Magnetic structures in Jana2020

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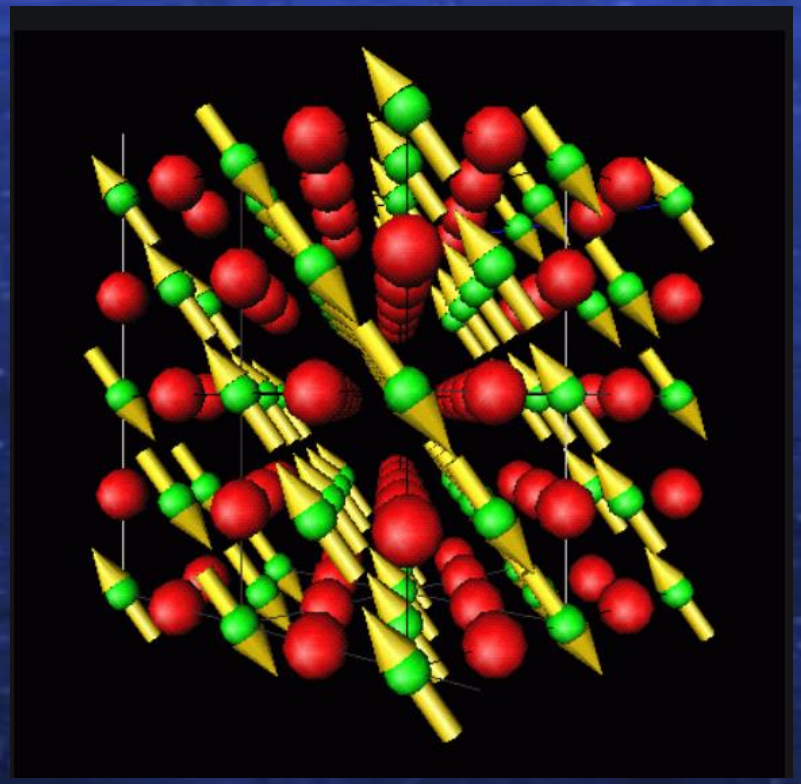
2024 International Workshop on Magnetic Crystallography
November 24-30, 2024, Dongguan, China

Overview

Jana2020 – Magnetic option:

- *Magnetic structure factors*
- *Representation analysis*
- *Handling symmetry*

Program features & workflow

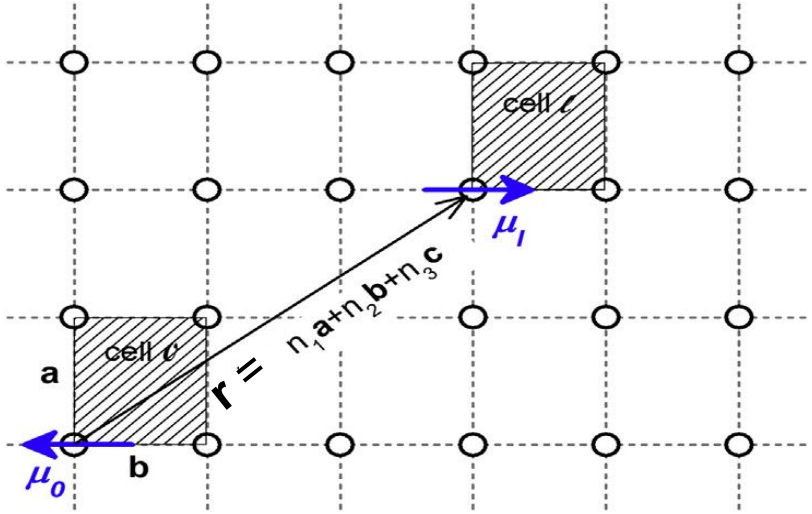


Magnetic structure factor

Whatever is the nature of the ordering, the moment distribution can be described by a periodic vector function:

$$\boldsymbol{\rho}_{mag}(\boldsymbol{r}) = \boldsymbol{\rho}_{mag}\left(\boldsymbol{r} + \sum_{i=1}^{3} n_i \boldsymbol{a}_i\right)$$

a_i stand for three lattice vectors of a Bravais lattice (3D crystal)

