

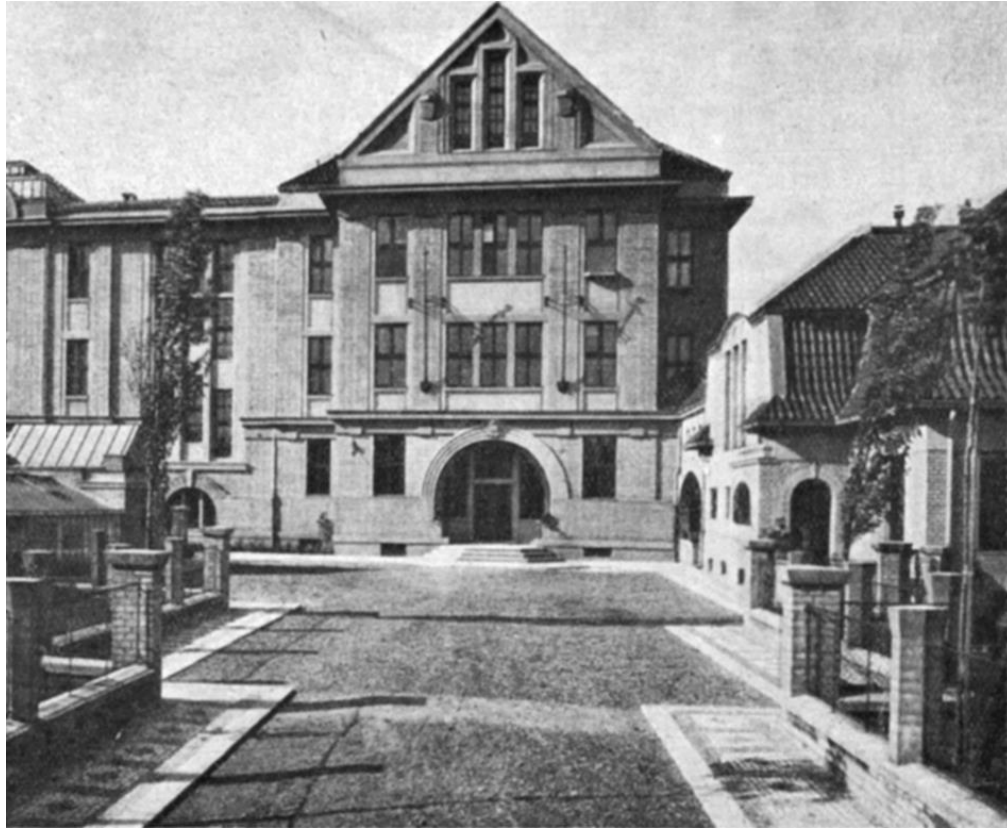
Jana2020

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

Václav Petříček, Michal Dušek, Lukáš Palatinus

Cinthia Antunes Corrêa

Institute of Physics, Prague 6, Cukrovarnická street



1923



2023

Since 1980...



History

1980 SDS

Program for solution and refinement of 3d structures

1984 Jana

Refinement program for modulated structures



Václav Petříček



Pierre Becker Philip Coppens

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

1998 Jana98

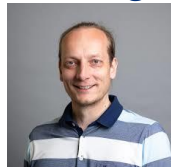
Improved Jana96. First widely used version. Graphical interface for DOS, DOS emulation and UNIX X11

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

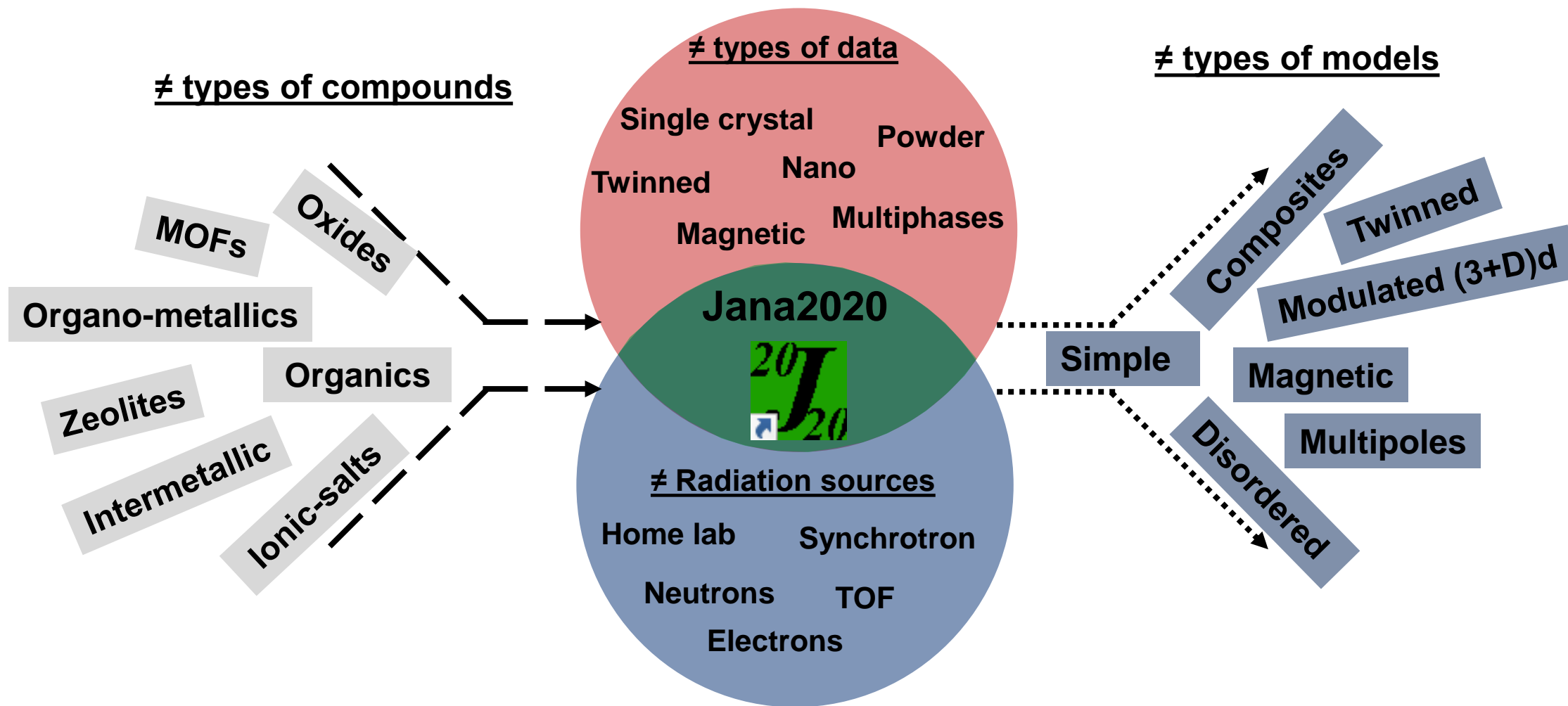
Michal Dušek



Lukáš Palatinus



What the program offers



Topics

Basic crystallography

Advanced tools

Commensurate structures

Incommensurate structures

Composite structures

Magnetic structures

Small organic and inorganic molecules

Complicated structures
Large, twinned, disordered, polytypic, ...

Minerals

Aperiodic structures

Magnetic structures

Micro and nano samples

Proteins

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

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 (<i>jana2000Pack.exe contains installation procedure</i>)	18/12/2007	jana2000Pack.exe.gz jana2000.tar.gz Debrogie'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 <i>Jana Cookbook cumulates examples from Jana workshops. The last version is always copied here together with input data. Raw data for electron diffraction examples are provided separately due to their size.</i>	----	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 Download Installation

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.

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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 (<i>jana2000Pack.exe contains installation procedure</i>)	18/12/2007	jana2000Pack.exe.gz jana2000.tar.gz Debrogie'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 <i>Jana Cookbook cumulates examples from Jana workshops. The last version is always copied here together with input data. Raw data for electron diffraction examples are provided separately due to their size.</i>	----	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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Download

Shortcuts: [Jana2006](#)
Jana2020: the latest version and Jana cookbook. Jana2006: development version. Jana2000: development version done automatically.

[Jana2020 for Windows](#)
[Jana2006 for Windows, STABLE](#)
[Jana2006 for Unix, STABLE](#)
[Jana2006 for Windows, LATEST](#)
[Jana2006 for Unix, LATEST](#)
[Jana2000 for Windows, FINAL](#)
[Jana2000 for Unix, FINAL](#)
(*jana2000Pack.exe contains installation procedure*)
[Manuals](#) (partially useful also for Jana2006)
[Cookbook](#)
Jana Cookbook cumulates examples from Jana workshops. The last version is always copied here together with input data. Raw data for electron diffraction examples are provided separately due to their size.

Registration

Jana2006 can be used free of charge but we are interested who is using it. Registered users are placed to our internal list and get e-mails about major updates.
Please note that registration for Jana2006 is not valid for Jana2020. Jana2020 has its own registration system available [here](#). Jana2020 is free only for academic users.

New registration: type your e-mail, choose a password and submit the registration.
Changes of existing registration: type your e-mail, password and submit. Forgotten password can be sent to your e-mail address.
Do not use precious passwords, this is not encrypted connection.

e-mail:
Password:

Jana2006 for Windows, 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 (<i>jana2000Pack.exe contains installation procedure</i>)	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 <i>Jana Cookbook cumulates examples from Jana workshops. The last version is always copied here together with input data. Raw data for electron diffraction examples are provided separately due to their size.</i>	----	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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[Create keyword](#) / [Index keywords](#)

Search in cookbook [Sort by revised](#) [Sort by example](#) [Sort by level](#)

Type a word(s) ...

Example 01.1: Zn Solution of a simple crystal structure from single crystal data Doc: Example 01.1 Zn.docx Pdf: Example 01.1 Zn.pdf Data: Data.zip Results: Results.zip	Show keywords ▾
Revised: Mar 20, 2024	
Example 02.1.1: PbSO4 Simple inorganic structure from powder Doc: Example 02.1.1_PbSO4.docx Pdf: Example 02.1.1_PbSO4.pdf Data: Data.zip Results: Results.zip	Show keywords ▾
Revised: Mar 20, 2024	
Example 02.2.2: LaPO4 Crystallite size by Fundamental approach Doc: Example_02.2.2_LaPO4.docx Pdf: Example_02.2.2_LaPO4.pdf Data: Data.zip Results: Results.zip	Show keywords ▾
Revised: Jan 1, 2022	
Example 03.1: AD3 Structure of a pseudo-merohedric twin Doc: Example 03.1 AD3.docx Pdf: Example 03.1 AD3.pdf Data: Data.zip Results: Results.zip	Show keywords ▾
Revised: Nov 21, 2023	
Example 03.2: PyNinit Twinned structure with partial overlaps of diffraction spots Doc: Example 03.2_PyNinit.docx Pdf: Example 03.2_PyNinit.pdf Data: Data.zip Results: Results.zip	Show keywords ▾
Revised: Nov 27, 2023	12

Where to get it

<http://jana.fzu.cz/>

Workshops



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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)

Institute of Physics
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16253 Praha 6
Czech Republic

Academy of Sciences | Institute of Physics
Dept of Structure Analysis | Laboratory of Crystallography
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CRYSTALLOGRAPHIC COMPUTING SYSTEM FOR STANDARD AND MODULATED STRUCTURES

Vaclav Petricek, Michal Dusek & Lukas Palatinus

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, Israel

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: satellite 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]

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

The screenshot displays the Jana2020 software interface. The central window, labeled "JanaDraw", shows a 3D ball-and-stick model of a crystal structure with yellow, red, and grey atoms. The left pane contains a "Refinement window" with a menu of options such as "Reflection file", "New Phases", "Edit structure parameters", "Structure solution", "Fourier synthesis", "Run Contour", "Import", "Refinement", "Distance calculation", "Draw structure", "CIF utilities", "Tools", "Edit file", "Files for MEM", "Export Structure to Recover files", "Matrix calculator", and "Run Jana2006". Below the menu are fields for "Active phase:" and "Data block:", and a "Delete rejected atoms" button. The right pane, labeled "Application controls", includes a "Rotate" section with radio buttons for "Picture axes", "Direct axes", and "Reciprocal axes", and sub-options for "Rotate in steps" and "Rotate continuously" with an "Angle step [deg]" field set to 5.000. Below this is a "View along" section with buttons for "a", "b", "c", "a*", "b*", and "c*", and a "Mode" dropdown set to "Basic" with a "Bond selection" checkbox. At the bottom, a "Lower toolbar" contains various icons for navigation and editing. The status bar at the very bottom shows: "Wizard OFF | Actual formula: C14 H13 N2 O6 Na S | 37 atoms in asymmetric unit | 548/0 atoms drawn/selected | 600/0 bonds drawn/selected |".

Refinement window

JanaDraw

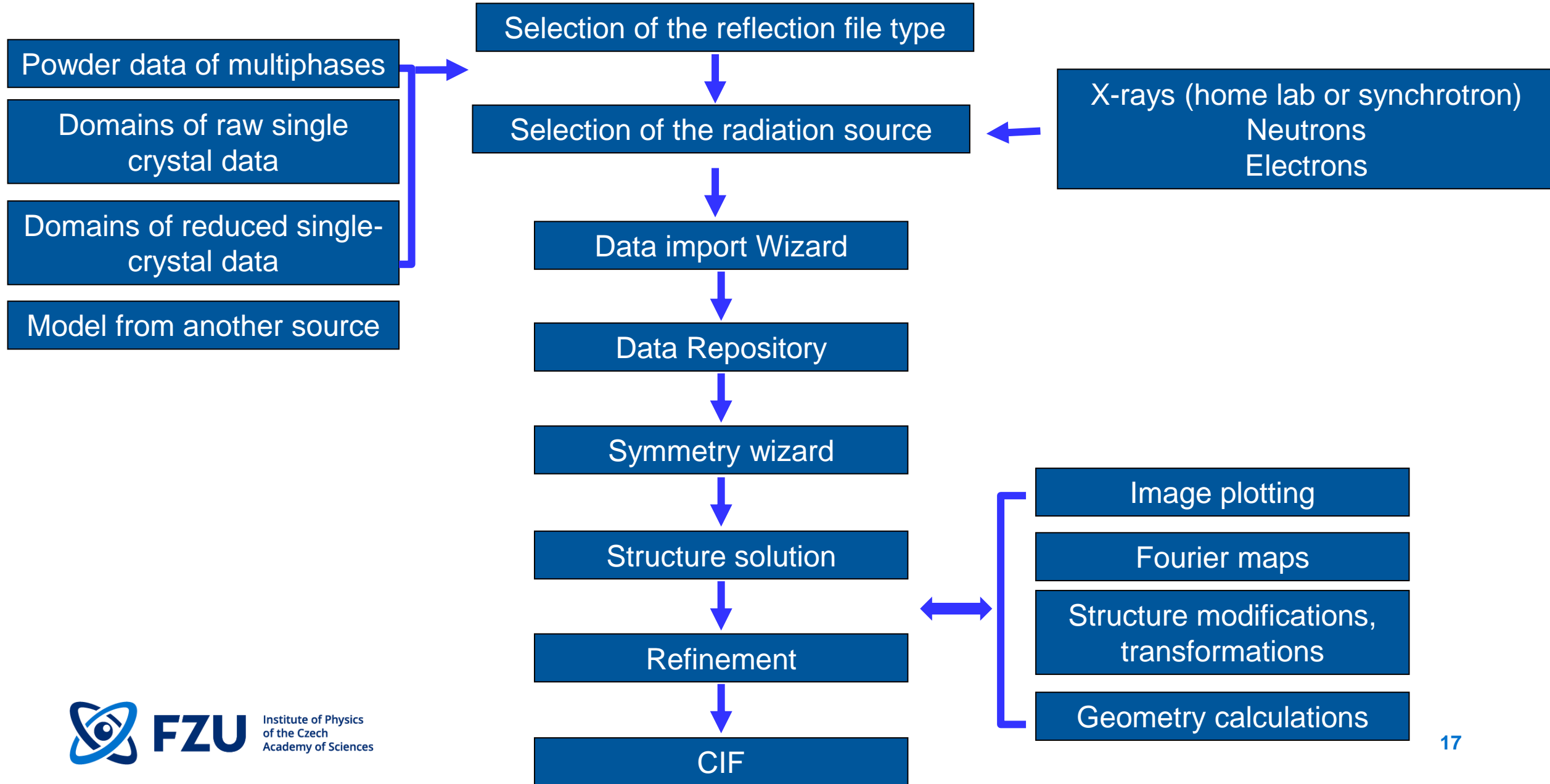
Application controls

Lower toolbar

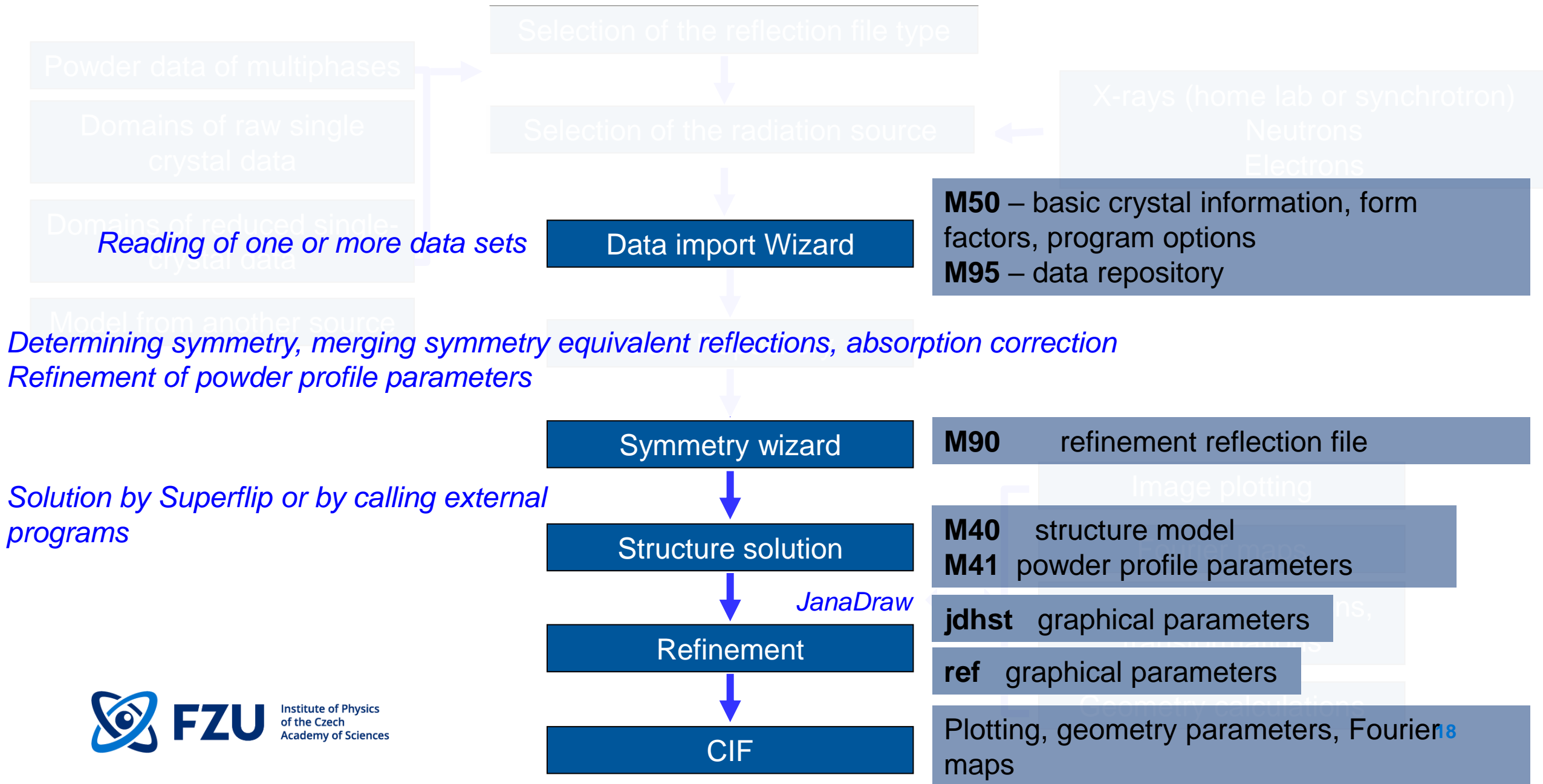
Jana2020 Interface

The screenshot shows the Jana2020 software interface. At the top, the title bar reads "Jana2020 - [D:\CookbookExamples\1.1_Zn\Data\Zn]". Below it is the "Main Menu bar" with options: Structure, Transformations, Settings, Tools, Help. The main window is titled "Main" and contains a toolbar with "Quick buttons" (a black square, a ring of atoms, a graph) and "Focus buttons" (a magnifying glass, a cube, a sphere, a double-headed arrow). On the left is the "Command tree" with a vertical list of icons and a corresponding list of commands: Reflection file, New Phases, Edit structure parameters, Structure solution, Fourier synthesis, Run Contour, Import, Refinement, Distance calculation, Draw structure, CIF utilities, Tools, Edit file, Files for MEM, Export structure to Recover files, Matrix calculator, Run Jana2006. On the right is the "Expanded Command tree" showing a detailed list of actions under "Reflection file": Import/modify reflection file, Run reimport in the silent mode, Make space group test, Create refinement reflection file, View listing from the merging process, Manual culling, Run statistic test - Wilson plot, List of observed vs. calculated intensities, and "New Phases". At the bottom right, there is a "Rotate" control panel with axes (x, y, z) and a "w along" slider. The bottom status bar displays: "Wizard OFF | Actual formula: C14 H13 N2 O6 Na 5 | 37 atoms in asymmetric unit | 548/0 atoms drawn/selected | 600/0 bonds drawn/selected |".

