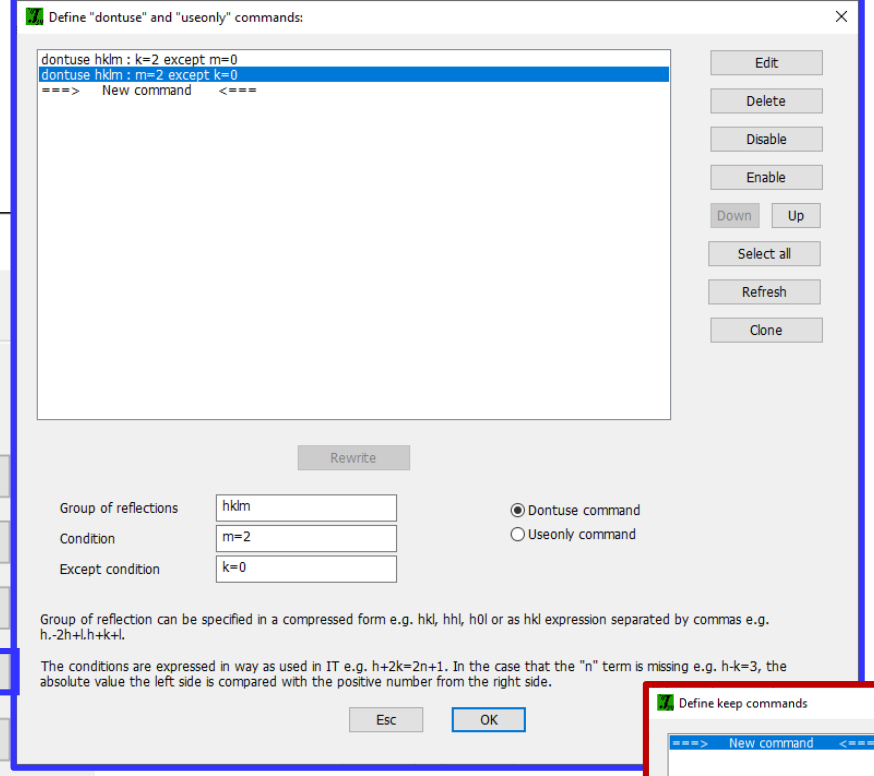


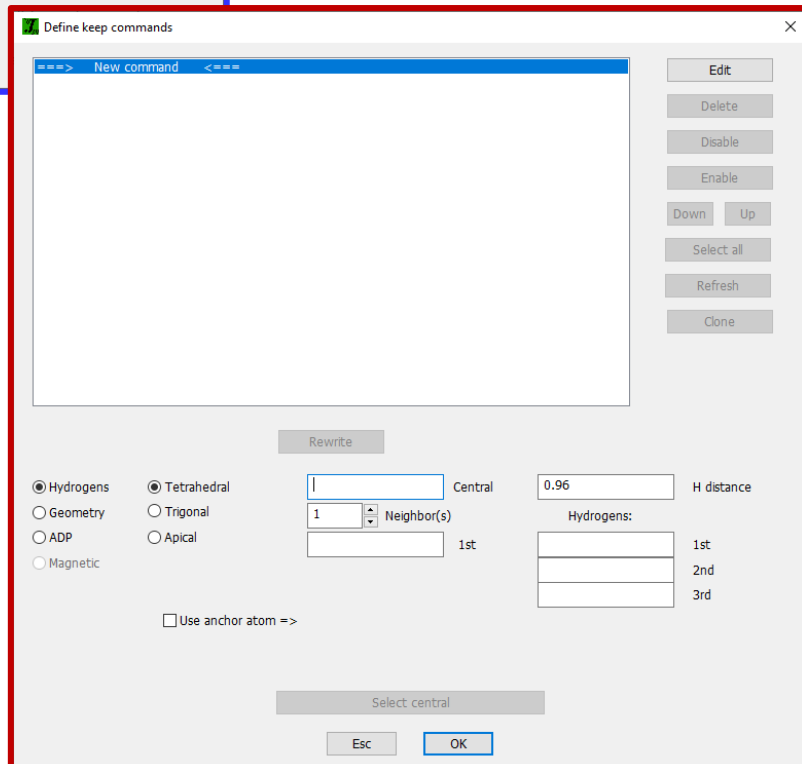




Refinement







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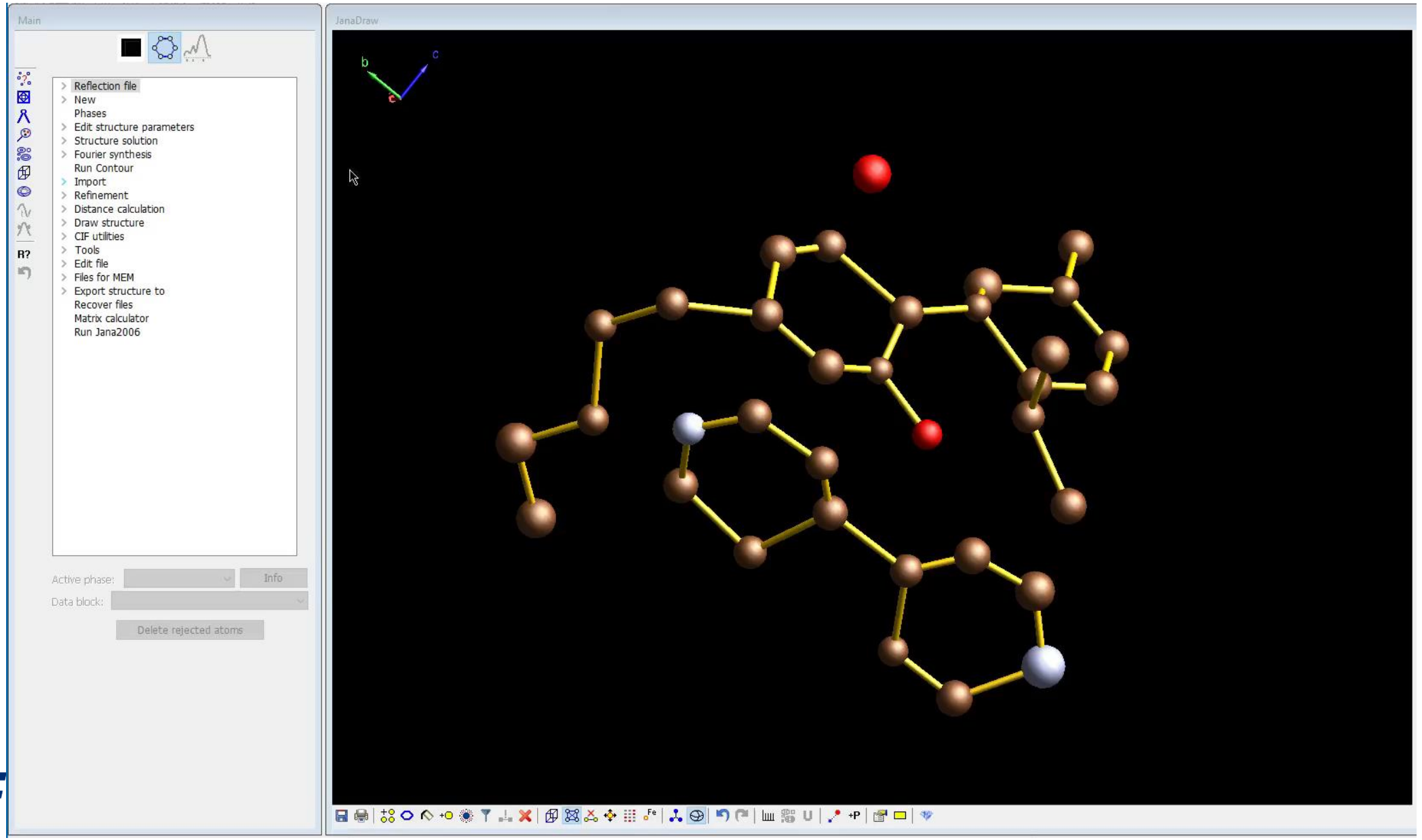
Adding hydrogen atoms - refinement



Refinement – output file .ref

D:\Conferences_Trips_Seminars\2024.06.22_Workshop_Knoxville-US_American Physical Society Meeting\Examples\K2V3O8\Data\K2V3O8.ref - Viewer

File Edit Search View Convert Options Help

Statistics as a function of sin(th)/lambda and structure factors

sin(th)/lambda

limits	0.427710	0.542082	0.624612	0.705653	0.776086	0.844663	0.923330	1.002003
number +	2288	2510	2508	2434	2321	2090	1791	1401
-	422	199	199	291	397	597	912	1307
together	2710	2709	2707	2725	2718	2687	2703	2708
av. wdIq	72.1241	43.1428	42.0990	22.9032	22.3219	15.0929	10.8331	8.2790
numerator +	7334.8	9398.1	11901.4	10081.5	11493.4	9770.7	8188.8	6757.8
-	-2026.2	-505.5	-787.9	-929.7	-1158.8	-1243.8	-1997.0	-3129.0
together	9361.0	9903.6	12689.3	11011.3	12652.2	11014.4	10185.8	9886.7
denominator	44826.5	44839.4	50416.4	47558.5	52921.4	51757.7	54842.6	58869.3
R factor	20.88	22.09	25.17	23.15	23.91	21.28	18.57	16.79

Groups by $\sin\theta/\lambda$

struct. factors

limits	4.2	5.6	7.0	9.7	17.9	27.6	41.6	170.6	unobs
number +	2852	2758	2587	2609	1843	1518	1554	1622	4317
-	0	0	2	48	847	1186	1156	1085	176
together	2852	2758	2589	2657	2690	2704	2710	2707	4493
av. wdIq	30.5060	40.0206	47.9993	56.2322	39.7918	3.9463	5.8902	13.6304	6.2657
numerator +	9430.0	13681.4	16069.6	19905.9	9993.4	1489.2	1798.3	2558.7	15988.9
-	0.0	0.0	-0.7	-38.7	-1414.2	-2523.6	-3160.6	-4639.9	-595.1
together	9430.0	13681.4	16070.3	19944.6	11407.6	4012.7	4959.0	7198.6	16584.0
denominator	9434.8	13711.5	16224.2	21757.9	36104.4	61654.8	93286.4	153858.3	18480.3
R factor	99.95	99.78	99.05	91.67	31.60	6.51	5.32	4.68	89.74

Groups by F

final check	sin(th)/lambda	structure factors
number +	17343	17343
-	4324	4324
together	21667	21667
numerator +	74926.5	74926.4
-	-11777.8	-11777.8
together	86704.3	86704.2
denominator	406031.8	406032.4
R-factor	21.35	21.35

Overall information

Refinement program page= 256
structure : 17:03:58 01-06-24

Statistics as a function of satellite indices

Satellite indices		+-(0,0)	+-(1,0)
number	+	5974	11369
	-	4324	0
together		10298	11369
av. wdIq		6.9	50.2
numerator	+	7227.1	67699.1
	-	-11777.8	0.0
together		19004.9	67699.1
denominator		338333.9	67699.1
R factor		5.62	100.00

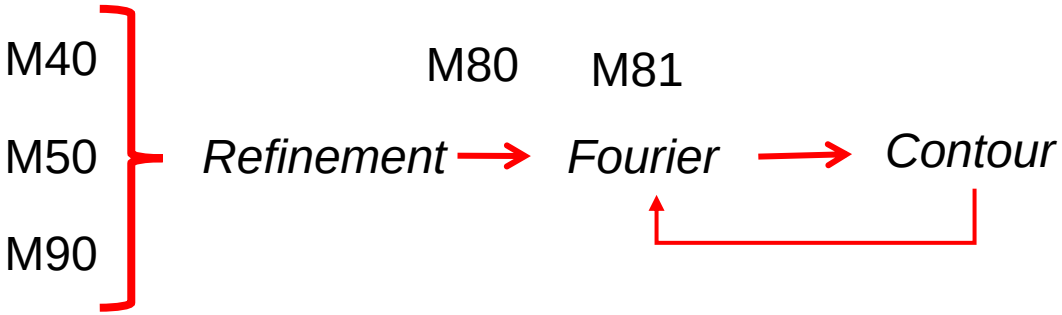
Satellites

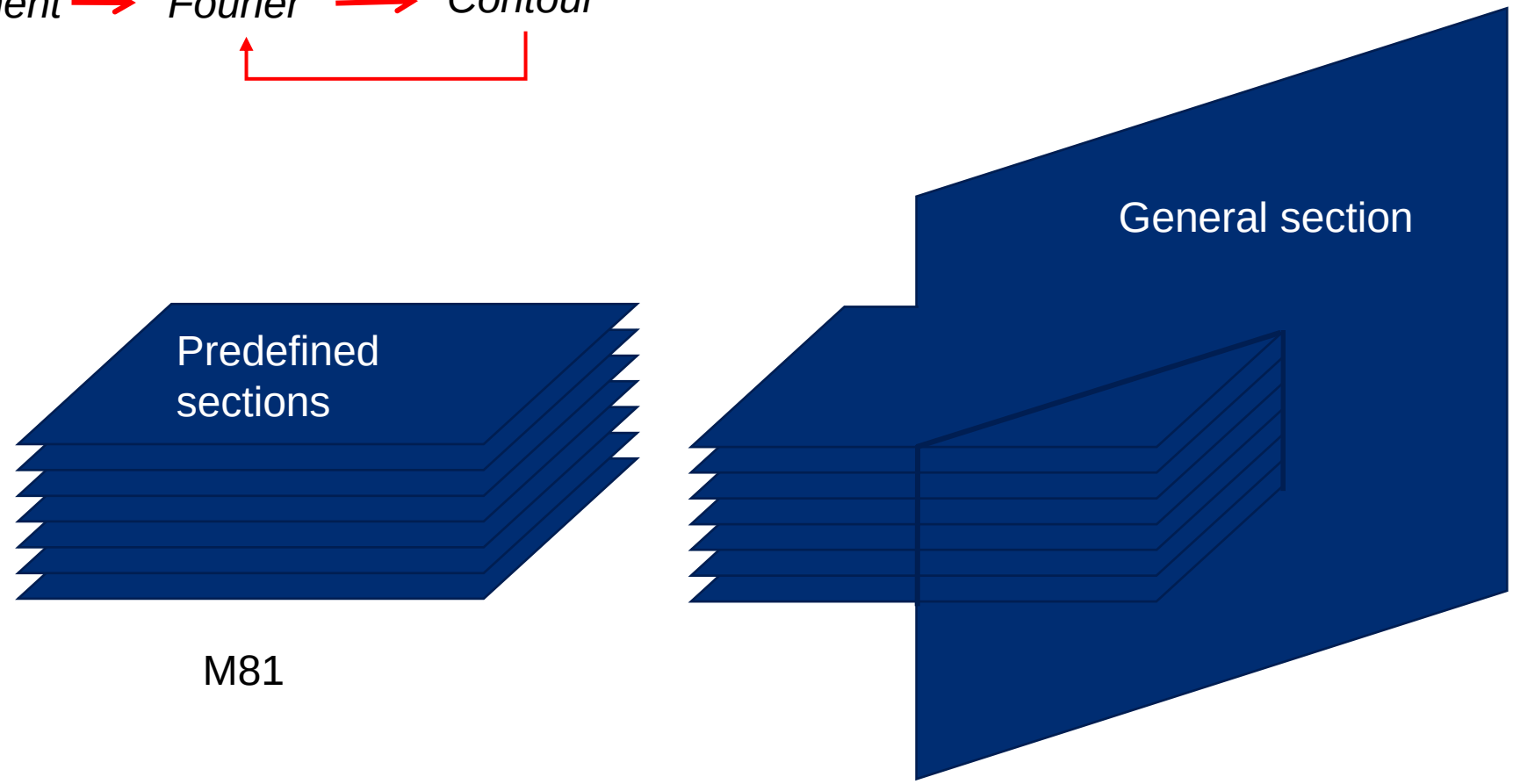
Last screen information window:

```
|R factors : [26160=21667+4493/55],    Damping factor:   1.0000          |
|GOF(obs)=  5.45    GOF(all)=  5.07                                      |
|R(obs)=  21.35    wR2(obs)= 35.77    R(all)=   24.33    wR2(all)= 36.44 |
|R factors for main reflections : [10570=10298+272]                     |
|R(obs)=   5.62    wR2(obs)= 12.64    R(all)=    5.80    wR2(all)= 12.71 |
|R factors for satellites +-(1,0) : [15590=11369+4221]                  |
|R(obs)= 100.00    wR2(obs)=100.00    R(all)=  100.00    wR2(all)=100.00 |
|Last wR2(all): 36.44                                                   |
|Maximum change/s.u. :    0.0089 for x[04]                              |
```