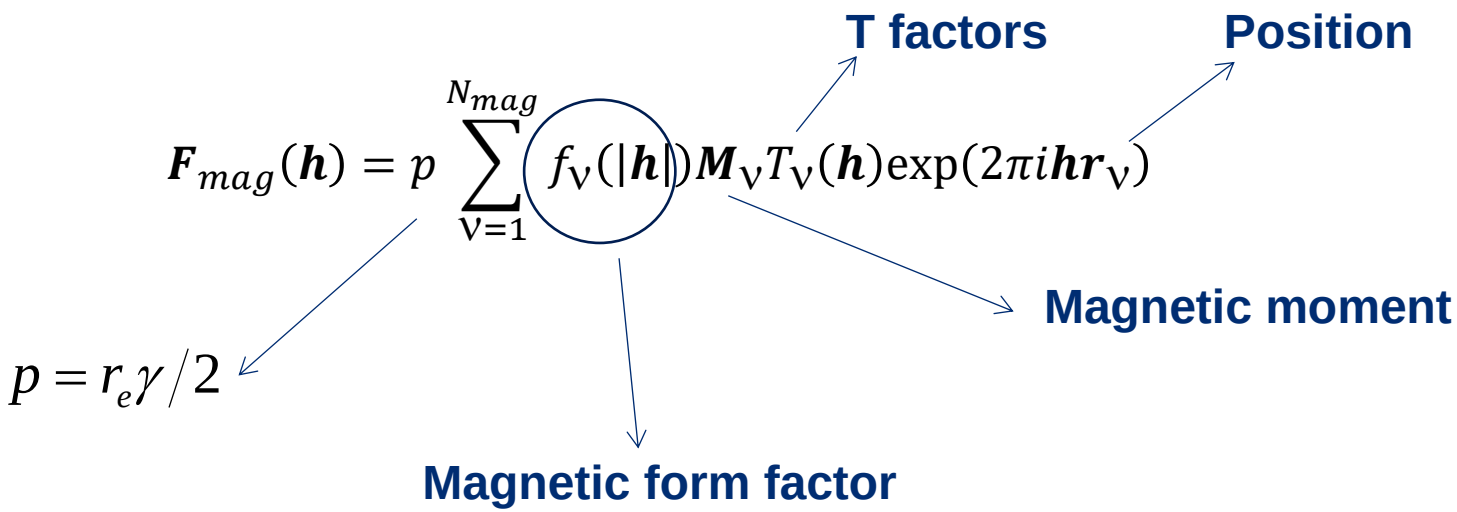


3D periodicity in ordering of magnetic moments → density of magnetic moments can be expressed as Fourier summation of magnetic structure factors:

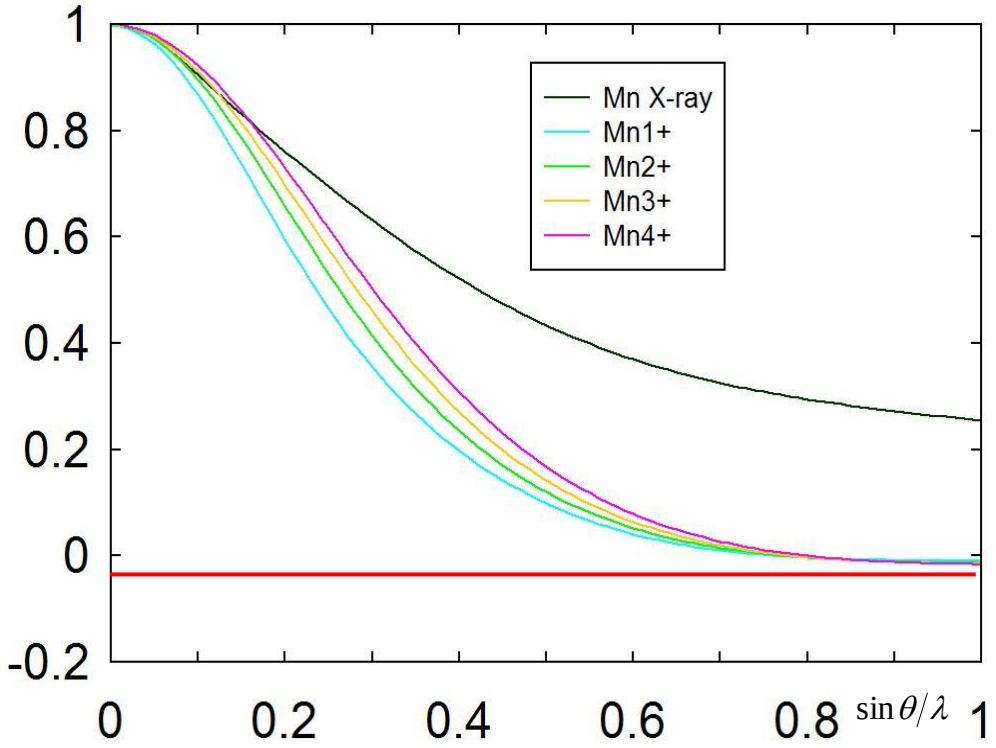
$$\boldsymbol{\rho}_{mag}(\boldsymbol{r}) = \sum_{\boldsymbol{h}} \boldsymbol{F}_{mag}(\boldsymbol{h}) \exp(-2\pi i \boldsymbol{h}\boldsymbol{r})$$

