Jana 2020

Margarida Henriques
Václav Petříček

FZU Fyzikální ústav Akademie věd České republiky

Magnetic Structure Determination from Neutron Diffraction Data
October 7th
ORNL

History

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.*

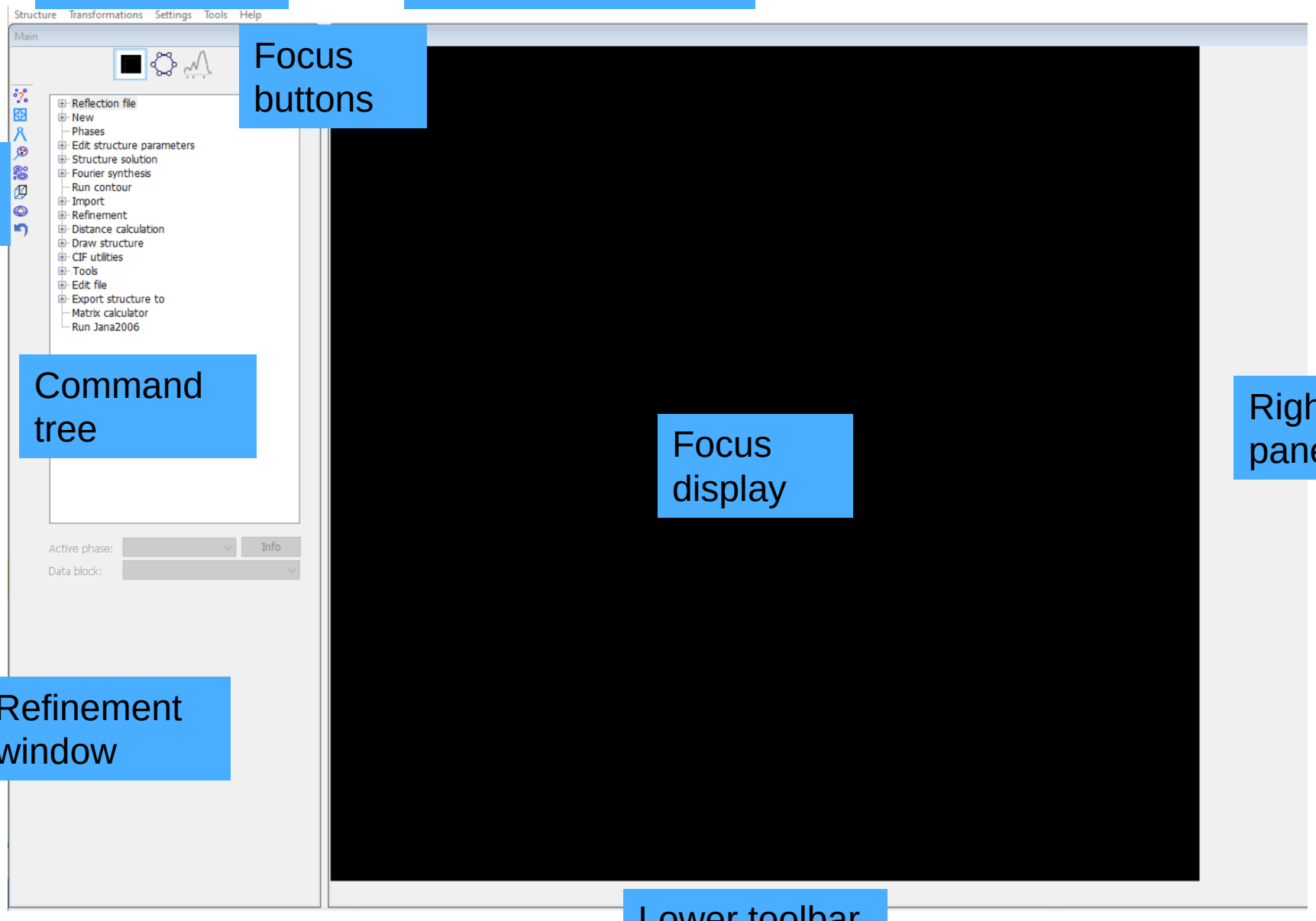
1998 Jana98 — *Improved Jana96. First widely used version. Graphical interface for DOS, DOS emulation, UNIX X11.*

2000 Jana2000 — *Support for powder data and multiphase refinement. Graphical interface for Win32 and UNIX X11.*

2006 Jana2006 — *Combination of data sources, magnetic structures, TOF data. Dynamical allocation of memory. Only for Windows.*

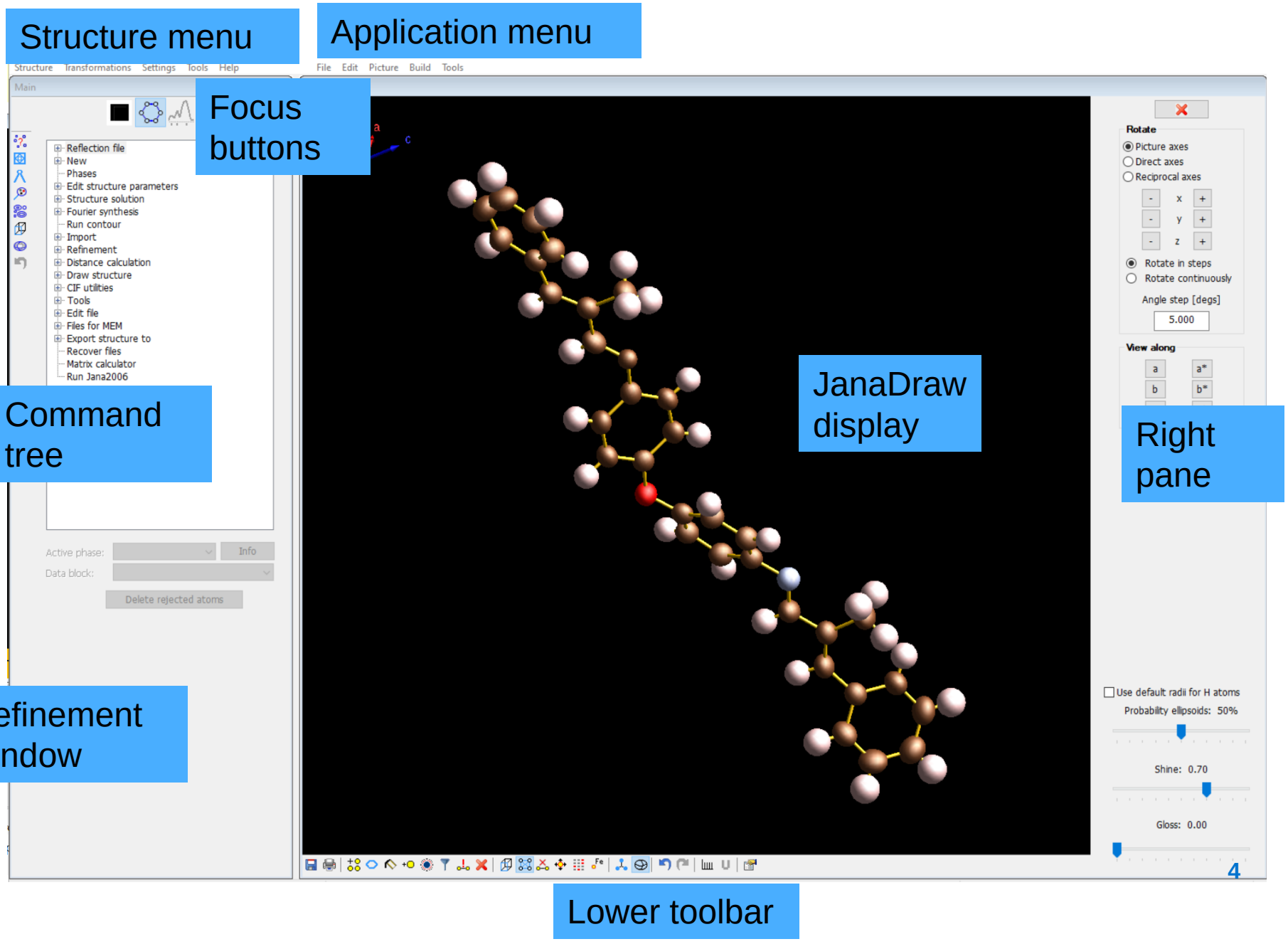
2020 Jana2020 — *New graphic interface and user-friendly approach.*

Jana2020



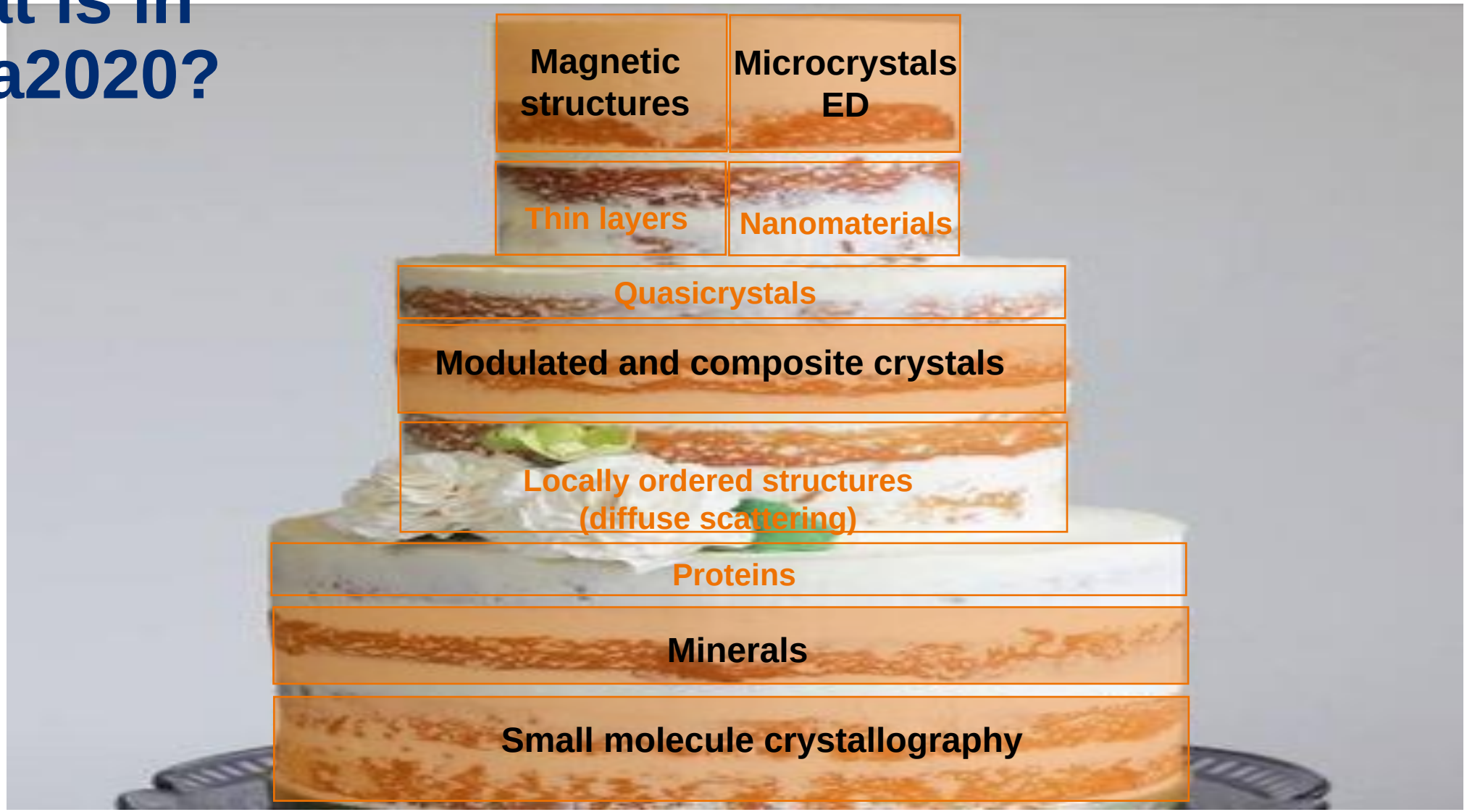
FZU Fyzikální ústav Akademie věd České republiky

Jana2020

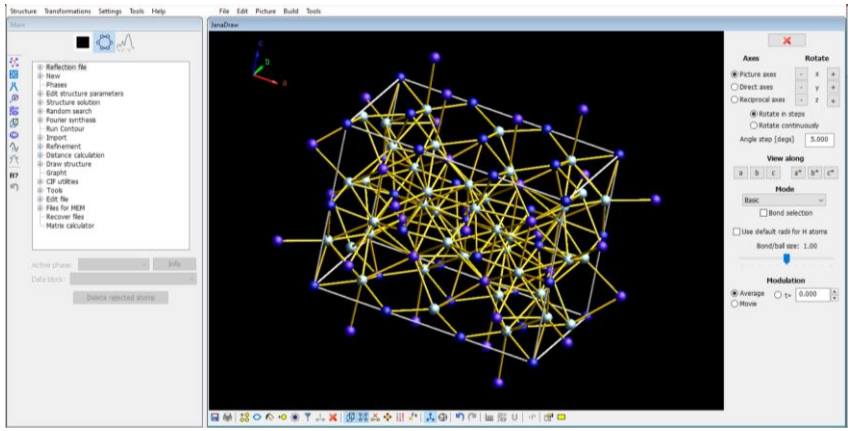


FZU Fyzikální ústav Akademie věd České republiky

What is in Jana2020?



Jana2020



1

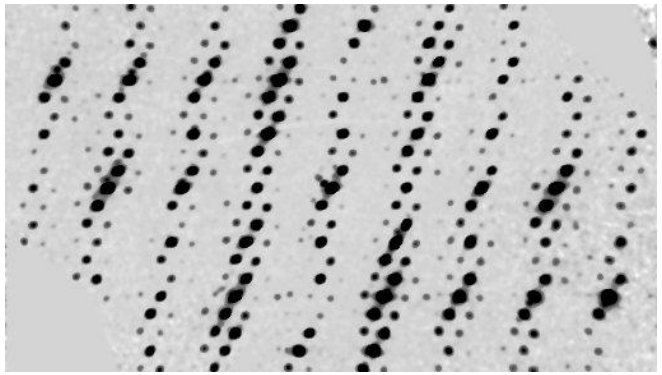
GENERIC FEATURES

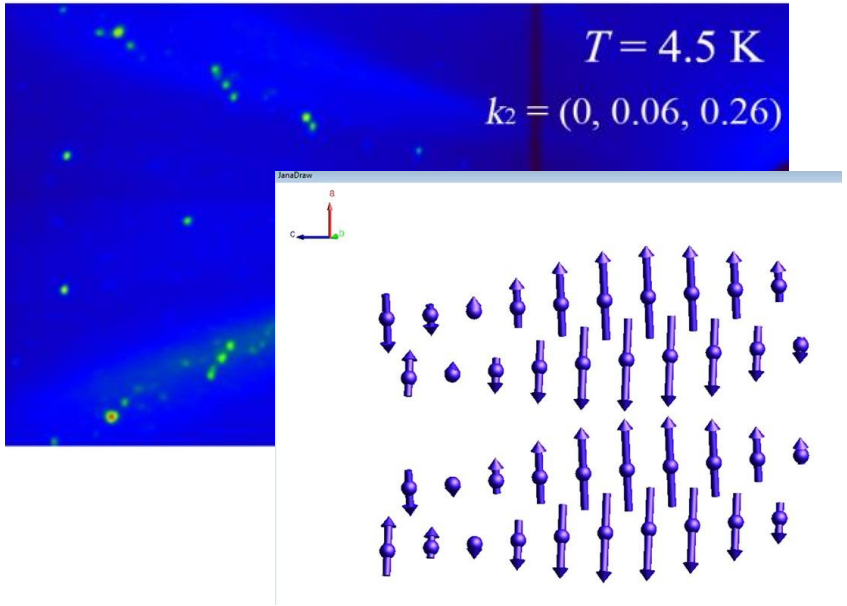
Generic crystallography

2

ADVANCED TOOLS

Structure solution and analysis of crystals from diffraction data in (3+n)D: twinned, modulated, composite structures