Software flow scheme



Software flow scheme and files created



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

Data import wizard

Specify type of the file to be imported

Single crystal:

- known diffractometer formats
- reflection file corrected for LP and absorption
- start with indexing procedure

Powder data:

- various CW formats
- various TOF/ED formats

Structure:

- from SHELX
- from CIF
- from SHELX embedded in CIF
- from Jana2020 embedded in CIF
- from XD
- from Jana2000

Magnetic parent structure:

- nuclear model interactively
- nuclear model from SHELX
- nuclear model from CIF
- nuclear model from Jana2006/Jana2020

Back Next Cancel

Data import wizard

Input data: single crystal, powder, TOF

Data import wizard

Data reduction file from:

Input file name: CsLiSO4.hkl Browse

Nonius-CCD

Bruker-CCD

Bruker-CCD (raw)

Oxford Diffraction-CCD

Rigaku-CCD

IPDS Stoe

D9-ILL, D23 or Trics-Zebra

HeDi

ILL-Vivaldi

ISIS SXD

TOPAZ, Corelli

Koala at ANSTO

SCD-LANL

Hasylab F1

Hasylab HUBER

Hasylab XDS

6T2 LBB

Pets electron diffractometer

SENJU TOF

Polarized neutrons

SHELX on I - abs.correction needed

Back Next Cancel

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

Data from different sources can be combined during refinements.

Define basic KUMA (OD, Rigaku) data file:

input from "cif_od" file

input from "sum" file

File name: CsLiSO4_red.sum Browse

Esc Ok

Data import wizard

Data import wizard [Close]

Complete/correct experimental parameters

Cell parameters:

Number of input indices:

Radiation:

X-rays

Neutrons

Electrons

Kalpha1/Kalpha2 doublet

Wavelength #1:

Wavelength #2:

I(#2)/I(#1):

Data collection details:

Temperature:

Polarization correction:

Circular polarization

Perpendicular setting

Parallel setting

Linearly polarized beam

Guinier camera

Monochromator parameters:

Perfectness:

Glancing angle:

Data import wizard

Data import wizard [Close]

Define the reference cell

Actual cell parameters of data block: 10.8945 10.8894 8.8048 90.001 90.024 119.946
Reference cell parameters derived from actual: 10.8945 10.8894 8.8048 90.001 90.024 119.946

Matrix calculator **Apply the transformation**

H= * h+ * k+ * l
K= * h+ * k+ * l
L= * h+ * k+ * l


Target dimension:

Twinning **Twinning matrices**

Number of domains:
Data related to domain#:
Multiply input F(hkl)/I(hkl) by
 Analyze overlaps by Jana tools instead of HKLF5

INFORMATION
All 11132 input reflections were properly handled
OK

Back **Next** **Cancel**



Name	Ext	Size
DIR		DIR
CsLiSO4.hkl		378 488
CsLiSO4_red.sum		78 864

Name	Ext	Size
DIR		DIR
CsLiSO4.hkl		378 488
CsLiSO4.i01		2 515 832
CsLiSO4.i51		161
CsLiSO4.m50		450
CsLiSO4_red.sum		78 864

Data import wizard

M50 – basic crystal information, form factors, program options

Name	Ext	Size
...		DIR
CsLiSO4.hkl		378 488
CsLiSO4.I01		2 515 832
CsLiSO4.I51		161
CsLiSO4.m50		430
CsLiSO4_red.sum		78 864

```
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 [X]

Define parameters for absorption and scaling procedure

None or done before importing

Correction for spherical sample Radius of the sphere:

Gaussian integration method Integration grid:

Empirical correction and/or frame scaling

Define absorption coefficient =>

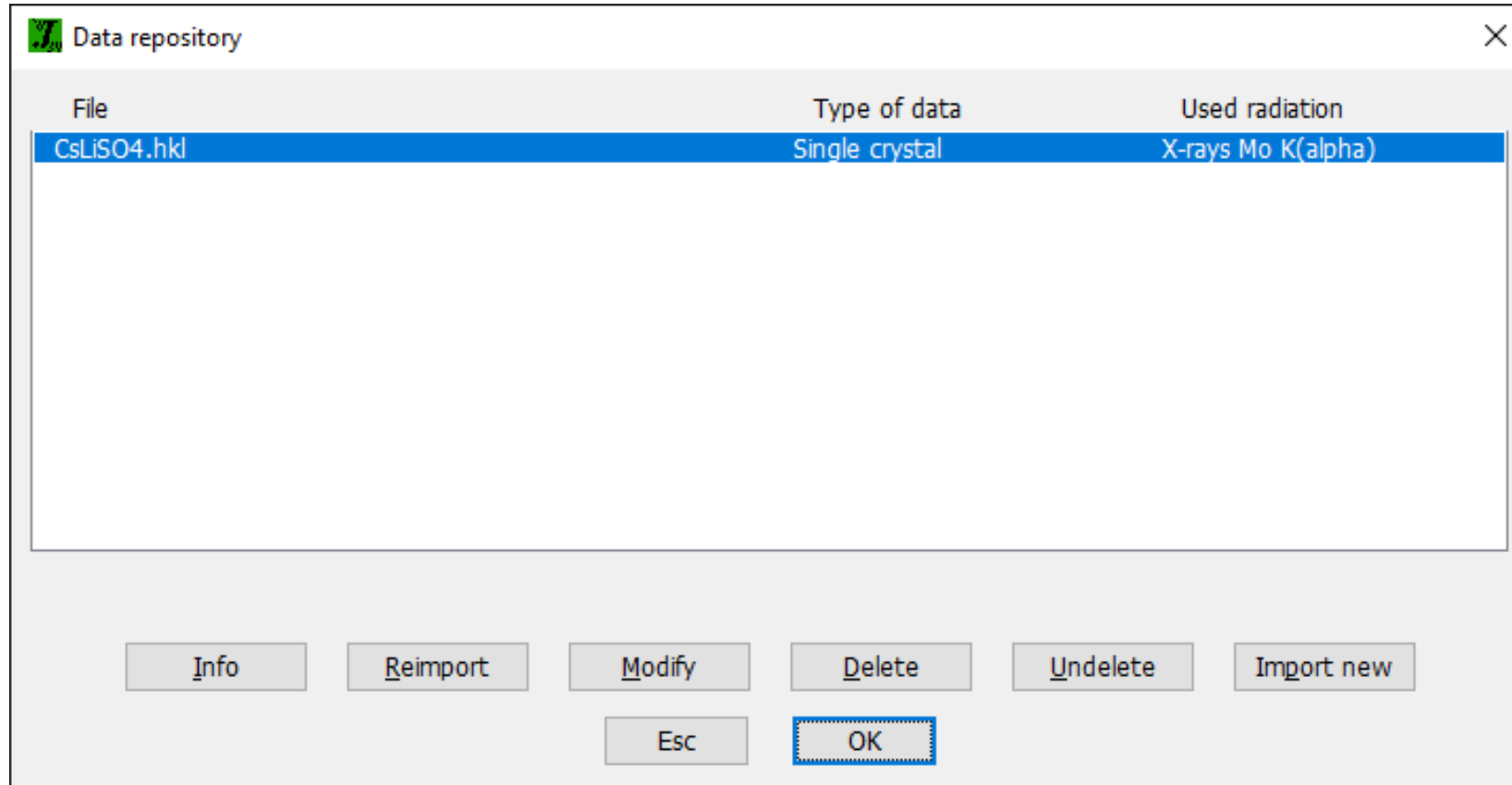
Define formula => Calculate absorption coefficient:

Number of formula units =>

INFORMATION

The data import wizard is complete. As a next step you can import another or modify the previously imported ones.

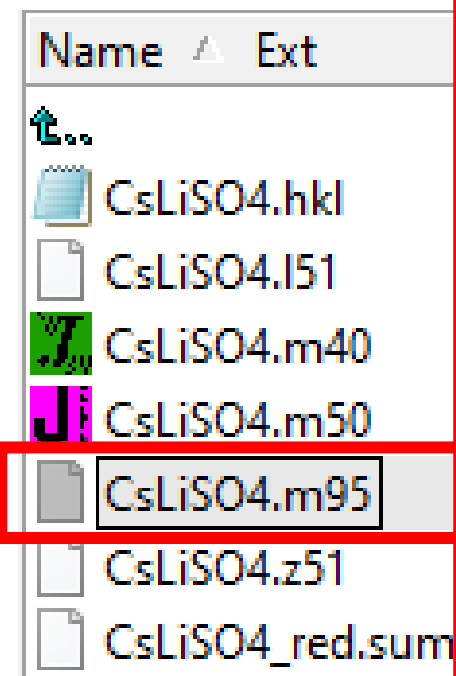
Data import wizard



Name	Ext	Size
↑..		DIR
CsLiSO4.hkl		378 488
CsLiSO4.I51		161
CsLiSO4.m40		657
CsLiSO4.m50		385
CsLiSO4.m95		2 516 633
CsLiSO4.z51		161
CsLiSO4_red.sum		78 864

Data import wizard

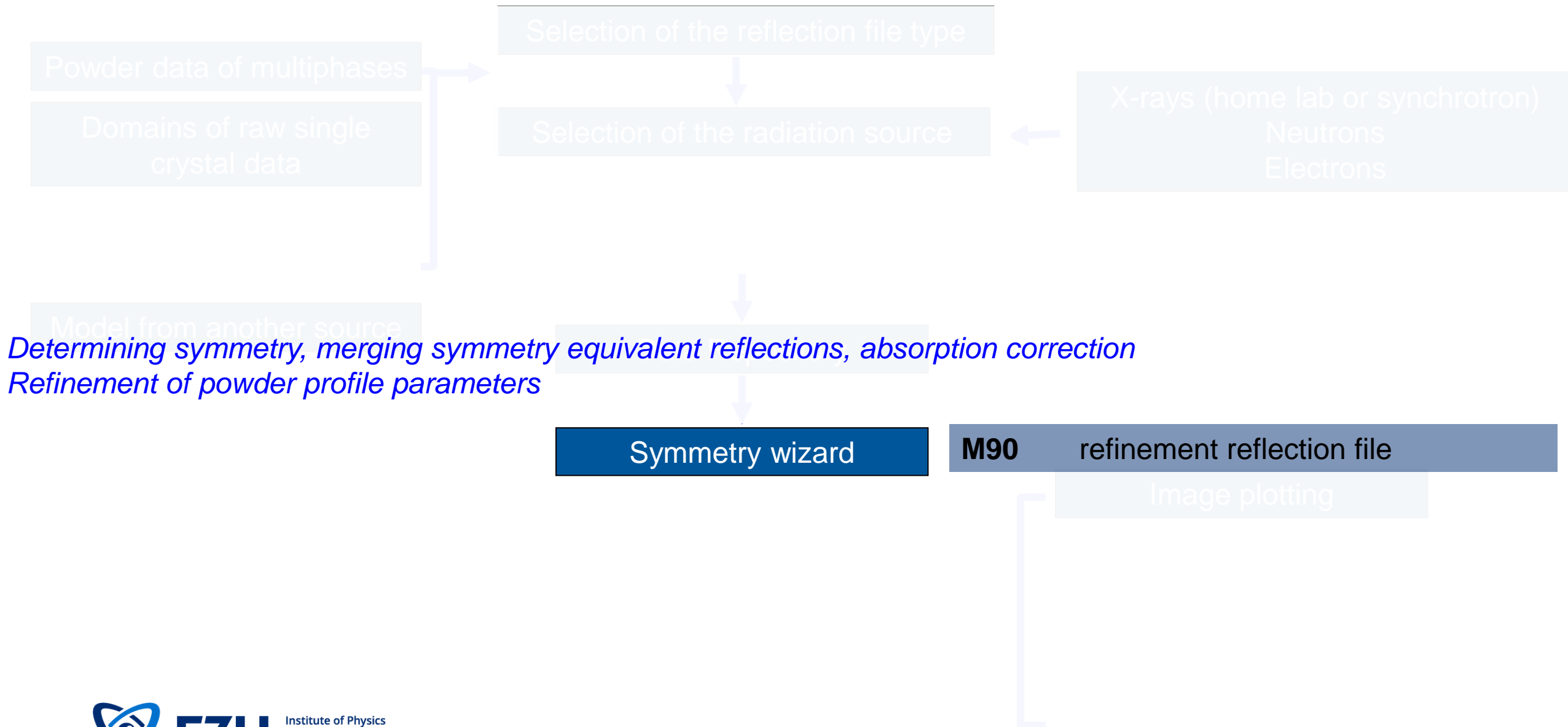
M95 – data repository



```
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
commcelled 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 corrrabs 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
celled 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
```



Software flow scheme and files created

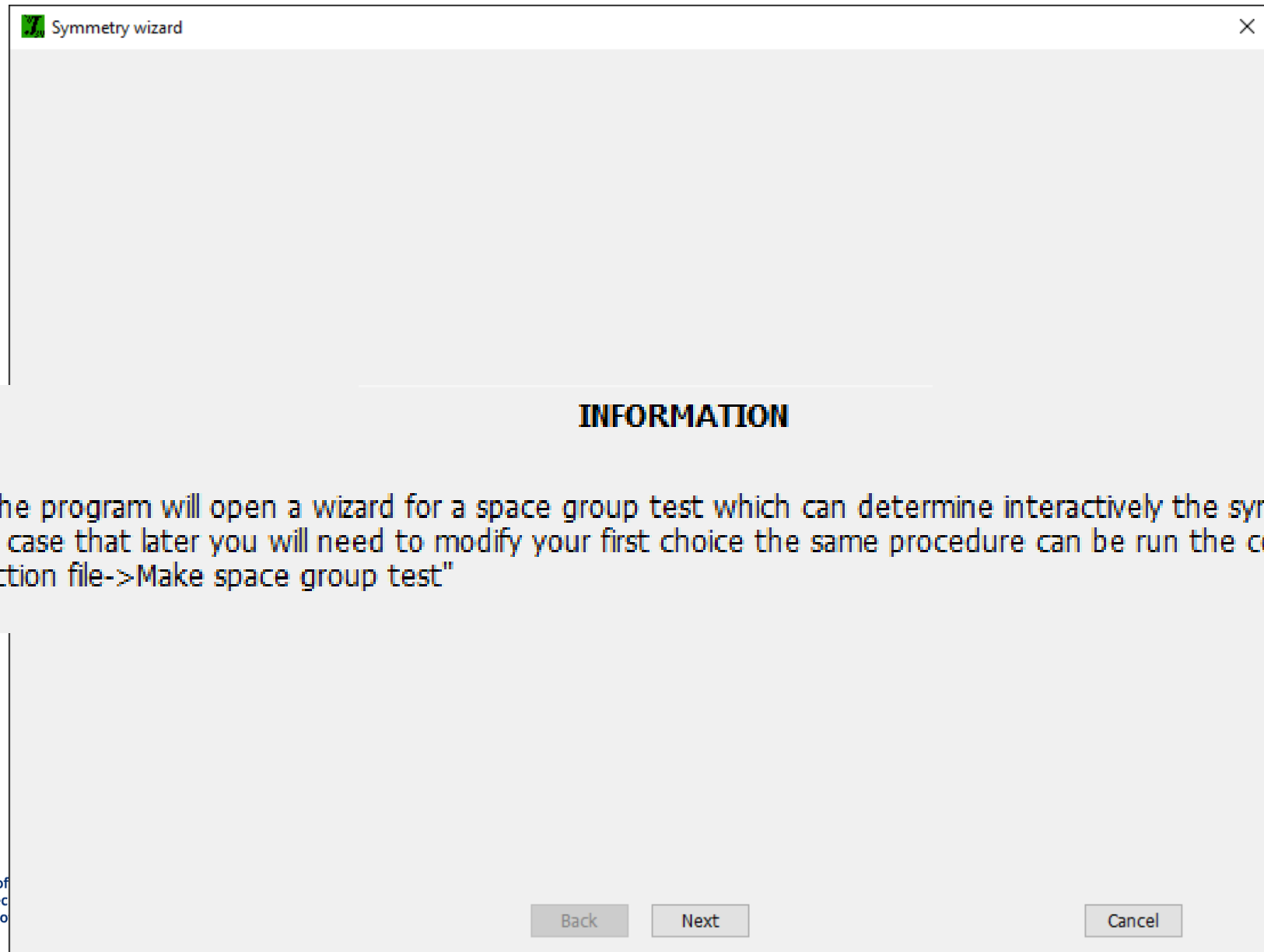


Symmetry wizard

*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

Symmetry wizard [X]

Start with data collection cell: 10.895 10.889 8.805 90.00 90.02 119.95

Search for higher symmetrical supercell (recommended)

Start with actual cell: 10.895 10.889 8.805 90.00 90.02 119.95

Keep old twin matrices

Tolerances for crystal system recognition:

Maximal deviation for cell lengths in Ang:

Maximal deviation for cell angles in degs:

Maximal deviation for modulation vector:

Tolerances for space group recognition:

Maximal ave(I/sig(I)) for systematic extinctions induced by cell centering:

Maximal ave(I/sig(I)) for systematic extinctions induced by other symmetry:

Symmetry wizard

Symmetry wizard

Select Laue point group

PointGroup	Axes	Rint(obs/all)	#averaged(obs/all)	Redundancy
-1	(-c,a+b,a)	5.68/5.74	2752/3790	2.937
2/m	(b,c,a)	6.31/6.37	1493/2026	5.495
2/m	(a+2b,-a,c)	5.68/5.74	2752/3790	2.937
2/m	(-a+b,a+b,-c)	5.68/5.74	2752/3790	2.937
2/m	(-2a-b,b,-c)	5.68/5.74	2752/3790	2.937
2/m	(a+b,-a+b,c)	5.68/5.74	2752/3790	2.937
2/m	(b,-2a-b,c)	5.68/5.74	2752/3790	2.937
2/m	(-a,a+2b,-c)	5.68/5.74	2752/3790	2.937
mmm	(2a+b,b,c)	6.31/6.37	1493/2026	5.495
mmm	(a-b,a+b,c)	6.31/6.37	1493/2026	5.495
mmm	(-a-2b,-a,-c)	6.31/6.37	1493/2026	5.495
-3	(a,b,c)	14.35/14.40	1012/1270	8.765
-31m	(a,b,c)	14.46/14.50	559/698	15.948
-3m1	(a,b,c)	14.46/14.51	618/740	15.043
6/m	(a,b,c)	14.46/14.51	543/682	16.323
6/mmm	(a,b,c)	14.51/14.56	344/425	26.193

Averages made from 7493/11132 reflections

Details

Introduce twin law for subgroups

Back Next Cancel

Symmetry wizard

Symmetry wizard ✕

Select cell centering

	Centering	#obs/#all	ave(I/sig(I))	
<input type="radio"/>	P	0/0	0.000/0.000	Details
<input type="radio"/>	A	823/1405	26.669/16.090	Details
<input type="radio"/>	B	823/1405	26.669/16.090	Details
<input checked="" type="radio"/>	C	0/0	0.000/0.000	Details
<input type="radio"/>	I	4521/5580	51.128/41.615	Details
<input type="radio"/>	R-obverse	n.a.	n.a.	Details
<input type="radio"/>	R-reverse	n.a.	n.a.	Details
<input type="radio"/>	F	823/1405	26.669/16.090	Details
<input type="radio"/>	X (1/2,0,0), ...	0/0	0.000/0.000	Details
<input type="radio"/>	X (1/3,0,0), ...	-----/-----	-----/-----	Details

Show/modify X centering

Warning: The cell centring need not be what you expect from the data collection as the program first transforms the cell to the reduced form.

Moreover, after your selection, the program makes another transformation whenever the centring is not the standard one.

Back Next Cancel

Symmetry wizard

Symmetry wizard

Select space group

Characteristics for systematically absent reflections

Space group	#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

Symmetry wizard ✕

Final step of the space group test

accept the space group in the standard setting:

Space group: Ccce
Cell parameters: 18.8654 10.8919 8.8048 90 90 90

Transformation matrix:

$$\begin{vmatrix} a' \\ b' \\ c' \end{vmatrix} = \begin{vmatrix} 1 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix} * \begin{vmatrix} a \\ b \\ c \end{vmatrix}$$

accept the space group transformed into the original cell:

Space group: ???
Cell parameters: 10.8945 10.8894 8.8048 90.001 90.024

discard the changes

Accept twinning matrices induced by the space group test

Symmetry wizard

Symmetry wizard

Final step of the space group test

accept the space group in the standard setting:

Space group: Ccce
Cell parameters: 18.8654 10.8919 8.8048 90 90 90

Transformation matrix:

$$\begin{pmatrix} a' \\ b' \\ c' \end{pmatrix} = \begin{pmatrix} 1 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix}$$

accept the space group transformed into the original cell:

Space group: ???
Cell parameters: 10.8945 10.8894 8.8048 90.001 90.024

discard the changes

Accept twinning matrices induced by the space group test

Back Finish Cancel

Name	Ext	Size
↑...		DIR
	CsLiSO4.hkl	378 488
	CsLiSO4.m40	835
	CsLiSO4.m50	733
	CsLiSO4.m95	2 516 642
	CsLiSO4.usd	17
	CsLiSO4_red.sum	78 864

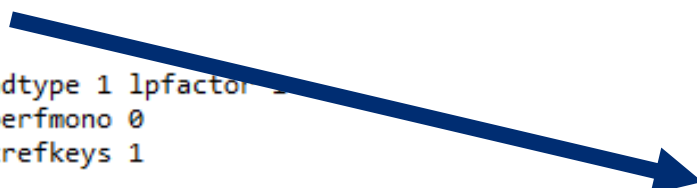
Symmetry wizard

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 1
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
```

Reflection file wizard

Reflection file wizard

Processing refinement reflection file for : Block1->Single crystal/X-rays/Mo K(alpha)

Reflections I < *sig(I) will be sorted as unobserved

Note: this limit is not used automatically by REFIN program Run in silent mode

use in output file E-format (recommended for data with large dynamical range)

Import statistics - obs/all

7493/11132 reflections read from input file
7492/11119 reflections written to output file
1/13 reflections rejected as systematically extinct.