Refinement results

Fourier maps





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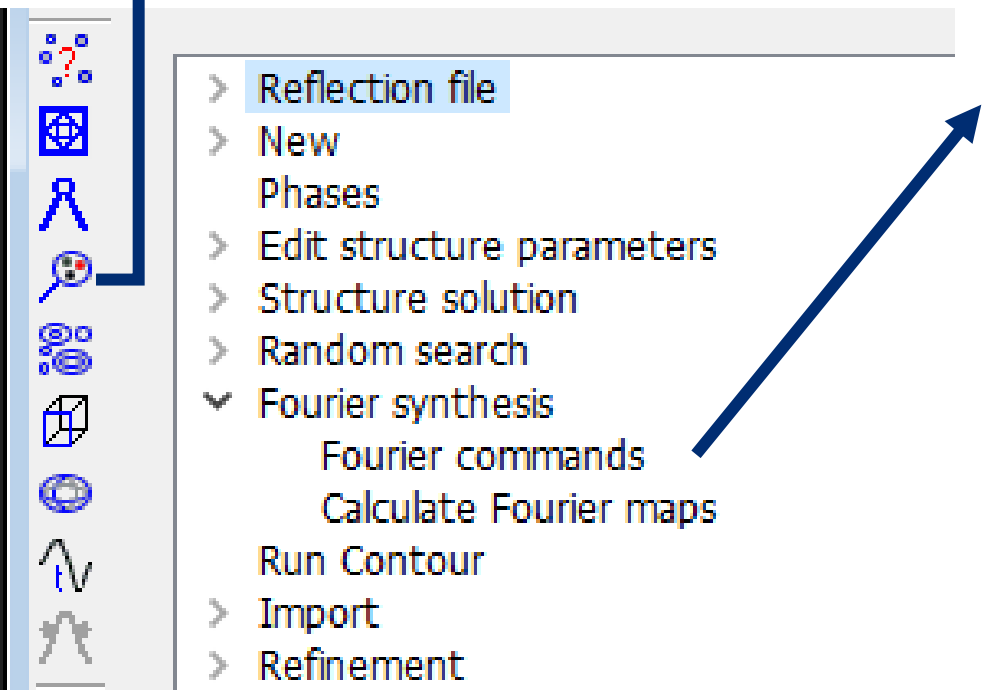
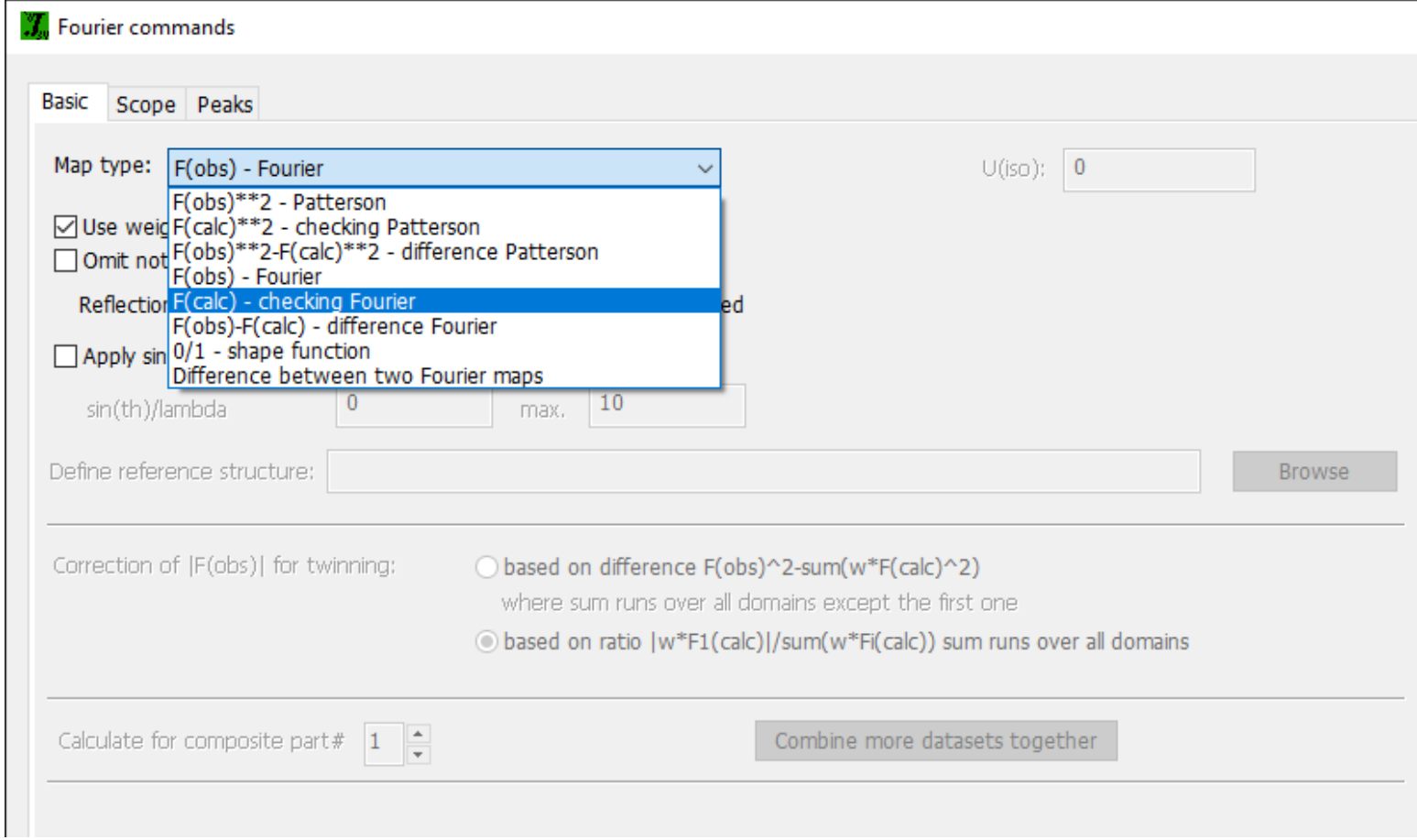
Contour can plot a predefined section, or it can calculate and plot general sections. For arbitrary general sections the predefined section must cover at least asymmetric unit of the elementary cell.

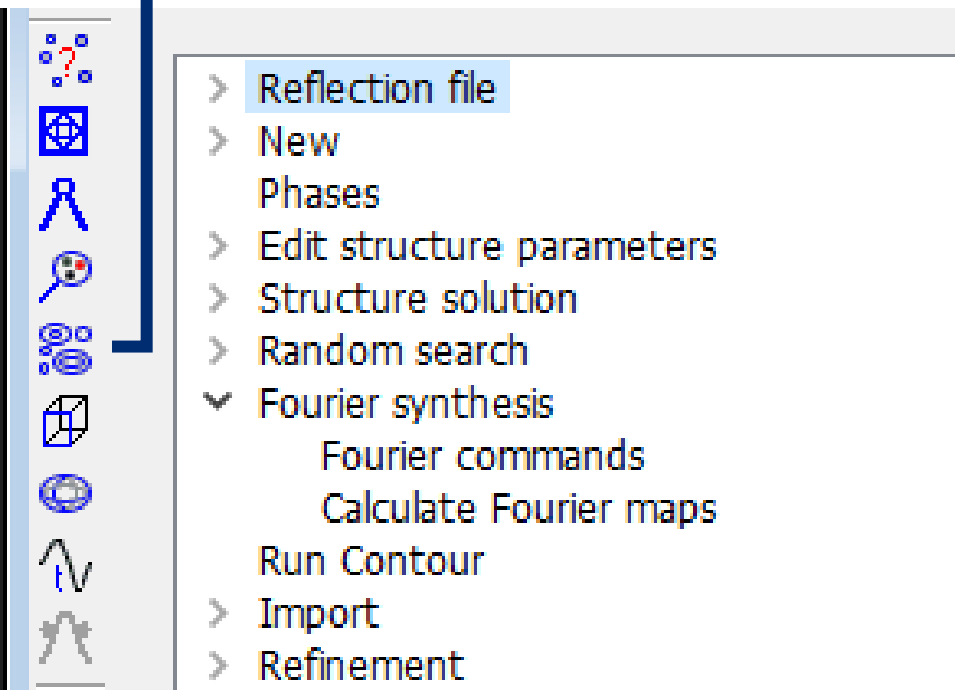
Fourier maps

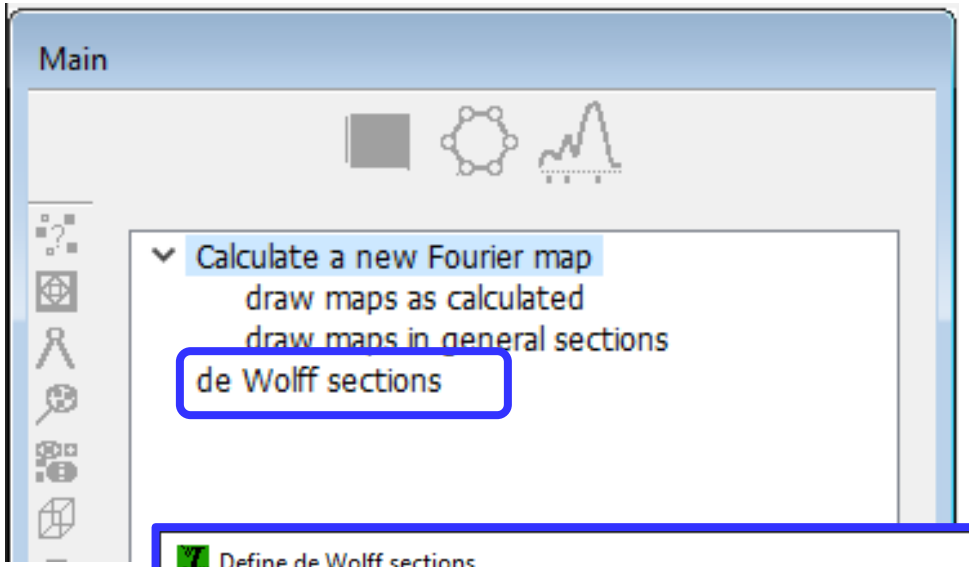


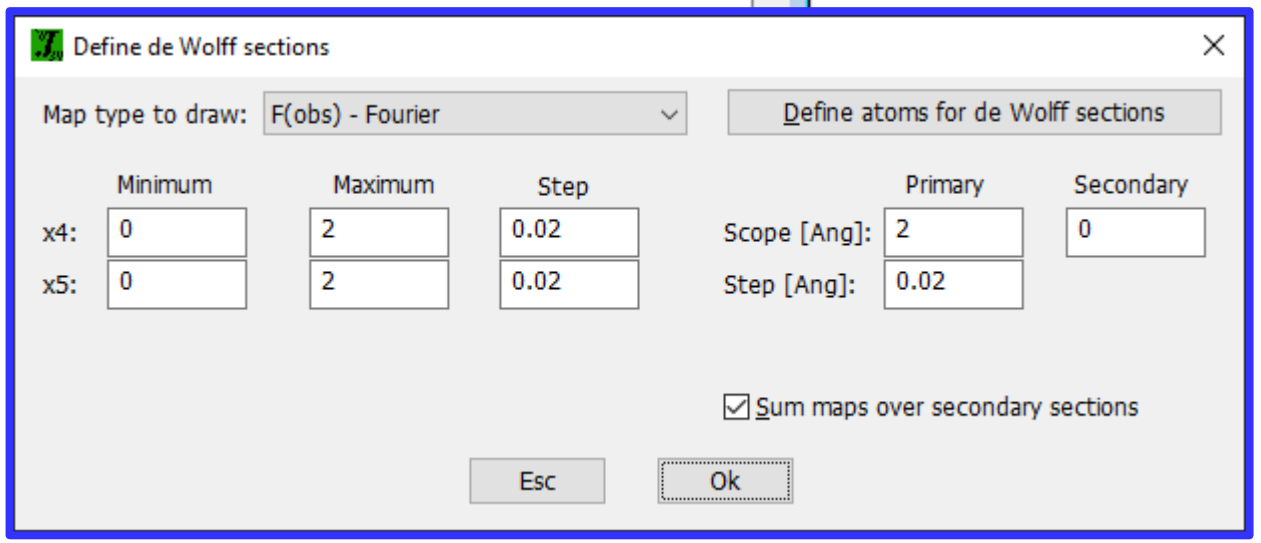


Contour can plot a predefined section, or it can calculate and plot general sections. For arbitrary general sections the predefined section must cover at least asymmetric unit of the elementary cell.

Fourier maps







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

Basic crystallography

- Radiation type selection
- Symmetry determination
- External call to structure solution by Charge flipping and Direct methods
- Tools for editing structure parameters
- Fourier calculation
- Tools for adding hydrogen atoms
- Constrains and Restraints

- JanaDraw
- Graphical tools for atomic parameters, refinement commands, bond distances, angles, etc.