3

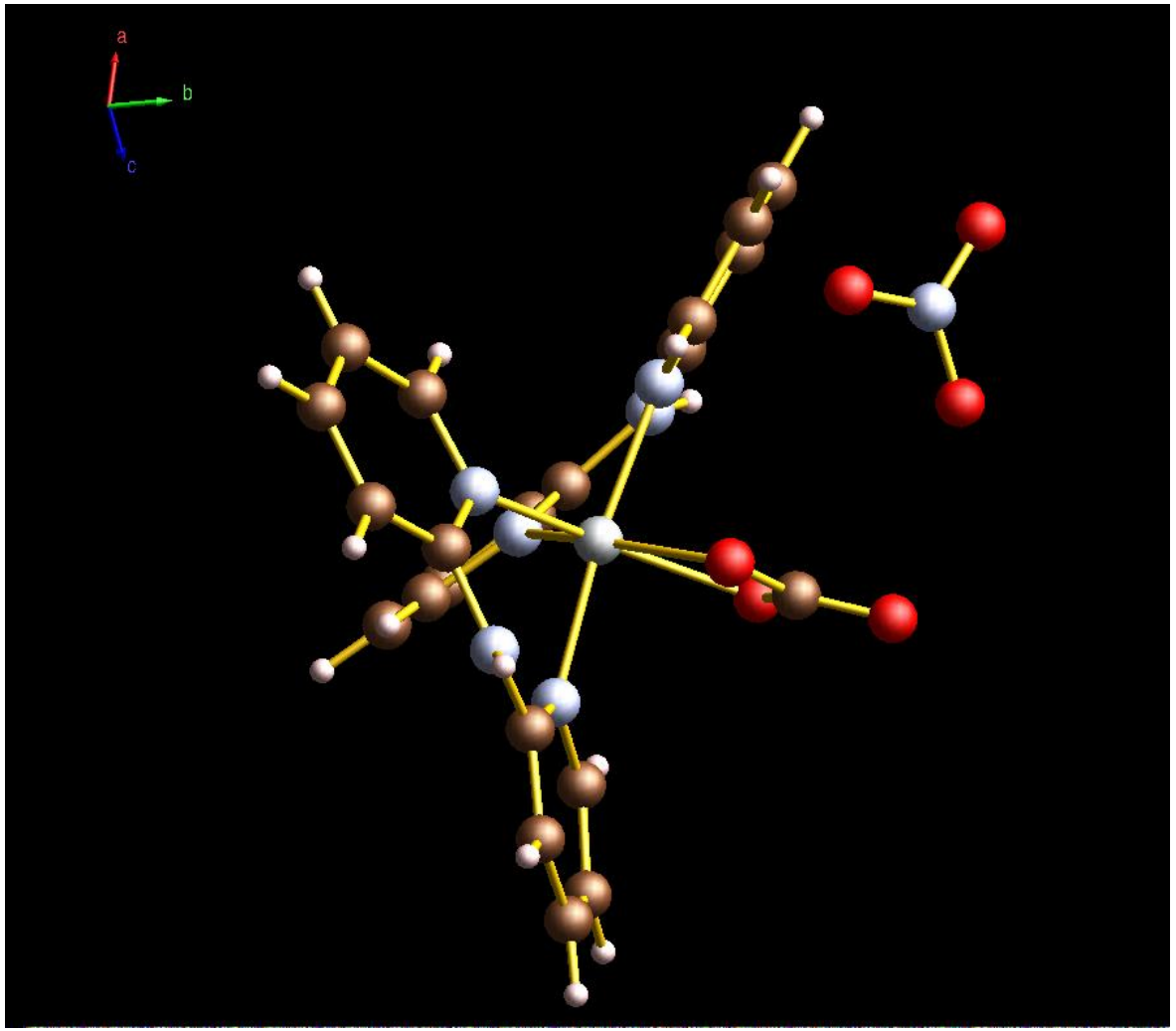
MAGNETIC OPTION

Solution and refinement of magnetic structures from powder and single crystal diffraction data sets

Jana2020

Regular structures

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



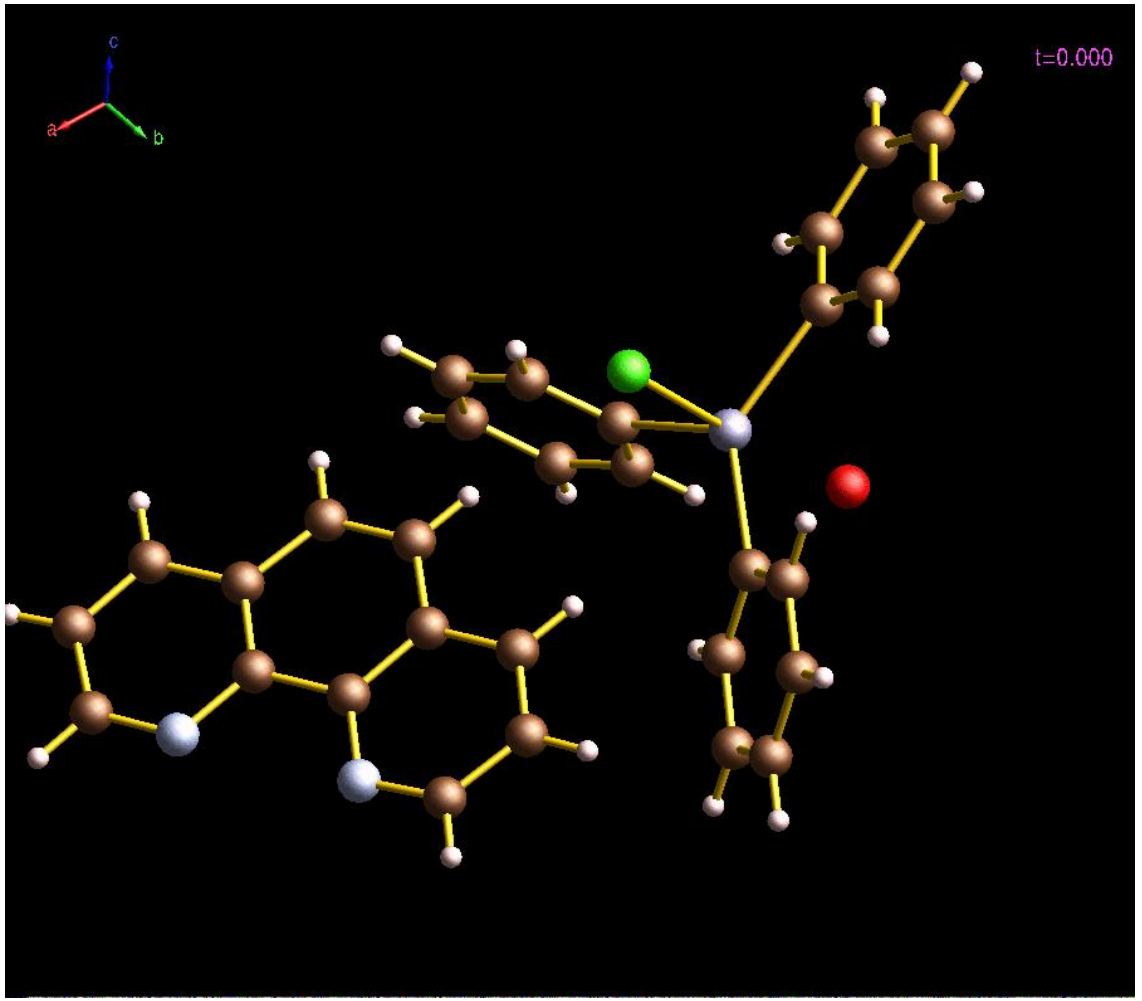
Jana2020

Modulated crystal structures

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

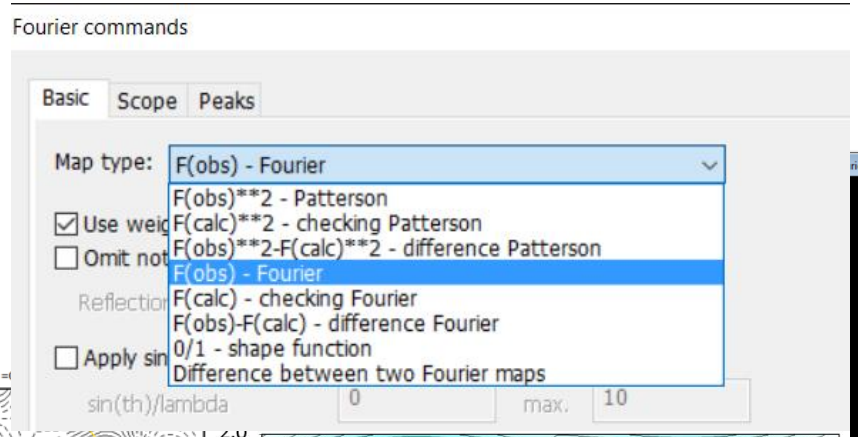
+

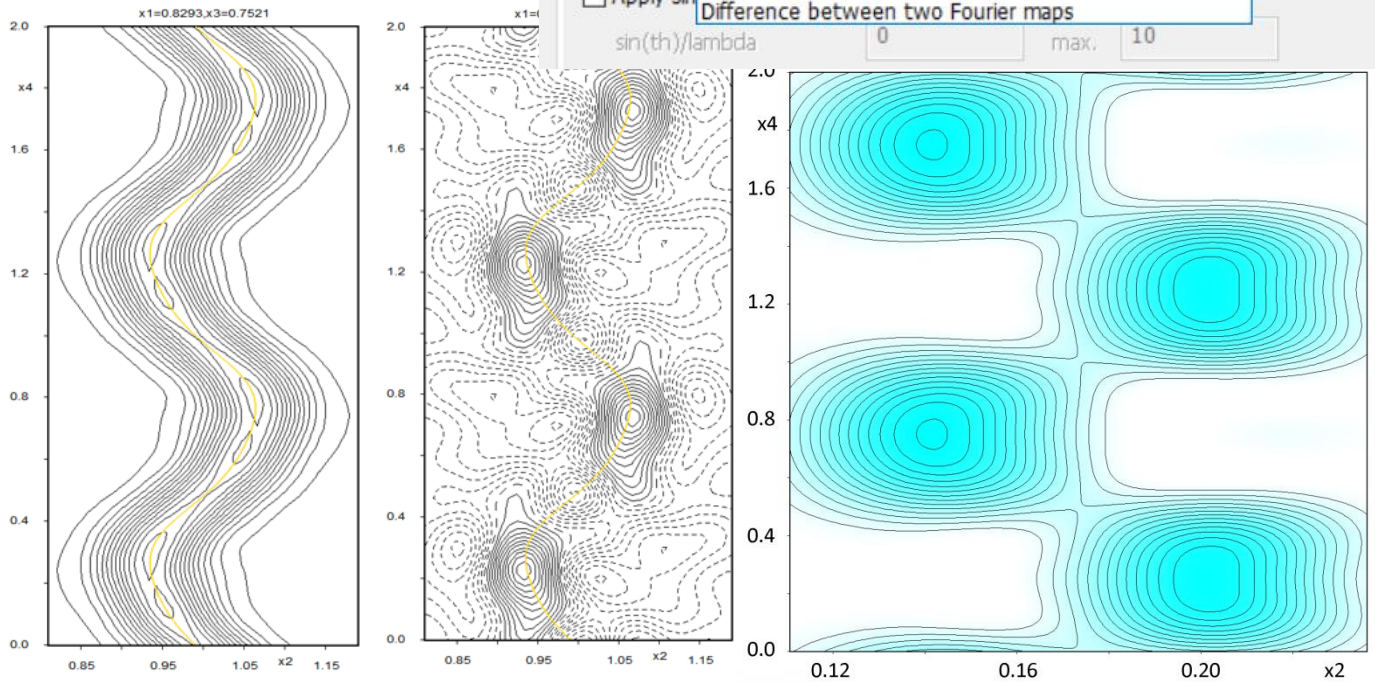
$$p(x_4) = p_0 + \sum_n \left(p_{s,n} sin2\pi n x_4 + p_{c,n} cos2\pi n x_4\right)$$

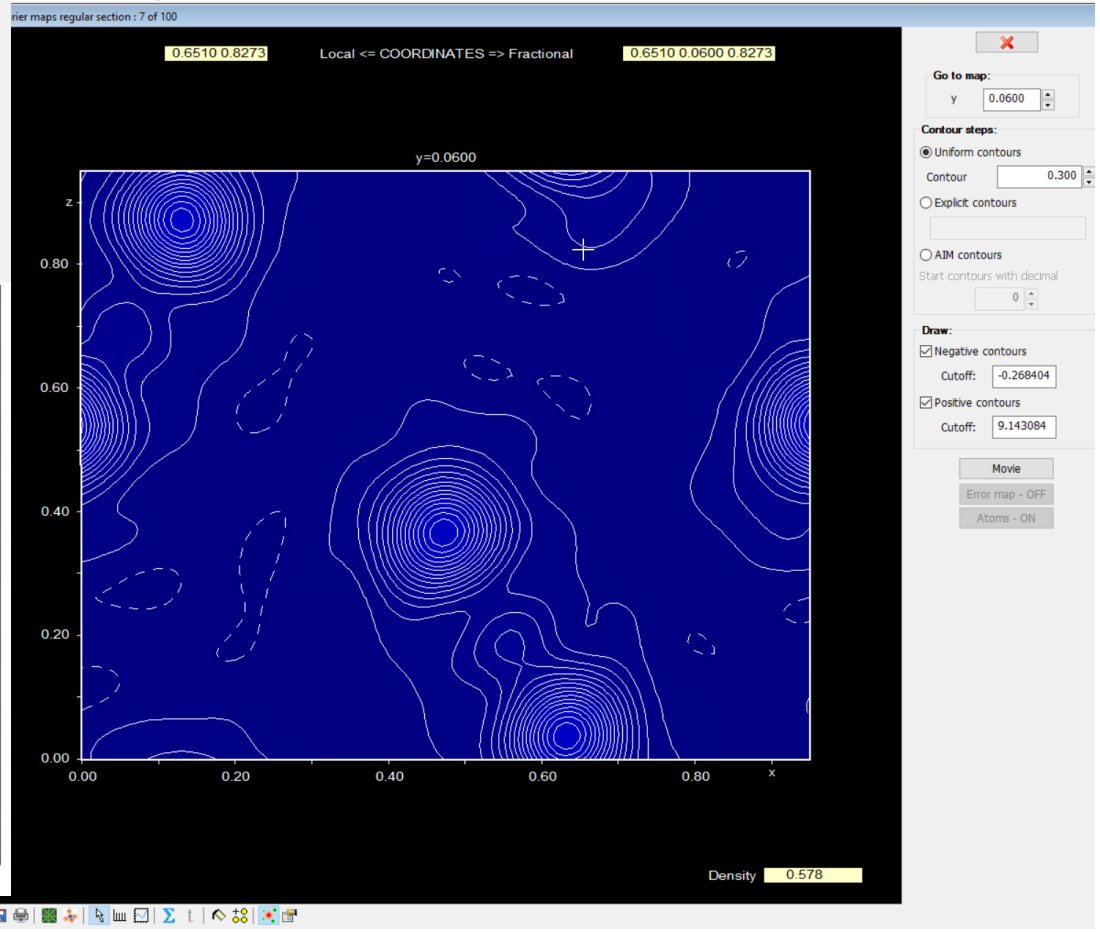


Jana2020: advanced tools (common for 3d and modulated structures)