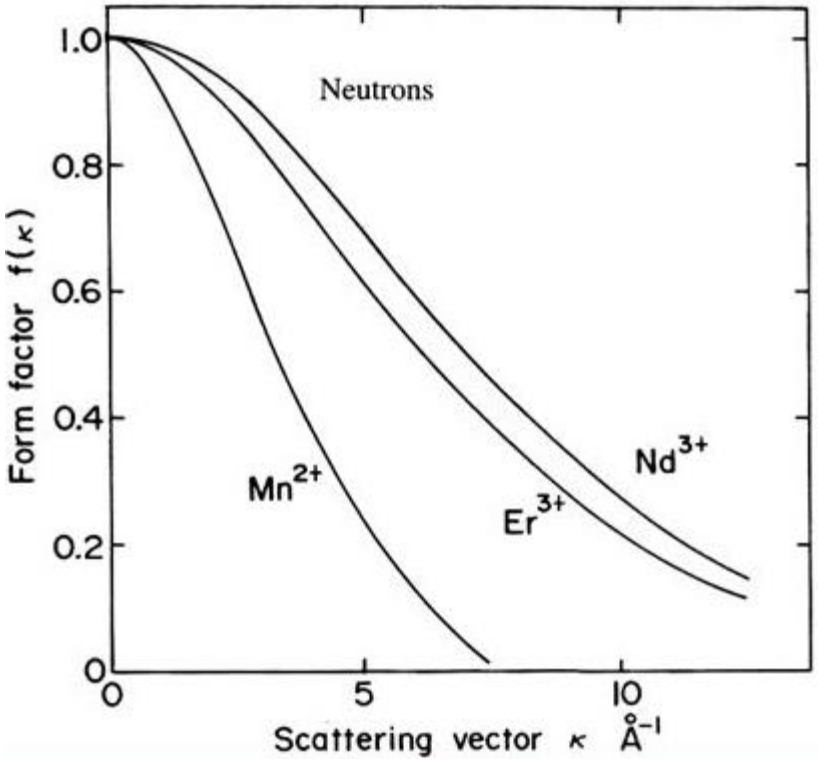
Magnetic structure factor (k=0)

The magnetic density can be divided into the individual contributions of magnetic atoms



Magnetic form factor





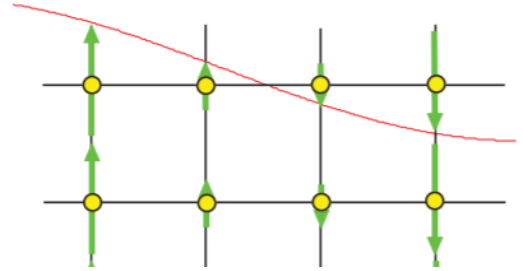
Magnetic structure factor (k≠ 0)

Modulated magnetic structures: **superspace approach**

[Wolf, P.M., Janner, A., Janssen, T. (1981) *Acta Cryst*. A**37**, 625–636]

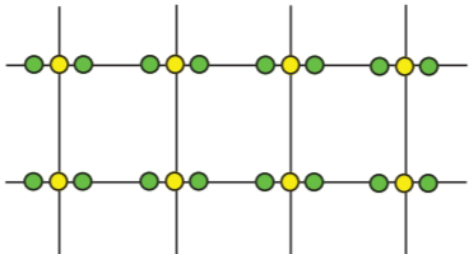
The generalized modulation of the spin for the atom ν is

$$\boldsymbol{M}_\nu = \boldsymbol{M}_{\nu,0} + \sum_m \boldsymbol{M}_{\nu,ms} \sin 2\pi m x_4 + \sum_m \boldsymbol{M}_{\nu,mc} \cos 2\pi m x_4$$



Kinematic theory of diffraction: satellite reflections of order *m*

$$\boldsymbol{F}_{mag}(\boldsymbol{h} \pm m\boldsymbol{k}) = p \sum_{\nu=1}^{N_{mag}} f_\nu(|\boldsymbol{h} \pm m\boldsymbol{k}|) \frac{\boldsymbol{M}_{\nu,mc} \pm i\boldsymbol{M}_{\nu,ms}}{2} T_\nu(\boldsymbol{h} \pm m\boldsymbol{k}) \exp(2\pi i[\boldsymbol{h} \pm m\boldsymbol{k}]\boldsymbol{r}_\nu)$$