OK

Summary of systematic absences

n(all) : 13, n(obs) : 1
Average(I/Sig(I)) : 0.98
List of the strongest reflections violating systematic absences:

h	k	l	I	sig(I)	I/sig(I)
0	0	-3	39.8	9.2	4.3

OK

Back Next Cancel

Reflection file wizard

Reflection file wizard

Processing refinement reflection file for : Block1->Single crystal/X-rays/Mo K(alpha)

Perform averaging
 Only sort and apply culling if activated
 Use non-averaged data

	h	k	l
The slowest varying index	<input type="radio"/>	<input type="radio"/>	<input checked="" type="radio"/>
The fastest varying index	<input checked="" type="radio"/>	<input type="radio"/>	

Full print Reflections $|I-I(\text{ave})| >$ *sig(I(ave)) will be printed
 Apply culling Reflections $|I-I(\text{ave})| >$ *sig(I(ave)) will be culled
 Apply $1/\text{sig}(I)^2$ weights in averaging
 Add center of symmetry in the averaging process
 Display graph sig(Icount)/sig(Istat)

Sigma(I(ave)) from:

Poisson
 Equivalentents
 Maximum from Poisson and equivalentents

Summary after averaging

Rint(obs/all) = 6.31/6.37 for 1492/2021 reflections
 averaged from 7492/11119 reflections

Redundancy = 5.502

h(min) = -23, h(max) = 23
 k(min) = 0, k(max) = 13
 l(min) = 0, l(max) = 11

R(obs/all) from e.s.d. of I : 0.67/ 0.89
 Information from culling : no reflection was culled
 Culled(fit)/Culled(man)/Culled(auto) : 0/0/0

OK

Reflection file wizard

Reflection file wizard

Processing refinement reflection file for : Block1->Single crystal/X-rays/Mo K(alpha)

Accept the new DatBlock and calculate coverage
 Accept the new DatBlock
 Discard the new DatBlock

Name	Ext	Size
↑..		DIR
CsLiSO4.hkl		378 488
CsLiSO4.i51		161
CsLiSO4.m40		835
CsLiSO4.m50		733
CsLiSO4.m89		92 920
CsLiSO4.m90		105 467
CsLiSO4.m95		2 516 642
CsLiSO4.rre		160 856
CsLiSO4.usd		17
CsLiSO4_MakeRefFile.i70		892
CsLiSO4_red.sum		78 864

Back Finish Cancel

Reflection file wizard

M90

refinement reflection file

Name	Ext	Size
..		DIR
CsLiSO4.hkl		378 488
CsLiSO4.I51		161
CsLiSO4.m40		835
CsLiSO4.m50		733
CsLiSO4.m89		92 920
CsLiSO4.m90		105 467
CsLiSO4.m95		2 516 642
CsLiSO4.rre		160 856
CsLiSO4.usd		17
CsLiSO4_MakeRefFile.I70		892
CsLiSO4_red.sum		78 864

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 diff scales 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

Structure solution

Solution by Superflip or by calling external programs


Structure solution

M40 structure model

M41 powder profile parameters

Structure solution

Main



- > Reflection file
- Phases
- > Edit structure parameters
- ▼ Structure solution
 - Run Superflip
 - Run Shelxt
- > Import
- > Refinement
- > CIF utilities
- > Tools
- > Edit file
- > Export structure to
 - Matrix calculator
 - Run Jana2006

Run Superflip

Basic commands | Advanced commands

Formula: Cs Li S O Phase: ▼

Formula units: 16 ▲ ▼ Calculate density Sum formula from structure model Show Periodic Table

Actual space group: Ccce Change the space group

use in le Bail decomposition structure information for already identified phases

allow manual editing of the command file before start

use previously prepared input file for Superflip

use old solution and reinterpret it

Repeat Superflip: Until the convergence detected Biso: 0

Repeat Superflip: Number of runs => 10 Maxcycles: 300000

Use local normalization

Use a specific random seed => 111

Define explicitly delta value => 0.9

Iteration scheme: CF For peak search use: EDMA - fixed composition

LDE EDMA - fixed number of atoms => 1

AAR EDMA - peak interpretation by Jana2020

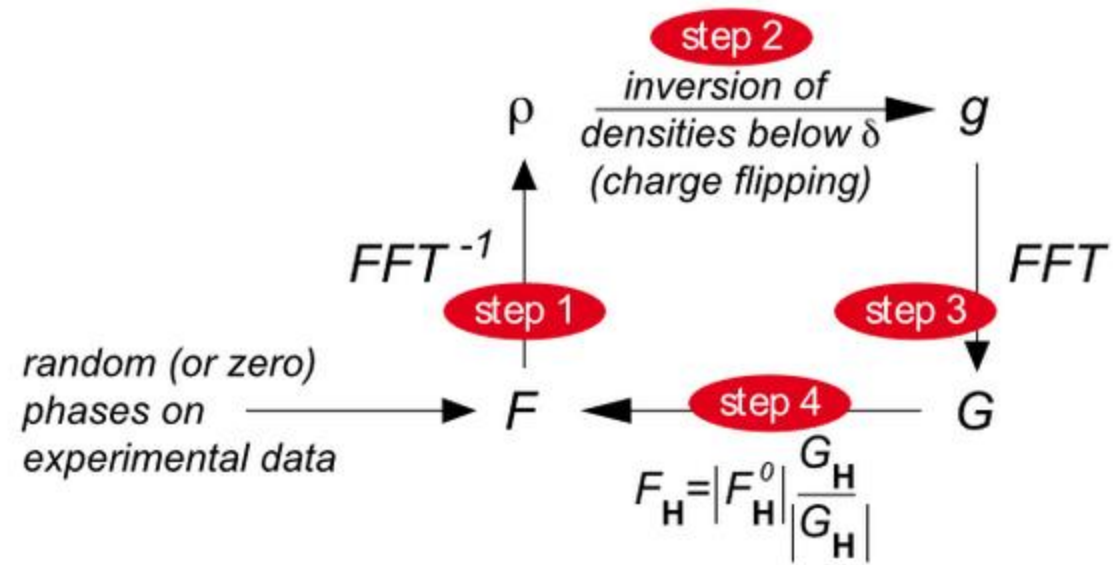
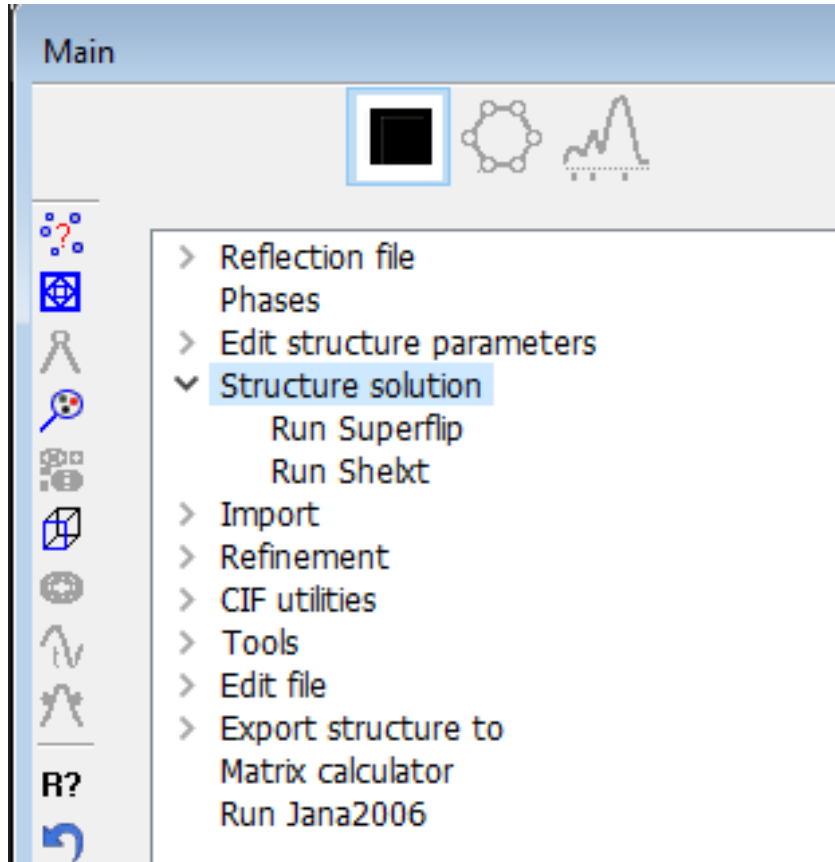
Starting model: Random phases Peaks from Jana2020

Patterson superposition map Peaks from Jana2020 but first run Fourier

Run Superflip Open the listing Draw structure Draw 3d map Draw deWolff maps


Accept last solution Quit

Structure solution



Structure solution

Main



- > Reflection file
- Phases
- > Edit structure parameters
- ▼ Structure solution
 - Run Superflip
 - Run Shelxt
- > Import
- > Refinement
- > CIF utilities
- > Tools
- > Edit file
- > Export structure to
 - Matrix calculator
 - Run Jana2006

Run Shelxt:

Formula: Cs Li S O Phase: ▼

Formula units: 16 ▲▼ Calculate density Show Periodic Table

Actual space group : Ccce Change the space group

use in le Bail decomposition structure information for already identified phases

Shelxt commands:

Space group	Orientation	R1	Rweak	Alpha	Formula
-------------	-------------	----	-------	-------	---------

Run SHELXT Open the listing Draw structure

Accept last solution Quit

Structure solution

M50 – basic crystal information, form factors, program options

Name Ext

- ..
- CsLiSO4.hkl
- CsLiSO4.inflip
- CsLiSO4.I51
- CsLiSO4.m40
- CsLiSO4.m50**
- CsLiSO4.m70
- CsLiSO4.m80
- CsLiSO4.m81
- CsLiSO4.m89
- CsLiSO4.m90
- CsLiSO4.m95
- CsLiSO4.rre
- CsLiSO4.sflog
- CsLiSO4.usd
- CsLiSO4_red.sum

```
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 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
```

Structure so

Number of atoms and molecules in the 1st composite part

Number of atoms and molecules in the 2nd composite part

M40 structure model

Name	Ext	Size
..		DIR
CsLiSO4.hkl		378 488
CsLiSO4.inflip		112 989
CsLiSO4.I51		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
0.037995 0.000000 0.000000 0.000000 0.000000 0.000000 0000000000
O5 4 1 0.500000 0.832000 0.500000 0.448000
0.037995 0.000000 0.000000 0.000000 0.000000 0.000000 0000000000
O6 4 1 0.500000 0.832000 0.500000 0.448000
0.037995 0.000000 0.000000 0.000000 0.000000 0.000000 0000000000
O7 4 1 0.500000 0.832000 0.500000 0.448000
0.037995 0.000000 0.000000 0.000000 0.000000 0.000000 0000000000
O8 4 1 0.500000 0.832000 0.500000 0.448000
0.037995 0.000000 0.000000 0.000000 0.000000 0.000000 0000000000
O9 4 1 0.500000 0.832000 0.500000 0.448000
0.037995 0.000000 0.000000 0.000000 0.000000 0.000000 0000000000
O10 4 1 0.500000 0.832000 0.500000 0.448000
0.037995 0.000000 0.000000 0.000000 0.000000 0.000000 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
Li2 2 1 1.000000 0.624000 0.577000 0.504000
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
atomic name
ADPs
occupancy
atomic position

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 0.000000 0.000000
Cs2
  
```

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

Data block:

Cell Radiation Profile Asymmetry/Diffractometer Sample/Experiment Corre

Peak-shape function

Gaussian
 Lorentzian
 Pseudo-Voigt
 Modified Lorentzian

Cutoff

GU
 GV
 GW
 GP

LX
 LXe
 LY
 LYe

Anisotropic strain broadening

None
 Axial method
 Tensor method

Broadening direction

Anisotropic particle broadening

None
 Axial method
 Spherical harmonics

Broadening direction

Esc

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

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

A. Leinweber 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 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:

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

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

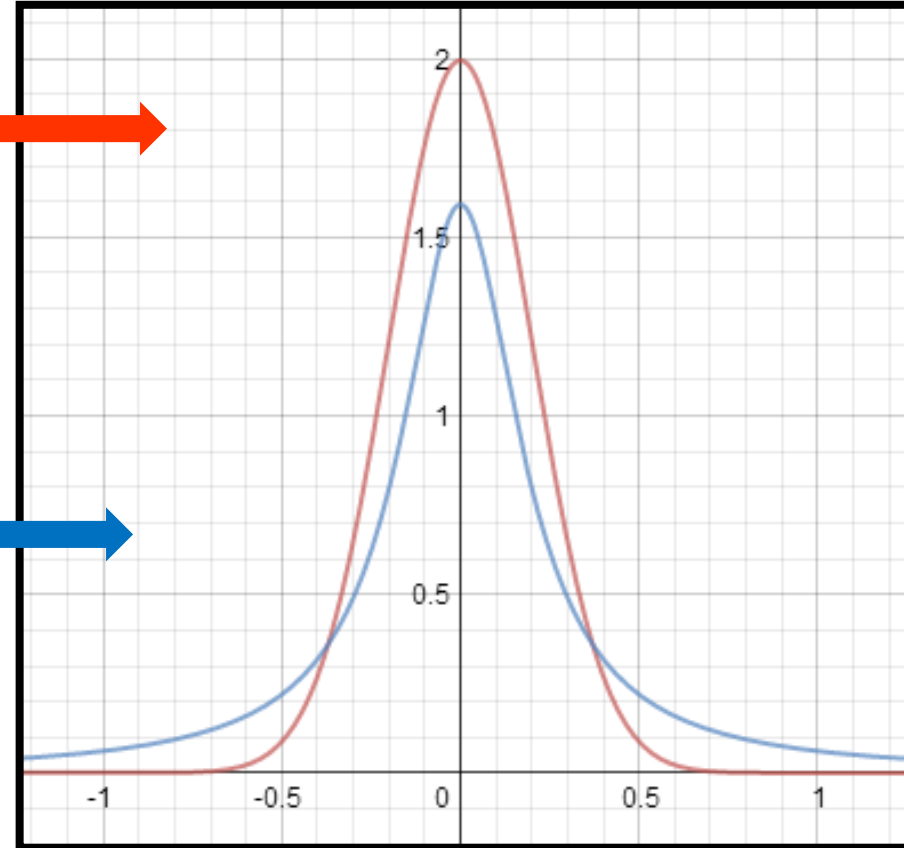
Where H_G is Full-Width at Half-Maximum

Lorentzian:

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

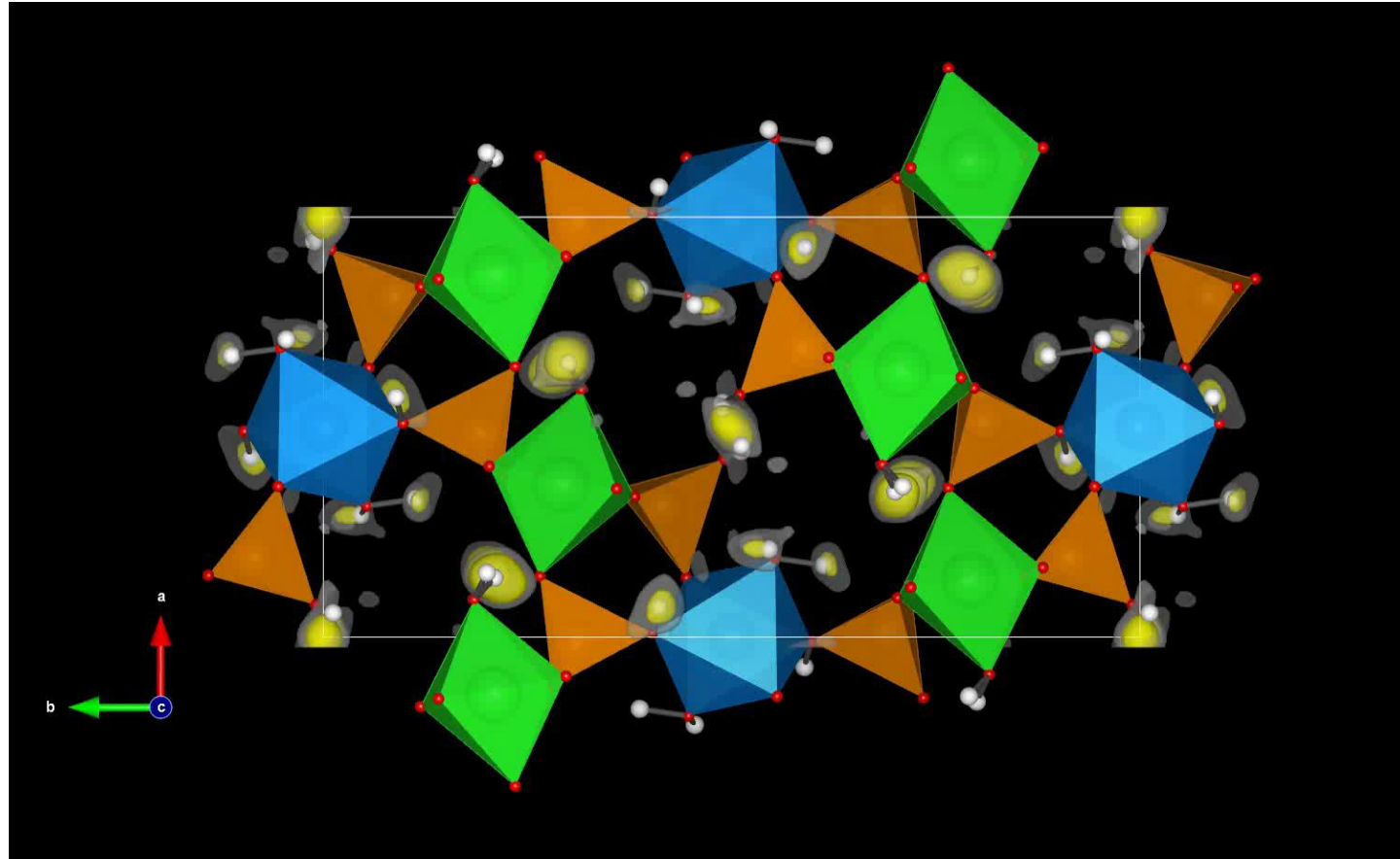
$$b_L = H_L$$

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



FZU

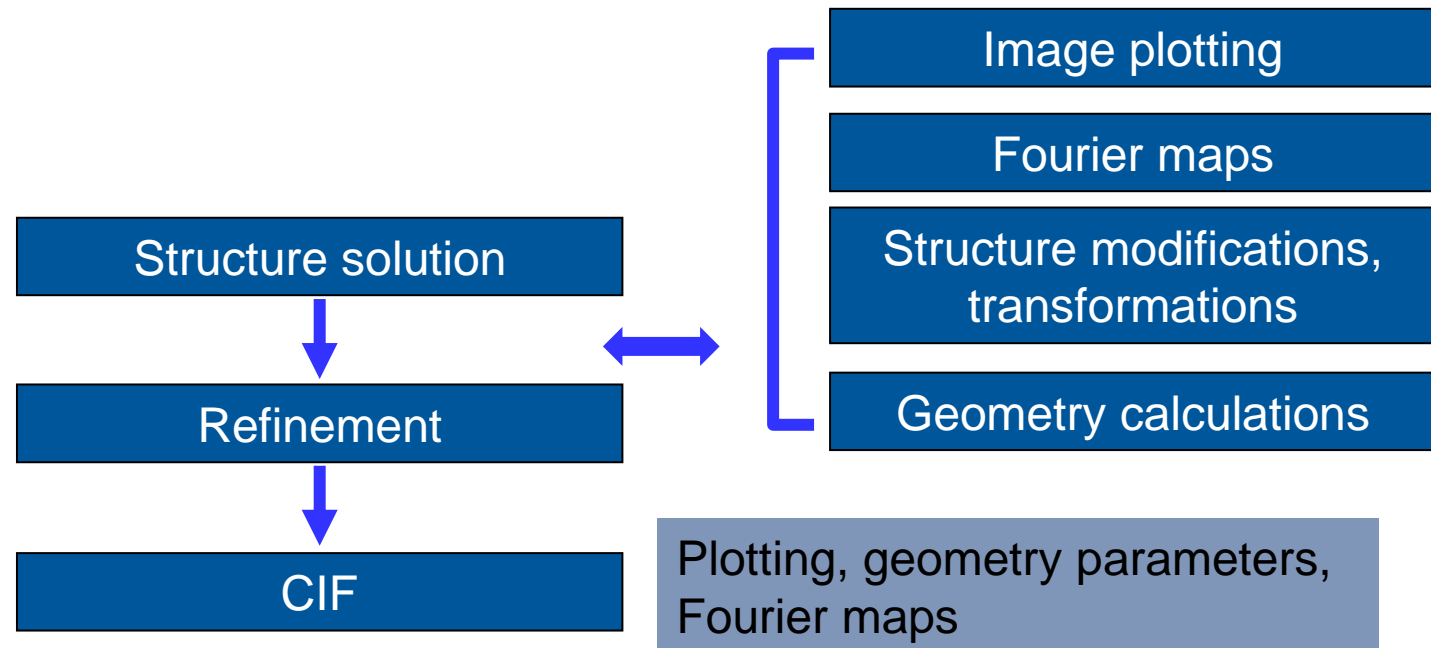
Institute of Physics
of the Czech
Academy of Sciences

L. Palatinus, C. A. Corrêa et al. *Acta Crystallographica B* **71**, 740-751 (2015).

L. Palatinus, V. Petříček, C. A. Corrêa. *Acta Crystallographica A* **71**, 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.

- > Reflection file
- > New Phases
- ▼ **Edit structure parameters**
 - Options
 - Edit basic parameters (cell, symmetry, etc.)
 - 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

Edit scale parameters

Data block: [dropdown]

TOverall 0 sclam/2 0 sc3lam 0

Maximal number of scales: 6

scale1 0.819623 scale2 0 scale3 0 scale4 0

scale5 0 scale6 0

Extinction correction

Data block: [dropdown]

Extinction model:

None Type 1 Gaussian Lorentzian

Isotropic - Becker_Coppens Type 2 Mixed

Anisotropic - Becker_Coppens SHELX model

Radius [cm]: used only if tbar not present on M90 file

Extinction parameters:

Giso 0.01 RhoIso 0.01

Refine all Fix all Reset

Esc OK

Edit twin fractions

Data block: [dropdown]

twvol2 0.07868 twvol3 0.282781

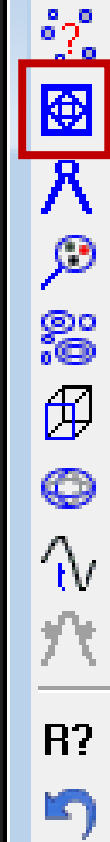
Four-fold axis in direction (0.352,0.000,1.000)

h'	0.0027	0.9877	0	h
k'	-1.0121	0.0024	0	k
l'	0.3518	-0.3465	0.9994	l

Refine all Fix all Reset

Esc OK

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 R_w is increased by 10% reduce the damping by a factor 2
After 3 cycles try to enlarge it back.

Check for convergence => stop if $\max(\text{change}/s.u.) < 0.05$ 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 $F(\text{obs})^{**2}$

Apply electroneutrality
 Simulation run
 After last cycle call Fourier

Correct for $\lambda/2$ effect
 Correct for 3λ 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 commands

Basic Select/Listing **Restrains/Constraints** Modulation/Twin Powder

Press the button to edit/create:

- Restrictions
- Equations
- Fixed commands
- Dontuse/Useonly command[2+0!]**
- Scale command
- Partial RFactors
- Distance restraints
- Angle restraints
- Torsion angle restraints
- Magnetic moment restraints
- Keep commands**

Define "dontuse" and "useonly" commands