- **Fourier analysis**

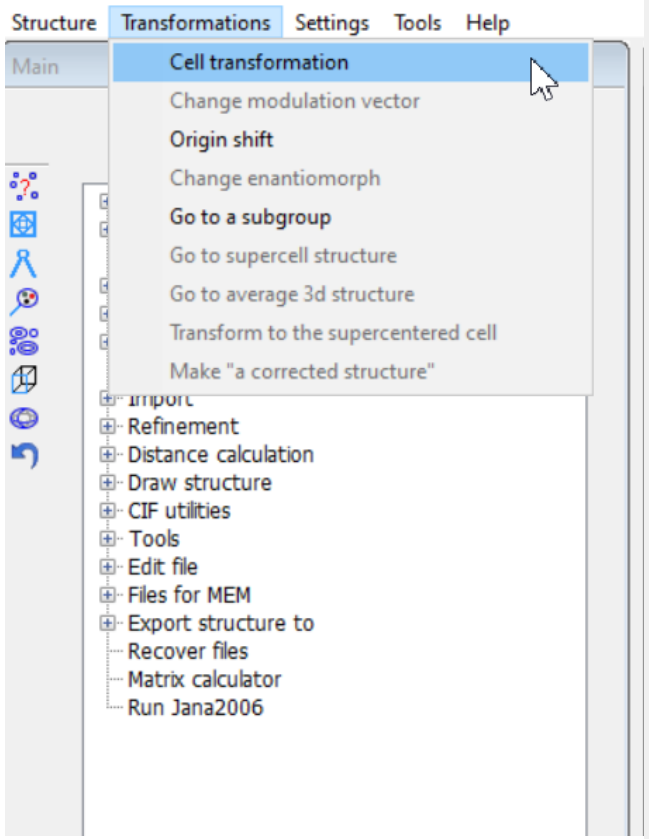


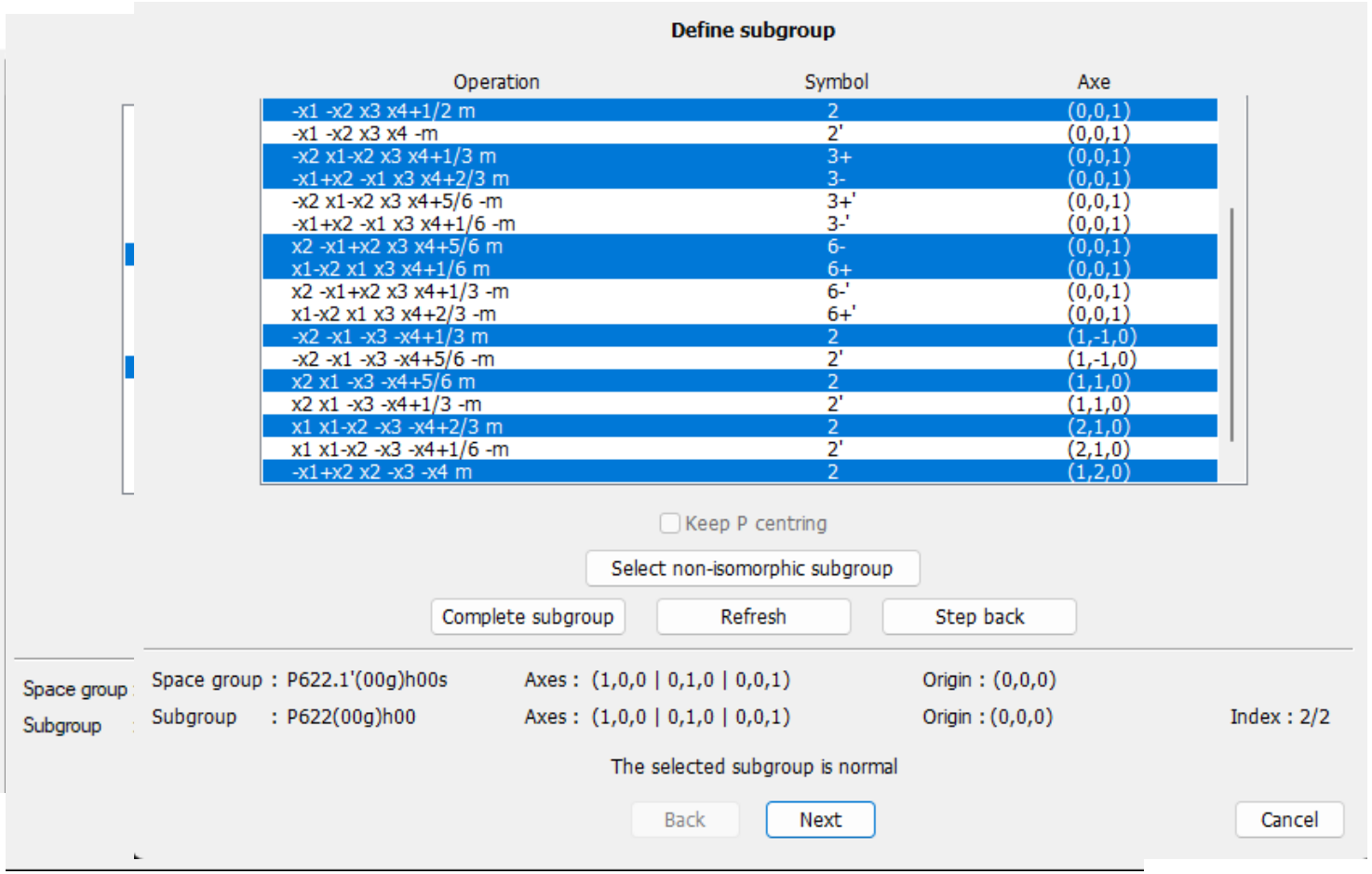




Jana2020: advanced tools

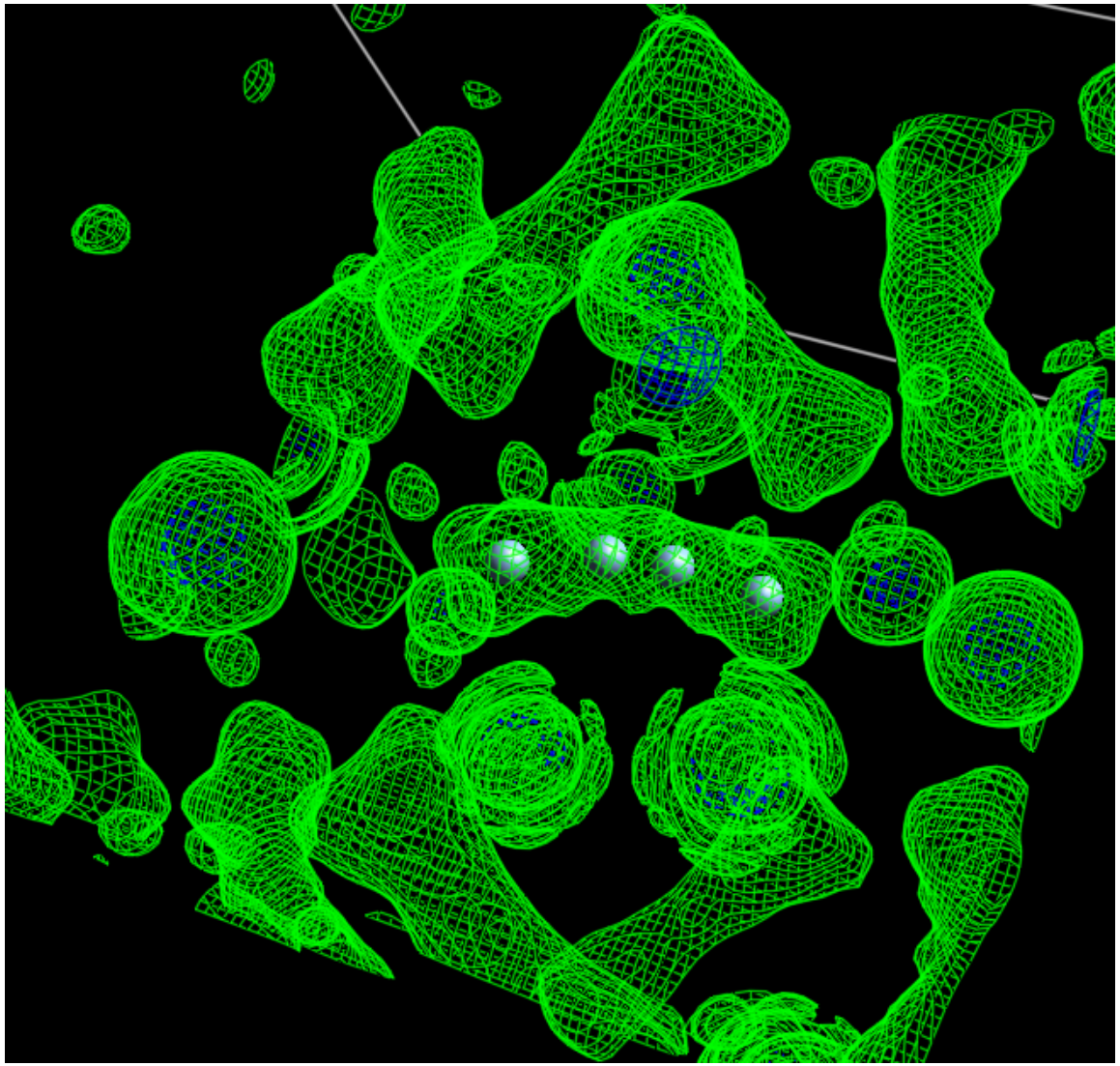
- **Transformation tools, group-subgroup relations**





Jana2020: advanced tools

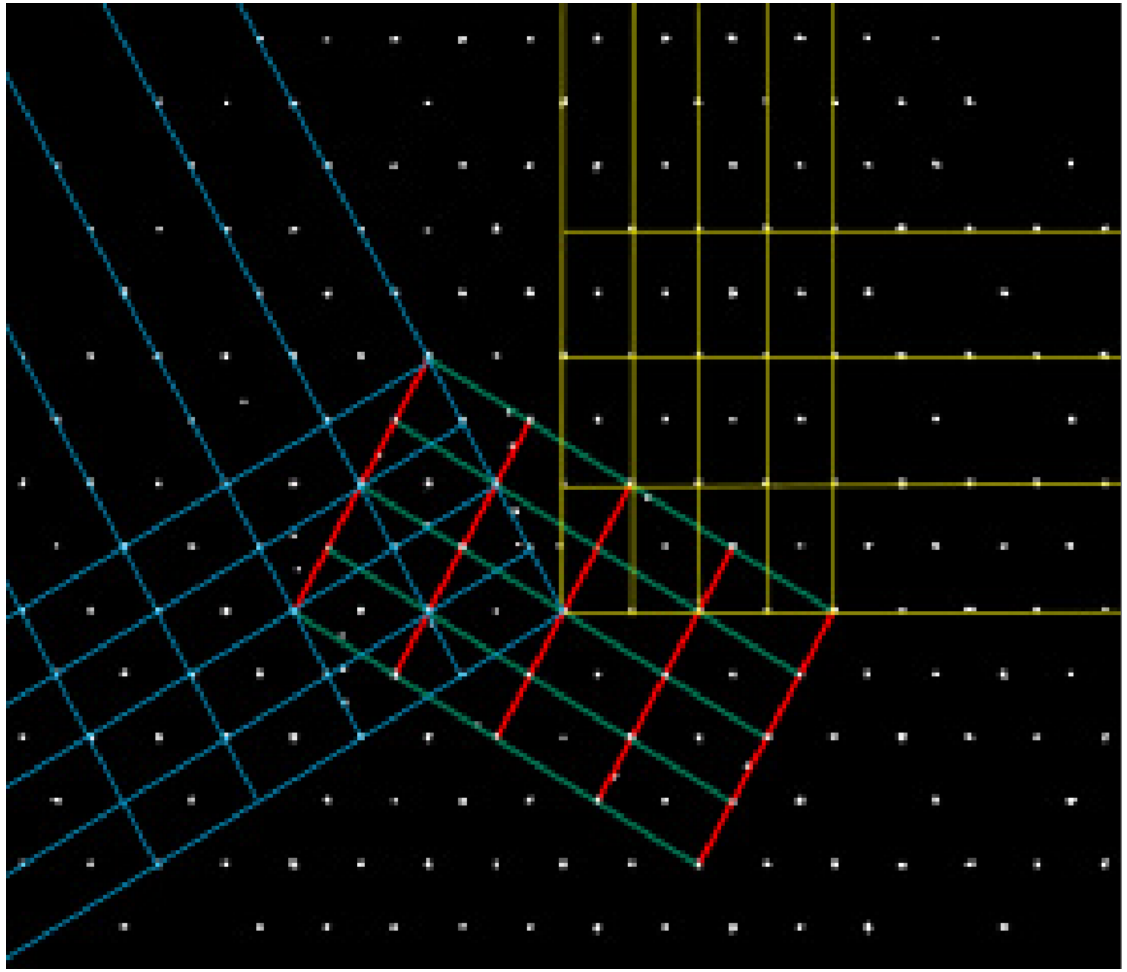
- **Disorder and “rigid body” approach**
  Anharmonic ADP



Jana2020: advanced tools

- **Twinning (merohedric or general), treating of overlapped reflections**

pseudo-merohedric three-fold twin



Jana2020

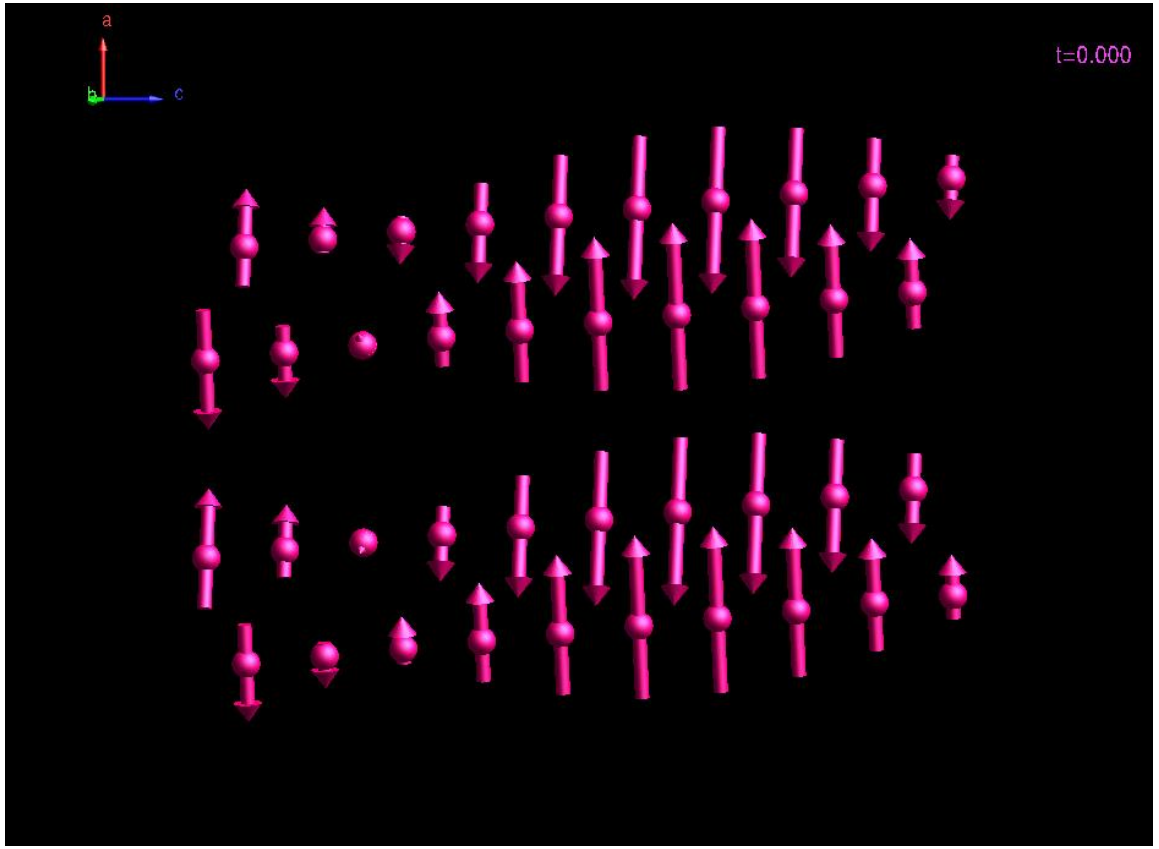
Magnetic structures

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

+

Magnetic moments

(commensurate/incommensurate)



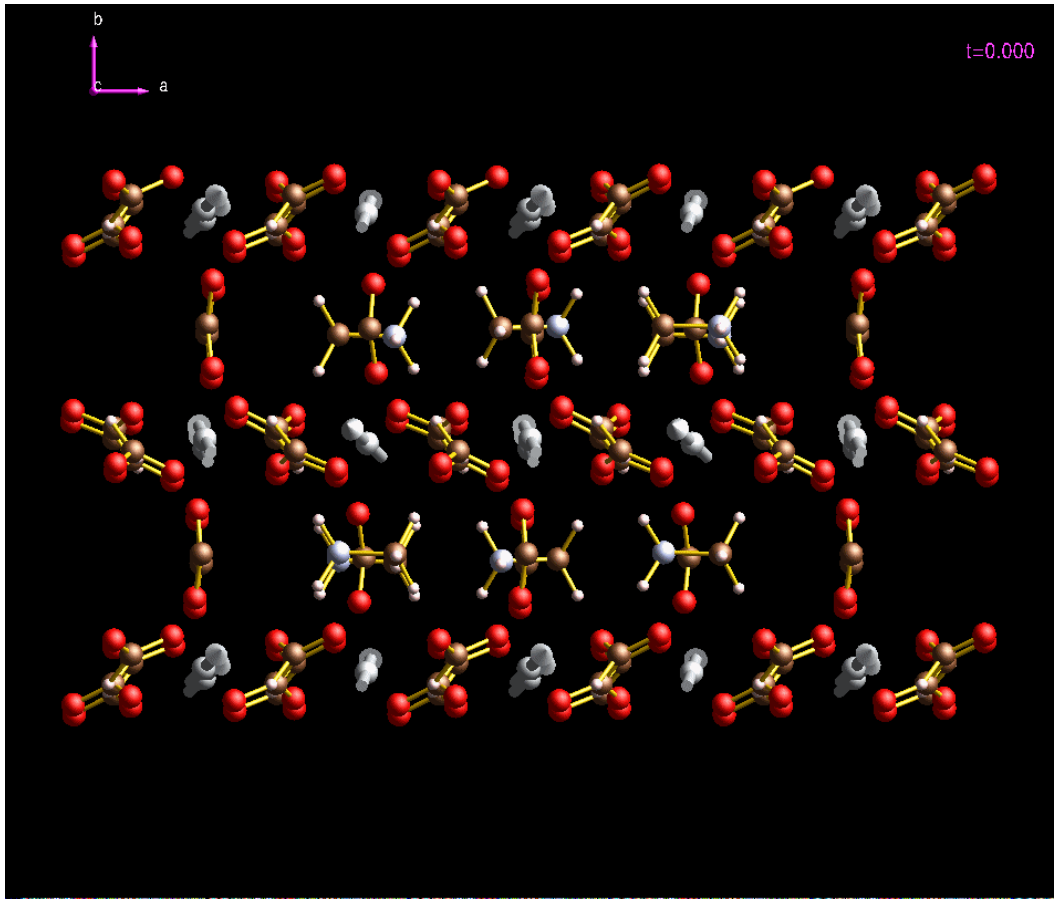
Jana2020

Magnetic structures

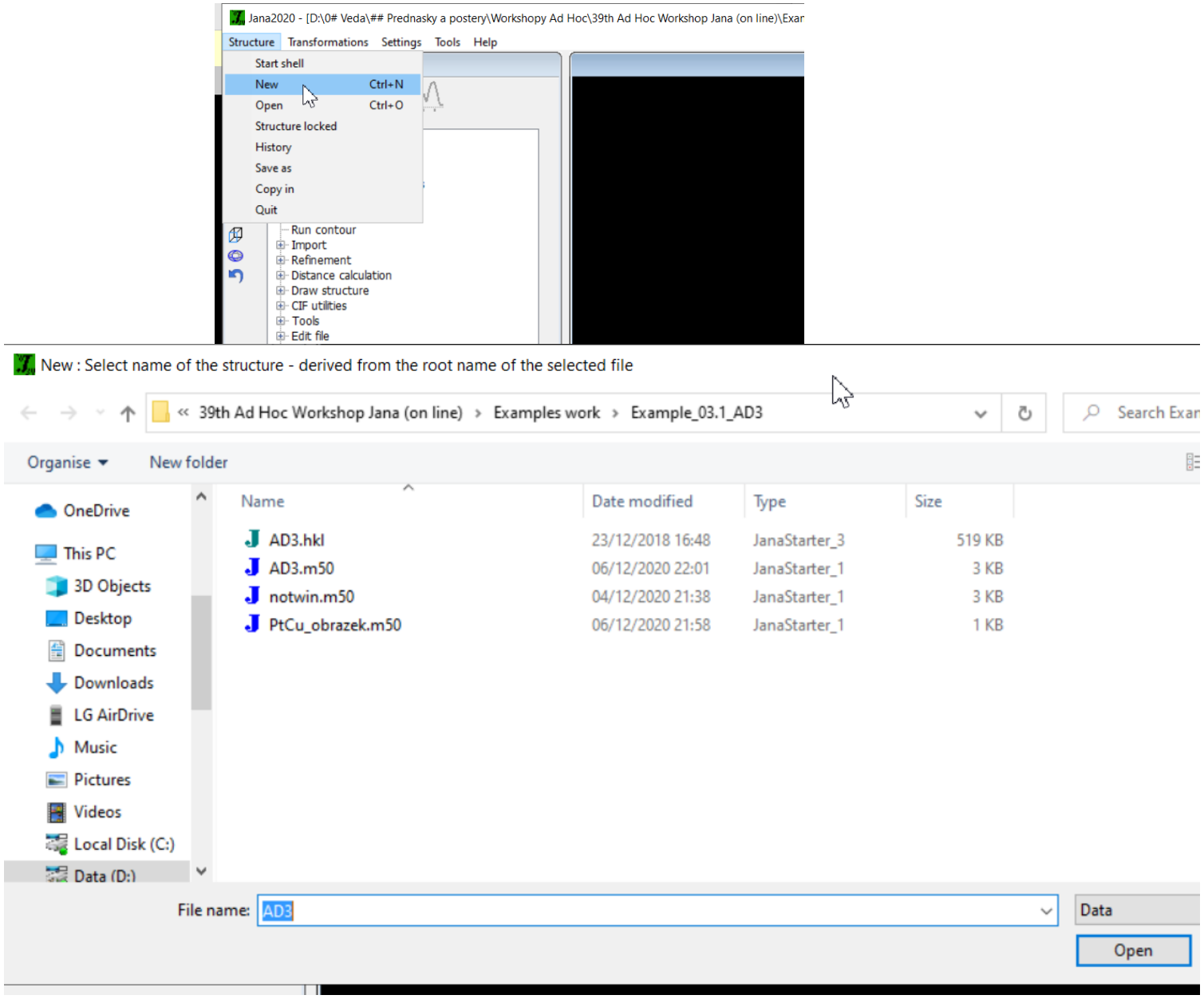
- Scale factor
- Extinction parameters
- Atomic site coordinates and occupancies
- ADPs (Temperature parameters)
- Magnetic moments