Intensity of diffraction

For an unpolarized beam, the detected intensity is

$$I_{mag}(\mathbf{h}) = Lp(\mathbf{h})A(\mathbf{h})E(\mathbf{h})\left[\left|\boldsymbol{F}_{mag}(\mathbf{h})\right|^{2} - \left\{\mathbf{e}.\boldsymbol{F}_{mag}(\mathbf{h})\right\}^{2}\right]$$

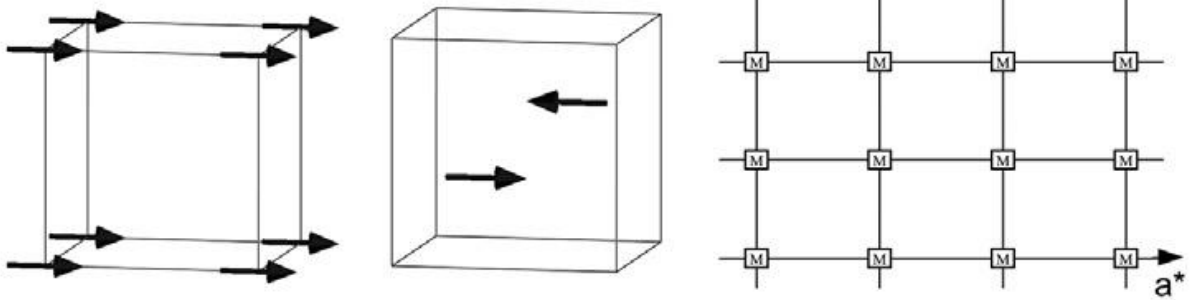
where **e** = **h**/|**h**| is the unit vector along the diffraction vector

As nuclear and magnetic diffraction are independent, detected intensity is composed of two contributions:

$$I(\mathbf{h}) = I_{nuc}(\mathbf{h}) + I_{mag}(\mathbf{h})$$

- Multiphase approach – nuclear and magnetic phases are used separately
- Combined nuclear+magnetic contributions used in a complete model

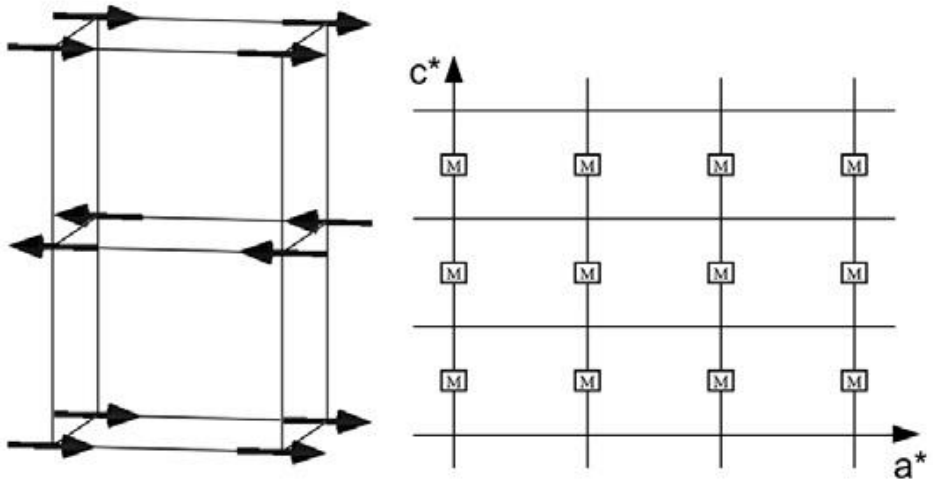
Magnetic diffraction



ferromagnet

k = 0
antiferromagnet

reciprocal space
k = 0 magnetic peaks

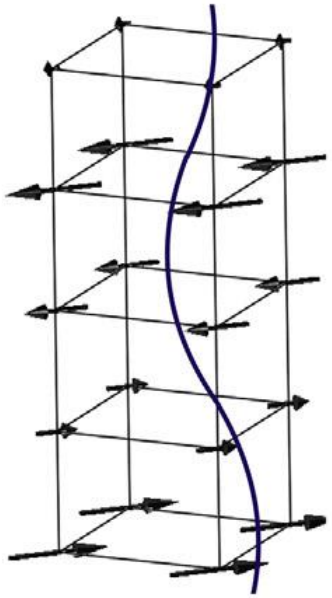


k = (0,0,½)
antiferromagnet

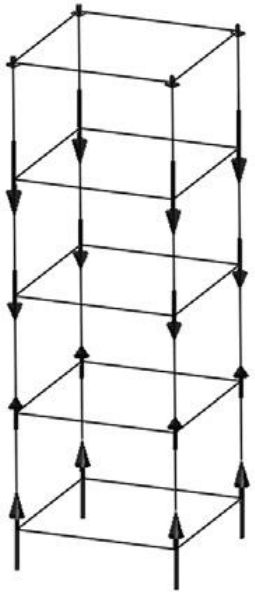
reciprocal space
k = (0,0,½)