```
====> New command <====  
dontuse hklm : k=2 except m=0  
dontuse hklm : m=2 except k=0
```

Edit
Delete
Disable
Enable
Down Up
Select all
Refresh
Clone

Rewrite

Group of reflections: hklm
Condition: m=2
Except condition: k=0

Dontuse command
 Useonly command

Group of reflection can be specified in a compressed form e.g. hkl, hhl, h0l or as hkl expression separated by commas e.g. h,-2h+l,h+k+l.

The conditions are expressed in way as used in IT e.g. h+2k=2n+1. In the case that the "n" term is missing e.g. h-k=3, the absolute value the left side is compared with the positive number from the right side.

Esc OK

Define keep commands

```
====> New command <====
```

Edit
Delete
Disable
Enable
Down Up
Select all
Refresh
Clone

Rewrite

Hydrogens
 Geometry
 ADP
 Magnetic

Tetrahedral
 Trigonal
 Apical

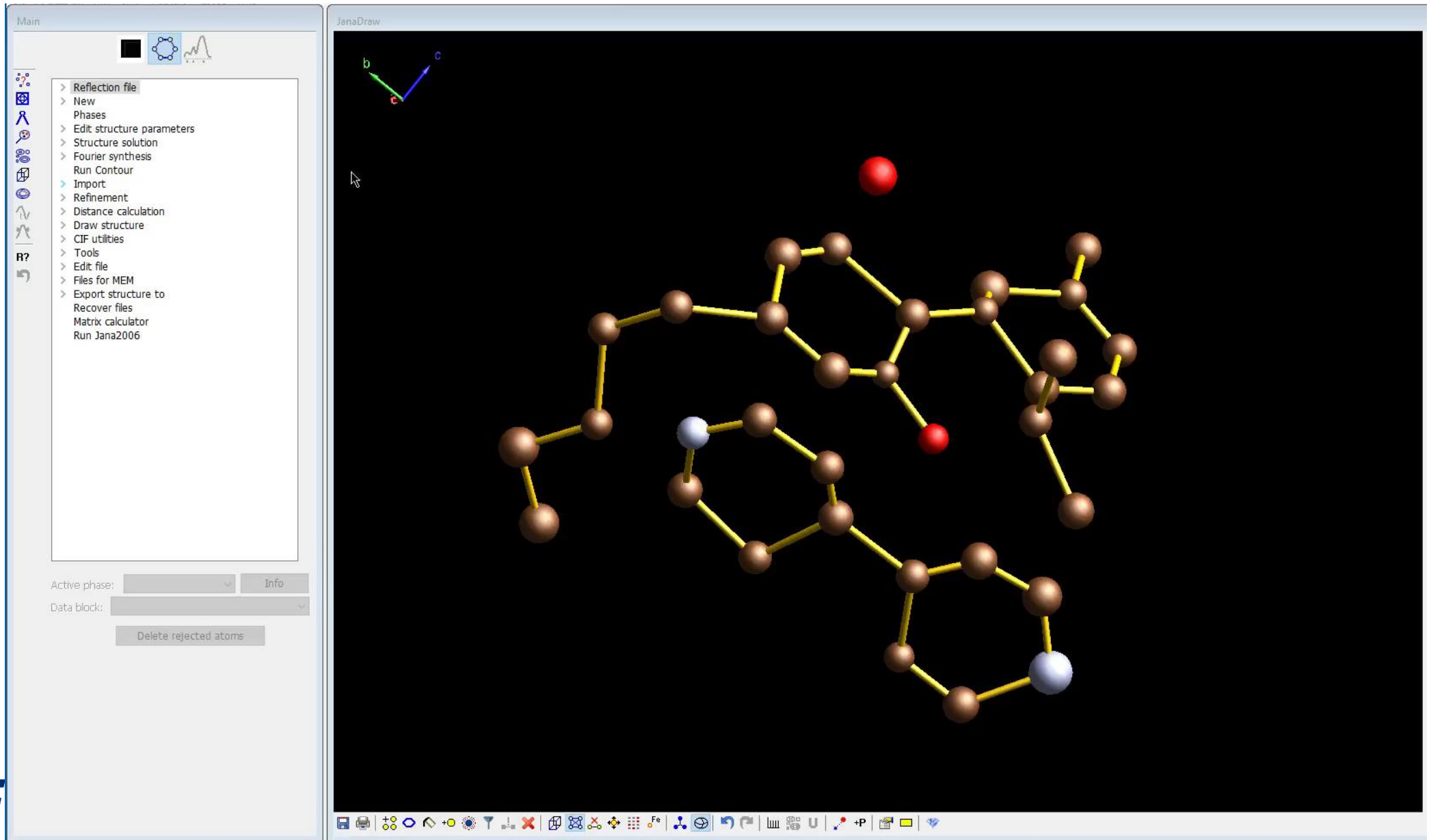
Central: 0.96 H distance
Neighbor(s): 1st
1st
2nd
3rd

Use anchor atom =>

Select central

Esc OK

Adding hydrogen atoms - refinement



The image displays the Jana software interface, which is used for crystallographic refinement. The main window, titled "JanaDraw", shows a 3D ball-and-stick model of a complex organic molecule. The atoms are represented by spheres: carbon (brown), oxygen (red), and nitrogen (blue). The bonds are shown as yellow sticks. The molecule is set against a black background. In the top-left corner of the main window, a 3D coordinate system is visible with axes labeled 'a', 'b', and 'c'. The left-hand side of the interface contains a menu titled "Main" with various options for file operations, structure solution, refinement, and drawing. Below the menu, there are fields for "Active phase:" and "Data block:", and a button labeled "Delete rejected atoms". At the bottom of the main window, there is a toolbar with various icons for navigation and manipulation of the model.

Main

- > Reflection file
- > New
- > Phases
- > Edit structure parameters
- > Structure solution
- > Fourier synthesis
- > Run Contour
- > Import
- > Refinement
- > Distance calculation
- > Draw structure
- > CIF utilities
- > Tools
- > Edit file
- > Files for MEM
- > Export structure to
- > Recover files
- > Matrix calculator
- > Run Jana2006

Active phase: Info

Data block:

Delete rejected atoms

JanaDraw



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 θ/λ

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 structure : page= 256 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:

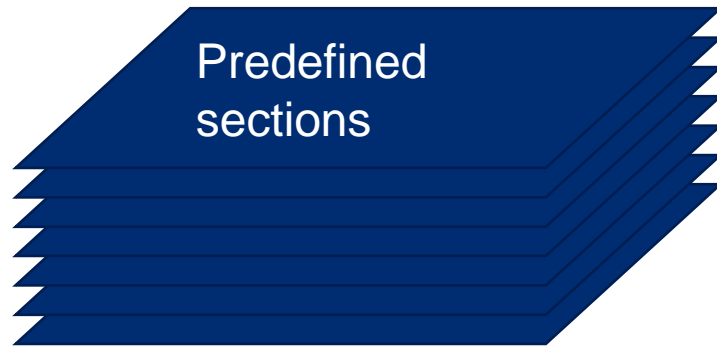
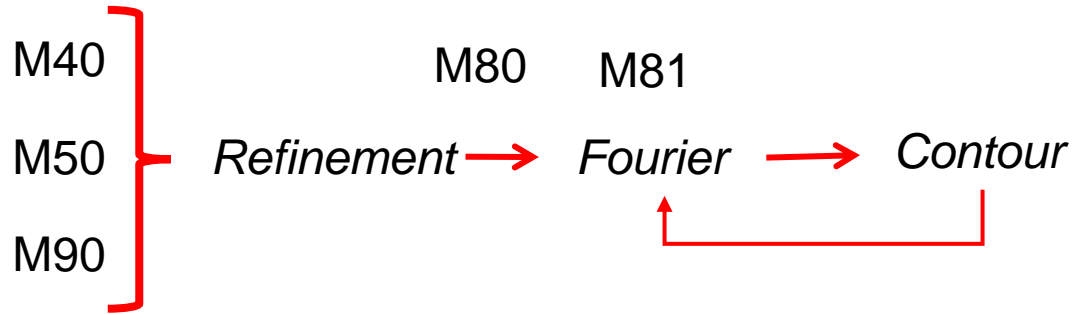
```