- Scale factor
- Atomic site coordinates and occupancies
- ADPs
- Extinction parameters

- CIF output

Advanced tools

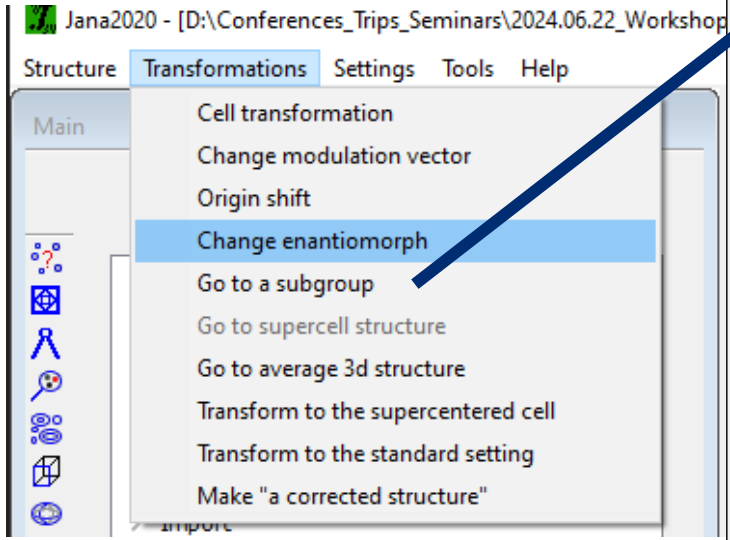
- Transformation tools, group-subgroup relations
- Twinning (merohedric, general), treating of overlapped reflections
- User equations and restrictions
- Fourier methods - Fourier sections and de Wolff sections

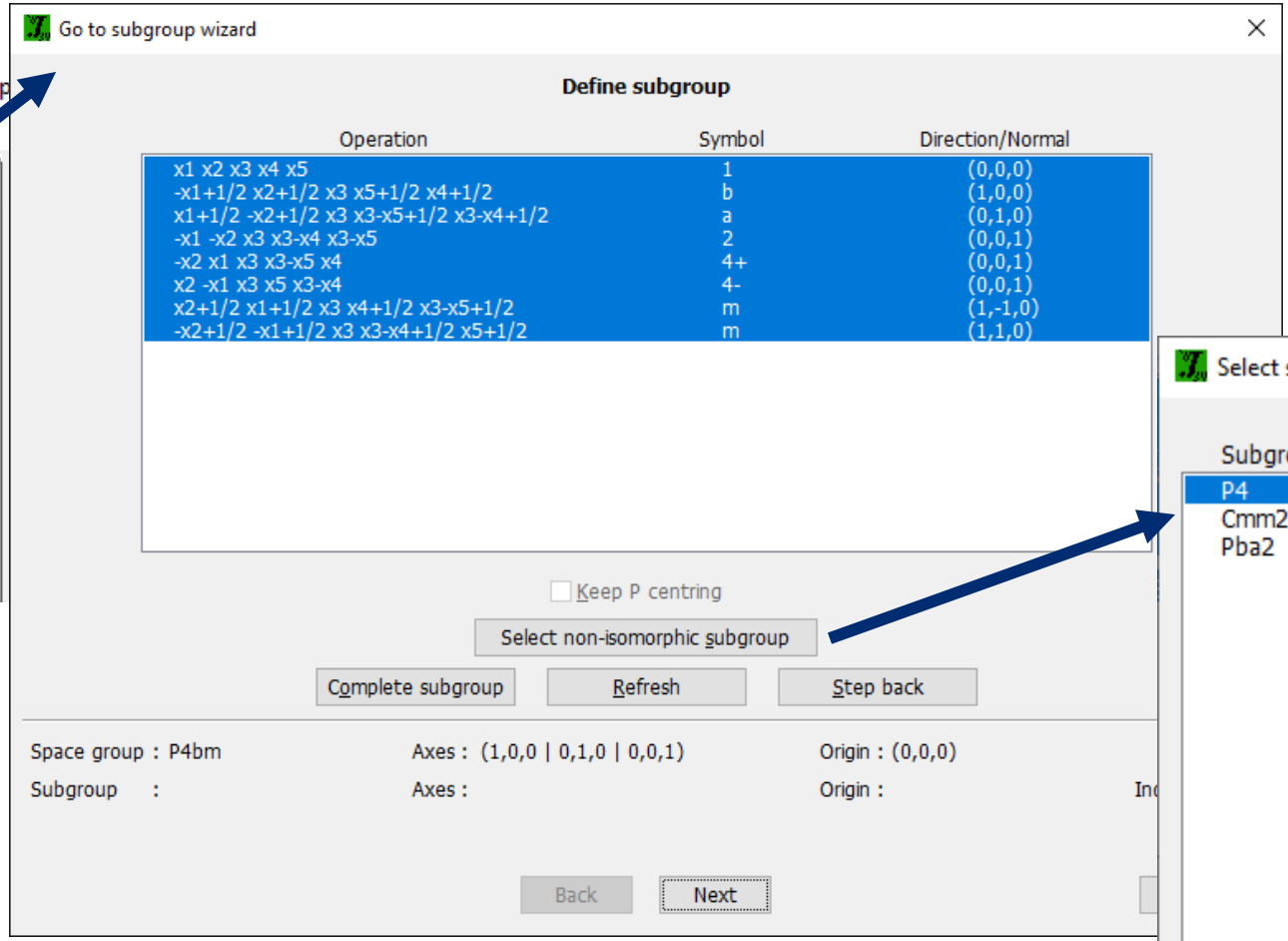
- Disorder
- Split atomic positions and introduces restrictions
- Rigid body approach, local symmetry
- Anharmonic ADPs

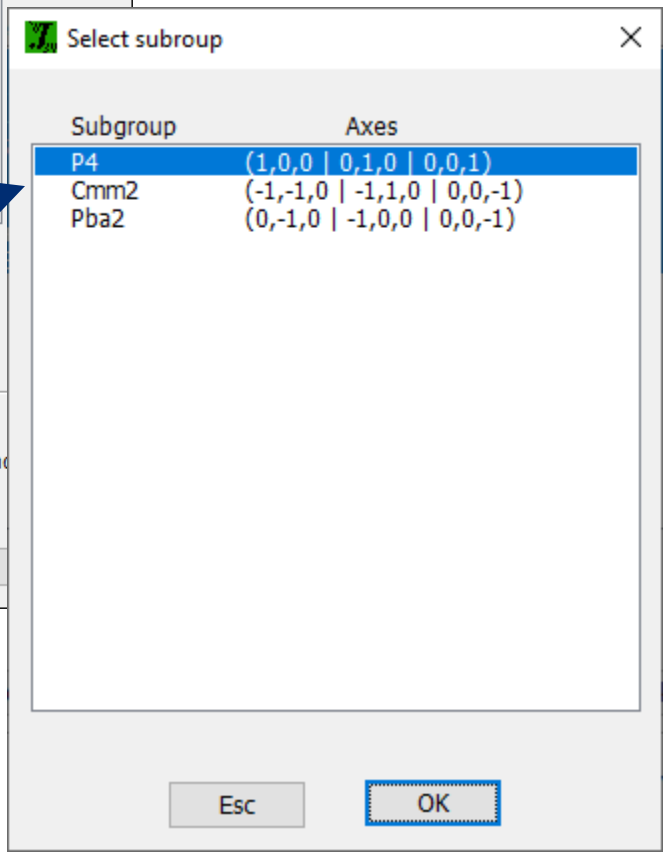
- Modulated and composite structures
- Several types of modulated functions
- Plotting of modulated parameters as a function of t
- Plotting of modulated structures
- Calculation of geometric parameters
- Visualization of the modulated structure in JanaDraw

- Multiphases for powder and single-crystal data
- Multipole refinement
- Cyclic refinement
- Fundamental approach
- Anisotropic strain broadening (generalized to satellites)

Advanced tools – Group-subgroup transformation







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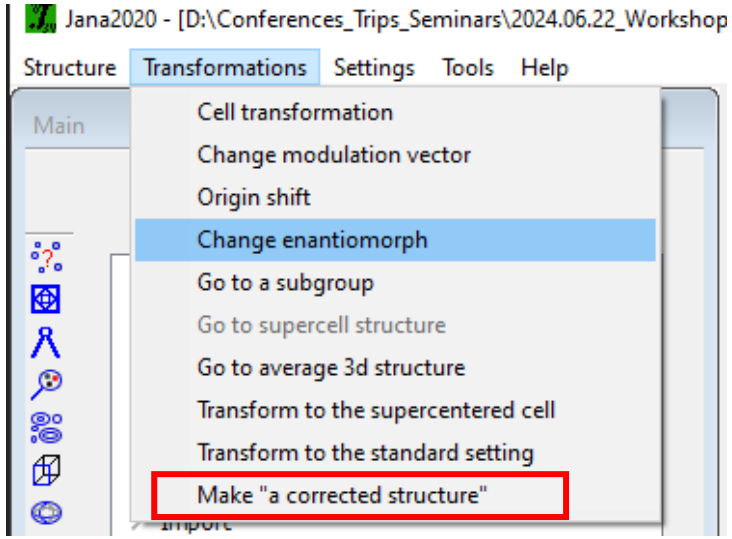
Advanced tools – Group-subgroup transformation

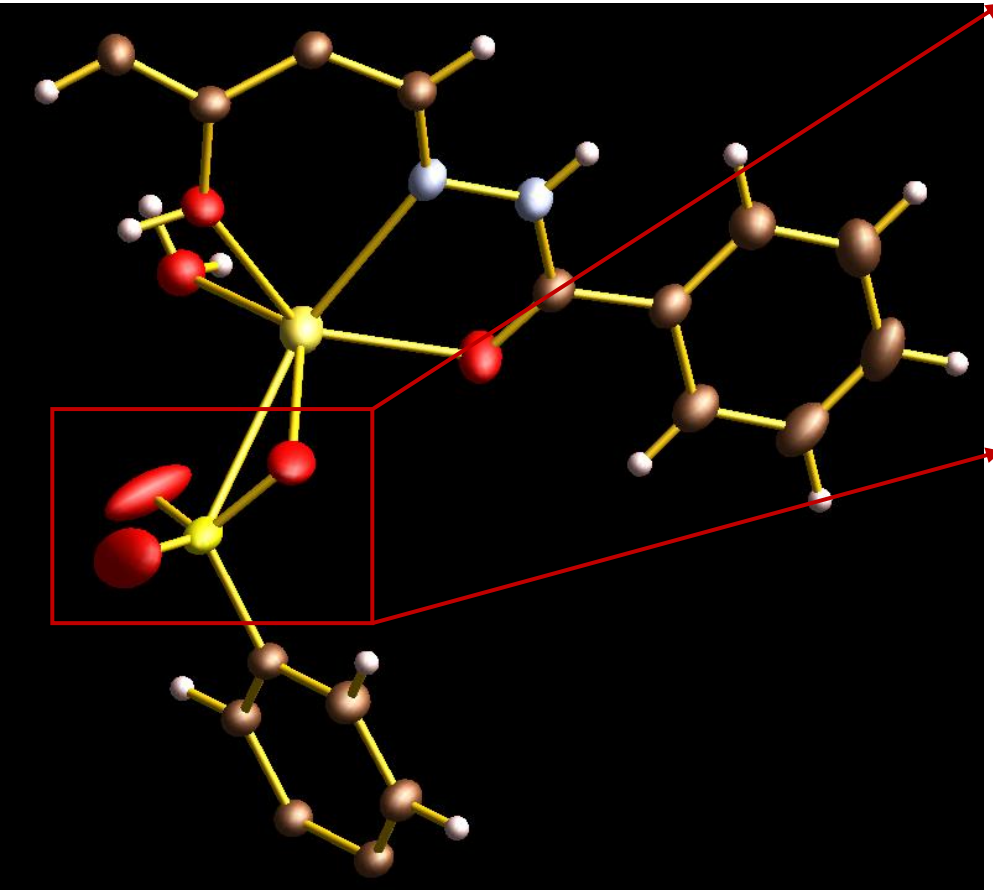


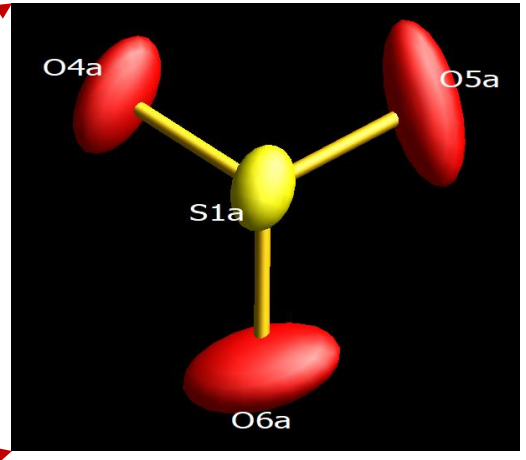
Make “a corrected structure” is used for TOF Laue single crystal data from ISIS SXD or TOPAZ. It applies individual scales and extinction correction and then it makes symmetry merging. This gives a more stable final refinement and more realistic GOF and R factors comparable with traditional data collections.

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 – Disorder, atom split, rigid body

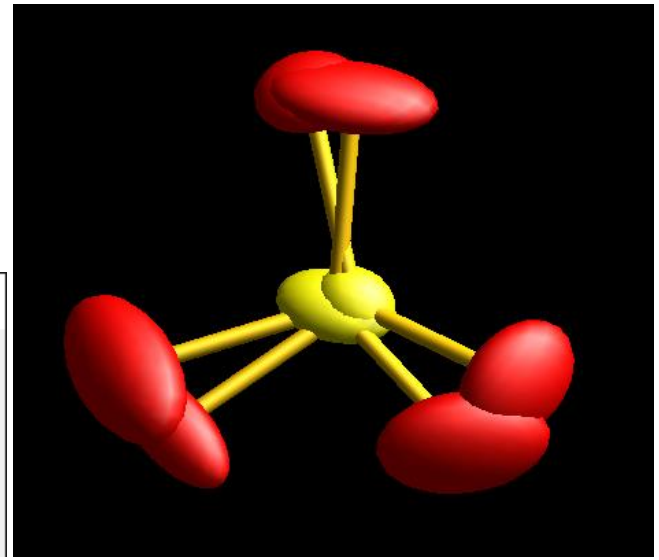




Information from refinement:

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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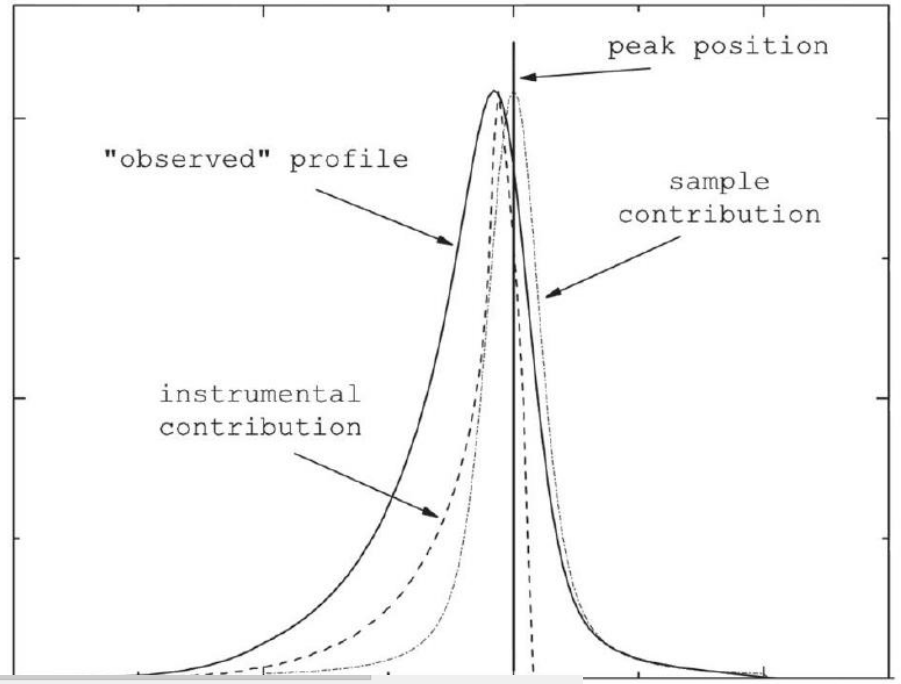
Advanced tools – Fundamental approach