+

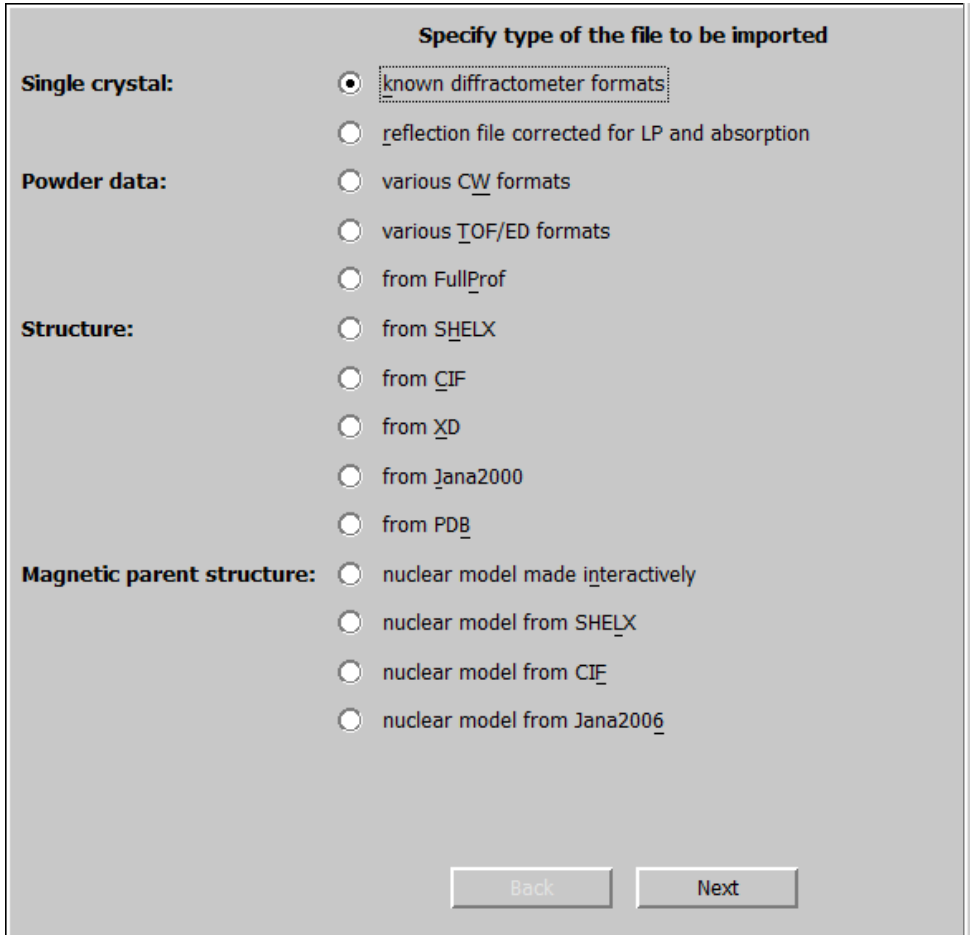
Modulation functions for the atomic parameters

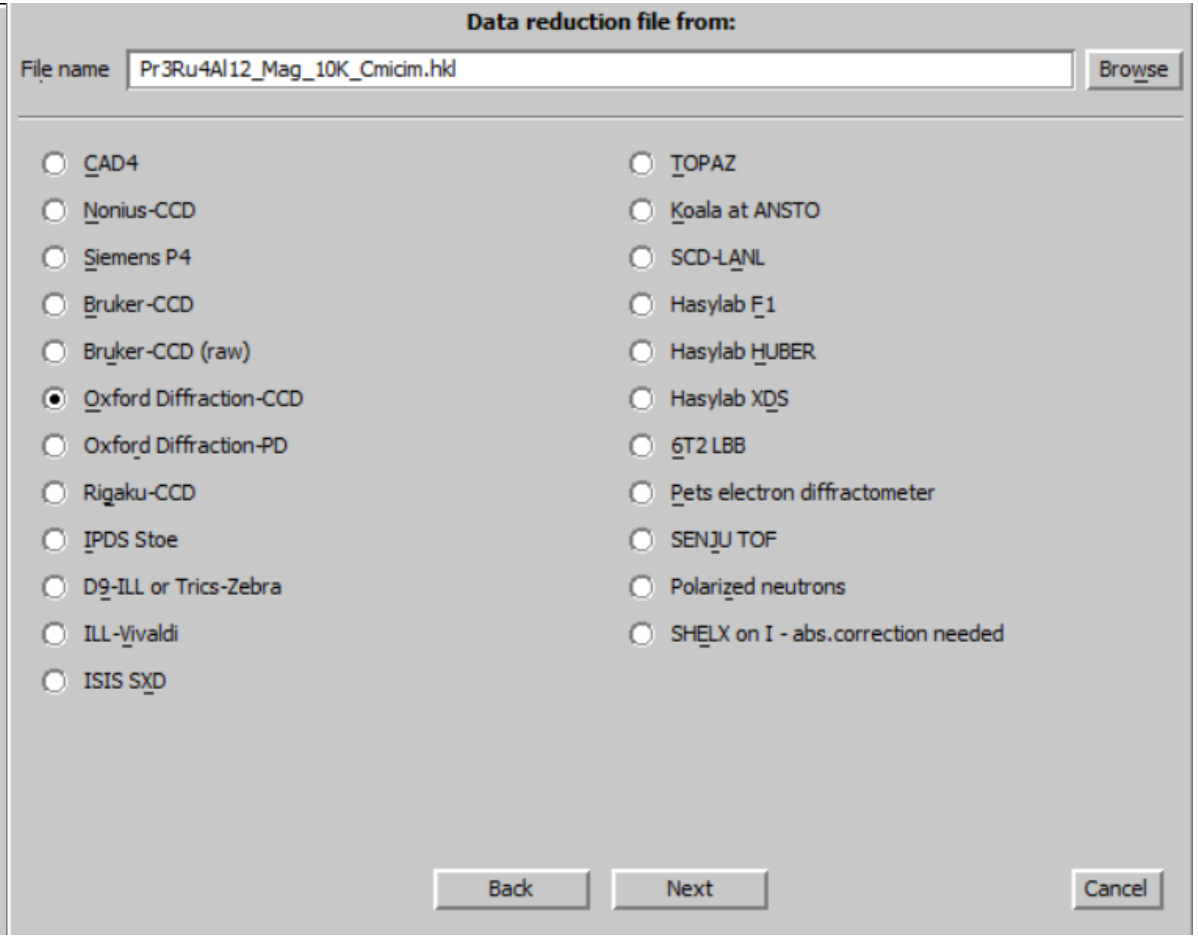


Jana2020


Jana2020 - [D:\0# Veda\## Prednasky a postery\Workshopy Ad Hoc\39th Ad Hoc Workshop Jana (on line)\Exar
Structure
Transformations
Settings
Tools
Help
Start shell
New Ctrl+N
Open Ctrl+O
Structure locked
History
Save as
Copy in
Quit
Run contour
Import
Refinement
Distance calculation
Draw structure
CIF utilities
Tools
Edit file
New : Select name of the structure - derived from the root name of the selected file
« 39th Ad Hoc Workshop Jana (on line) › Examples work › Example_03.1_AD3
Search Exar
Organise
New folder
OneDrive
This PC
3D Objects
Desktop
Documents
Downloads
LG AirDrive
Music
Pictures
Videos
Local Disk (C:)
Data (D:)
Name
Date modified
Type
Size
AD3.hkl 23/12/2018 16:48 JanaStarter_3 519 KB
AD3.m50 06/12/2020 22:01 JanaStarter_1 3 KB
notwin.m50 04/12/2020 21:38 JanaStarter_1 3 KB
PtCu_obrazek.m50 06/12/2020 21:58 JanaStarter_1 1 KB
File name: AD3
Data
Open

Jana2020


Specify type of the file to be imported
Single crystal:
known diffractometer formats
reflection file corrected for LP and absorption
Powder data:
various CW formats
various TOF/ED formats
from FullProf
Structure:
from SHELX
from CIF
from XD
from Jana2000
from PDB
Magnetic parent structure:
nuclear model made interactively
nuclear model from SHELX
nuclear model from CIF
nuclear model from Jana2006
Back
Next


Data reduction file from:
File name
Pr3Ru4Al12_Mag_10K_Cmicim.hkl
Browse
CAD4
Nonius-CCD
Siemens P4
Bruker-CCD
Bruker-CCD (raw)
Oxford Diffraction-CCD
Oxford Diffraction-PD
Rigaku-CCD
IPDS Stoe
D9-ILL or Trics-Zebra
ILL-Vivaldi
ISIS SXD
TOPAZ
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

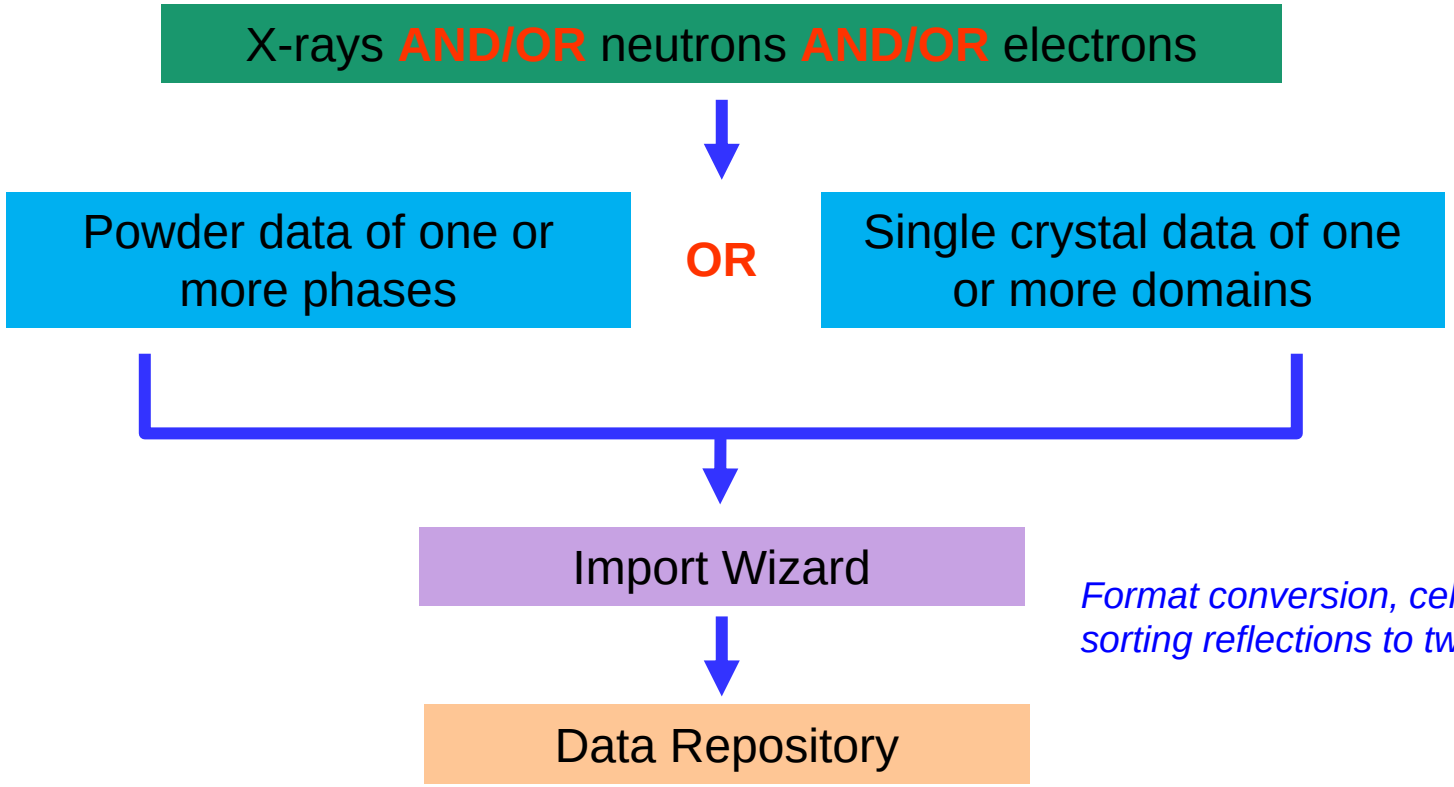
Jana2020 data

Input data: single crystal, powder, CW, TOF

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

Data from different sources can be combined during refinements.

Jana2020



Format conversion, cell transformation, sorting reflections to twin domains

Data repository

File	Type of data	Used radiation
sad_Cu.hkl	I(hkl) imported	X-rays 1.3817
sad_Zn.hkl	I(hkl) imported	X-rays 1.2843
sad_Zr.hkl	I(hkl) imported	X-rays 0.6889
SLO_100K_JANASXD_li.int	Single crystal	Neutrons TOF

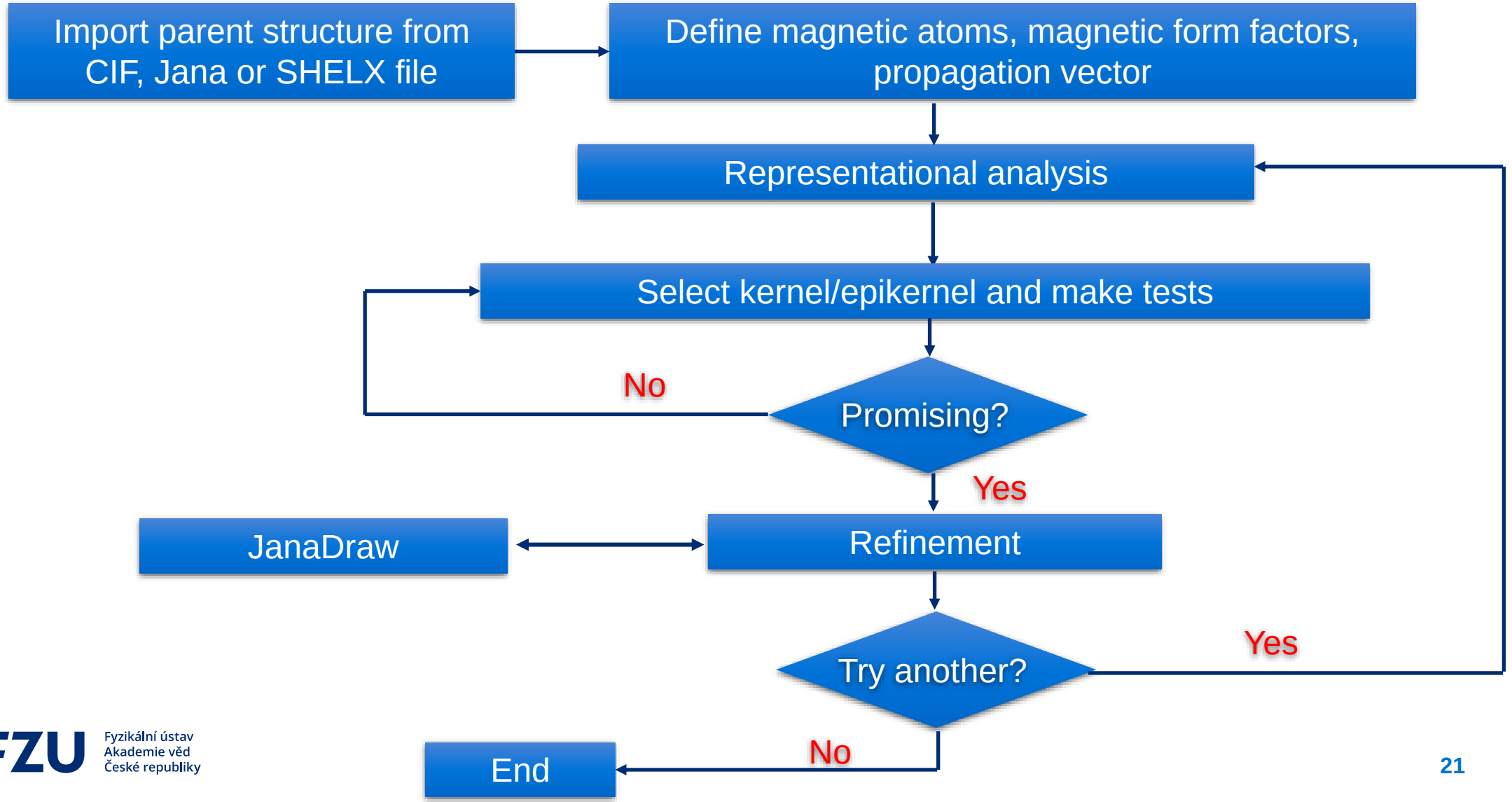
Jana2020: handling symmetry

- Performs symmetry tests by analyzing the reflection files for powder and/or single-crystal data.
- Superspace approach is implemented for (3+d) d=1,2,3 modulated systems.
- It handles any “reasonable” non-standard setting, including non-standard centrings.
- Site symmetry restrictions are generated automatically from the symmetry operations (including modulation, magnetic, and multipole parameters).
- Systematic extinctions are derived analytically
- Support for twinning in the crystal – merohedral, reticular, ….
- Interactive procedure for transforming the structure to lower symmetry.
- Local symmetry can be applied to individual atoms and to (rigid body) groups