-----
|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]
-----

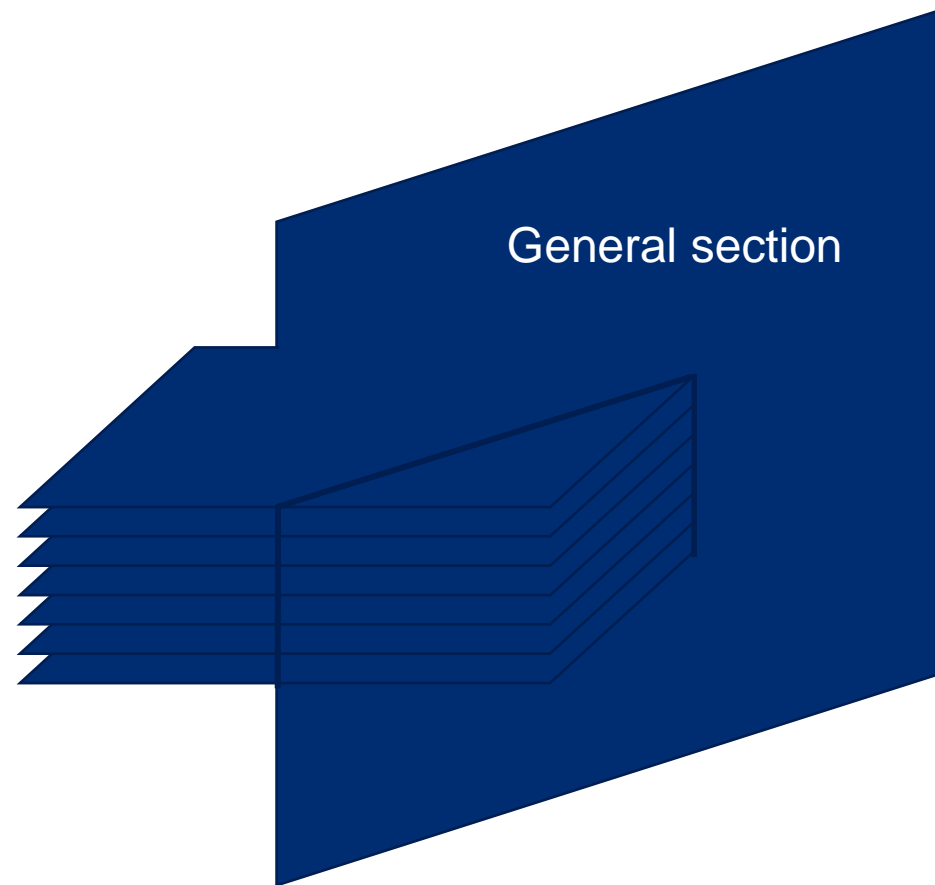
```

Refinement results

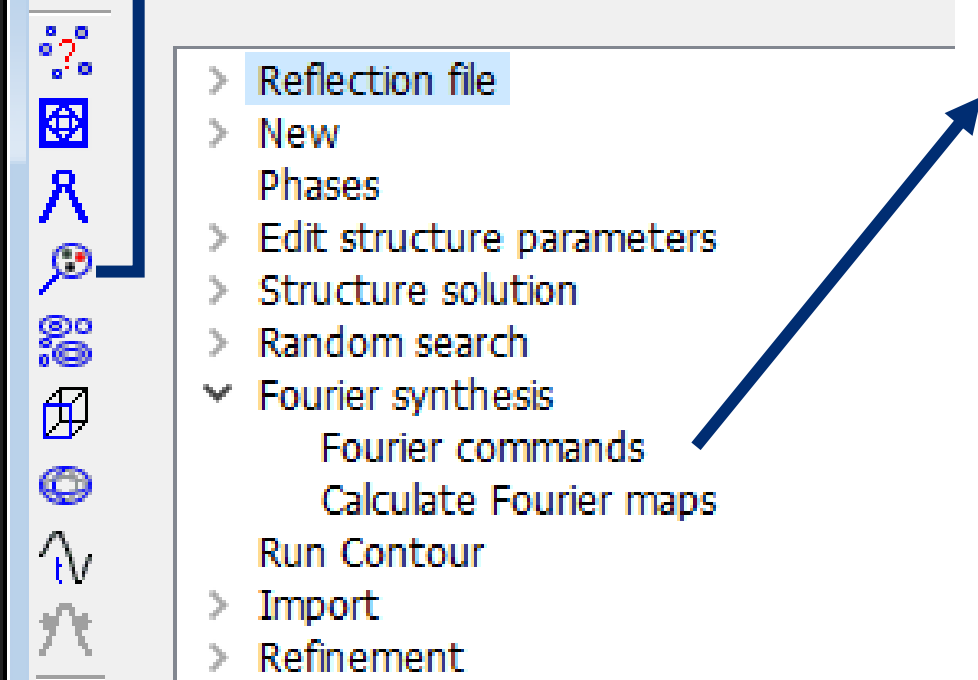
Fourier maps



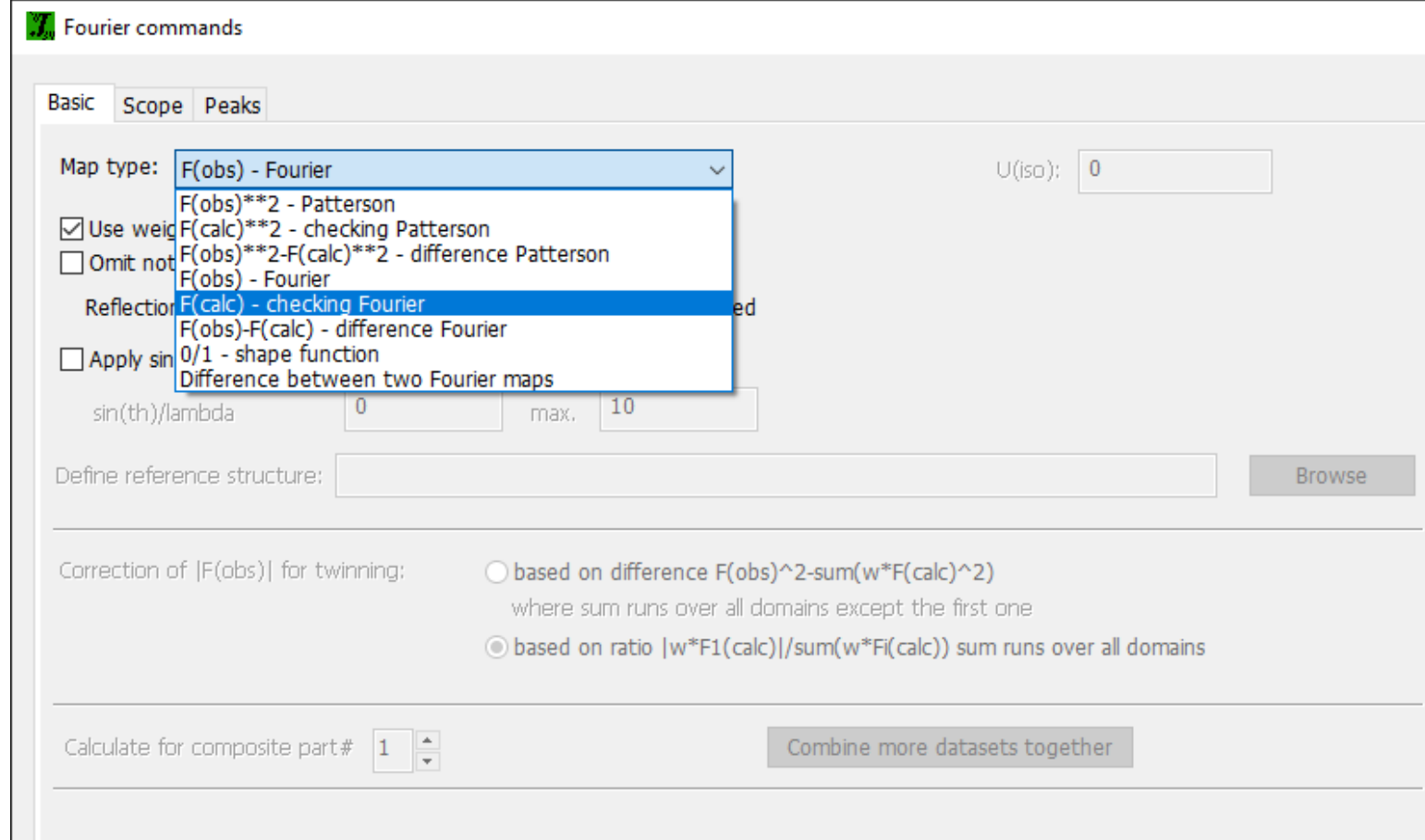
M81



Fourier maps



- > Reflection file
- > New
- Phases
- > Edit structure parameters
- > Structure solution
- > Random search
- Fourier synthesis
 - Fourier commands
 - Calculate Fourier maps
- Run Contour
- > Import
- > Refinement



Fourier commands

Basic Scope Peaks

Map type: **F(obs) - Fourier**

- F(obs)**2 - Patterson
- F(calc)**2 - checking Patterson
- F(obs)**2-F(calc)**2 - difference Patterson
- F(obs) - Fourier
- F(calc) - checking Fourier**
- F(obs)-F(calc) - difference Fourier
- 0/1 - shape function
- Difference between two Fourier maps

Reflection: **F(calc) - checking Fourier**

sin(th)/lambda: 0 max. 10

Define reference structure: **Browse**

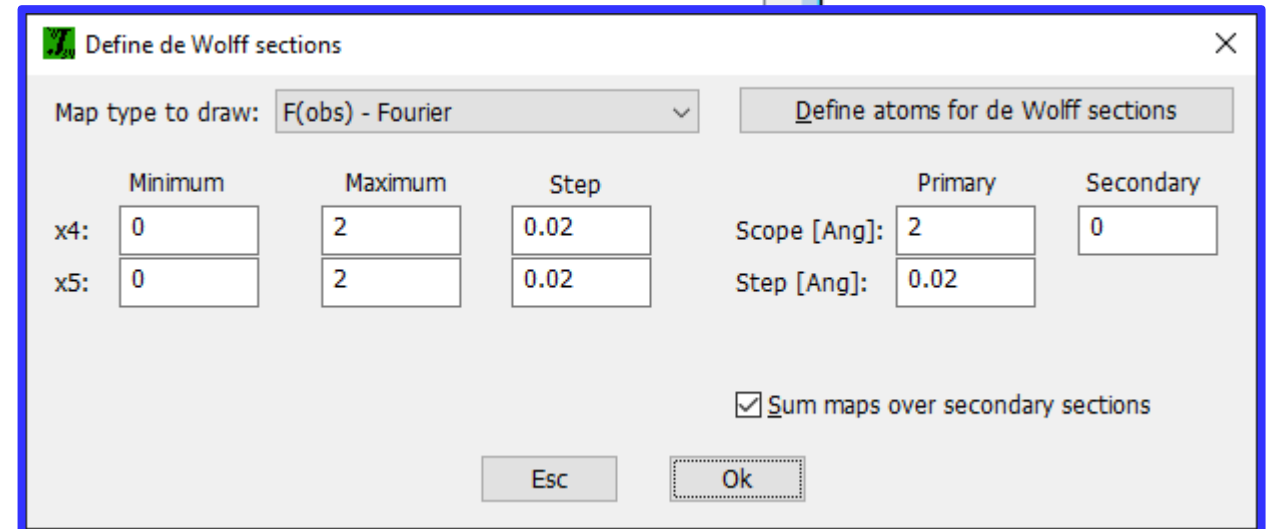
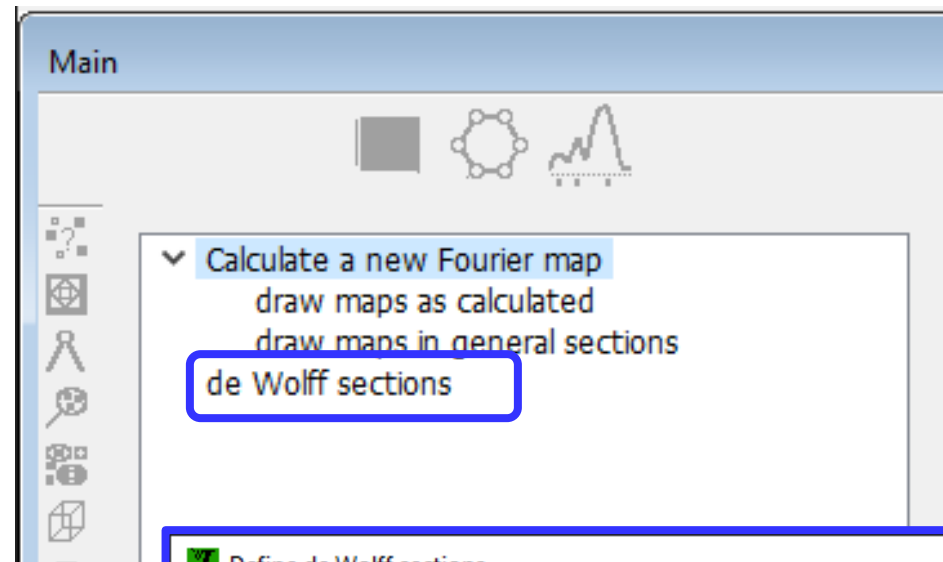
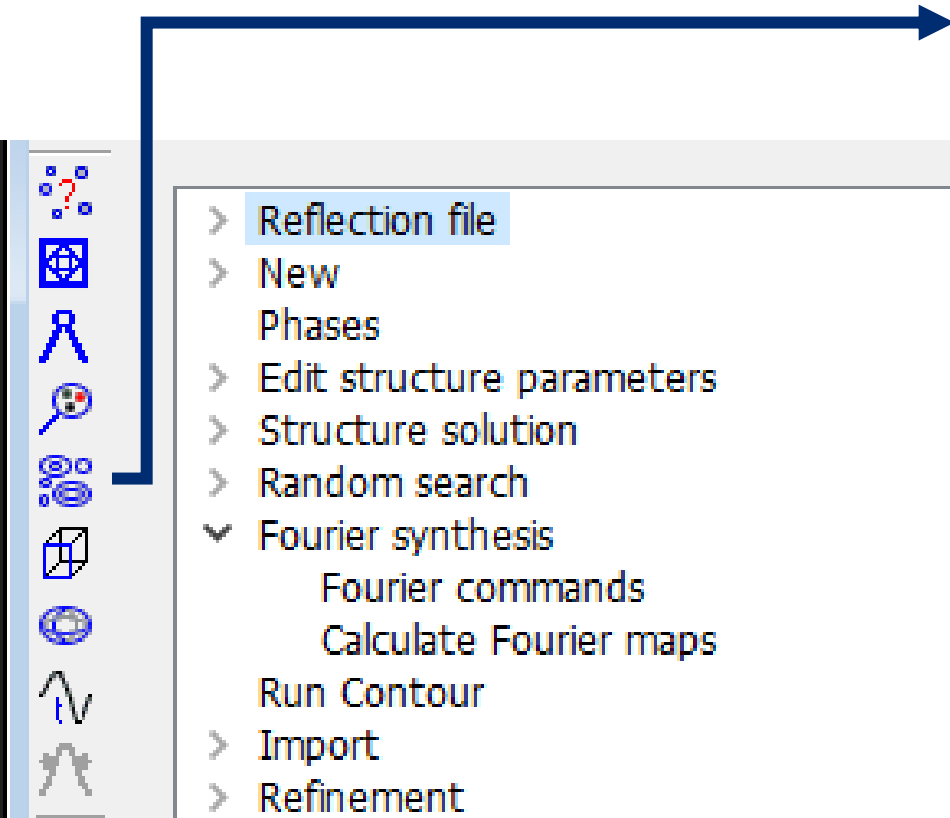
Correction of |F(obs)| for twinning:

- based on difference $F(\text{obs})^2 - \sum(w \cdot F(\text{calc})^2)$
where sum runs over all domains except the first one
- based on ratio $|w \cdot F_1(\text{calc})| / \sum(w \cdot F_i(\text{calc}))$ sum runs over all domains

Calculate for composite part #: 1 **Combine more datasets together**

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



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

The image shows a software interface with a menu and two dialog boxes. The menu is titled 'Jana2020 - [D:\Conferences_Trips_Seminars\2024.06.22_Workshop]' and has a 'Transformations' tab selected. The 'Go to a subgroup' option is highlighted. The 'Go to subgroup wizard' dialog box is open, showing a table of operations and their symbols. The 'Select subgroup' dialog box is also open, showing a list of subgroups and their axes. Arrows indicate the flow from the menu to the wizard and then to the subgroup selection.

Go to subgroup wizard

Operation	Symbol	Direction/Normal
x1 x2 x3 x4 x5	1	(0,0,0)
-x1+1/2 x2+1/2 x3 x5+1/2 x4+1/2	b	(1,0,0)
x1+1/2 -x2+1/2 x3 x3-x5+1/2 x3-x4+1/2	a	(0,1,0)
-x1 -x2 x3 x3-x4 x3-x5	2	(0,0,1)
-x2 x1 x3 x3-x5 x4	4+	(0,0,1)
x2 -x1 x3 x5 x3-x4	4-	(0,0,1)
x2+1/2 x1+1/2 x3 x4+1/2 x3-x5+1/2	m	(1,-1,0)
-x2+1/2 -x1+1/2 x3 x3-x4+1/2 x5+1/2	m	(1,1,0)

Keep P centring

Select non-isomorphic subgroup

Complete subgroup Refresh Step back

Space group : P4bm Axes : (1,0,0 | 0,1,0 | 0,0,1) Origin : (0,0,0)

Subgroup : Axes : Origin :

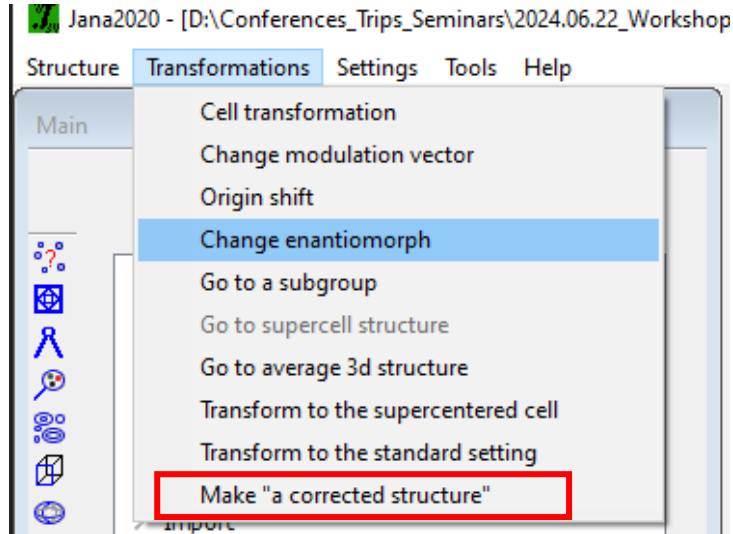
Back Next

Select subgroup

Subgroup	Axes
P4	(1,0,0 0,1,0 0,0,1)
Cmm2	(-1,-1,0 -1,1,0 0,0,-1)
Pba2	(0,-1,0 -1,0,0 0,0,-1)

Esc OK

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
```

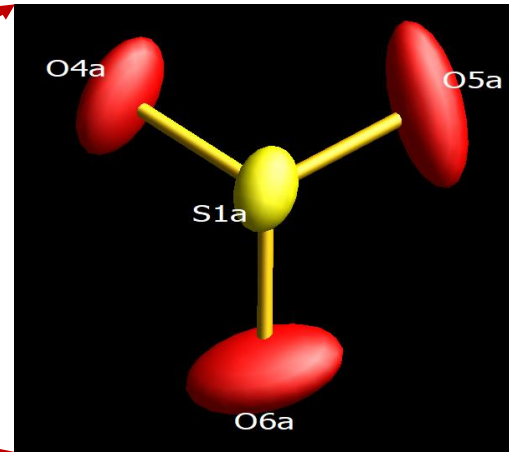
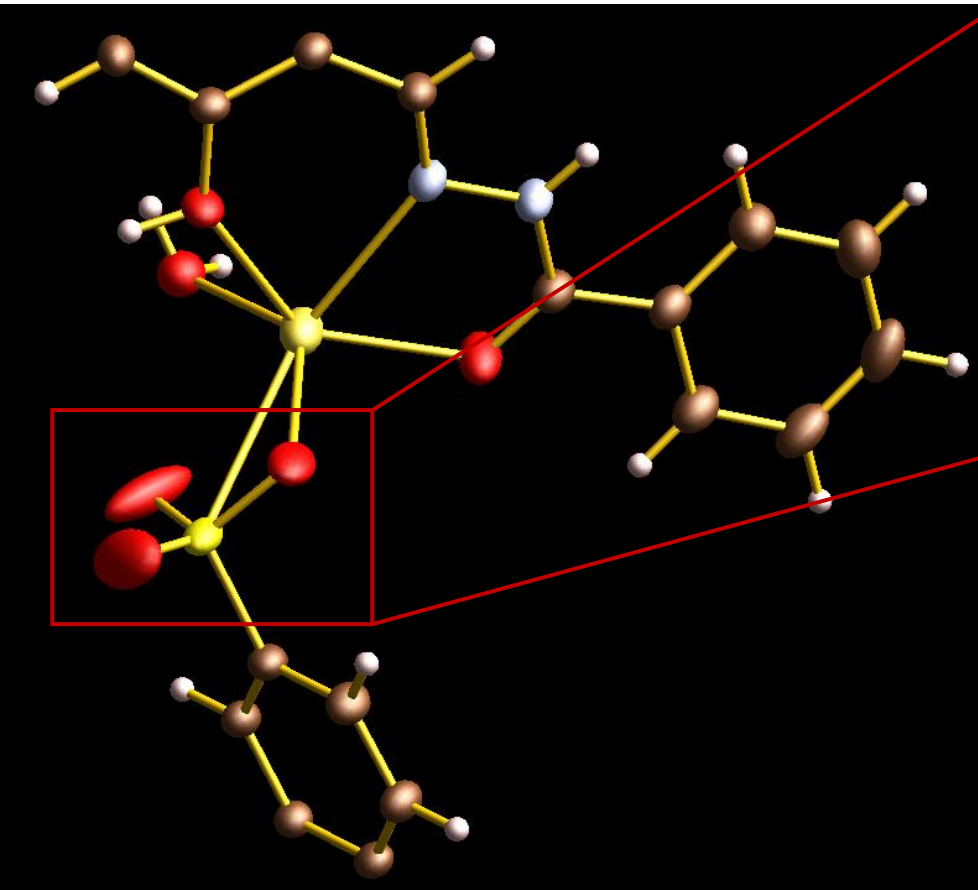
```
keep ADP riding C13 1.2 H1c13 H2c13 H3c13
```



FZU

Institute of Physics
of the Czech
Academy of Sciences

Advanced tools – Disorder, atom split, rigid body



Information from refinement:

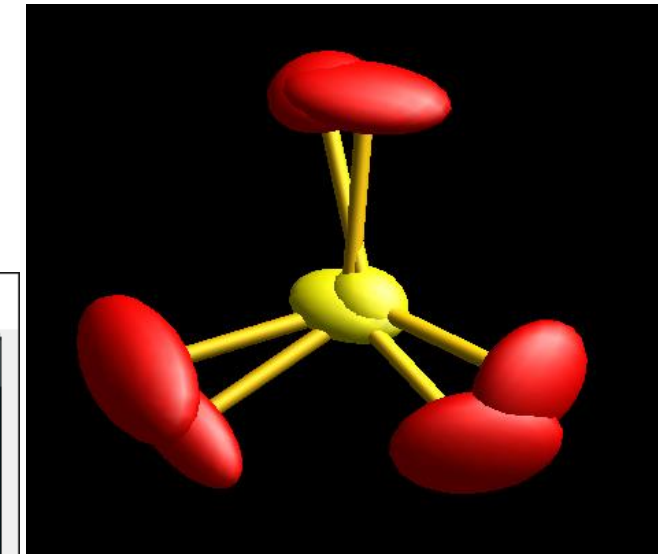
RFactors overview

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]