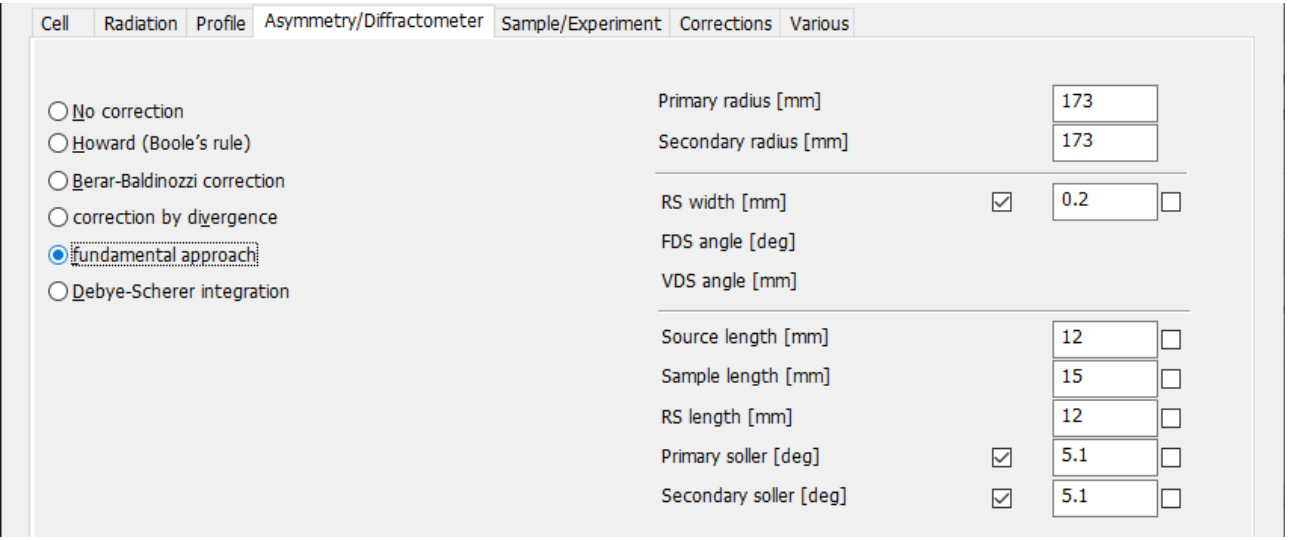
Final profile — Sample contribution — Instrumental contribution

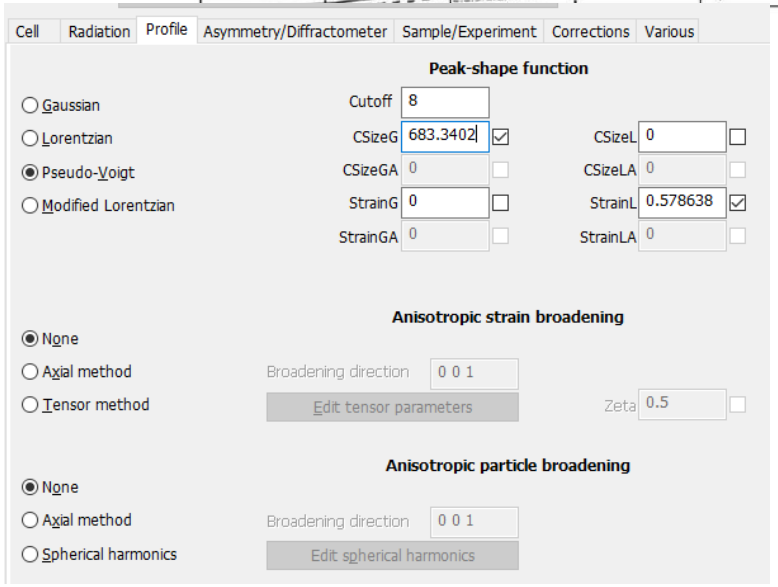
$$H(2\theta) = F(2\theta) \otimes G(2\theta)$$

crystalline size and stress

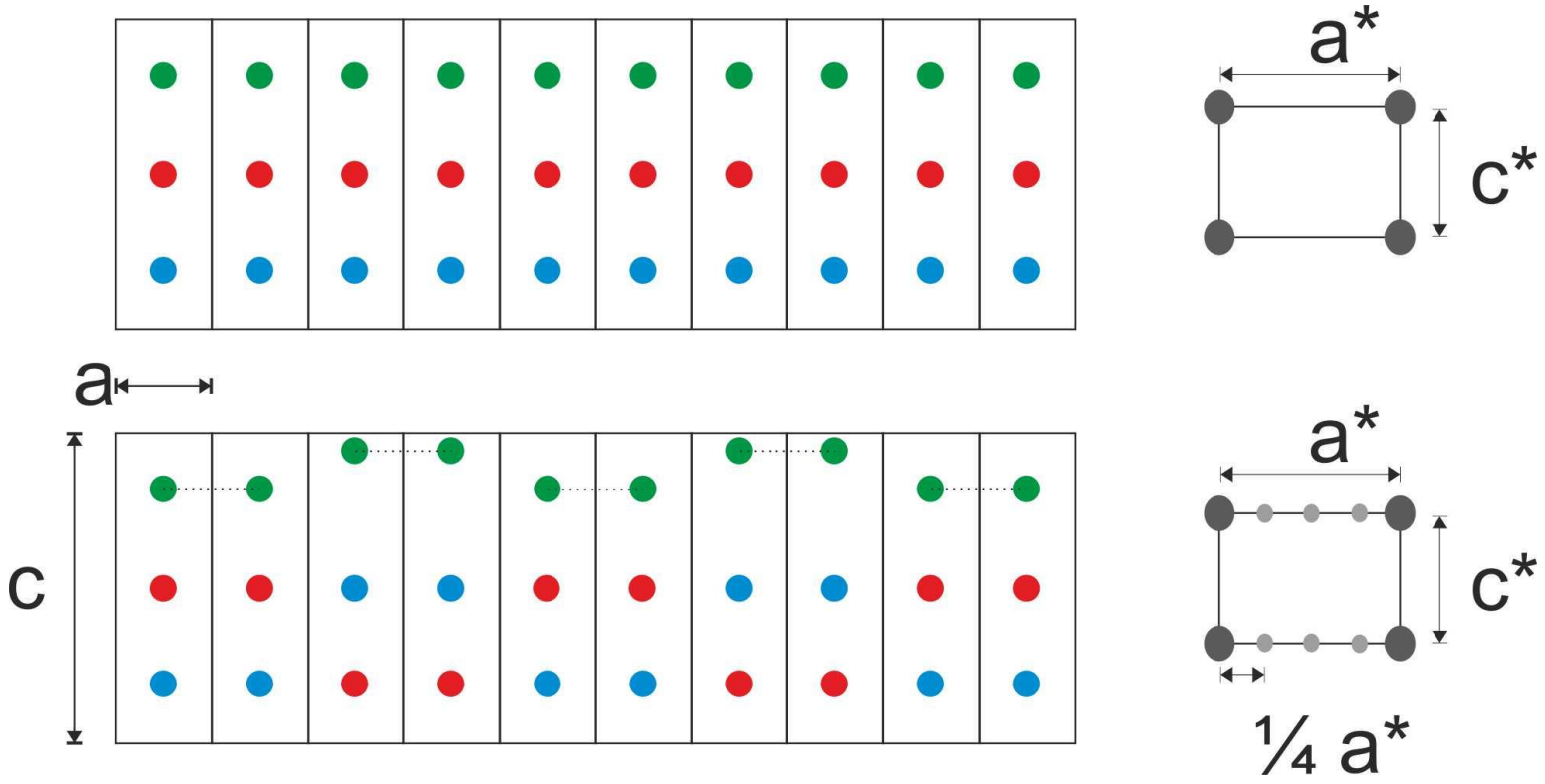
optics sample holder detector source





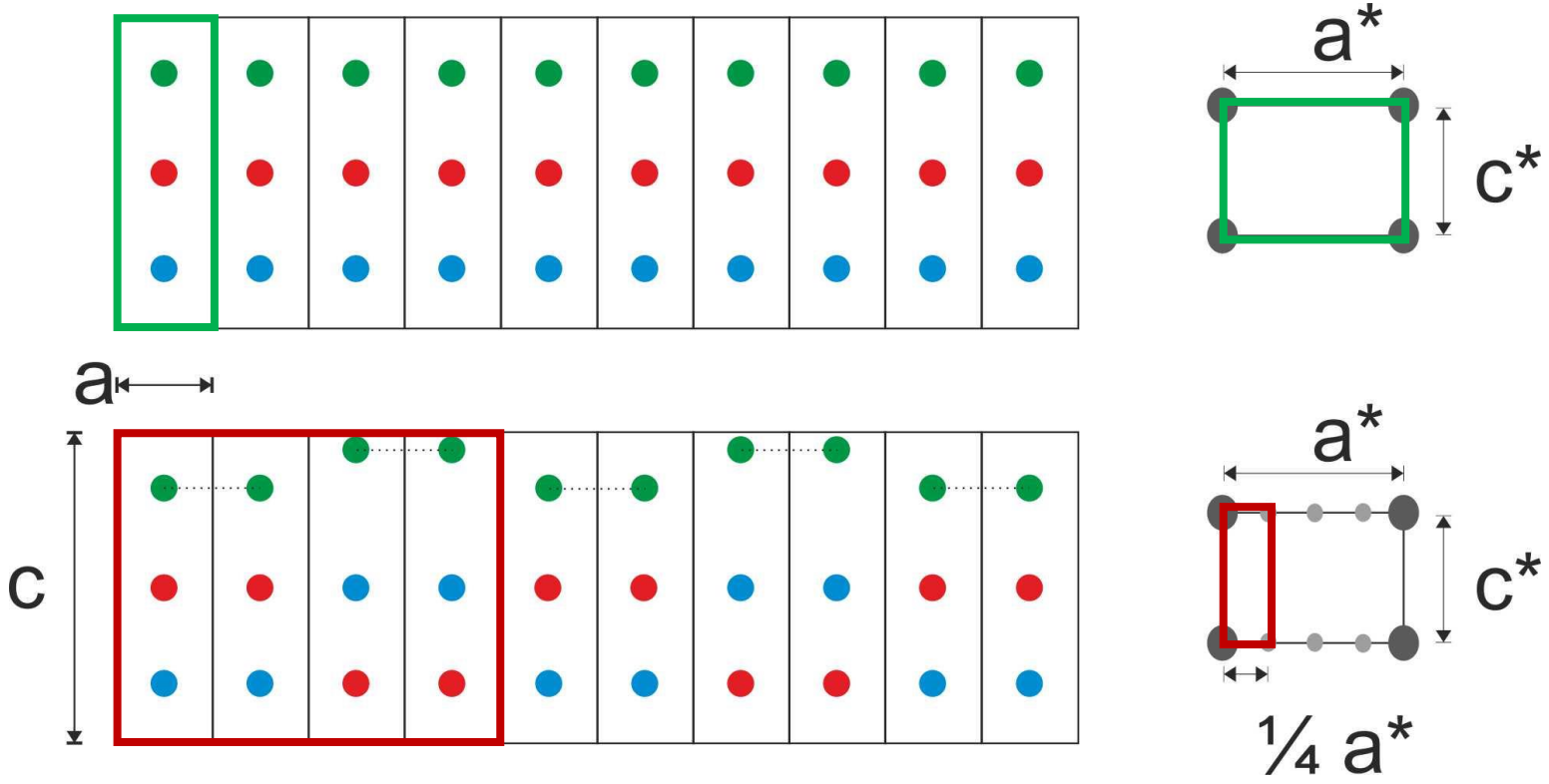


Advanced tools – modulated structures



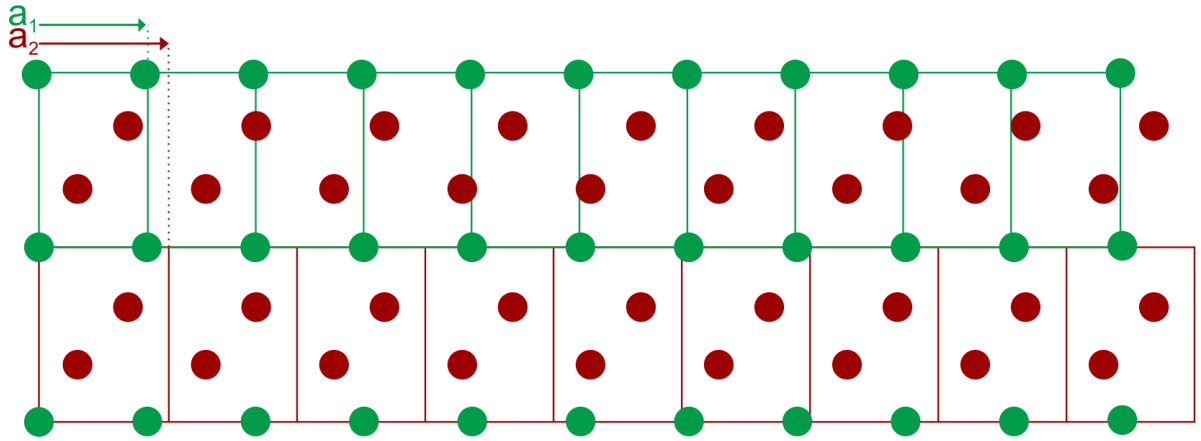
Modulation vector with rational components

Advanced tools – modulated structures



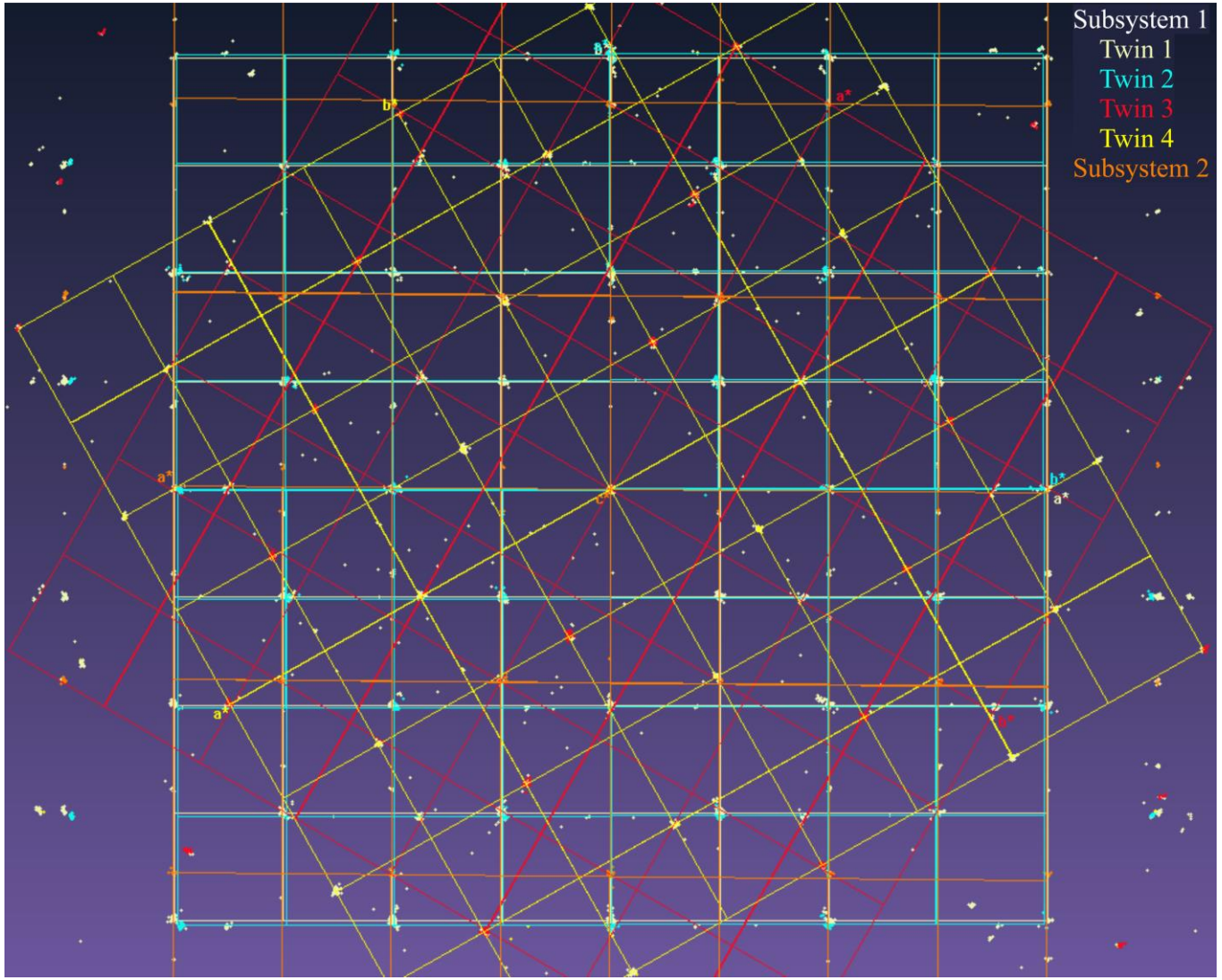
Modulation vector with (ir)rational components – (in)commensurate modulated structure