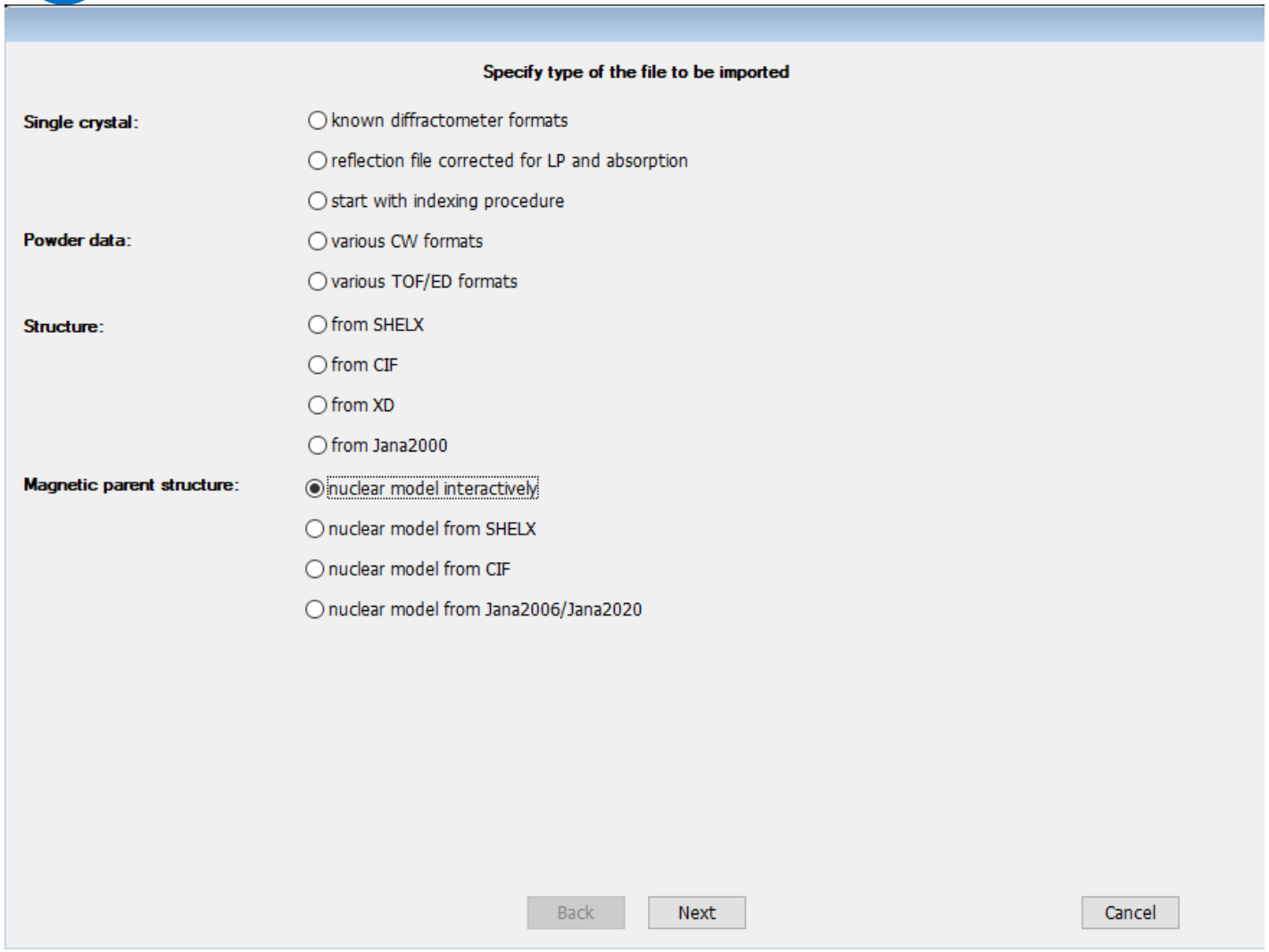
Jana2020: magnetic option

- For calculation of the structure factors the program uses MS(S)G
- It calculates both (mag+nuclear) contributions in parallel and combines them accordingly
- It offers a wizard mode to create a “parent” structure which can be used to test different groups (can be interrupted to go any other way)
- There is a simple tool for RA which can help you to test different possible space groups (calculated for the set of active irreps in the structure)
- For graphic visualization
  - JanaDraw
  - calls “VESTA” or it creates an input file for other programs

Jana2020: magnetic option



Jana2020

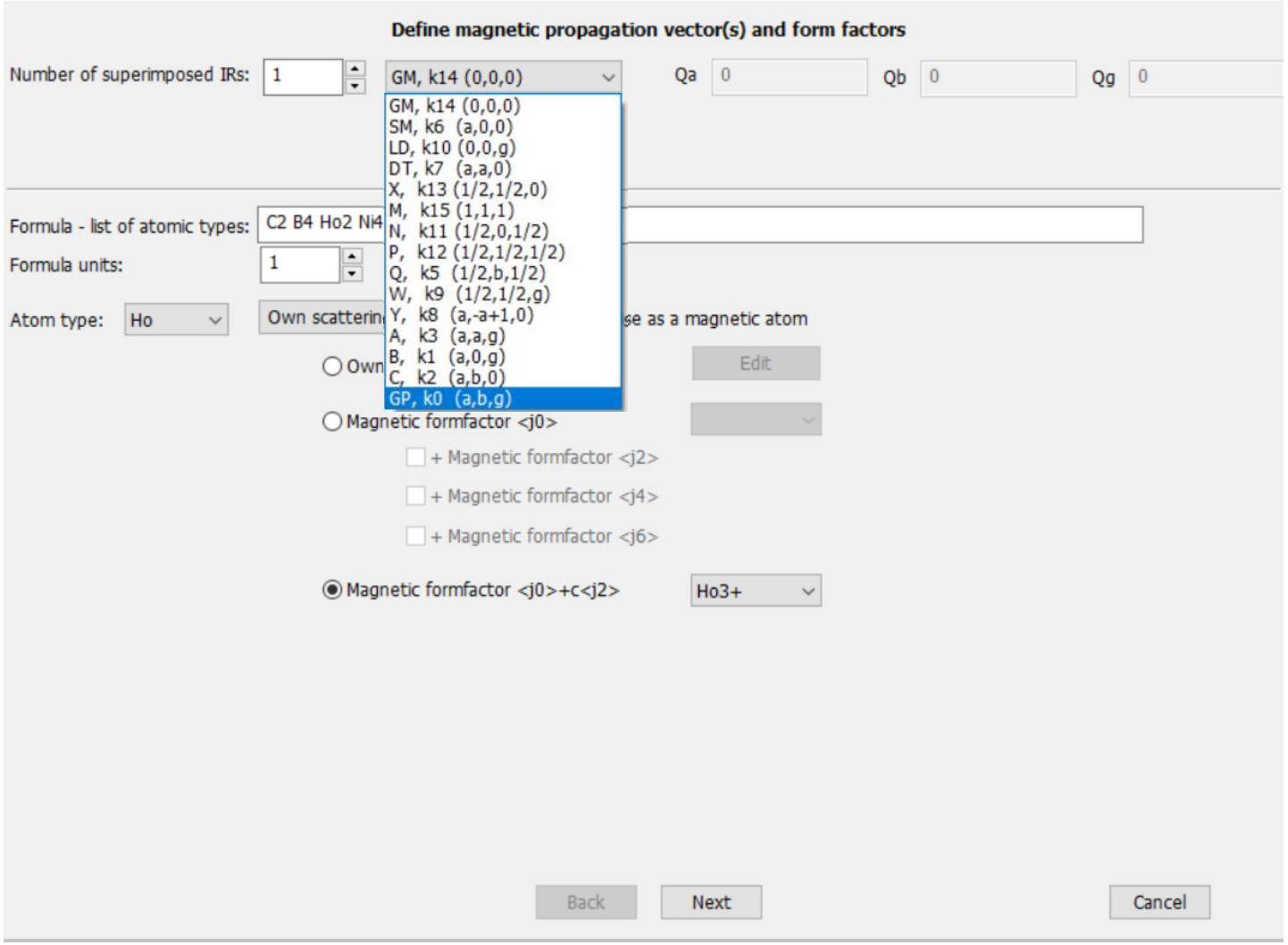


For magnetic structures from powder data, the import wizard goes through:

- Data import
- Profile refinement by le Bail method
- Rietveld refinement
- Representation analysis

Jana2020: magnetic option

Defining propagation vectors and magnetic atoms



FZU Fyzikální ústav Akademie věd České republiky

Jana2020: magnetic option

Representation analysis

List of irreps and correspoding kernel symmetries:

Representation	Dimension	Shubnikov space group	Axes	Origin shift	
mGM1+	1	P63/mmc	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0)	Details
mGM2+	1	P63/mm'c'	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0)	Details
mGM3+	1	P63'/m'mc'	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0)	Details
mGM4+	1	P63'/m'm'c	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0)	Details
mGM5+	2	P21/m	(-1,0,0 | 0,0,-1 | 0,-1,0)	(0,0,0)	Details
mGM6+	2	P21'/m'	(-1,0,0 | 0,0,-1 | 0,-1,0)	(0,0,0)	Details
mGM1-	1	P63/m'm'c'	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0)	Details
mGM2-	1	P63/m'mc	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0)	Details
mGM3-	1	P63'/mm'c	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0)	Details
mGM4-	1	P63'/mmc'	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0)	Details
mGM5-	2	P21/m'	(-1,0,0 | 0,0,-1 | 0,-1,0)	(0,0,0)	Details
mGM6-	2	P21'/m	(-1,0,0 | 0,0,-1 | 0,-1,0)	(0,0,0)	Details

Jana2020: magnetic option

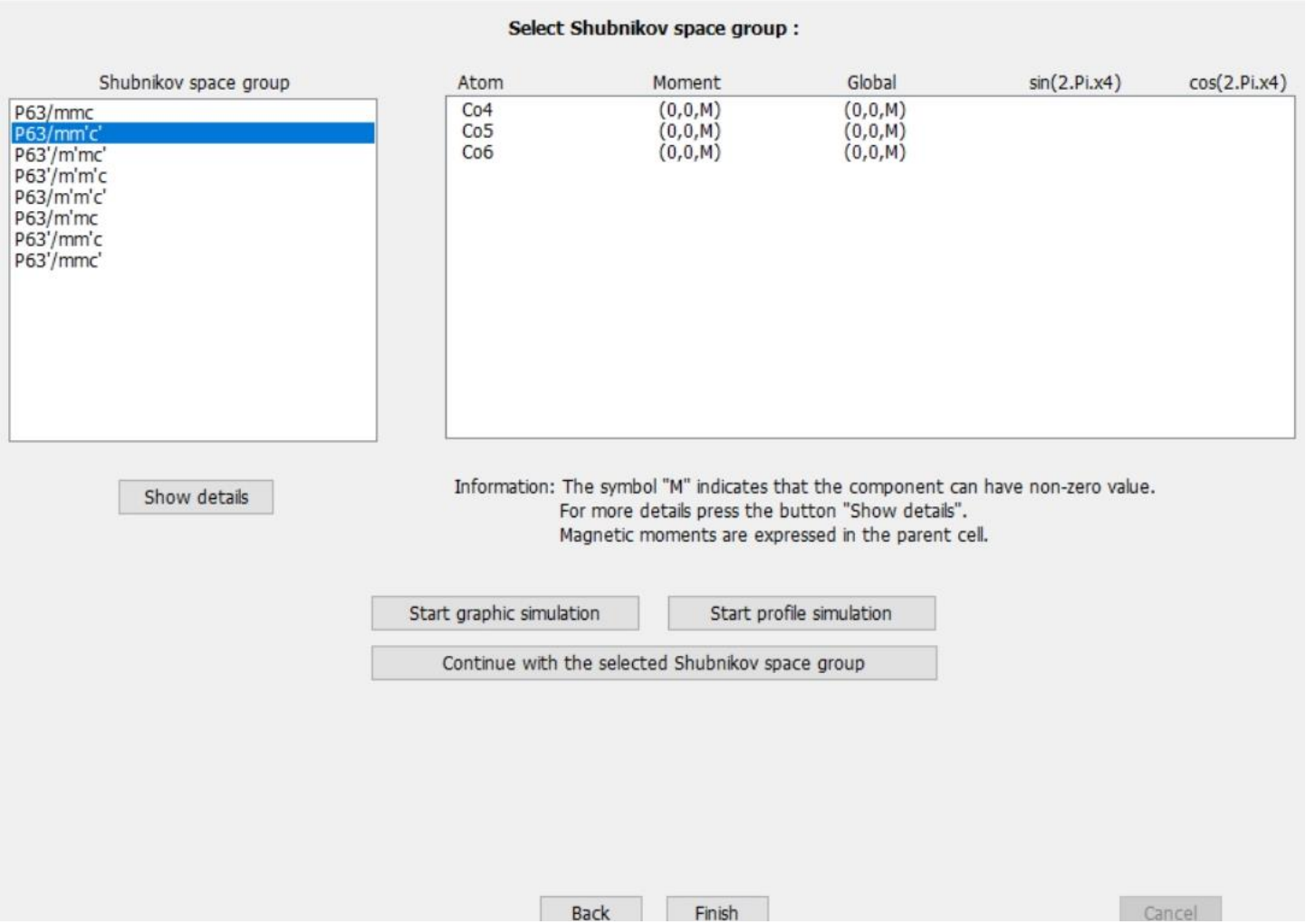
List of kernels and epikernels (isotropy subgroups)

List of kernels and epikernels:

Shubnikov space group	Axes	Origin shift	Representation	ODP-
P63/mmc	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0)	mGM1+	(a)
P63/mm'c'	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0)	mGM2+	(a)
P63'/m'mc'	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0)	mGM3+	(a)
P63'/m'm'c	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0)	mGM4+	(a)
P63/m'm'c'	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0)	mGM1-	(a)
P63/m'mc	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0)	mGM2-	(a)
P63'/mm'c	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0)	mGM3-	(a)
P63'/mmc'	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0)	mGM4-	(a)
Cmcm	(-1,0,0 | -1,-2,0 | 0,0,1)	(0,0,0)	mGM5+	(a,0)
Cm'c'm	(-1,0,0 | -1,-2,0 | 0,0,1)	(0,0,0)	mGM5+	(0,a)
Cmc'm'	(-1,0,0 | -1,-2,0 | 0,0,1)	(0,0,0)	mGM6+	(0,a)
Cm'cm'	(-1,0,0 | -1,-2,0 | 0,0,1)	(0,0,0)	mGM6+	(a,0)
Cm'cm	(-1,0,0 | -1,-2,0 | 0,0,1)	(0,0,0)	mGM6-	(0,a)
Cmc'm	(-1,0,0 | -1,-2,0 | 0,0,1)	(0,0,0)	mGM6-	(a,0)
Cm'c'm'	(0,1,0 | 2,1,0 | 0,0,-1)	(0,0,0)	mGM5-	(a,0)
Cmcm'	(0,1,0 | 2,1,0 | 0,0,-1)	(0,0,0)	mGM5-	(0,a)
P21/m	(-1,0,0 | 0,0,-1 | 0,-1,0)	(0,0,0)	mGM5+	(a,b)
P21'/m'	(-1,0,0 | 0,0,-1 | 0,-1,0)	(0,0,0)	mGM6+	(a,b)
P21/m'	(-1,0,0 | 0,0,-1 | 0,-1,0)	(0,0,0)	mGM5-	(a,b)
P21'/m	(-1,0,0 | 0,0,-1 | 0,-1,0)	(0,0,0)	mGM6-	(a,b)

Jana2020: magnetic option

Testing a kernel/epikernel ‘family’



Jana2020: magnetic option

List of irreps and correspoding kernel symmetries:

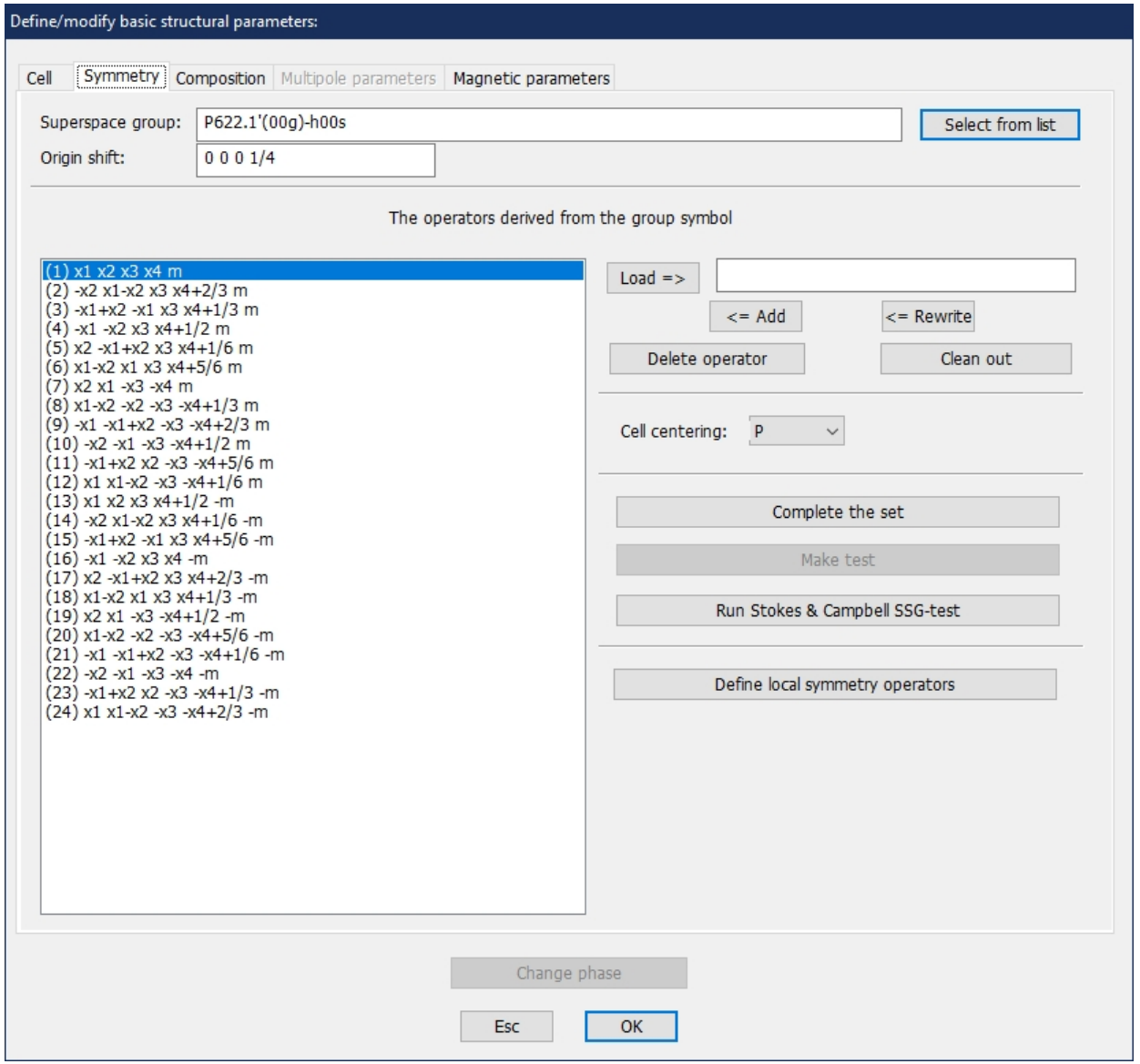
Representation	Dimension	Shubnikov superspace group	Axes	Origin shift	
mDT1	2	P6/mmm.1'(00g)0000s	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0,0)	Details
mDT2	2	P6/mmm.1'(00g)00sss	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0,0)	Details
mDT3	2	P6/mmm.1'(00g)s00ss	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0,0)	Details
mDT4	2	P6/mmm.1'(00g)s0s0s	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0,0)	Details
mDT5	4	P2.1'(0b0)0s	(-1,0,0 | 0,0,-1 | 0,-1,0)	(0,0,0,0)	Details
mDT6	4	P2.1'(0b0)ss	(-1,0,0 | 0,0,-1 | 0,-1,0)	(0,0,0,0)	Details

Select Magnetic superspace group :

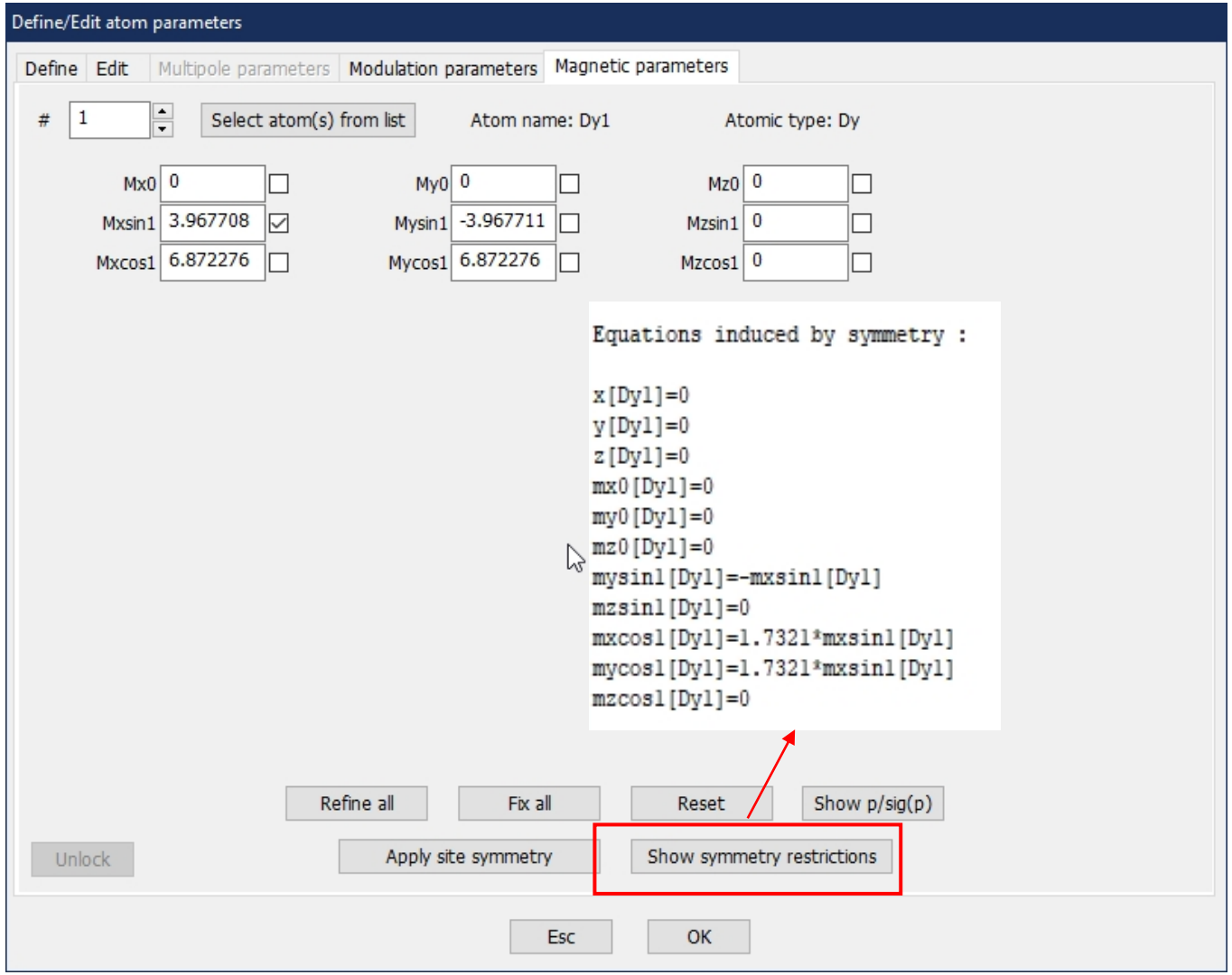
Magnetic superspace group
P622.1'(00g)t00s
P622.1'(00g)-h00s

Atom	Moment	Global	sin(2.Pi.x4)	cos(2.Pi.x4)
Dy1	(0,0,0)	(0,0,0)	(M,M,0)	(M,M,0)
Mn1	(0,0,0)	(0,0,0)	(M,M,0)	(M,M,0)

Jana2020: magnetic option

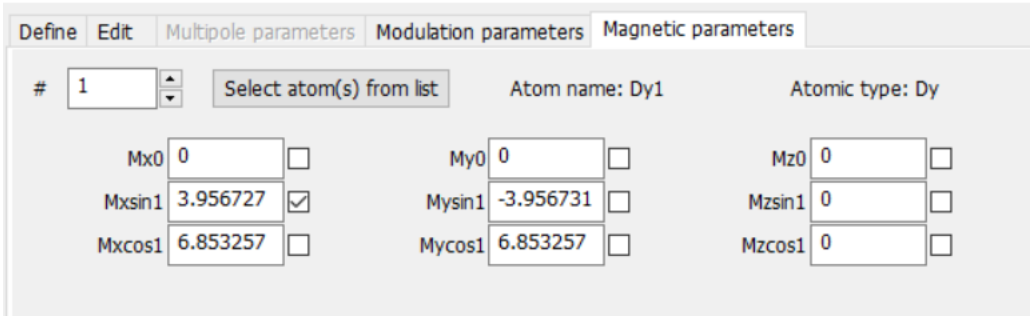


Jana2020: magnetic option

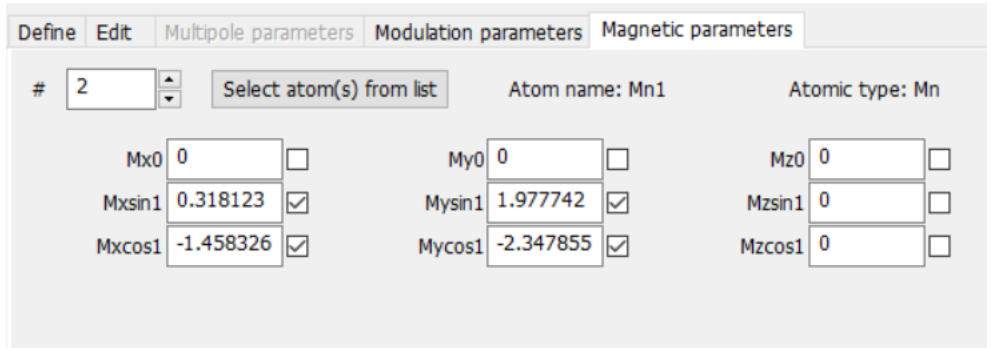


Jana2020: magnetic option

Define/Edit atom parameters



Define/Edit atom parameters

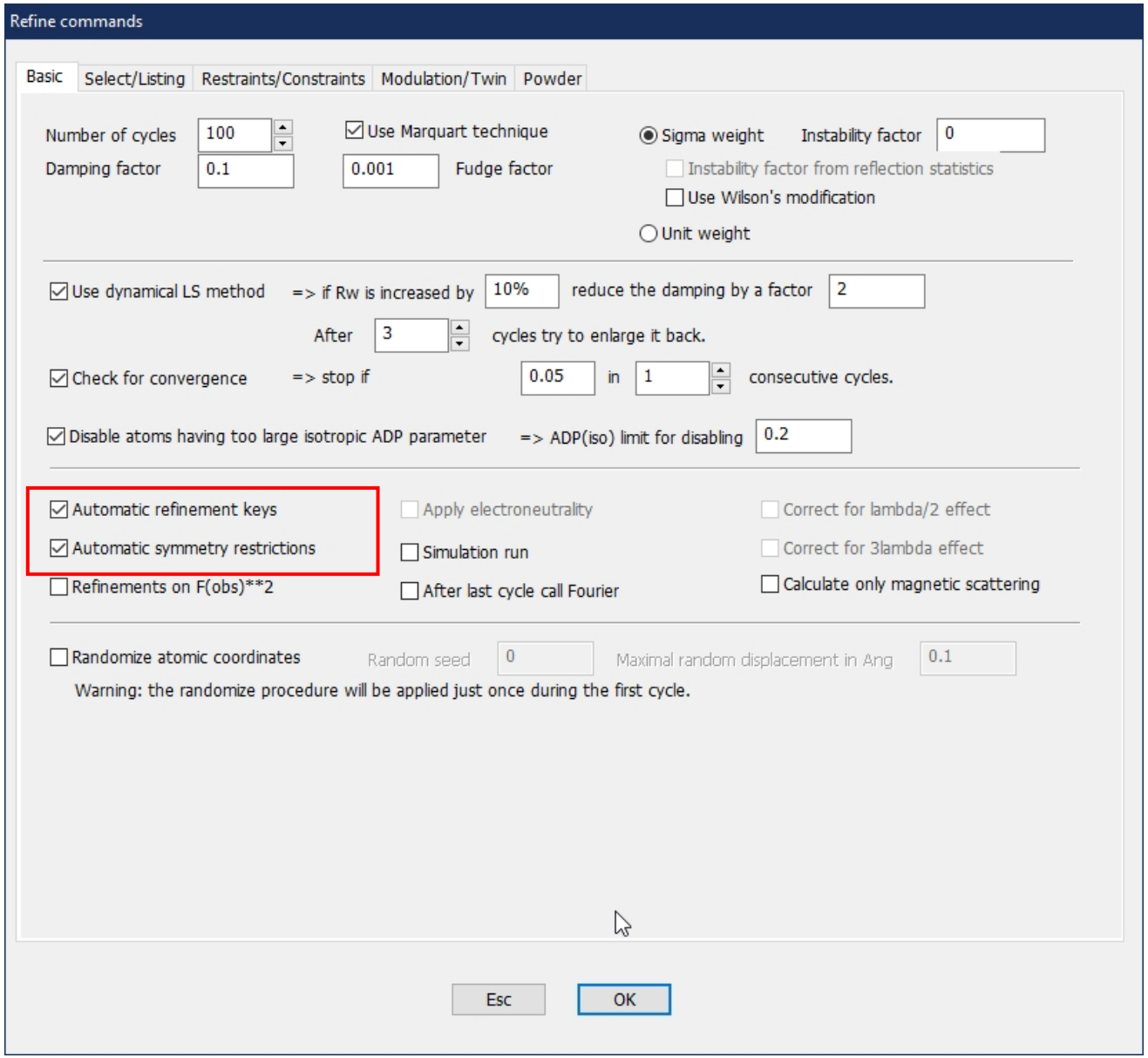


Refinement file

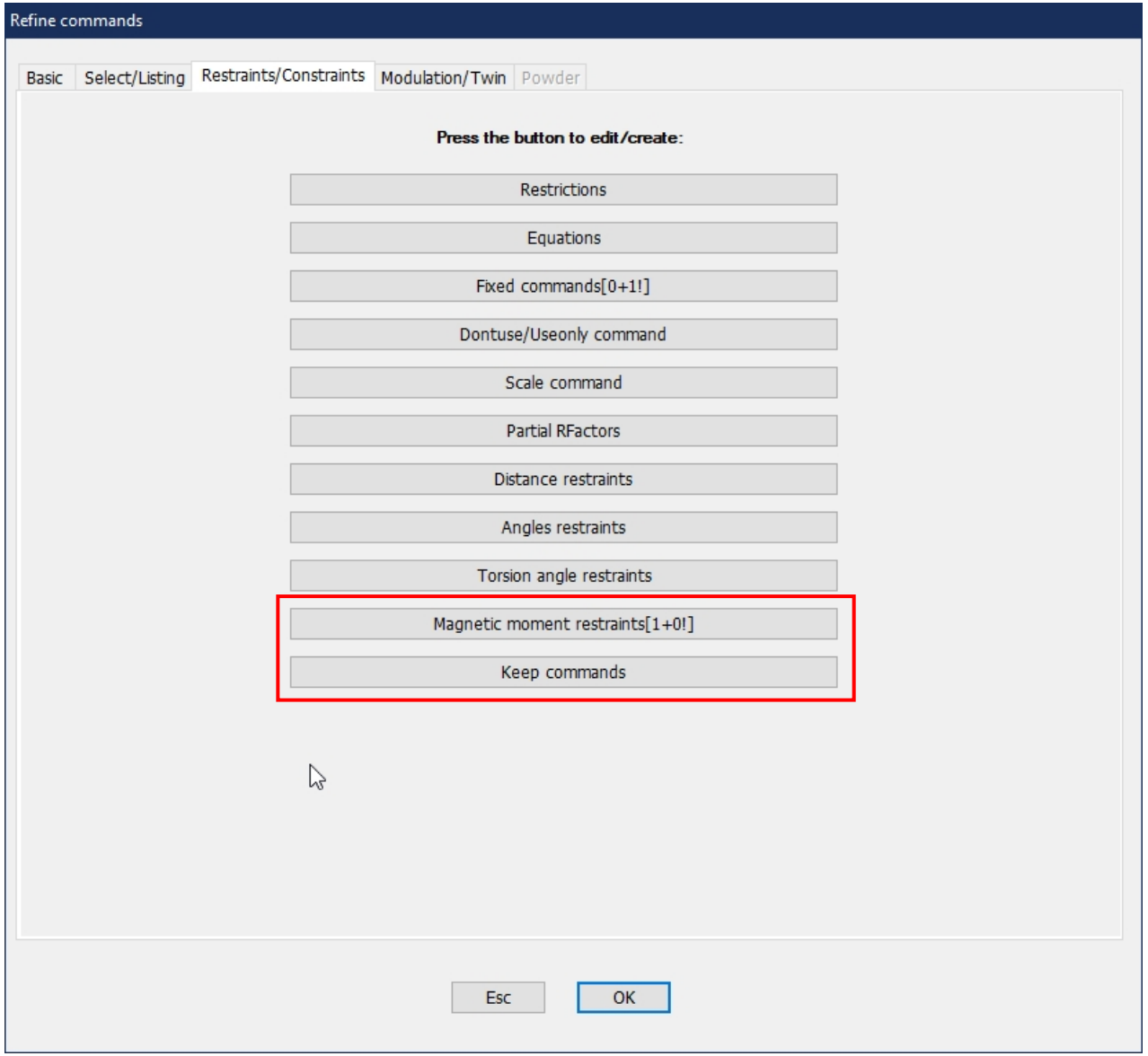
```
y[Dy1]=0
z[Dy1]=0
mx0[Dy1]=0
Refinement program
structure :

my0[Dy1]=0
mz0[Dy1]=0
mysin1[Dy1]=-mxsin1[Dy1]
mzsin1[Dy1]=0
mxcos1[Dy1]=1.7321*mxsin1[Dy1]
mycos1[Dy1]=1.7321*mxsin1[Dy1]
mzcos1[Dy1]=0
x[Mn1]=0.5
y[Mn1]=0
mx0[Mn1]=0
my0[Mn1]=0
mz0[Mn1]=0
mzsin1[Mn1]=0
mzcos1[Mn1]=0
x[Ge1]=0.33333
y[Ge1]=0.66667
z[Ge1]=0
x[Ge2]=0.33333
y[Ge2]=0.66667
z[Ge2]=0.5
x[Ge3_1]=0
y[Ge3_1]=0
```