Advanced tools – Fundamental approach

Final profile

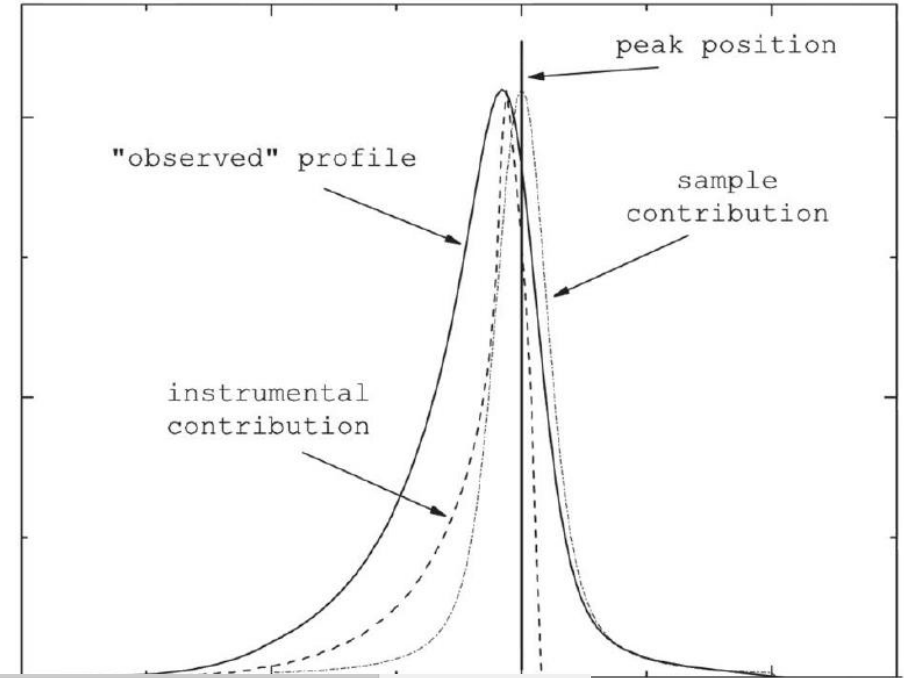
Sample contribution

Instrumental contribution

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

crystalline size
and stress

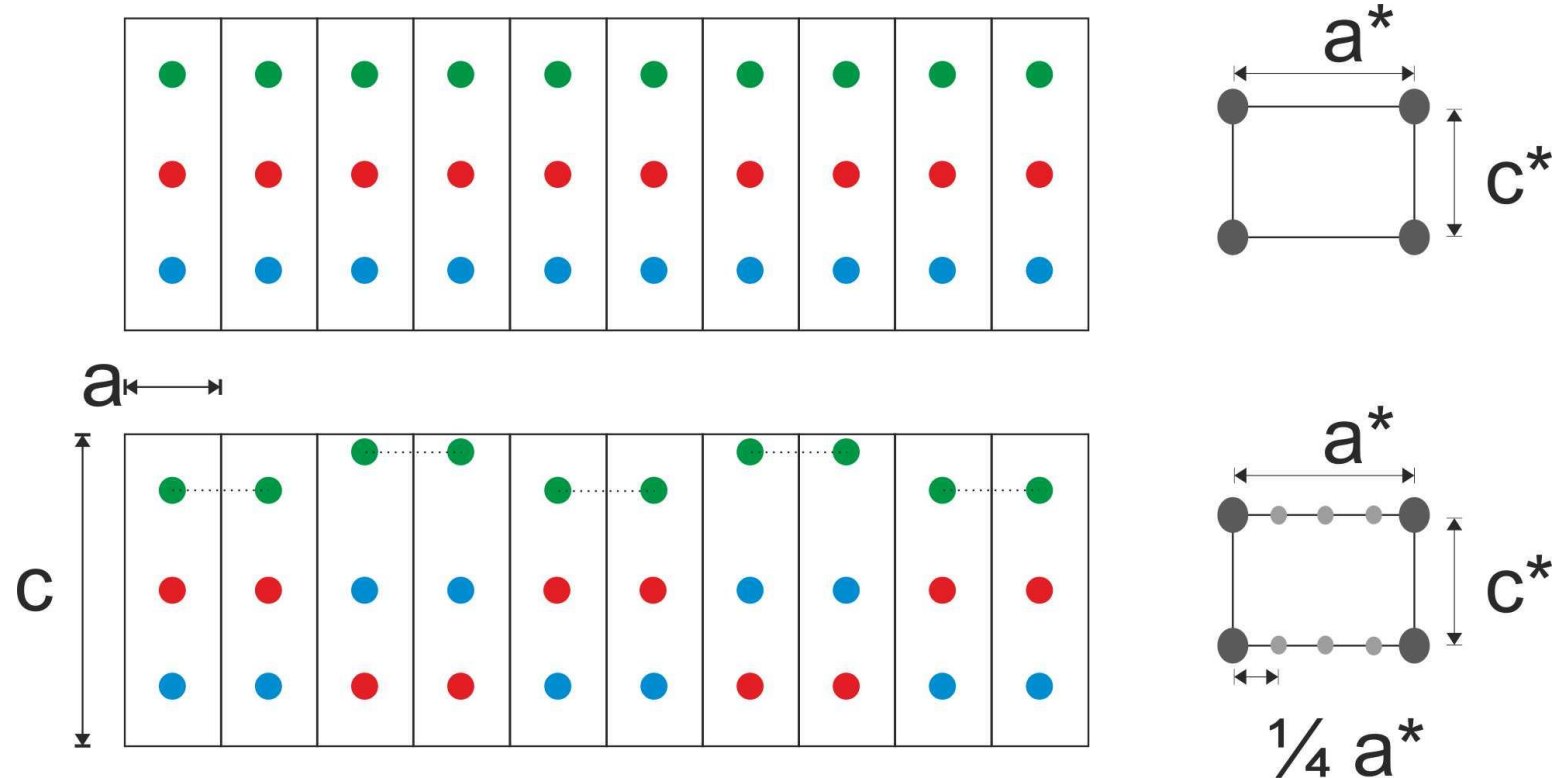
optics
sample holder
detector
source



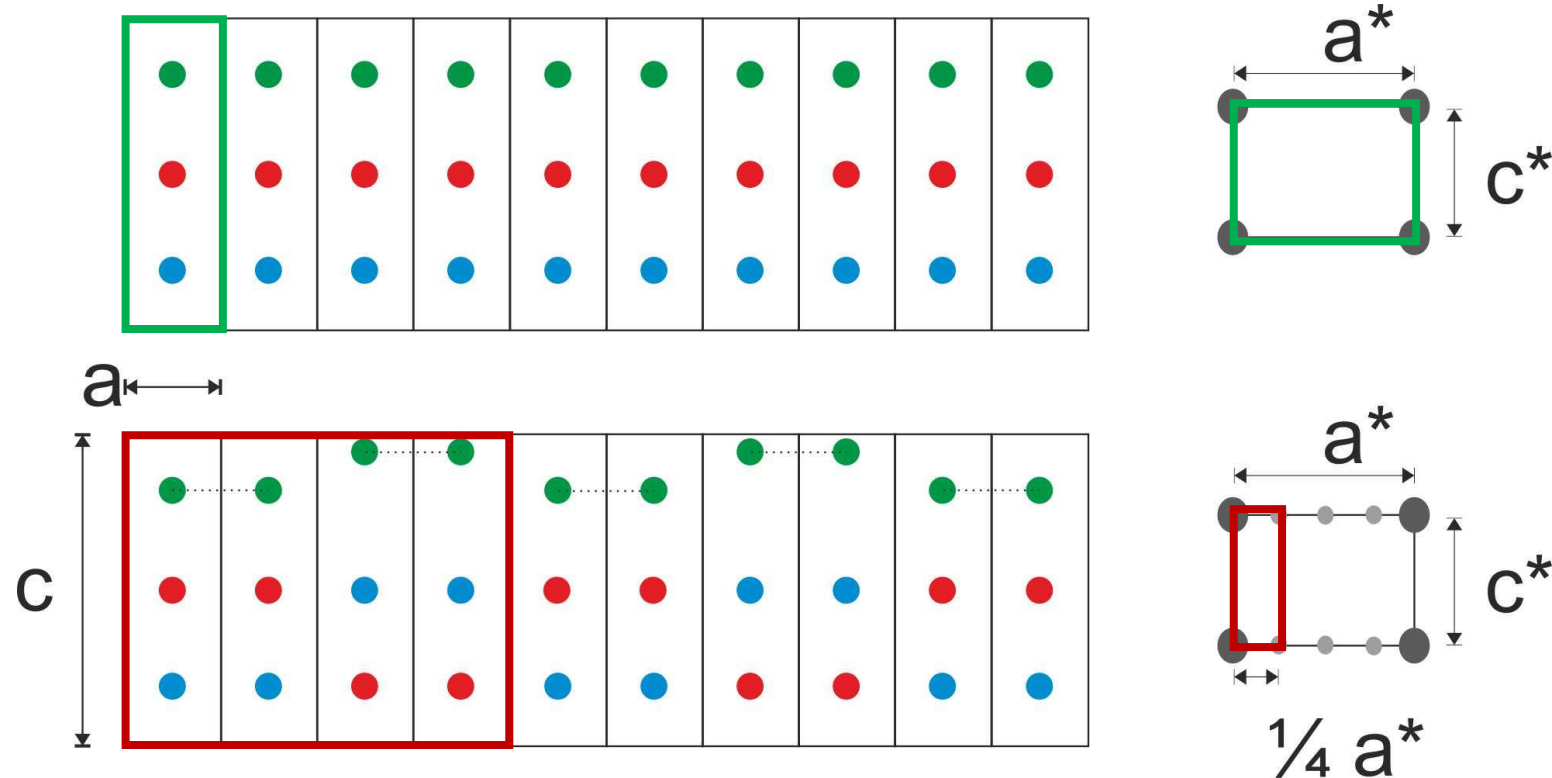
Cell	Radiation	Profile	Asymmetry/Diffractometer	Sample/Experiment	Corrections	Various
<input type="radio"/> No correction <input type="radio"/> Howard (Boole's rule) <input type="radio"/> Berar-Baldinozzi correction <input type="radio"/> correction by divergence <input checked="" type="radio"/> fundamental approach <input type="radio"/> Debye-Scherrer integration						
			Primary radius [mm]	<input type="text" value="173"/>		
			Secondary radius [mm]	<input type="text" value="173"/>		
			RS width [mm]	<input checked="" type="checkbox"/>	<input type="text" value="0.2"/>	<input type="checkbox"/>
			FDS angle [deg]			
			VDS angle [mm]			
			Source length [mm]	<input type="text" value="12"/>	<input type="checkbox"/>	
			Sample length [mm]	<input type="text" value="15"/>	<input type="checkbox"/>	
			RS length [mm]	<input type="text" value="12"/>	<input type="checkbox"/>	
			Primary soller [deg]	<input checked="" type="checkbox"/>	<input type="text" value="5.1"/>	<input type="checkbox"/>
			Secondary soller [deg]	<input checked="" type="checkbox"/>	<input type="text" value="5.1"/>	<input type="checkbox"/>

Cell	Radiation	Profile	Asymmetry/Diffractometer	Sample/Experiment	Corrections	Various
Peak-shape function						
<input type="radio"/> Gaussian <input type="radio"/> Lorentzian <input checked="" type="radio"/> Pseudo-Voigt <input type="radio"/> Modified Lorentzian						
		Cutoff	<input type="text" value="8"/>			
		CSizeG	<input type="text" value="683.3402"/>	<input checked="" type="checkbox"/>	CSizeL	<input type="text" value="0"/>
		CSizeGA	<input type="text" value="0"/>	<input type="checkbox"/>	CSizeLA	<input type="text" value="0"/>
		StrainG	<input type="text" value="0"/>	<input type="checkbox"/>	StrainL	<input checked="" type="checkbox"/>
		StrainGA	<input type="text" value="0"/>	<input type="checkbox"/>	StrainLA	<input type="text" value="0"/>
Anisotropic strain broadening						
<input checked="" type="radio"/> None <input type="radio"/> Axial method <input type="radio"/> Tensor method						
		Broading direction	<input type="text" value="0 0 1"/>			
		<input type="button" value="Edit tensor parameters"/>		Zeta	<input type="text" value="0.5"/>	<input type="checkbox"/>
Anisotropic particle broadening						
<input checked="" type="radio"/> None <input type="radio"/> Axial method <input type="radio"/> Spherical harmonics						
		Broading direction	<input type="text" value="0 0 1"/>			
		<input type="button" value="Edit spherical harmonics"/>				

Advanced tools – modulated structures

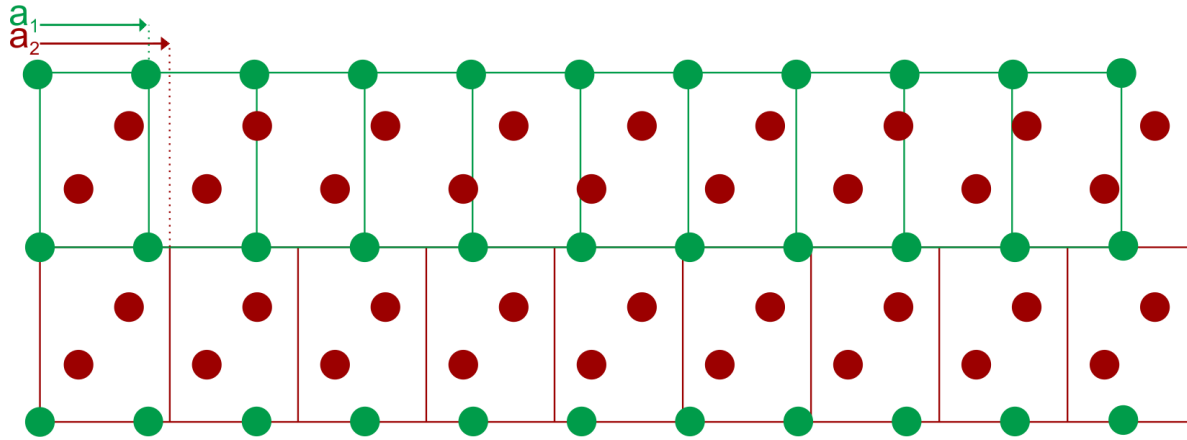


Advanced tools – modulated structures



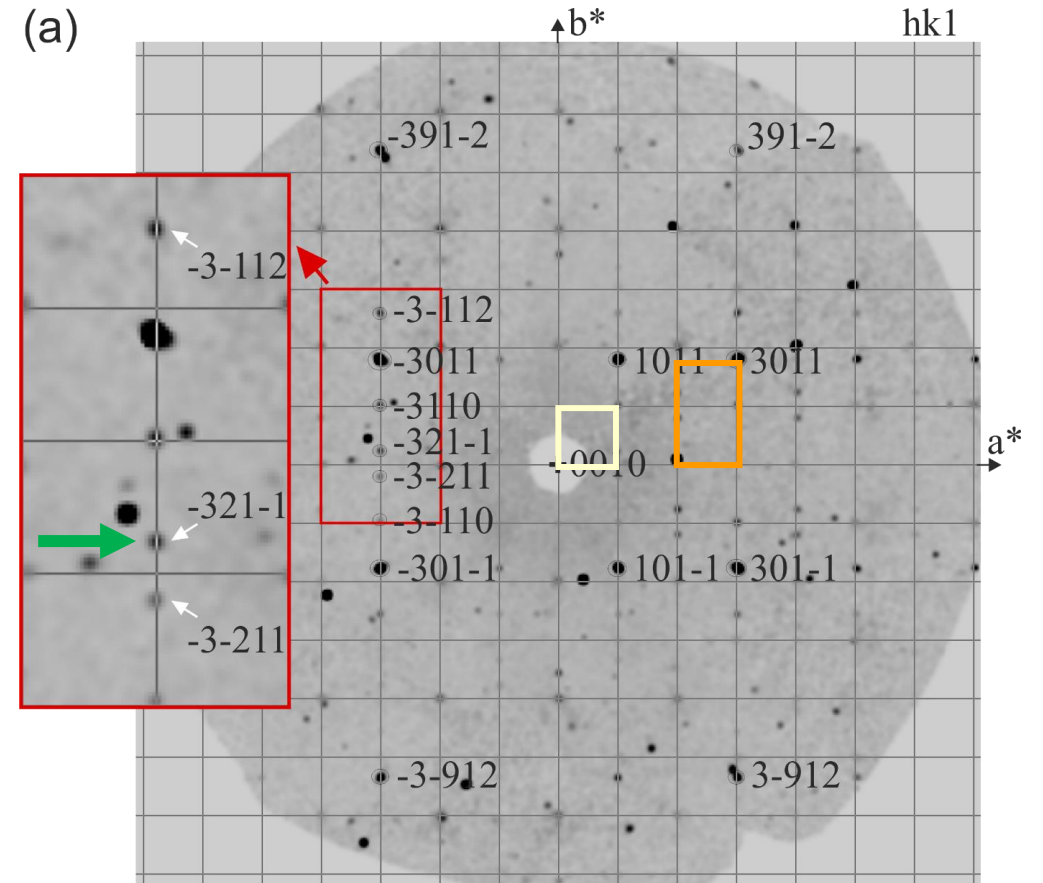
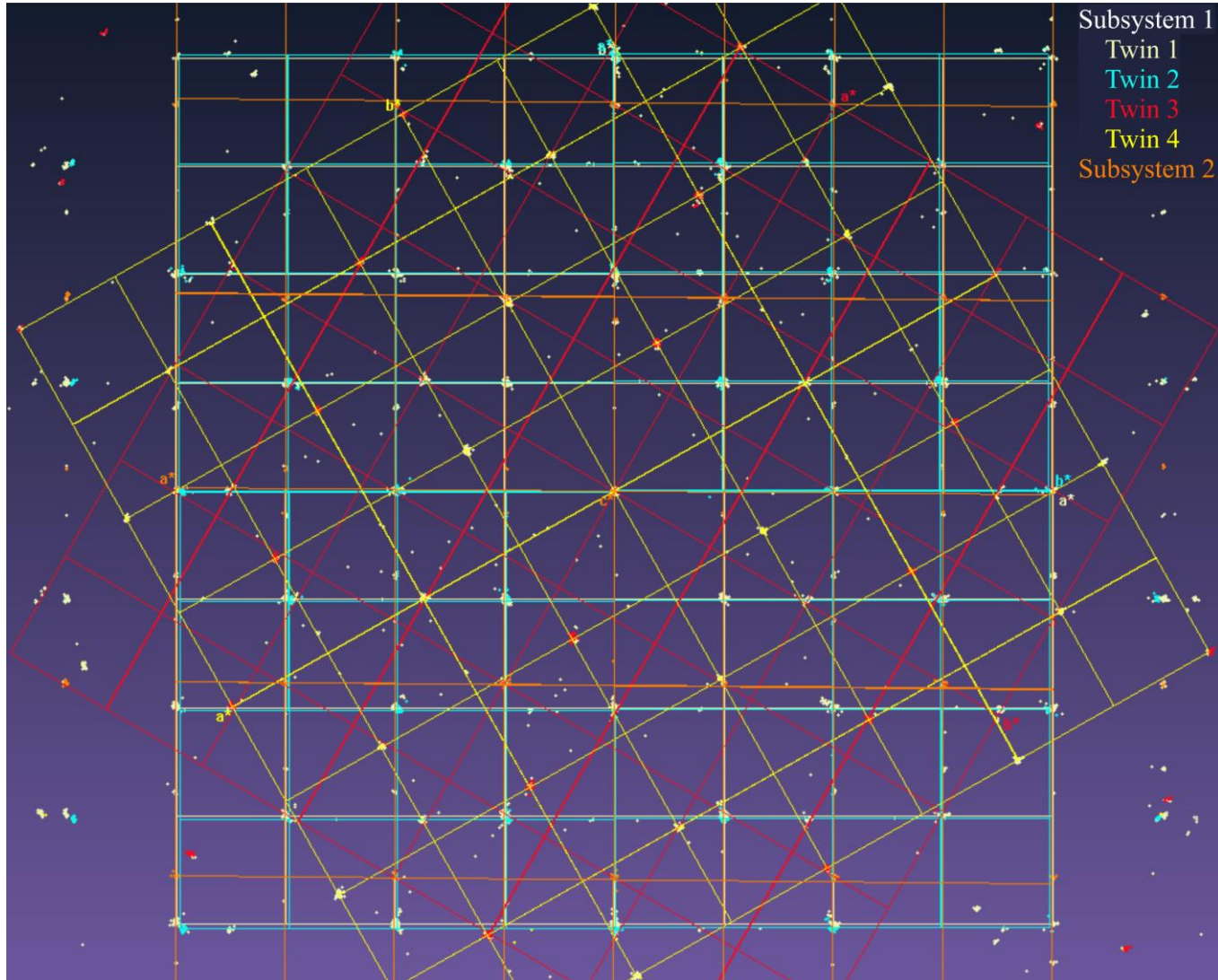
Modulation vector with (ir)rational components – (in)commensurate modulated structure

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

Edit basic parameters (cell, symmetry, etc.)