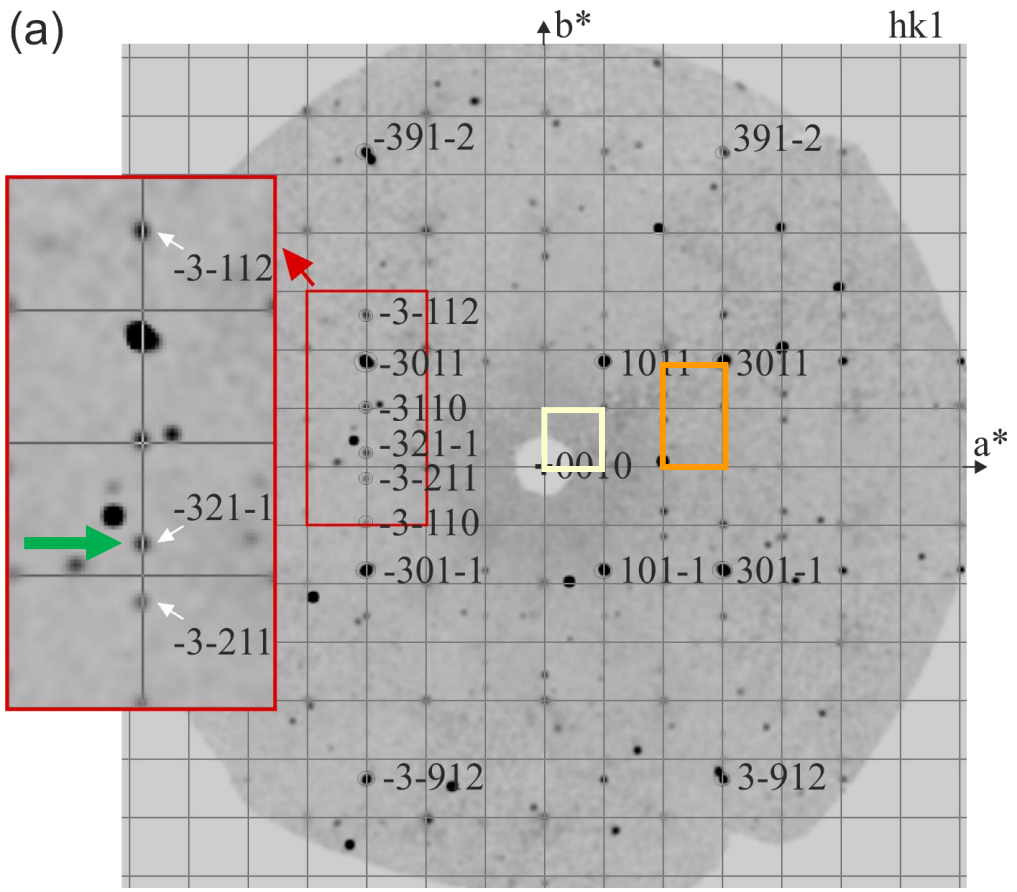
Advanced tools – composites



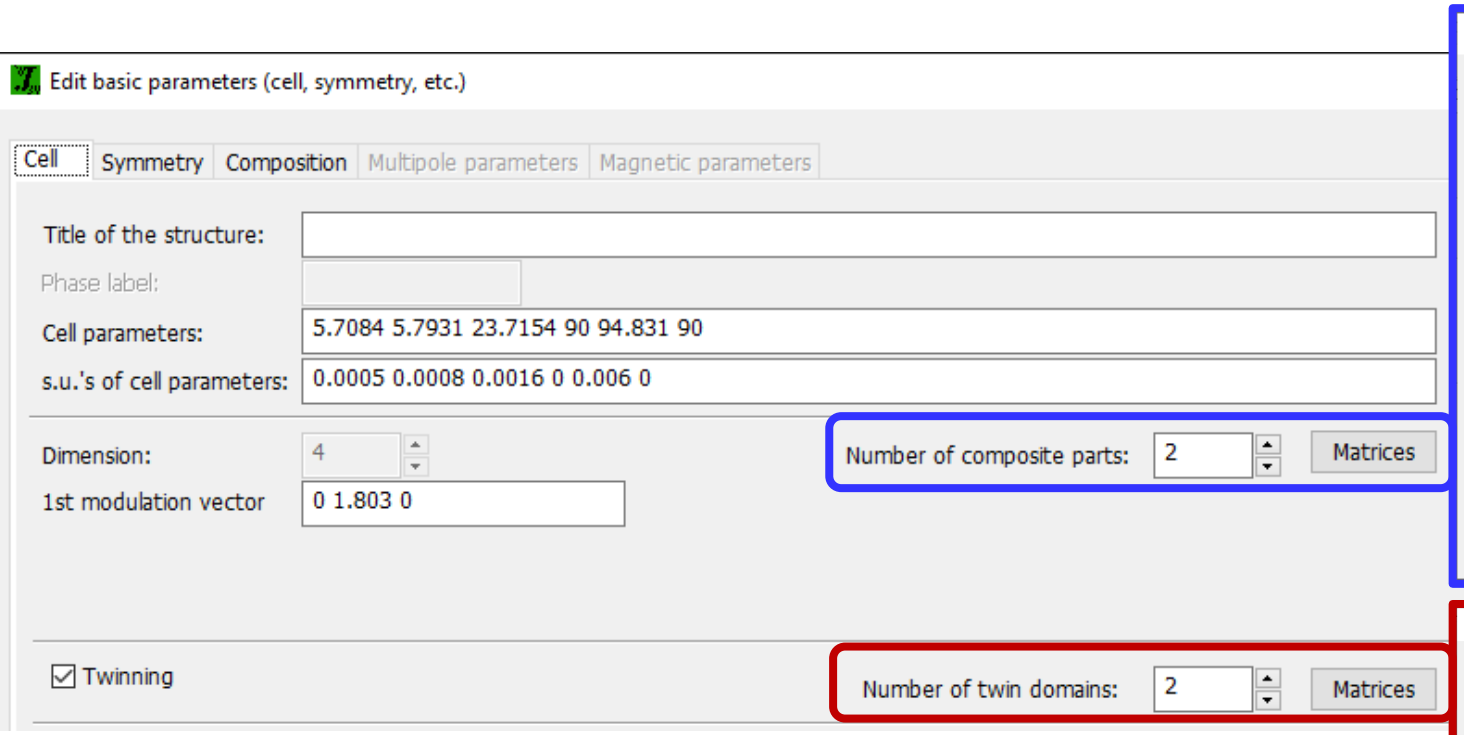
We can find two coexisting lattices, which cannot be described by a simple common supercell -> incommensurate composites

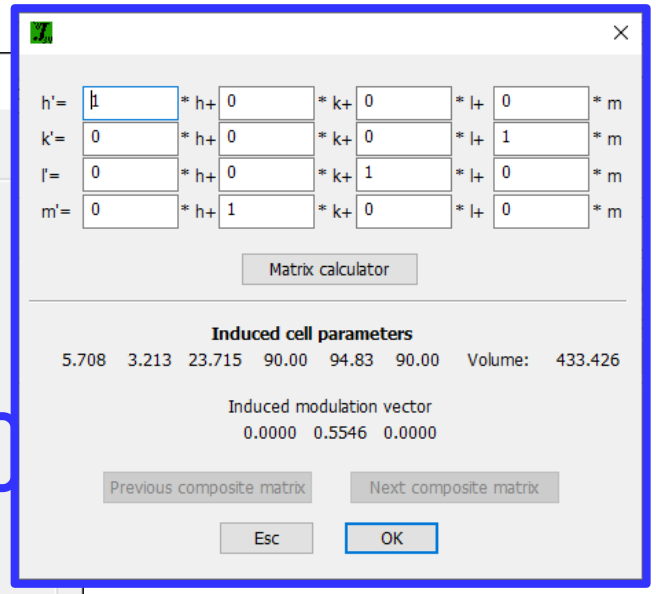
Advanced tools – Twins, composites

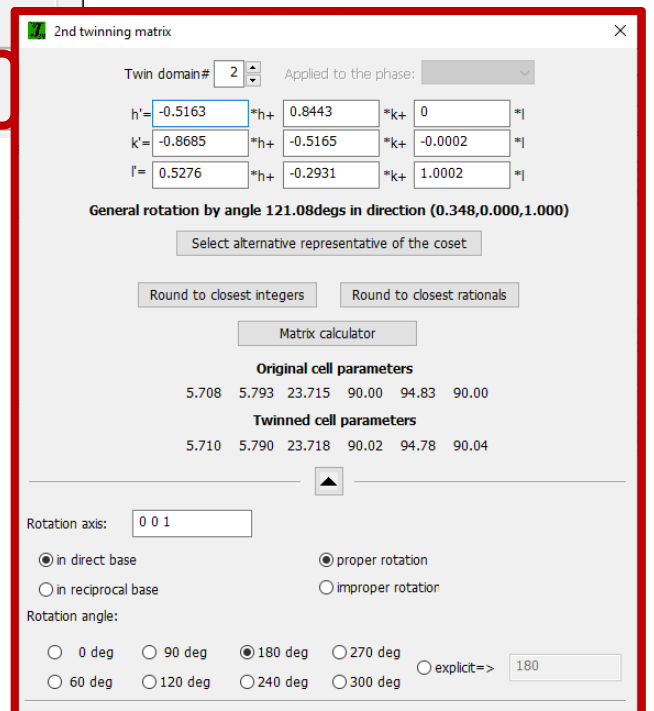




Advanced tools – Twins, composites







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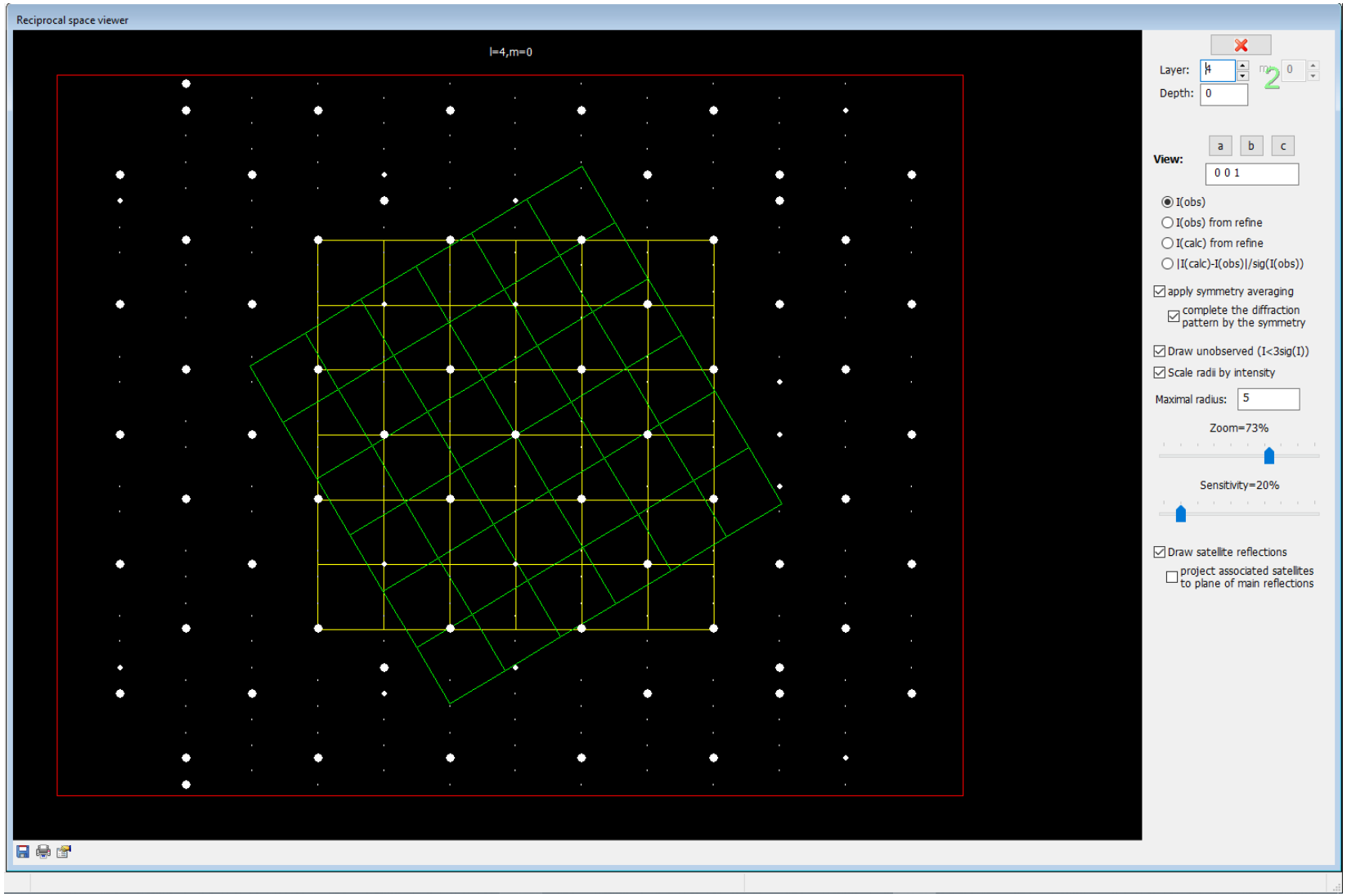
Advanced tools – Twins, composites