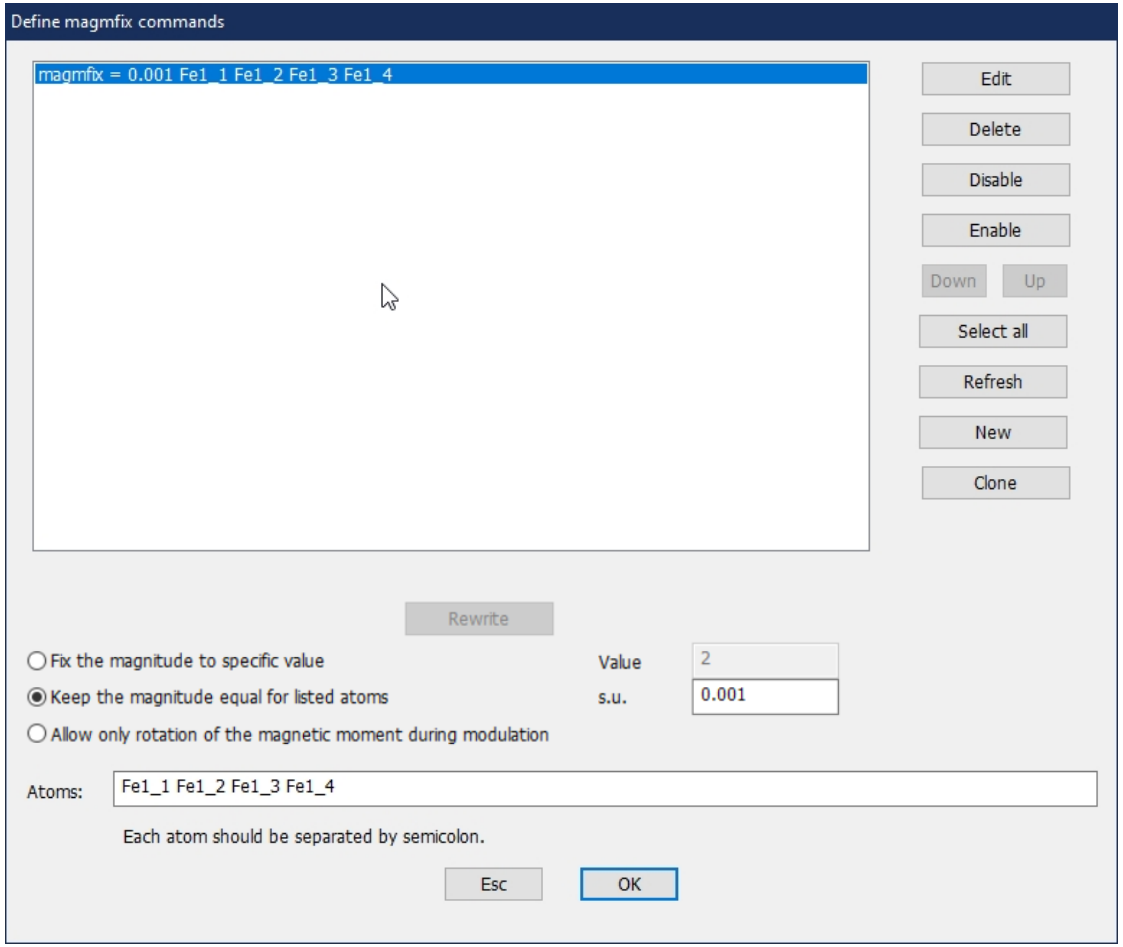
Jana2020

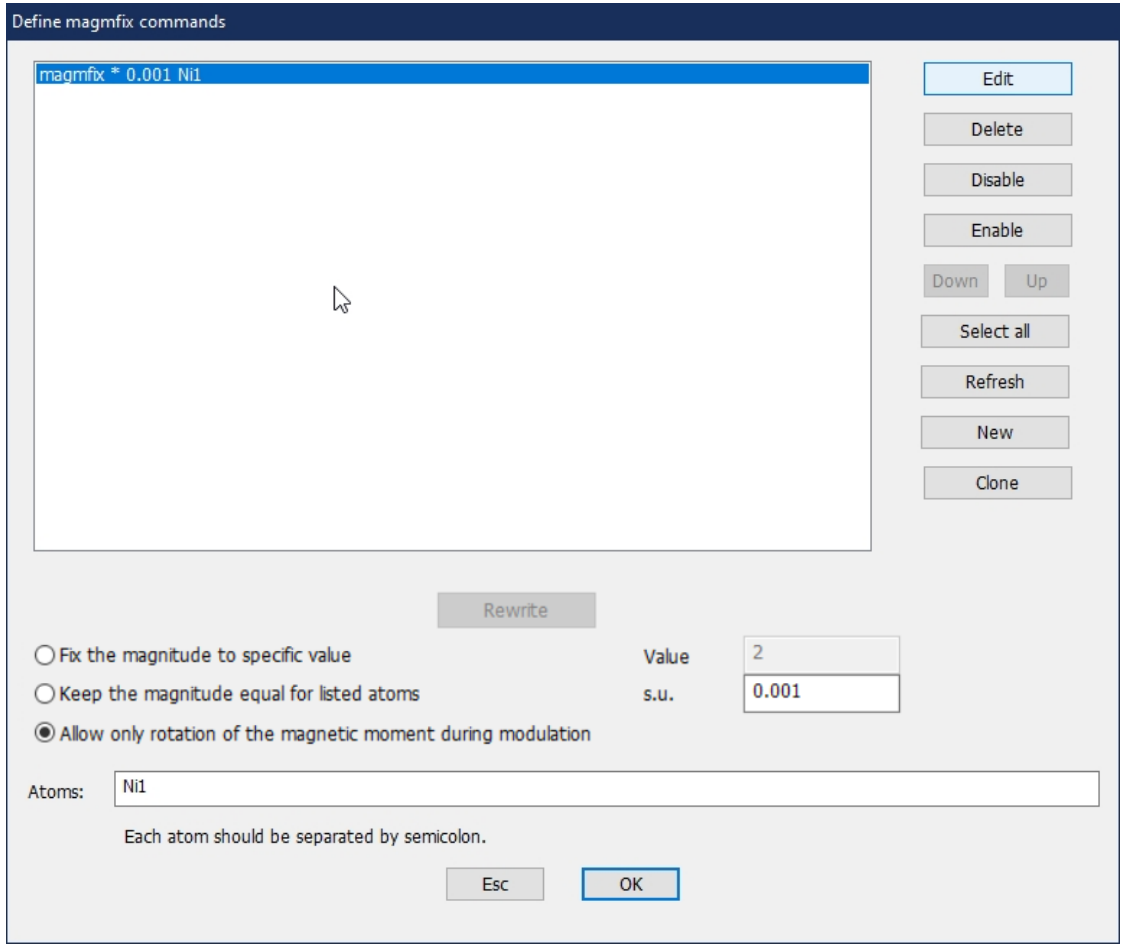

Refine commands
Basic
Select/Listing
Restraints/Constraints
Modulation/Twin
Powder
Number of cycles
100
Use Marquart technique
Sigma weight
Instability factor
0
Damping factor
0.1
0.001
Fudge factor
Instability factor from reflection statistics
Use Wilson's modification
Unit weight
Use dynamical LS method
=> 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
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

Jana2020

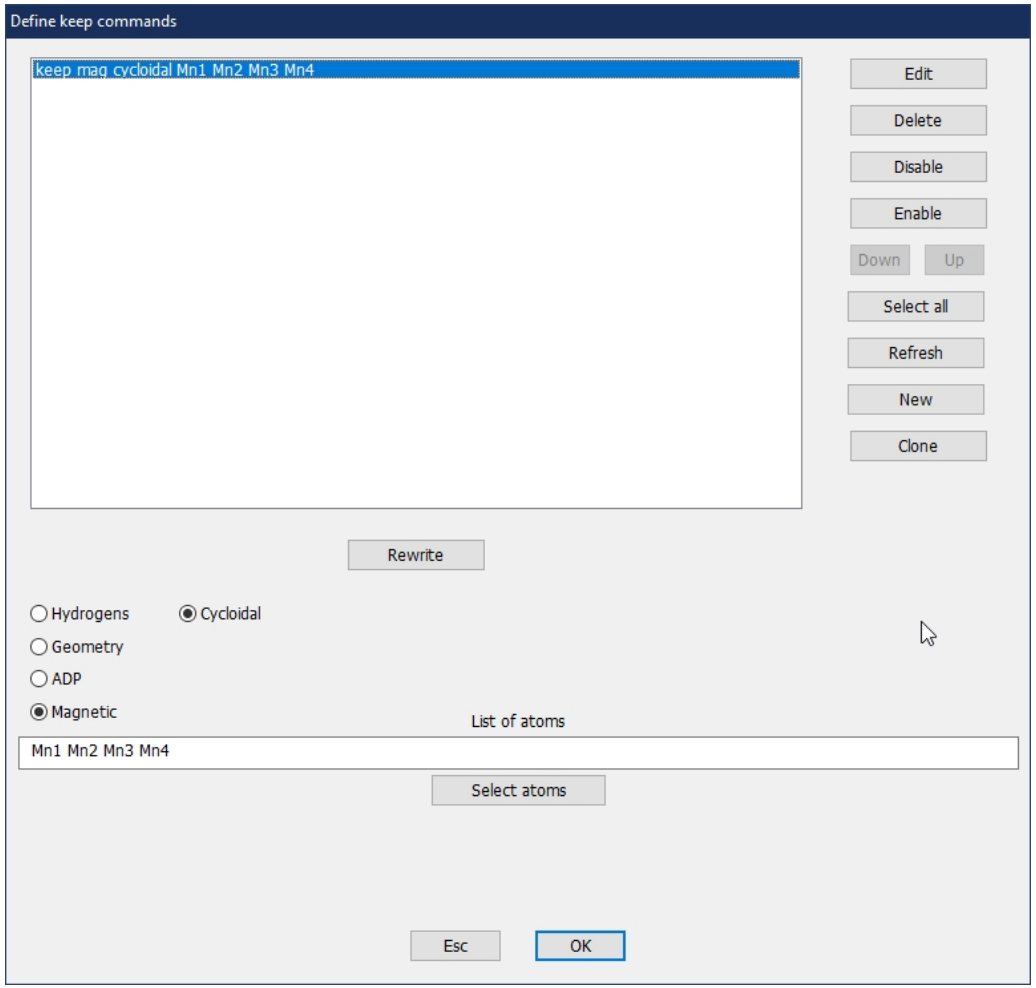

Refine commands
Basic
Select/Listing
Restraints/Constraints
Modulation/Twin
Powder
Press the button to edit/create:
Restrictions
Equations
Fixed commands[0+1!]
Dontuse/Useonly command
Scale command
Partial RFactors
Distance restraints
Angles restraints
Torsion angle restraints
Magnetic moment restraints[1+0!]
Keep commands
Esc
OK