Cell Symmetry Composition Multipole parameters Magnetic parameters

Title of the structure:

Phase label:

Cell parameters:

s.u.'s of cell parameters:

Dimension:

1st modulation vector

Twinning

5.7084 5.7931 23.7154 90 94.831 90

0.0005 0.0008 0.0016 0 0.006 0

4

0 1.803 0

Number of composite parts: 2

Matrices

Number of twin domains: 2

Matrices

Matrix calculator

h'	=	1	*	h_+	0	*	k_+	0	*	l_+	0	*	m
k'	=	0	*	h_+	0	*	k_+	0	*	l_+	1	*	m
l'	=	0	*	h_+	0	*	k_+	1	*	l_+	0	*	m
m'	=	0	*	h_+	1	*	k_+	0	*	l_+	0	*	m

Induced cell parameters
5.708 3.213 23.715 90.00 94.83 90.00 Volume: 433.426

Induced modulation vector
0.0000 0.5546 0.0000

Previous composite matrix Next composite matrix

Esc OK

2nd twinning matrix

Twin domain# 2 Applied to the phase:

h'	=	-0.5163	*	h_+	0.8443	*	k_+	0	*	l_+	*
k'	=	-0.8685	*	h_+	-0.5165	*	k_+	-0.0002	*	l_+	*
l'	=	0.5276	*	h_+	-0.2931	*	k_+	1.0002	*	l_+	*

General rotation by angle 121.08degs in direction (0.348,0.000,1.000)

Select alternative representative of the coset

Round to closest integers Round to closest rationals

Matrix calculator

Original cell parameters
5.708 5.793 23.715 90.00 94.83 90.00

Twinned cell parameters
5.710 5.790 23.718 90.02 94.78 90.04

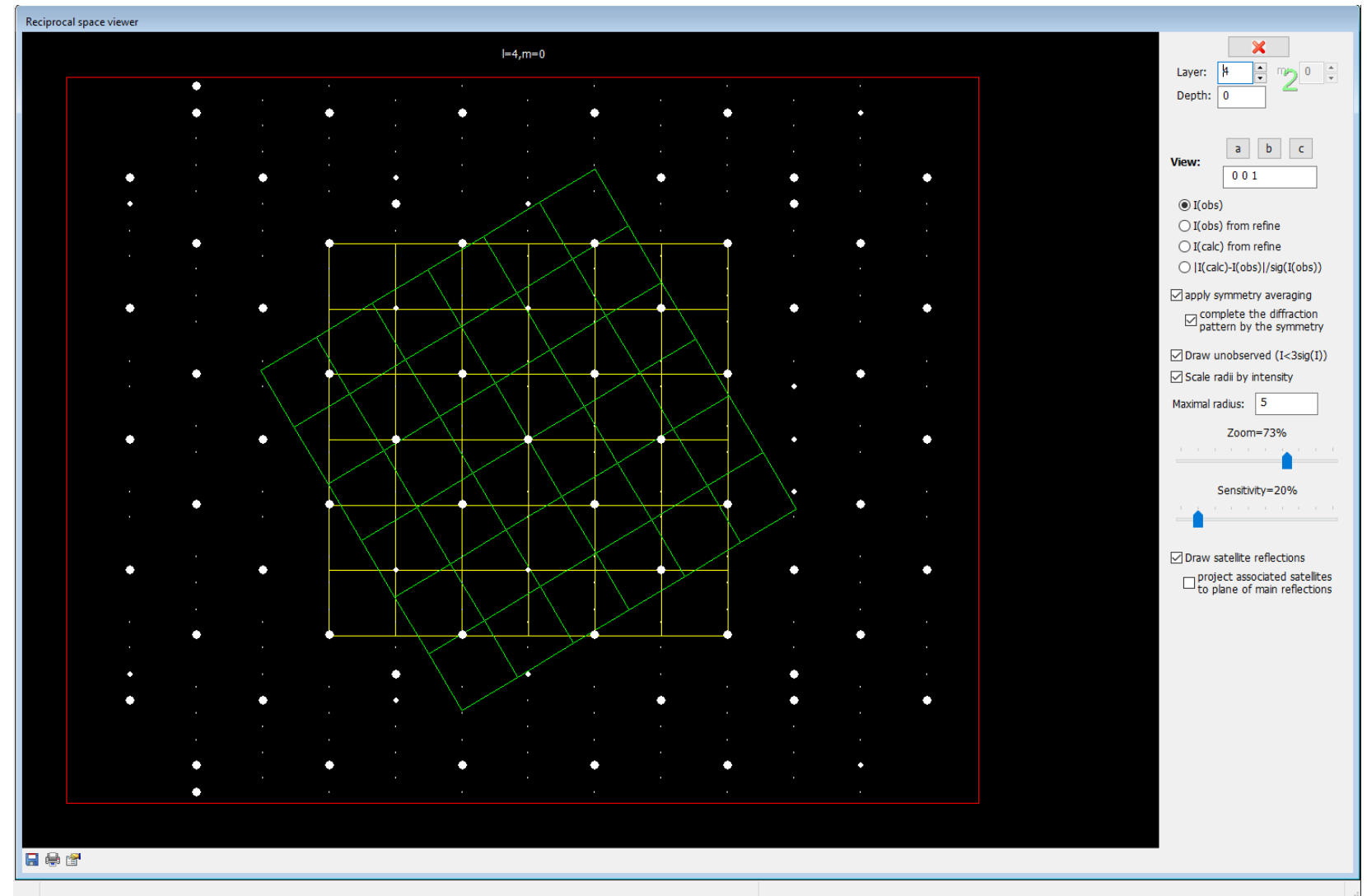
Rotation axis: 0 0 1

in direct base proper rotation
 in reciprocal base improper rotation

Rotation angle:
 0 deg 90 deg 180 deg 270 deg 300 deg
 60 deg 120 deg 240 deg explicit=> 180

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
- Graph
- > 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



Advanced tools – modulated structures

Edit basic parameters (cell, symmetry, etc.)

Cell Symmetry Composition Multipole parameters Magnetic parameters

Title of the structure:

Phase label:

Cell parameters: 8.89103 8.89103 5.1949 90 90 90

s.u.'s of cell parameters: 0.0001 0.0001 0 0 0 0

Dimension: 5 Number of components:

1st modulation vector: 0.314476 0.314476 1/2

2nd modulation vector: -0.314476 0.314476 1/2

Twinning Number of twin domains:

Commensurate case

Use simple supercell TZero:

Edit basic parameters (cell, symmetry, etc.)

Cell Symmetry Composition Multipole parameters Magnetic parameters

Superspace group: Xc(0b0)0

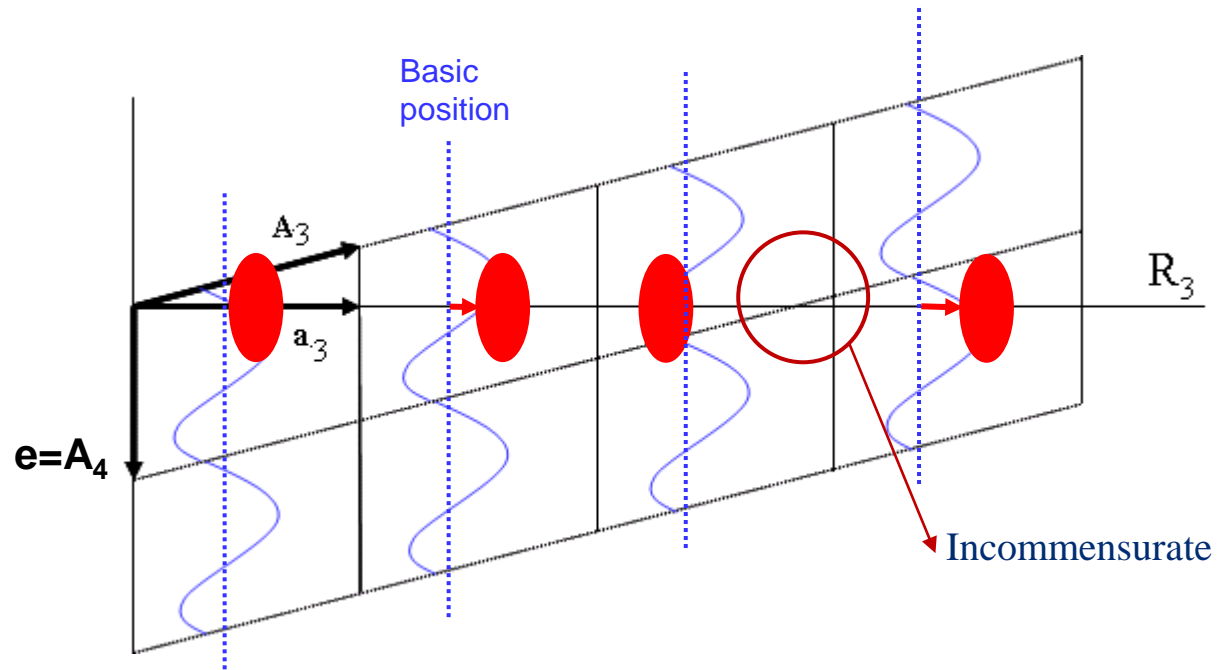
Origin shift: 0 0 0 0

The operators derived from the group symbol

(1) $x_1 \ x_2 \ x_3 \ x_4$
(2) $x_1 \ -x_2 \ x_3+1/2 \ -x_4$

Cell centering: X

Modulated structures



$$p(x_4) = p_0 + \sum_n (p_{s,n} \sin 2\pi n x_4 + p_{c,n} \cos 2\pi n x_4)$$

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 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 \mathbf{r} of an atom is the sum of the basic structure position and the modulation function \mathbf{u} .

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

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

Define/Edit atom parameters

Define Edit Multipole parameters Modulation parameters Magnetic parameters

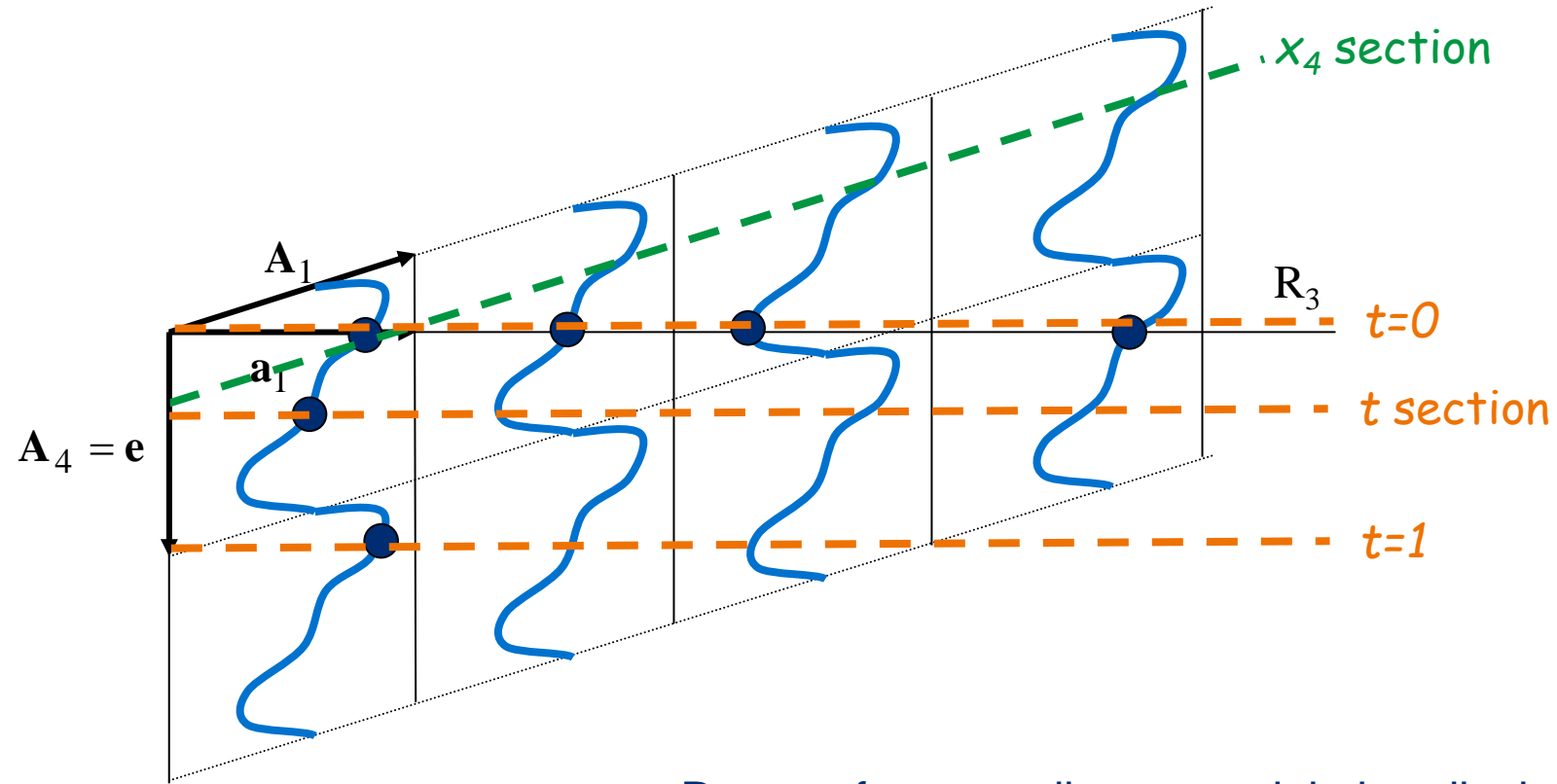
7 Select atom(s) from list Atom name: S4 Atomic type: S

Parameter: Position

xsin1	0.005255	<input checked="" type="checkbox"/>	ysin1	0.006119	<input checked="" type="checkbox"/>	zsin1	-0.002461	<input checked="" type="checkbox"/>
xsin2	0.003522	<input checked="" type="checkbox"/>	ysin2	0.009053	<input checked="" type="checkbox"/>	zsin2	0.002373	<input checked="" type="checkbox"/>
xcos1	-0.00338	<input checked="" type="checkbox"/>	ycos1	-0.000766	<input checked="" type="checkbox"/>	zcos1	0.000298	<input checked="" type="checkbox"/>
xcos2	0.005517	<input checked="" type="checkbox"/>	ycos2	0.001621	<input checked="" type="checkbox"/>	zcos2	0.002529	<input checked="" type="checkbox"/>

Modulated structures

Modulation parameters as function of t



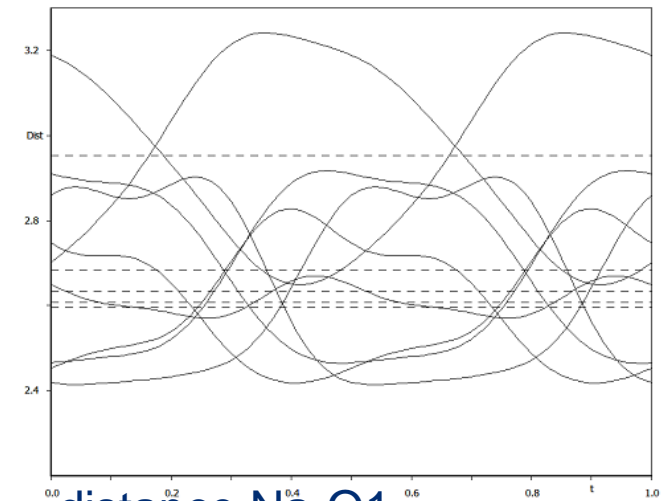
$$x_4 = t + \bar{\mathbf{r}} \cdot \mathbf{q}$$

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 a_3 , not A_3 .

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

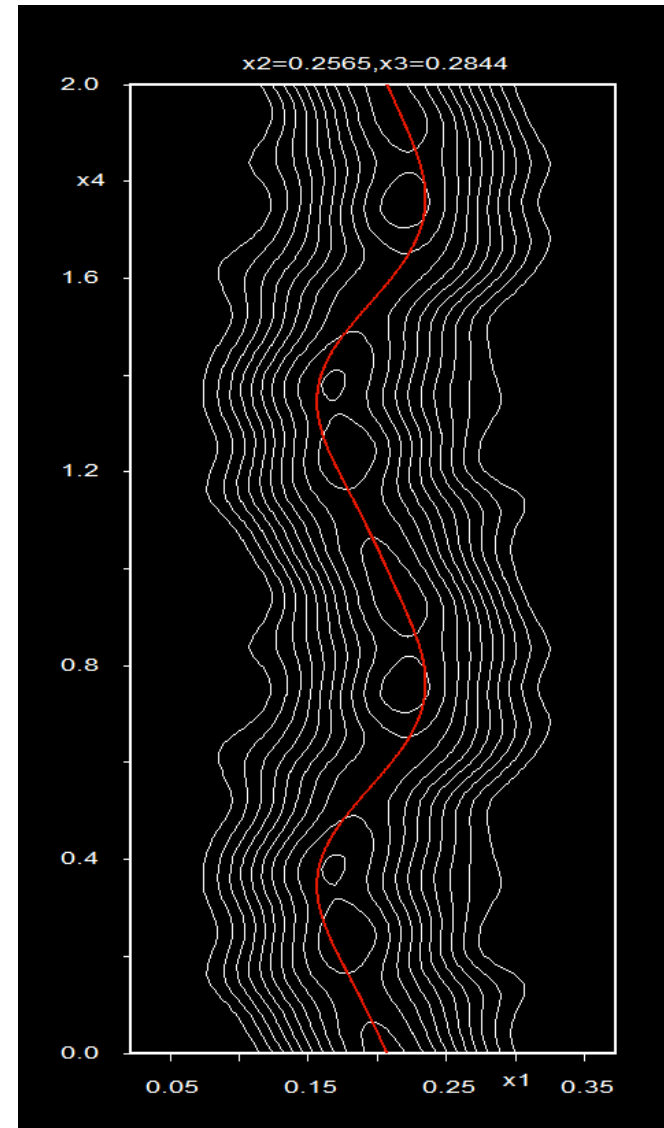
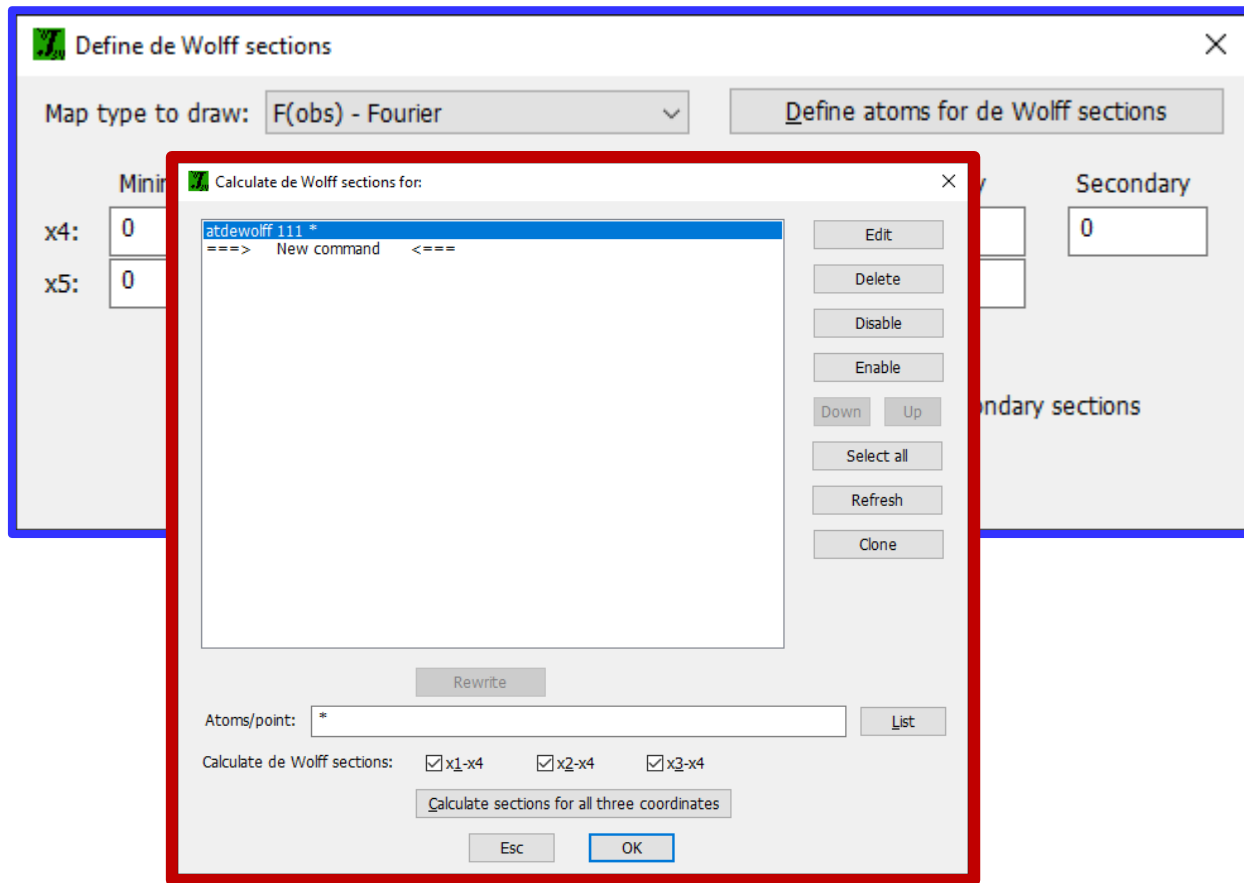
Graph



distance Na-O1

Cookbook example 5.2

Advanced tools – Fourier sections

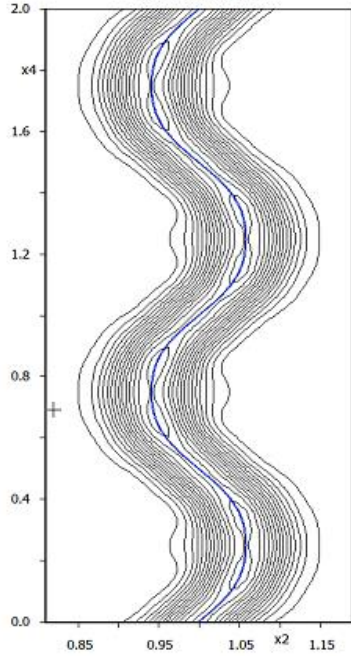


Checking results in
Fourier:

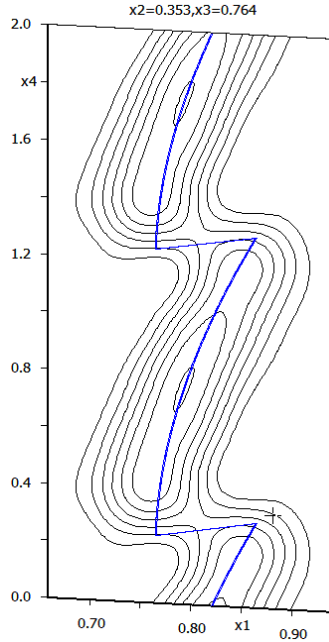
A_1 - A_4 Fourier sections

Modulated structures - Special modulation functions

Displacive modulation

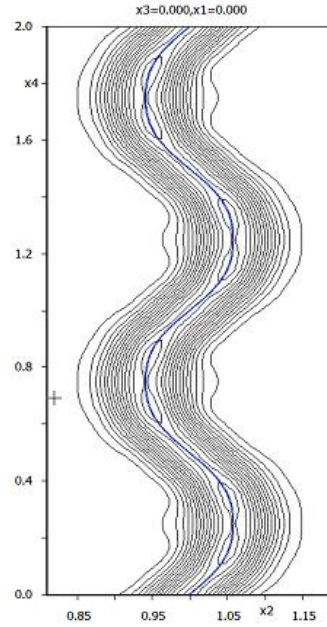


harmonic

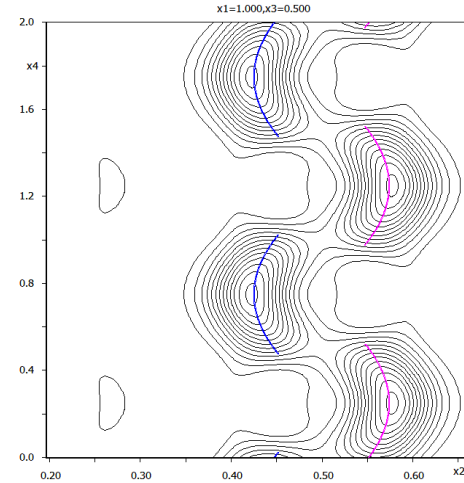


Saw-tooth

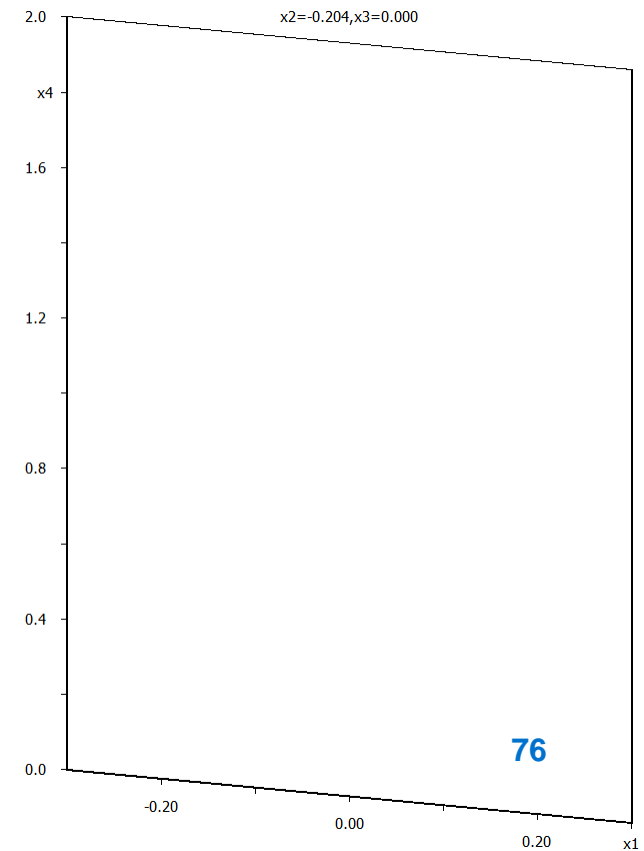
Occupational modulation



harmonic



Crenel



Define/Edit atom parameters

Define Edit Multipole parameters Modulation parameters Magnetic parameters

1 Select atom(s) from list Atom Pb1 Atomic type: Pb

ADP parameter(s):

- isotropic
- harmonic (anisotropic)
- anharmonic
- Use TLS

Modulation waves:

Occupancy: 0 use crenel occupancy from interval <0,1>

Position: 2 use saw-tooth use zig-zag

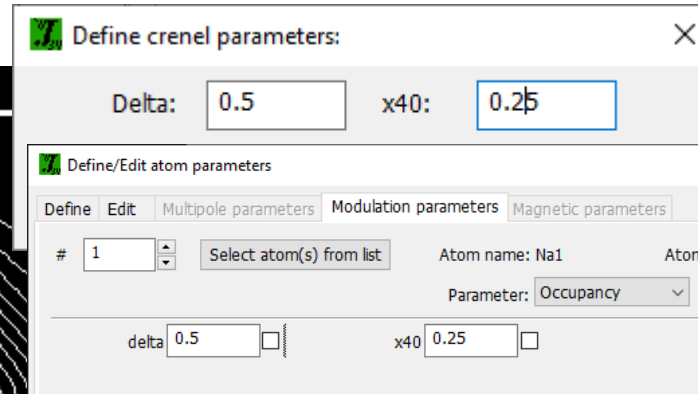
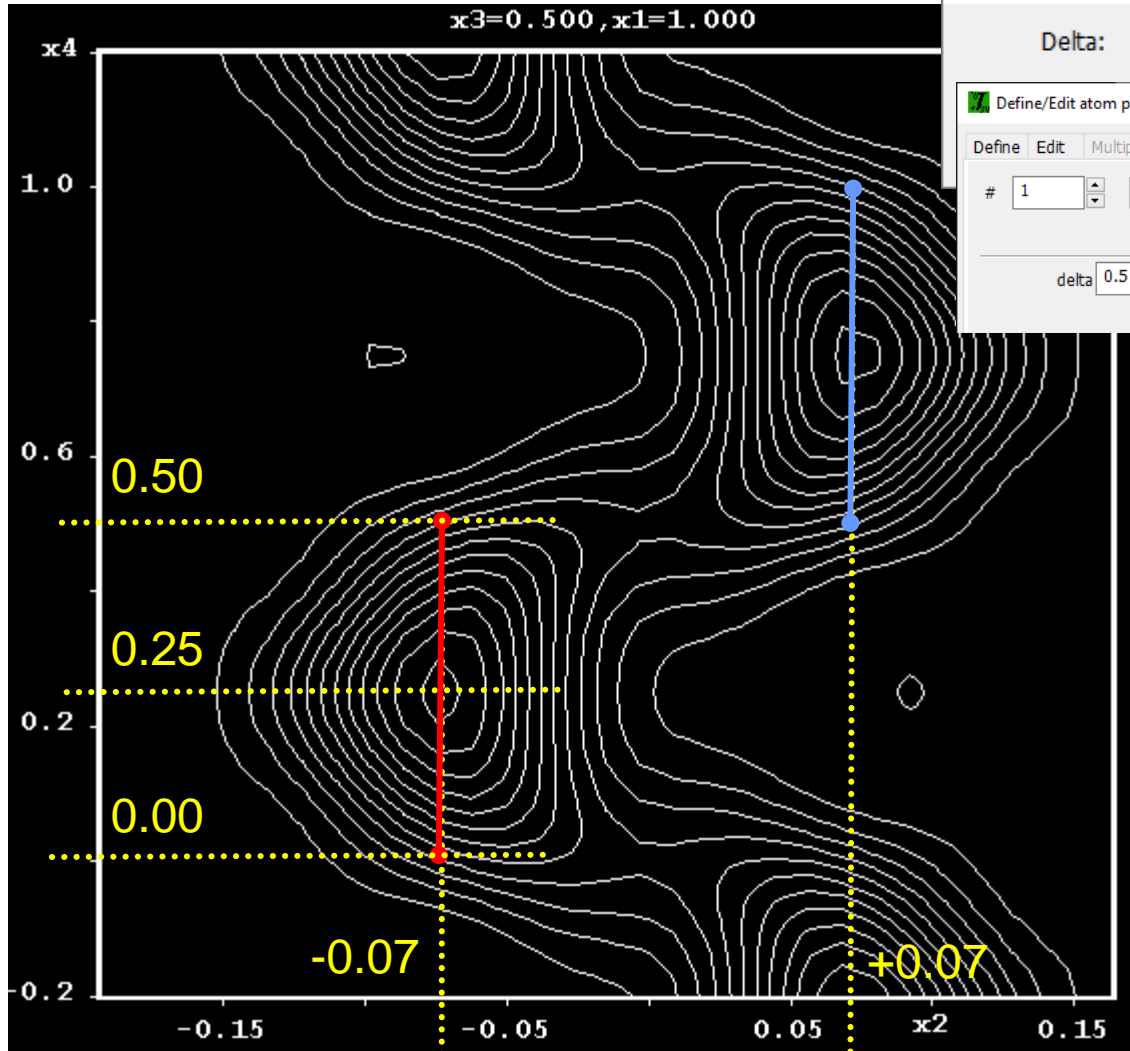
ADP 2nd: 2

Type of modulation functions:

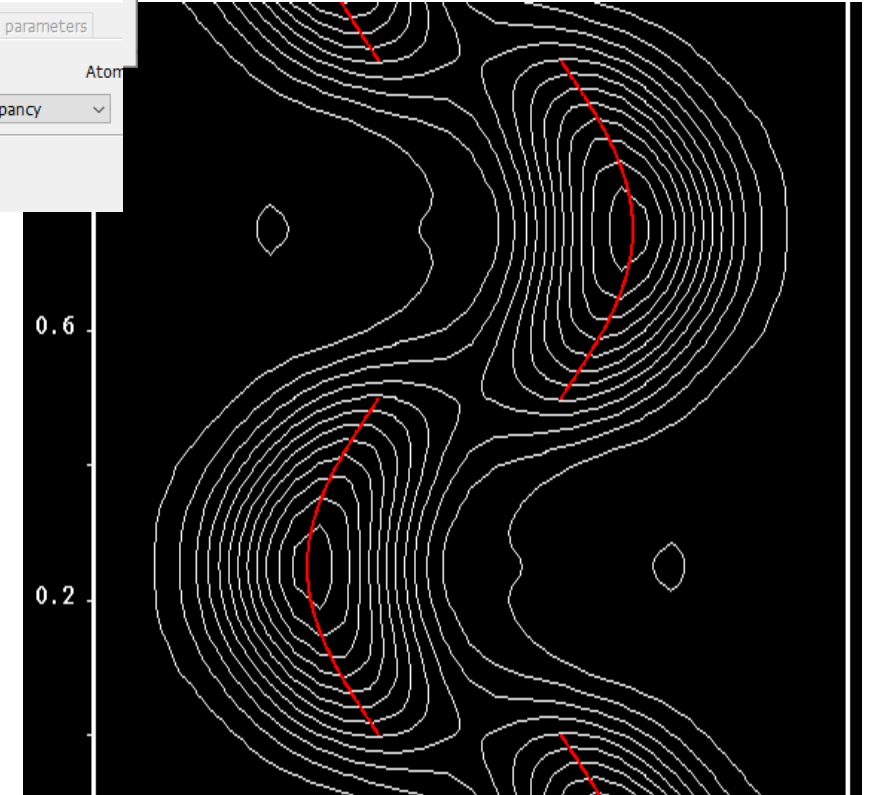
- harmonics in interval (0,1)
- harmonics in interval (0,1) orthogonalized to crenel interval
- Legendre polynomials in crenel interval
- x-harmonics in crenel interval

Selection limit for harmonics:

Modulated structures - Parameters of crenel function

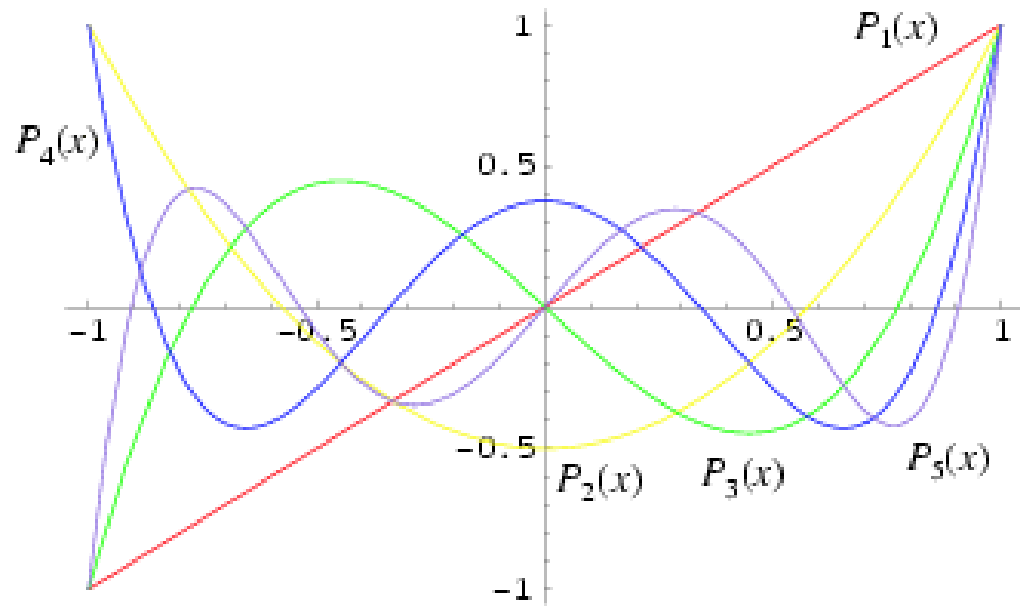


width and center of the crenel function



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

Modulated structures – Combination of functions



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

$$P_0(x) = 1$$

$$P_1(x) = x$$

$$P_2(x) = \frac{1}{2}(3x^2 - 1)$$

$$P_3(x) = \frac{1}{2}(5x^3 - 3x)$$

$$P_4(x) = \frac{1}{8}(35x^4 - 30x^2 + 3)$$

$$P_5(x) = \frac{1}{8}(63x^5 - 70x^3 + 15x)$$

$$P_6(x) = \frac{1}{16}(231x^6 - 315x^4 + 105x^2 - 5)$$

The additional modulation is expressed by Legendre polynomials

$$\mathbf{r}_v = \mathbf{r}_{v,0} + \sum_n \mathbf{U}_{vn}^s \sin(2\pi n x_4) + \mathbf{U}_{vn}^c \cos(2\pi n x_4)$$

$$\mathbf{r}_v = \mathbf{r}_{v,0} + \sum_n \mathbf{S}_{vn}^o P_n^o [2(x_4 - x_{40})/\Delta] + \mathbf{S}_{vn}^e P_n^e [2(x_4 - x_{40})/\Delta]$$

with harmonic waves

with Legendre polynomials

“o” and “e” indicate odd and even member. The first polynomial, 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.

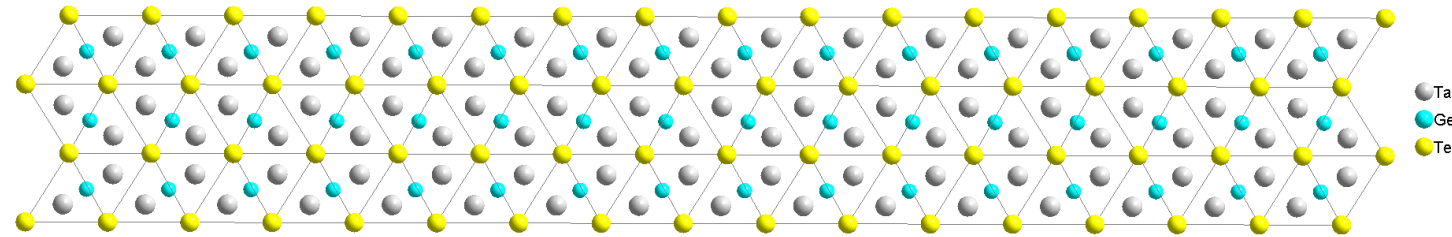
Results presentation

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:

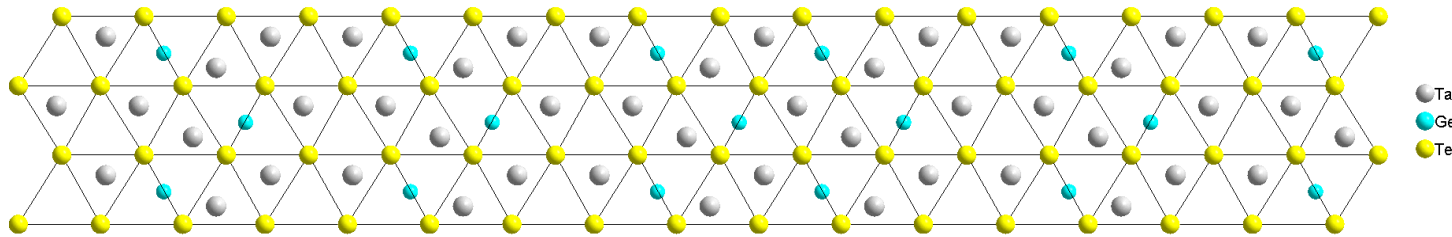
The same example as for the crenel function - $\text{TaGe}_{0.354}\text{Te}$

F. Boucher, M. Evain & V. Petříček, (1996). *Acta Cryst.*, B52, 100

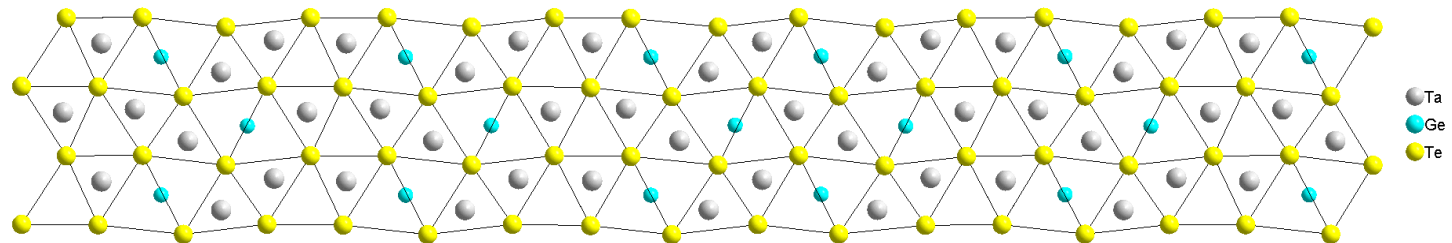
Average structure



Only occupational modulation



Final result

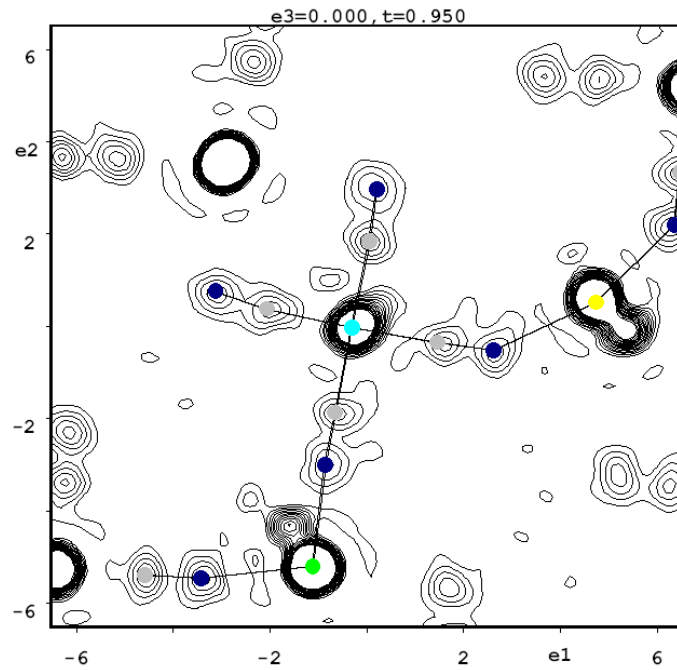


FZU

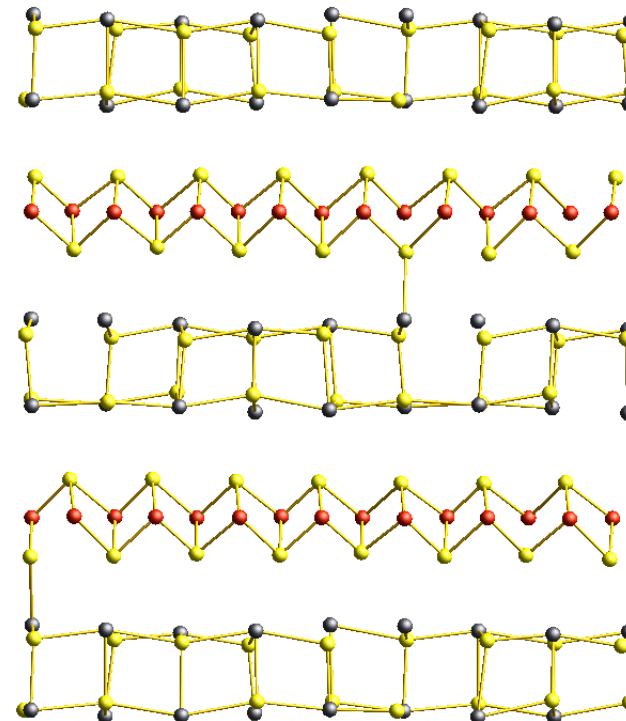
Institute of Physics
of the Czech
Academy of Sciences

Results presentation

Fourier maps as a movie



JanaDraw movie



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

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Thank you for your attention!