- 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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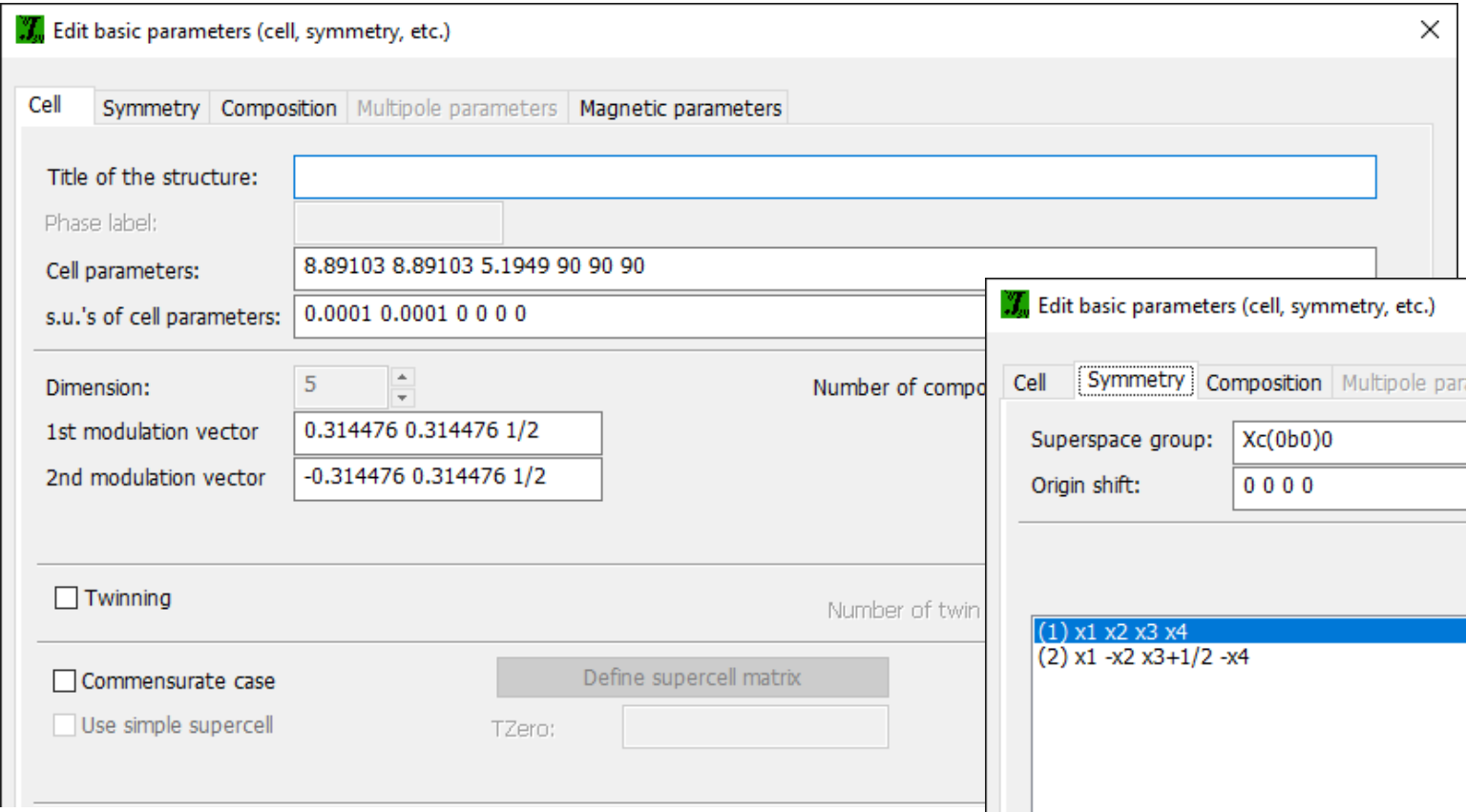
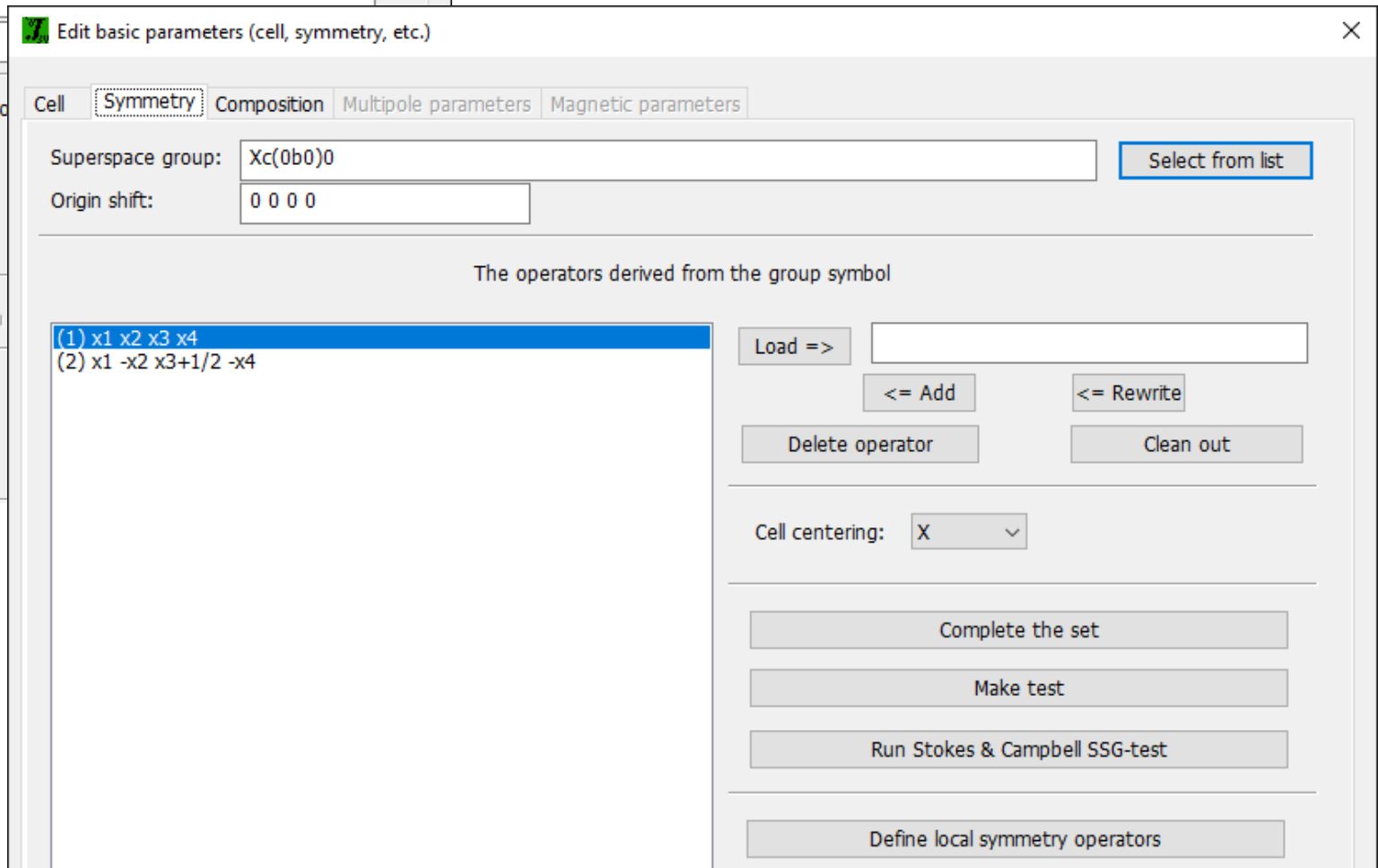
Advanced tools – modulated structures





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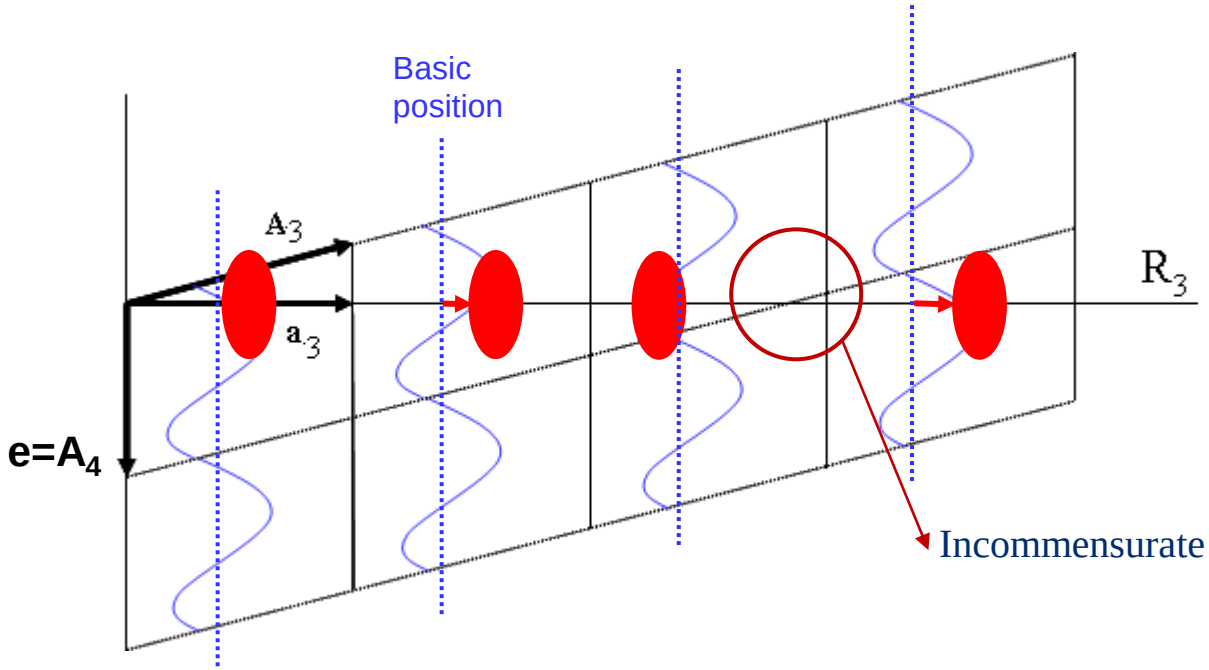
Modulated structures



Harmonic modulation from arbitrary displacements

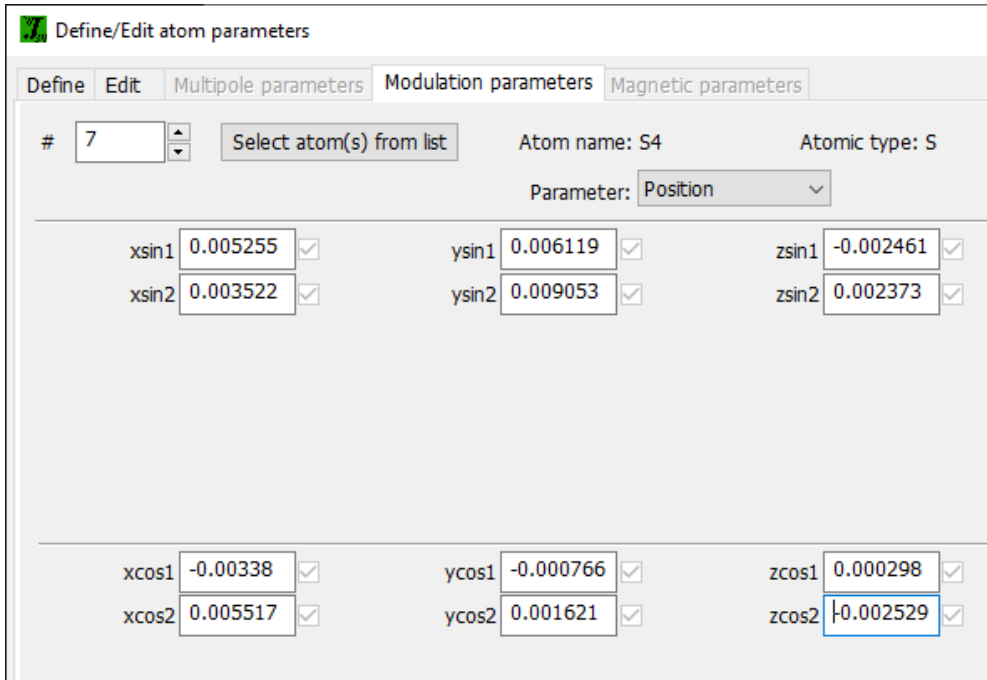
The atom is displaced from its basic position by a periodic modulation function that can be expressed as a Fourier expansion. In the first approximation intensities of satellites reflections up to order *m* are determined by modulation waves of the same order.
The position r of an atom is the sum of the basic structure position and the modulation function u.

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

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

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

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



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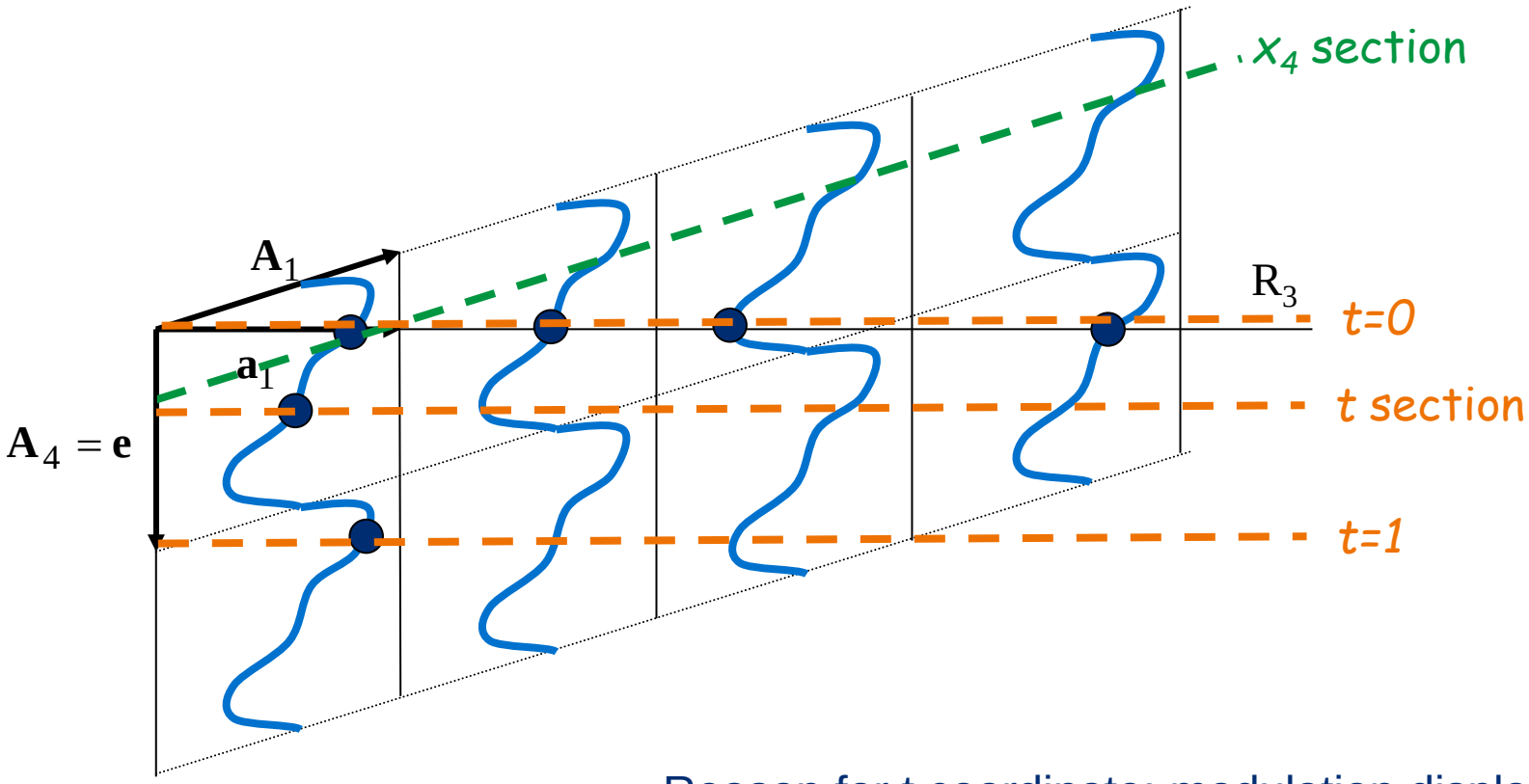
p -> site occupancy, position, ADP parameters

Modulated structures

Modulation parameters as function of t



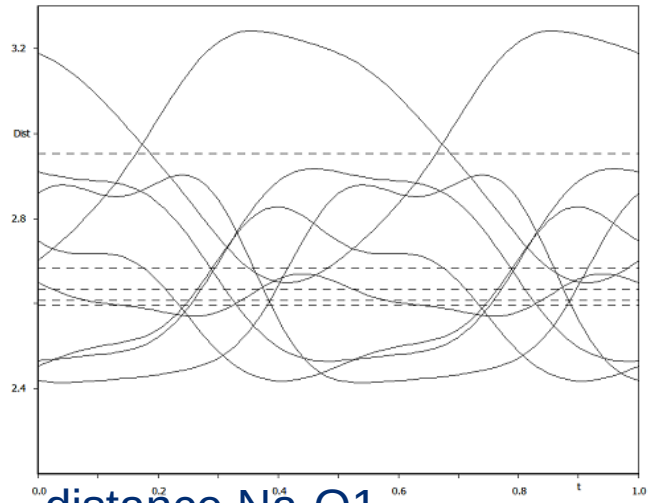
$$x_4 = t + \bar{\mathbf{r}} \cdot \mathbf{q}$$

The parameter t is a real number describing the initial phase of the wave. It plays a central role in the superspace analysis of aperiodic crystals

Reason for t coordinate: modulation displacement from the basic position is calculated in the real space, i.e. along a3, not A3.