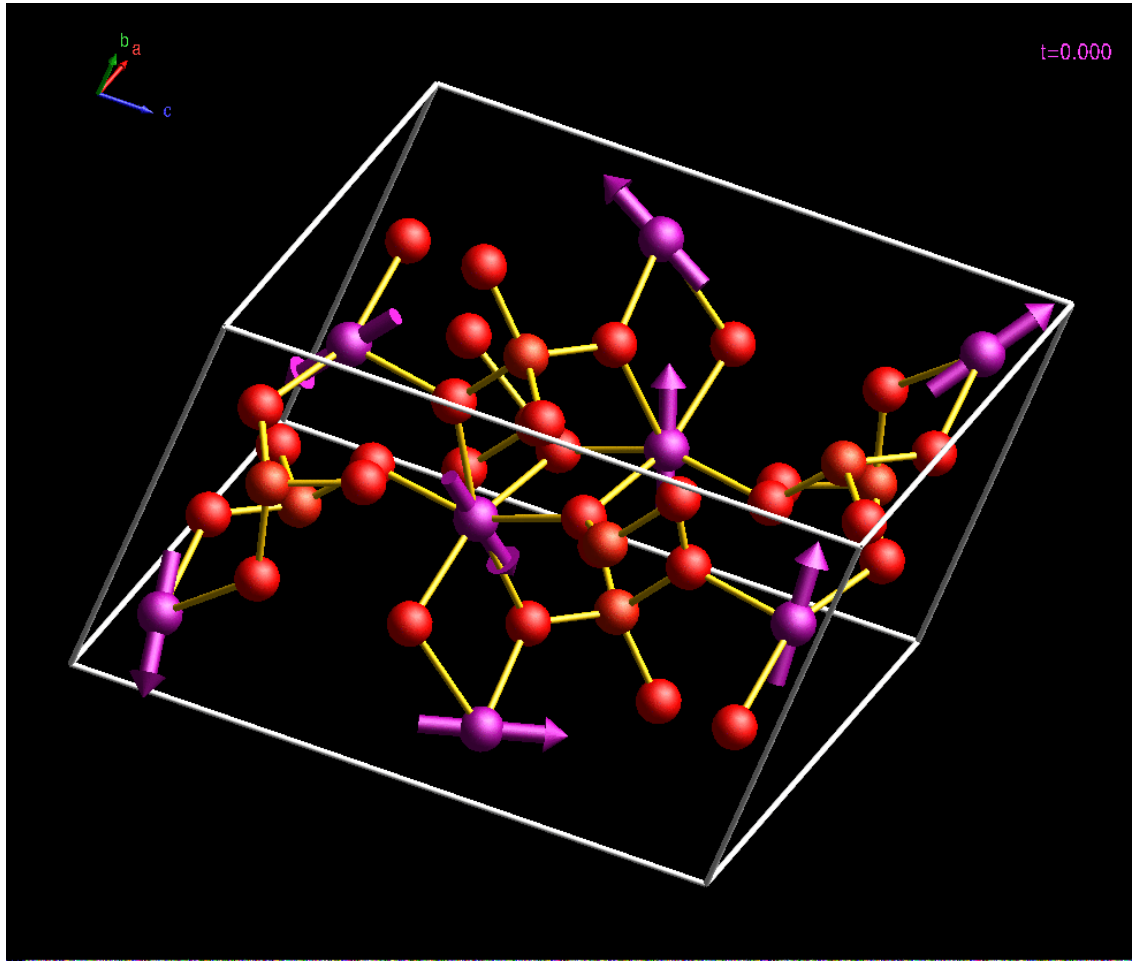
Jana2020: magnetic option



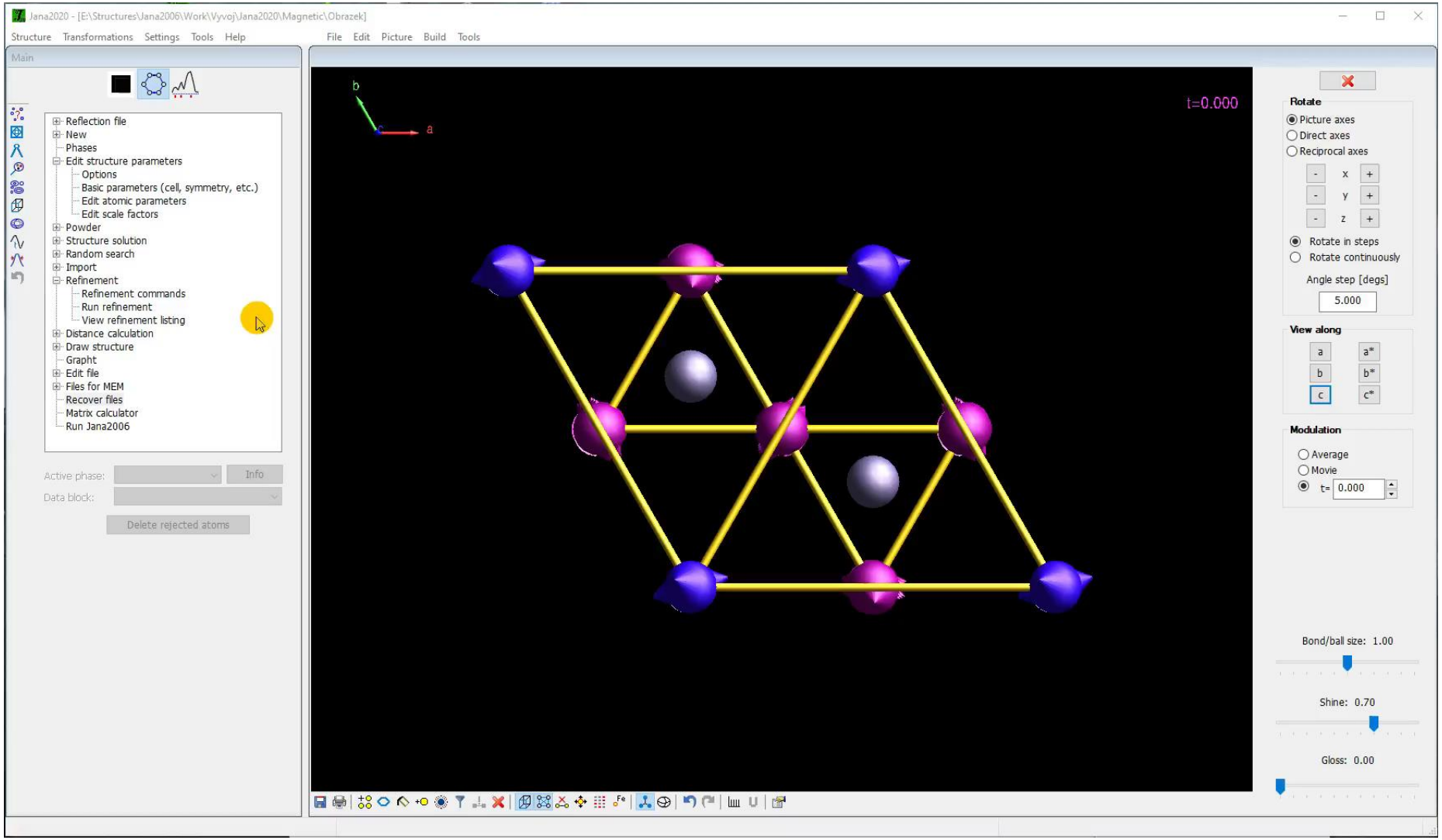


Jana2020: magnetic option



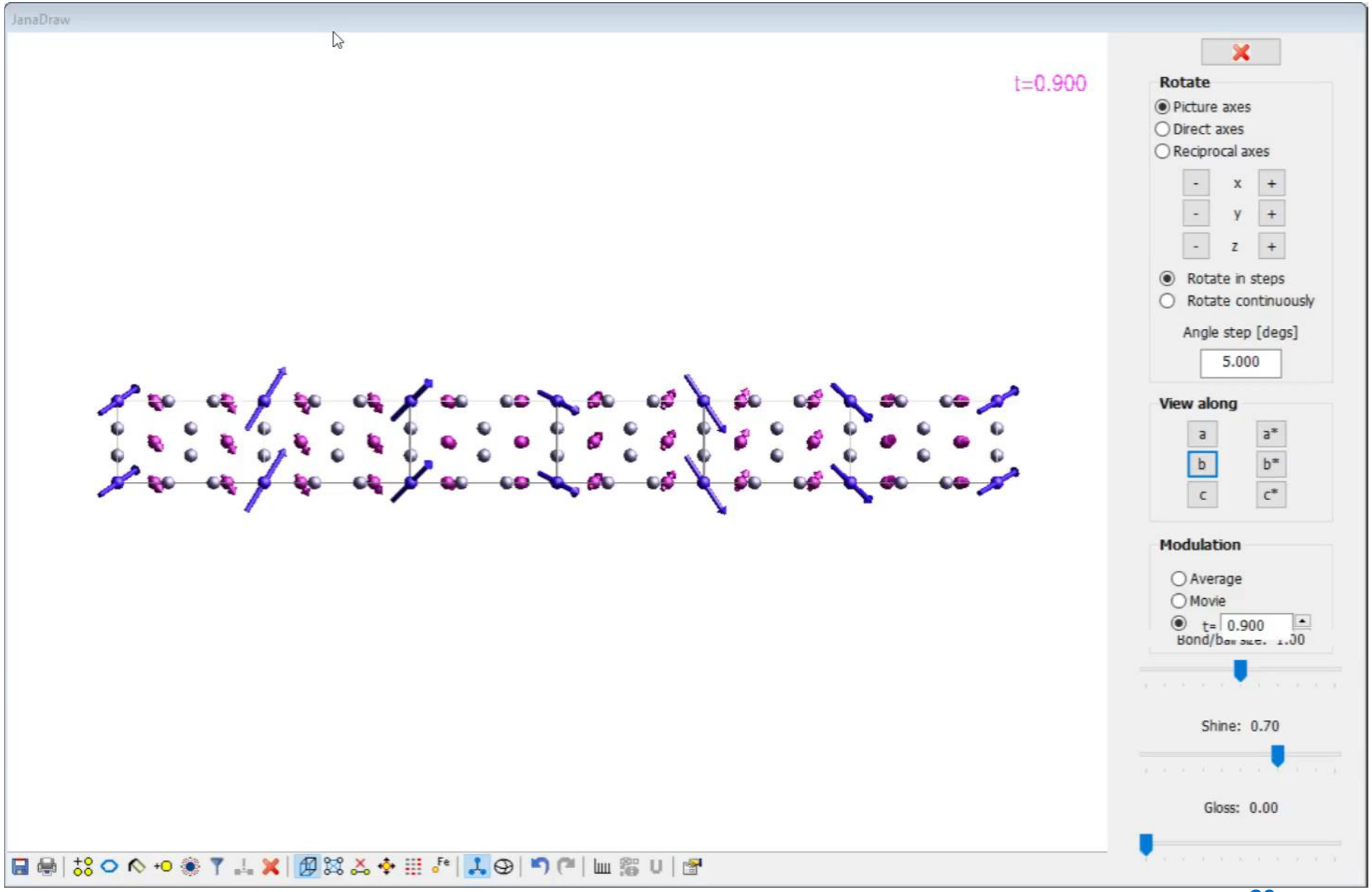


Jana2020: magnetic option



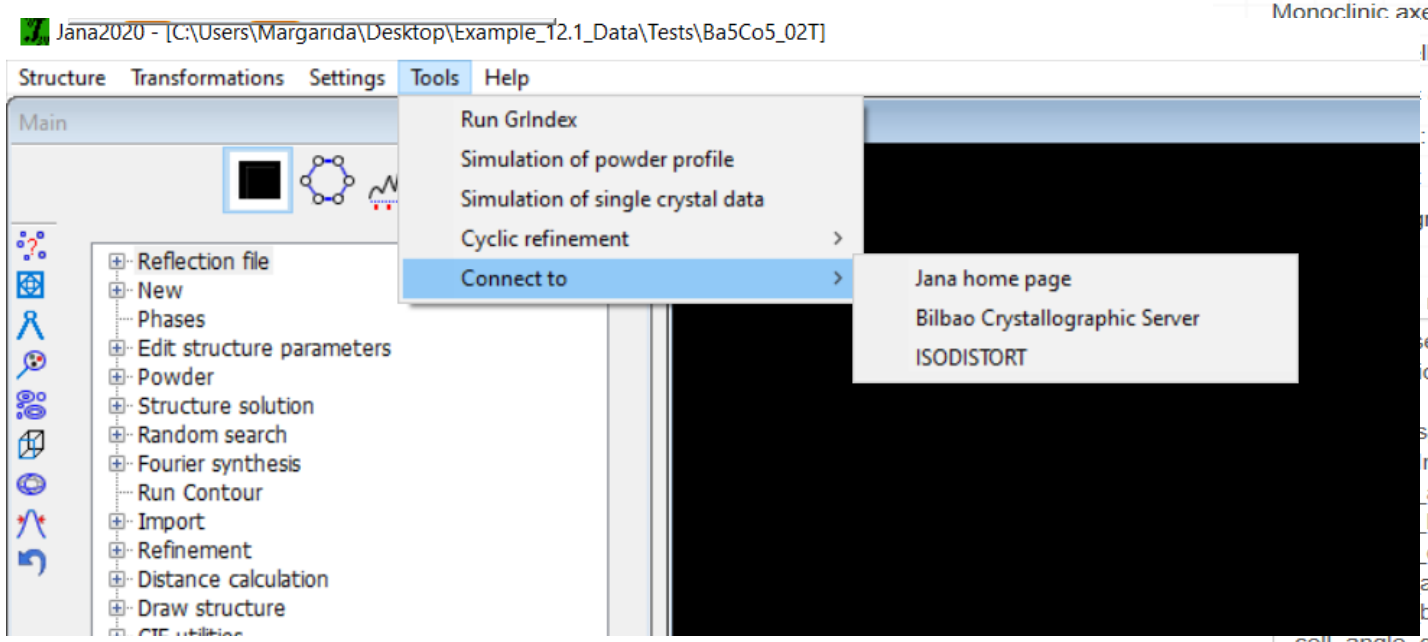
Jana2020

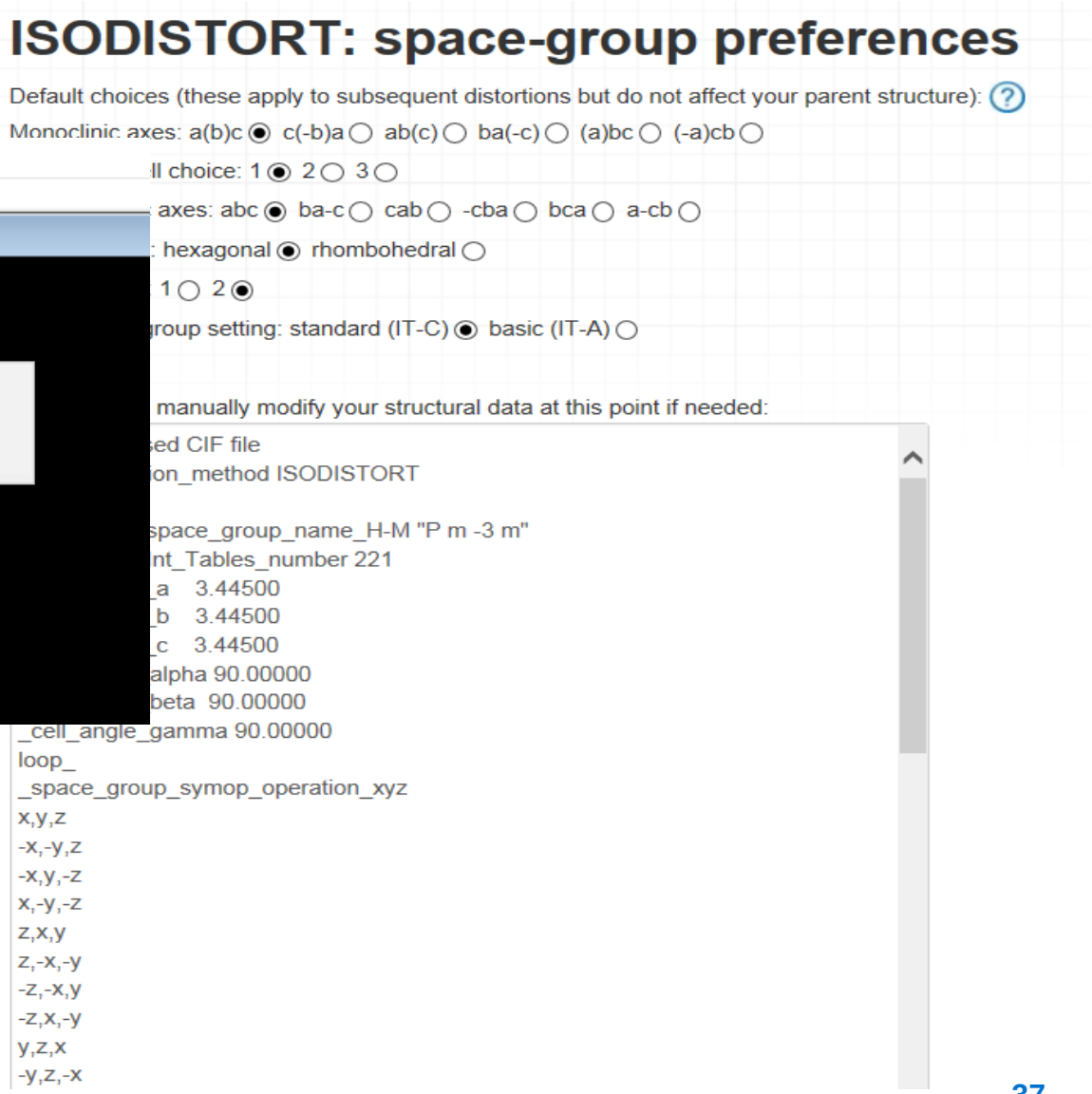
JanaDraw



FZU Fyzikální ústav Akademie věd České republiky

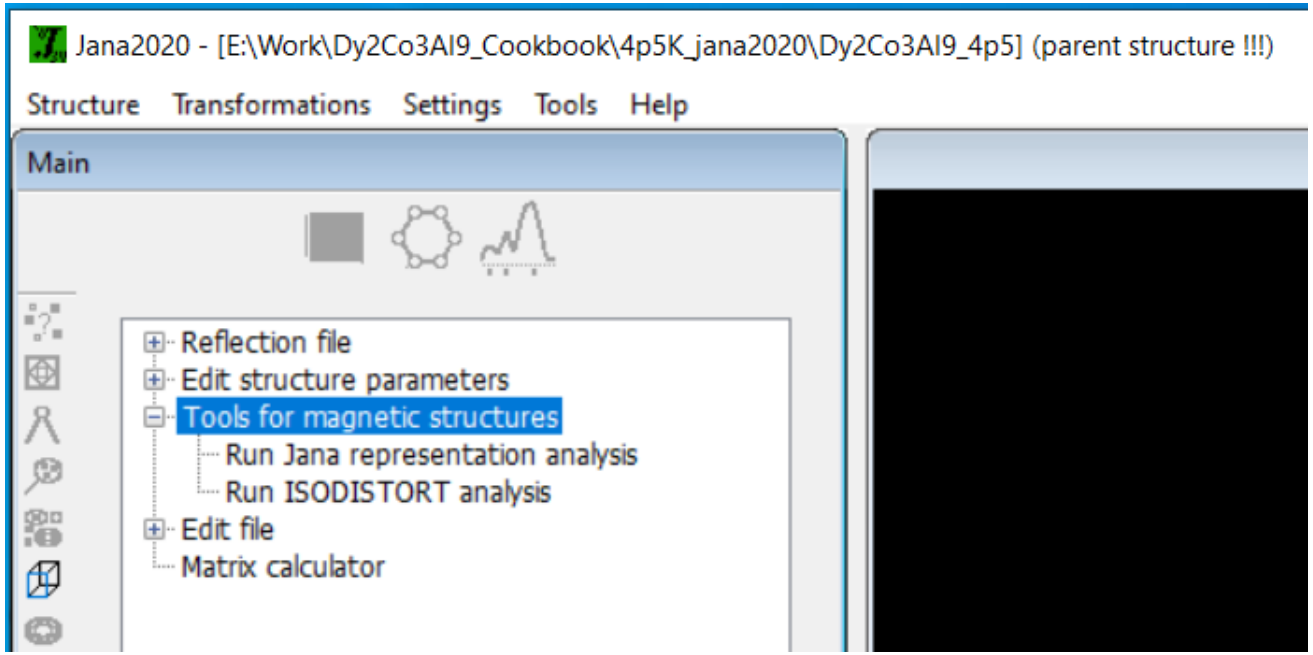
Jana2020: magnetic option





Jana2020: magnetic option

ISODISTORT



Jana2020

http://jana.fzu.cz/

jana.fzu.cz

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

CRYSTALLOGRAPHIC COMPU

Vaclav

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

News

June 19 - 24, 2022 APERI
Crystals: Sapporo, Japan

May 23 - 27, 2022 5th interna

August 22 - 30, 2020 The 25t

IUCr 25 Highlights related to
Magnetic structures
Aperiodic structures
Satellite workshop on aperi

August 20 - 21, 2020 Worksh
Prague, Czech Republic

May 31 - June 9, 2019 Magne

March 11 - 13, 2019 Jana bas

December 10 - 13, 2018 Jana

October 26-27, 2017 Worksh

August 11, 2016 Deadline for

July 4-8, 2015 3rd Internati
April 2016

October 28, 2015 Maintena
Download area. It cumulates
electron diffraction.

January 24, 2015 APERIODI

May 01, 2014 New reference
Z. Kristallogr. 229(5), 345-352

March 12, 2014 Zeitschrift f
present and previous issues until June 30,2014.

jana.fzu.cz

Jana system is a freeware but we are interested who is using it. We would like our users to **register**. Registered users get e-mails about major updates.

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

Jana2006 for UNIX: porting of Jana2006 to UNIX is in progress but it is not yet finished.
User manuals: not yet available. The old manuals for Jana98 and Jana2000 are still partially useful.

Program	Version string	Download from jana.fzu.cz
Jana2020 for Windows	30/05/2022	**jana2020Inst.msi**
Jana2006 for Windows, STABLE	23/05/2022	**janainst.msi**
Jana2006 for Unix, STABLE	- - - -	not available
Jana2006 for Windows, LATEST	23/05/2022	**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)

FZU Fyzikální ústav Akademie věd České republiky

Jana2020

jana-login.fzu.cz/cookbook

Example 12.1: Ba5Co5 | Simple antiferromagnetic structure (k = 0) from powder data — Show keywords ▼

Docx: 12.1_Ba5Co5_Vaclav.docx Pdf: 12.1_Ba5Co5_Vaclav.pdf Data: Data.zip Results: Results.zip

Revised: Apr 15, 2022

Example 12.2: Ba6Co6 | Commensurate magnetic structure from powder data — Show keywords ▼

Docx: Example 12.2_Ba6Co6.docx Pdf: Example 12.2_Ba6Co6.pdf Data: Data.zip Results: Results.zip

Revised: Apr 17, 2022

Example 12.3: PrSrMnO | Commensurate magnetic structure from powder data — Show keywords ▼

Docx: Example 12.3_PrSrMnO.docx Pdf: Example 12.3_PrSrMnO.pdf Data: Data.zip Results: Results.zip

Revised: Jul 3, 2021

Example 12.4: MnWO4 | Incommensurate magnetic structure from powder data — Show keywords ▼

Docx: Example 12.4_MnWO4.docx Pdf: Example 12.4_MnWO4.pdf Data: Data.zip Results: Results.zip

Revised: Apr 17, 2022

Example 12.5: HoNi | Commensurate magnetic structure from single-crystal data — Show keywords ▼

Docx: Example 12.5_HoNi.docx Pdf: Example 12.5_HoNi.pdf Data: Data.zip Results: Results.zip

Revised: Apr 18, 2022

Example 12.6: ISODISTORT | Communication between Jana2020 and ISODISTORT — Show keywords ▼

Docx: Example 12.6_ISODISTORT.docx Pdf: Example 12.6_ISODISTORT.pdf Data: Data.zip Results: Results.zip

Revised: Apr 22, 2022

Thank you!

FZU Fyzikální ústav Akademie věd České republiky