Due to translation periodicity all possible modulation displacements occur between t=0 and 1.

Graph



distance Na-O1

Cookbook example 5.2

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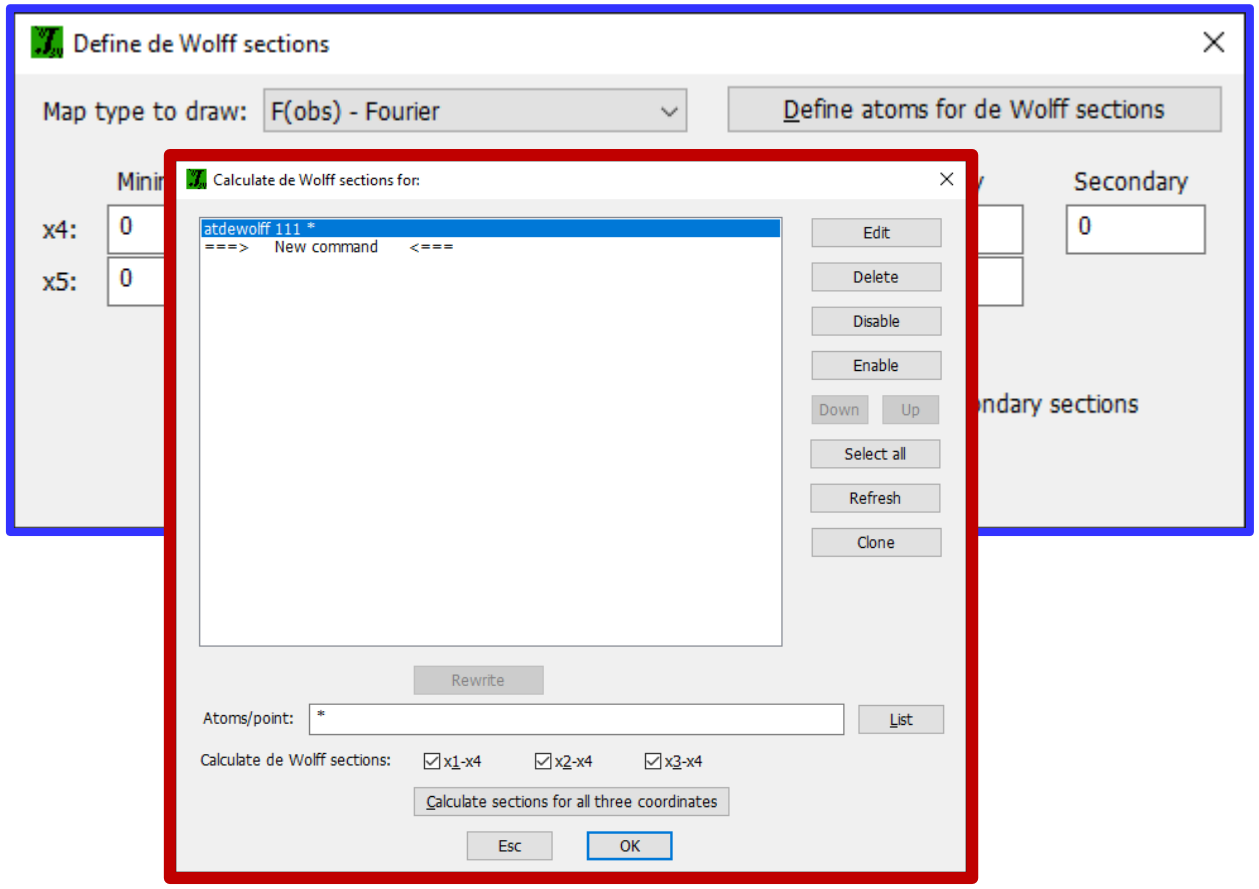
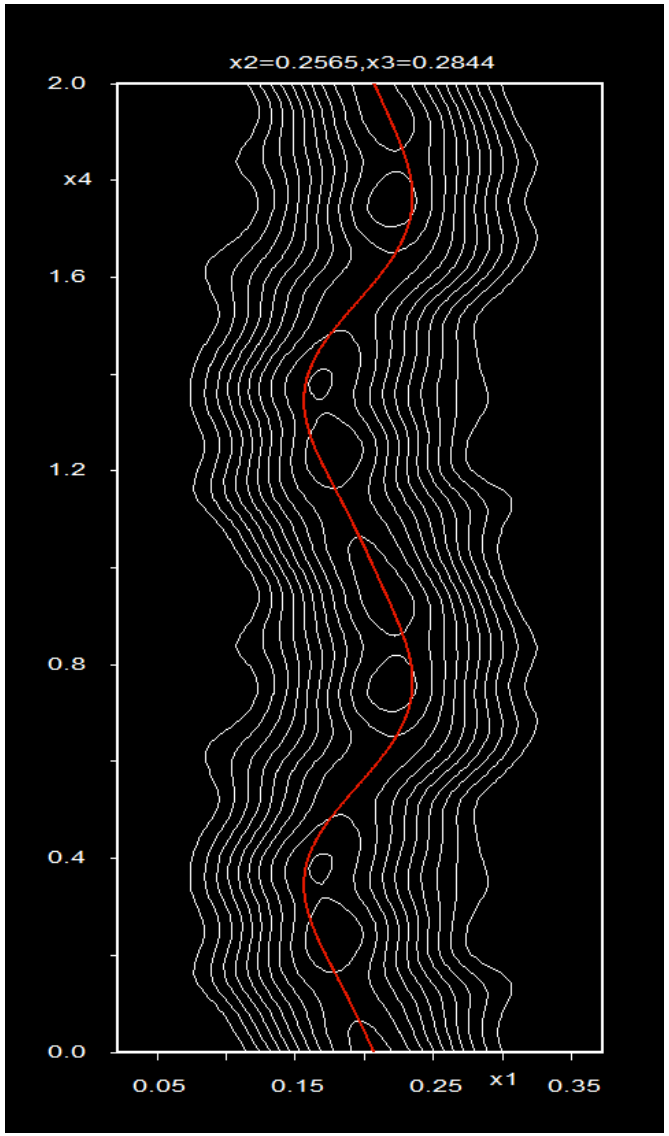
Advanced tools – Fourier sections





Checking results in Fourier:

A_i-A_4 Fourier sections

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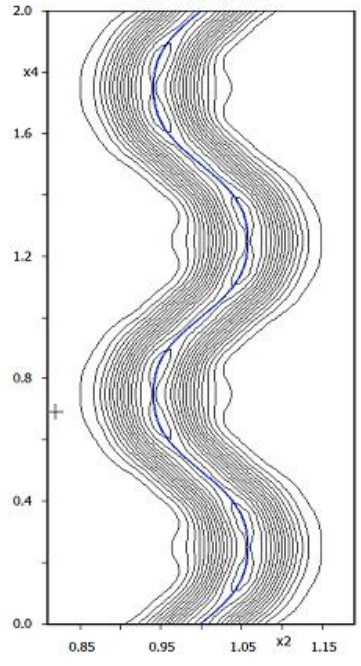
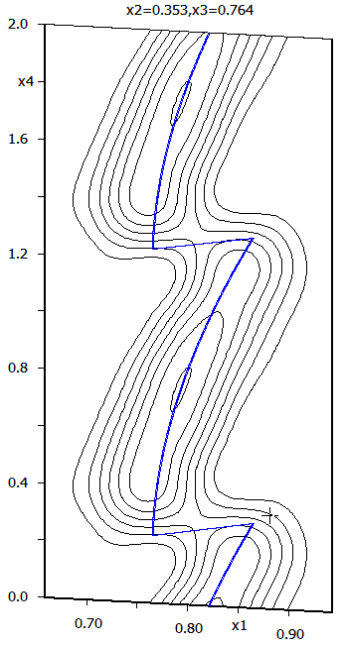
Modulated structures - Special modulation functions

Displacive modulation

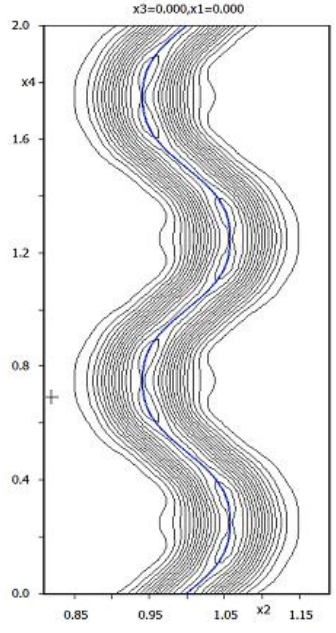


harmonic

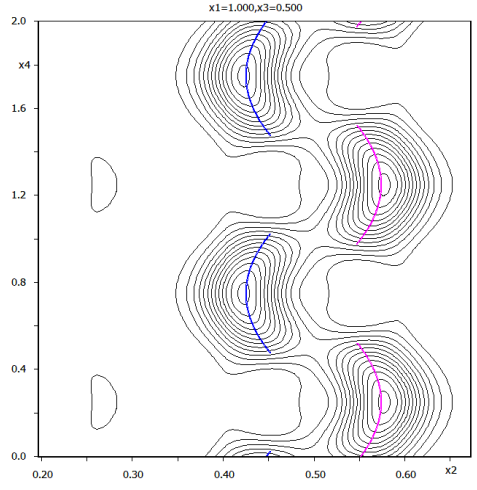


Saw-tooth

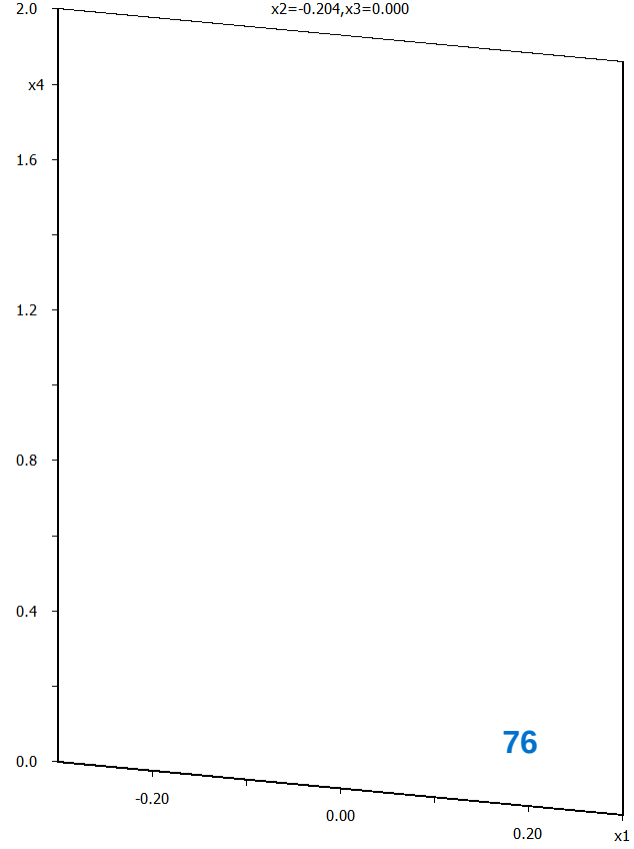
Occupational modulation

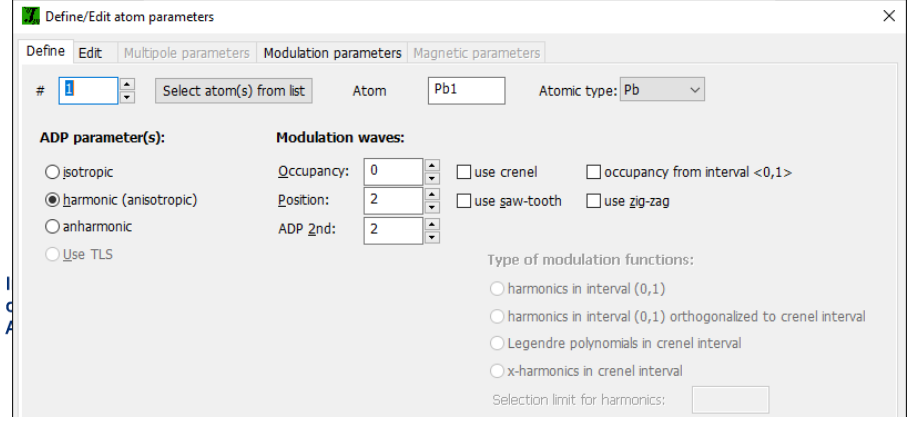


harmonic

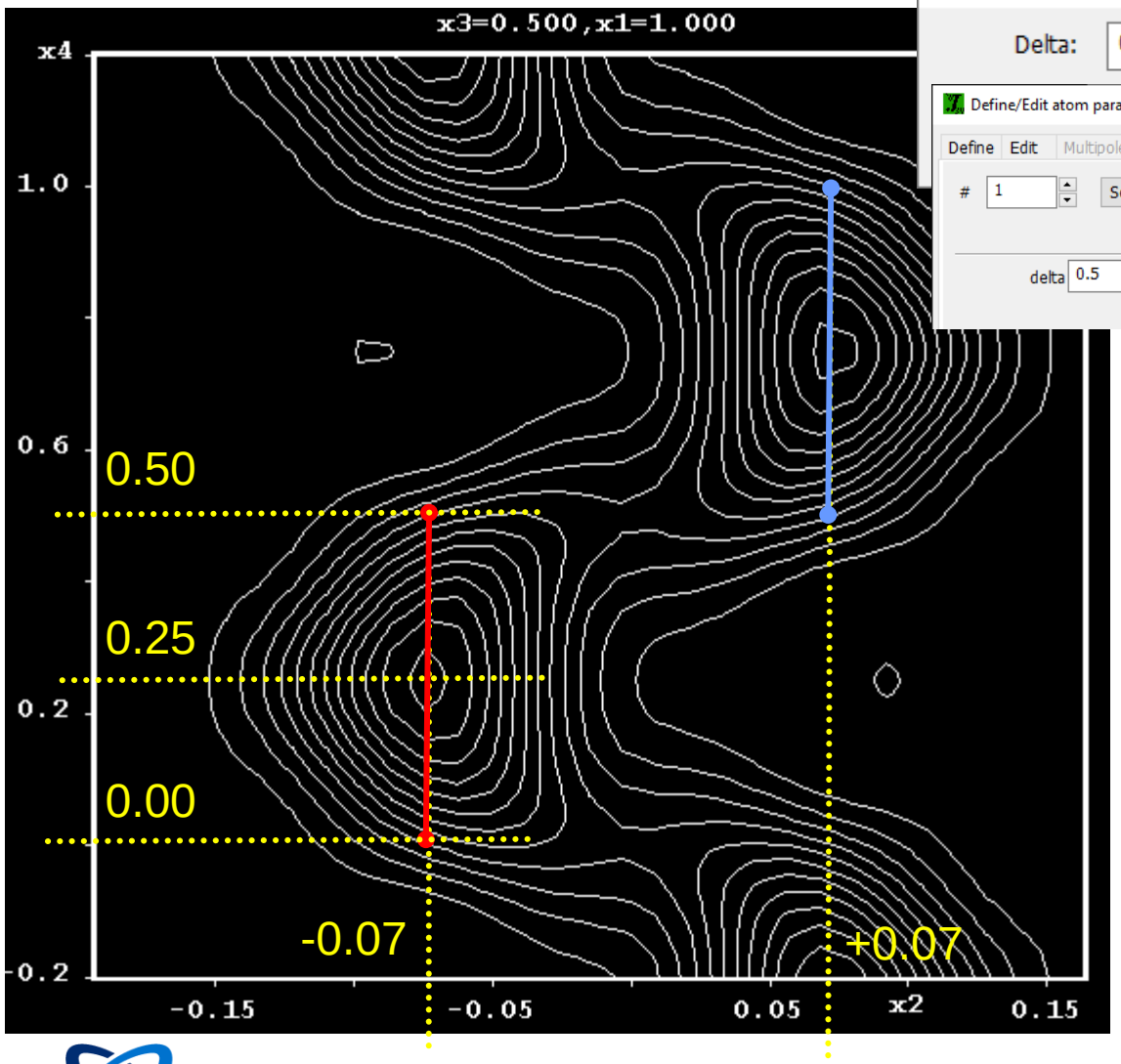


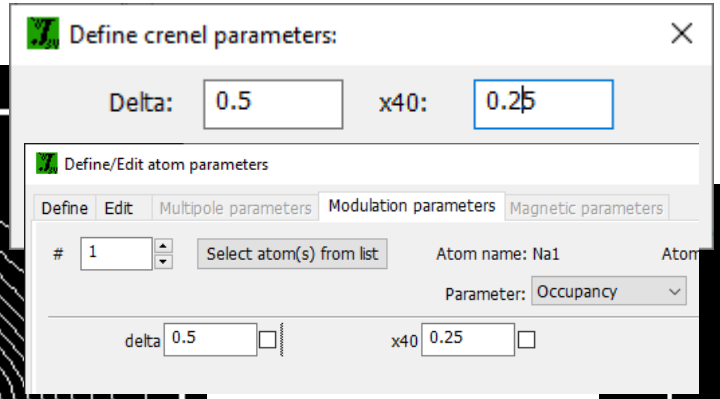
Crenel



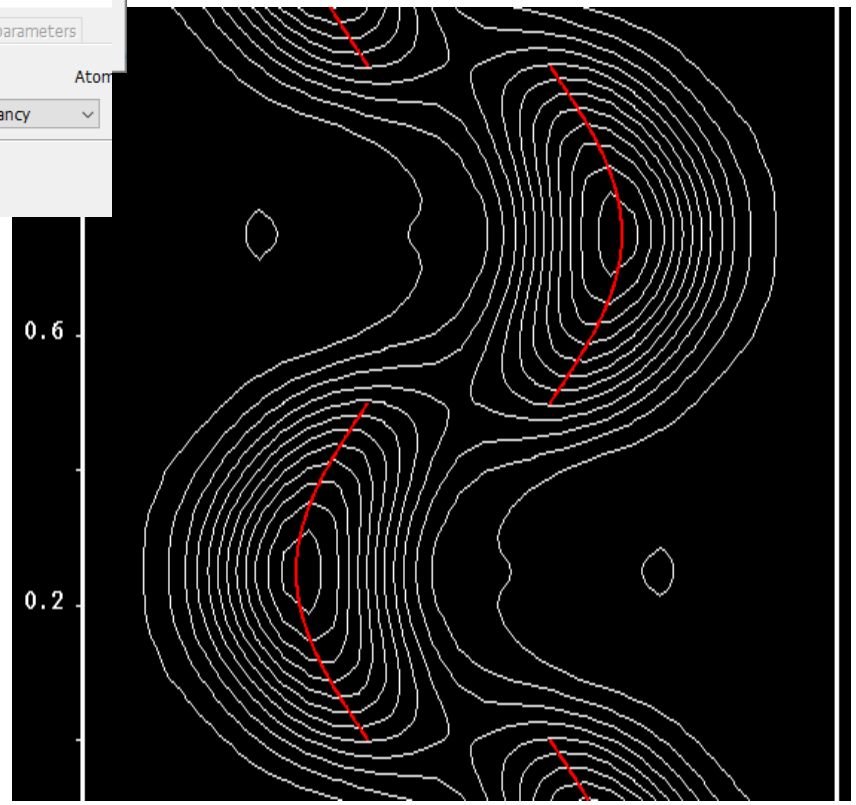


Modulated structures - Parameters of crenel function





width and center of the crenel function



Crenel function combined with modulation of position (Cookbook example 5.3.1)

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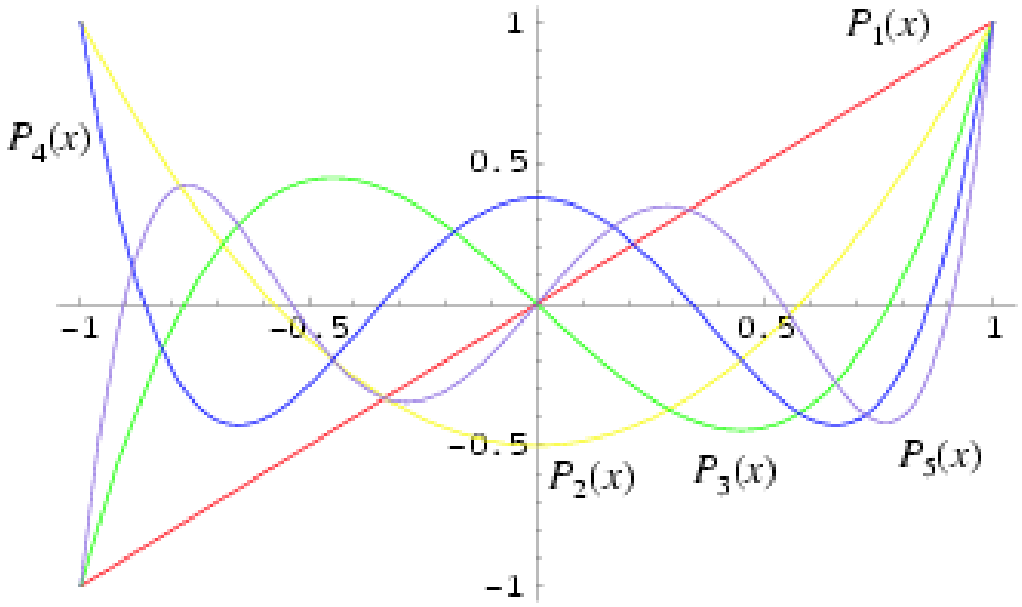
Modulated structures – Combination of functions



$$P_n(z) = \frac{1}{2\pi i}\oint \left(1 - 2tz + t^2\right)^{-1/2} t^{-n-1} dt$$

$$P_0(x) = 1$$
$$P_1(x) = x$$
$$P_2(x) = \tfrac{1}{2}\left(3x^2 - 1\right)$$
$$P_3(x) = \tfrac{1}{2}\left(5x^3 - 3x\right)$$
$$P_4(x) = \tfrac{1}{8}\left(35x^4 - 30x^2 + 3\right)$$
$$P_5(x) = \tfrac{1}{8}\left(63x^5 - 70x^3 + 15x\right)$$
$$P_6(x) = \tfrac{1}{16}\left(231x^6 - 315x^4 + 105x^2 - 5\right)$$

The additional modulation is expressed by Legendre polynomials

$$\mathbf{r}_\nu = \mathbf{r}_{\nu,0} + \sum_n \mathbf{U}^s_{\nu n} \sin\left(2\pi n x_4\right) + \mathbf{U}^c_{\nu n} \cos\left(2\pi n x_4\right)$$

with harmonic waves

$$\mathbf{r}_\nu = \mathbf{r}_{\nu,0} + \sum_n \mathbf{S}^o_{\nu n} P^o_n\left[2\left(x_4 - x_{40}\right)/\Delta\right] + \mathbf{S}^e_{\nu n} P^e_n\left[2\left(x_4 - x_{40}\right)/\Delta\right]$$

with Legendre polynomials

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"o" and "e" indicate odd and even member. The first polynom, i.e. $P_1{}^o$, defines a line. The three coefficients of $P_{1x}{}^o$, $P_{1y}{}^o$ and $P_{1z}{}^o$ are refined either to crenel or sawtooth shape.

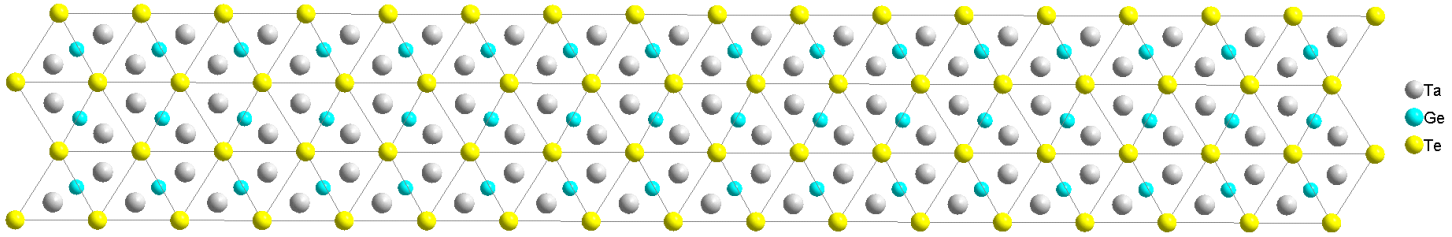
Results presentation

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:

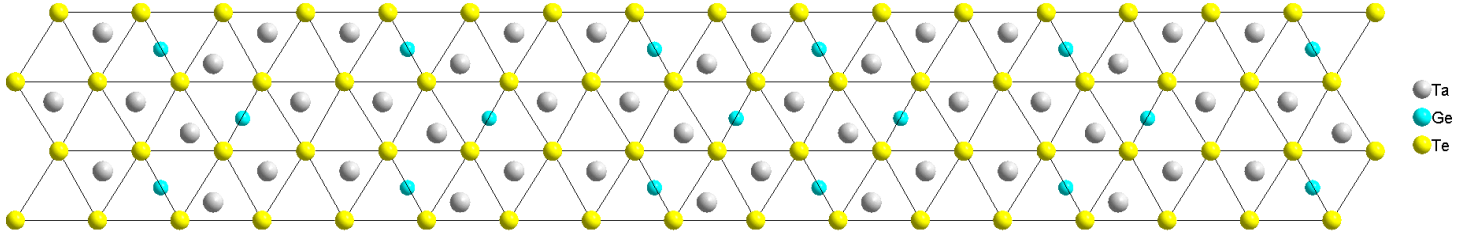
The same example as for the crenel function - $TaGe_{0.354}Te$

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

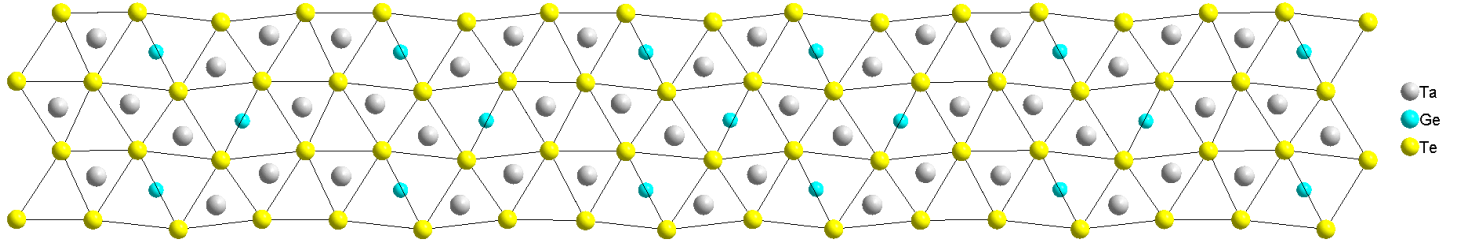
Average structure



Only occupational modulation



Final result



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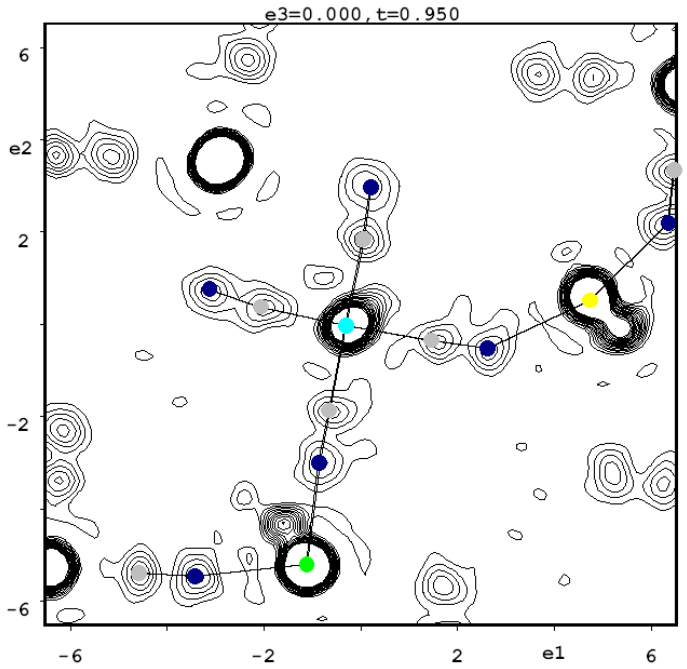
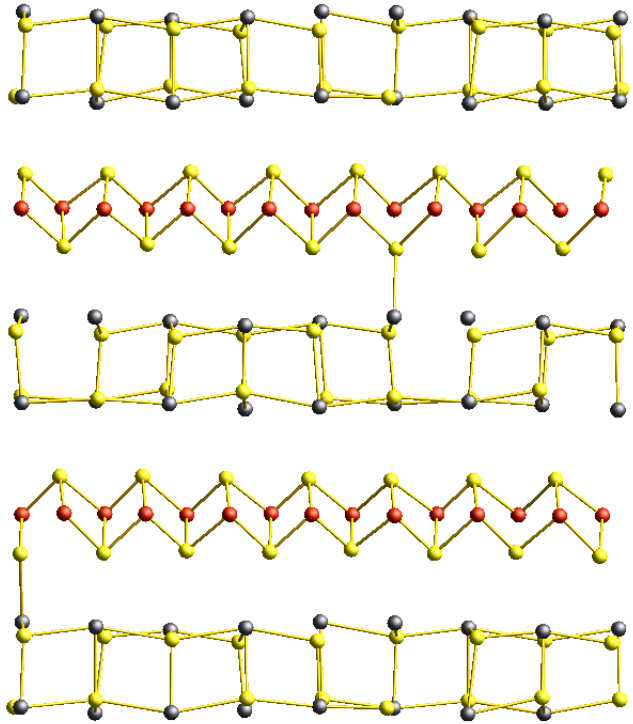
Results presentation

Fourier maps as a movie



JanaDraw movie



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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 6th 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 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!