E. Ressouche, Collection SFN 13 (2014) 02001

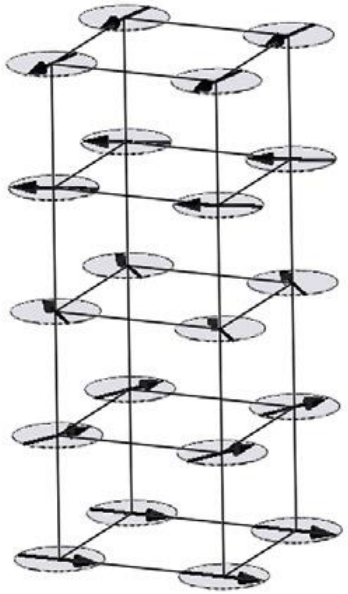
Magnetic diffraction



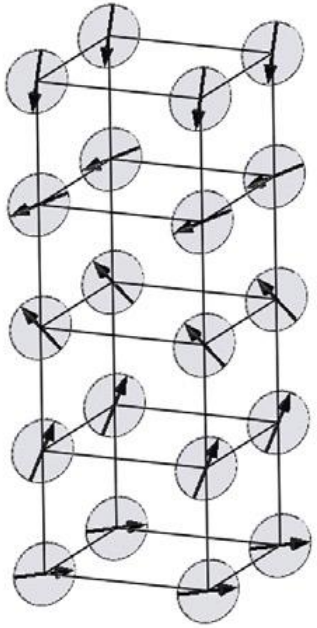
transverse
spin density wave



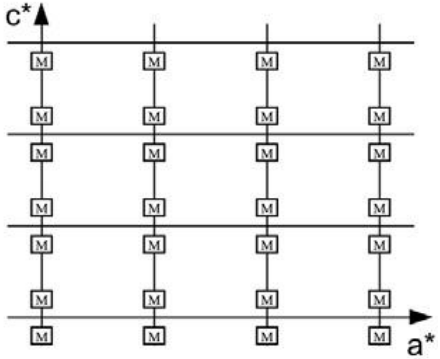
longitudinal
spin density wave



circular helix



circular cycloid

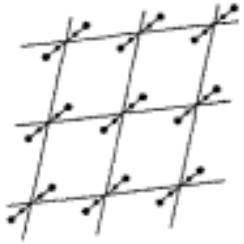


reciprocal space
±k = (0,0,±ξ)

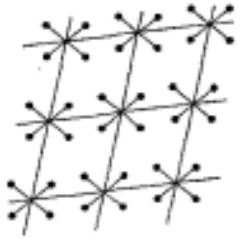
k = kx, ky, kz



1k,3k,…

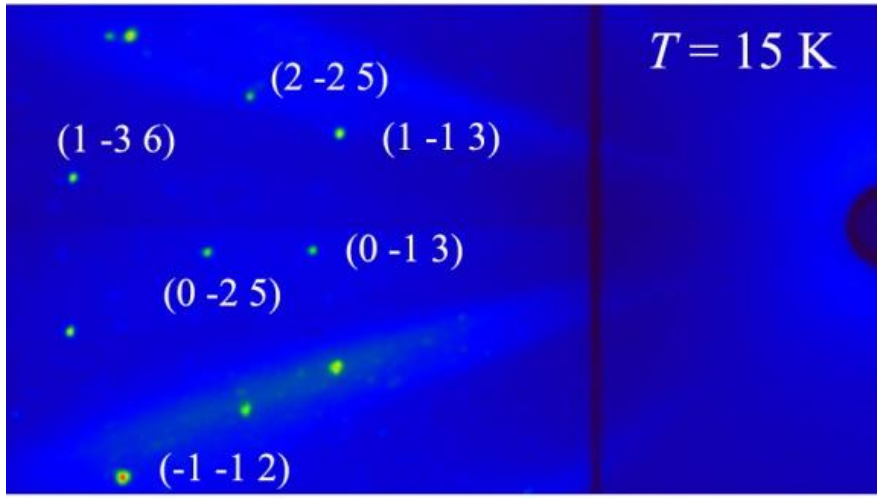


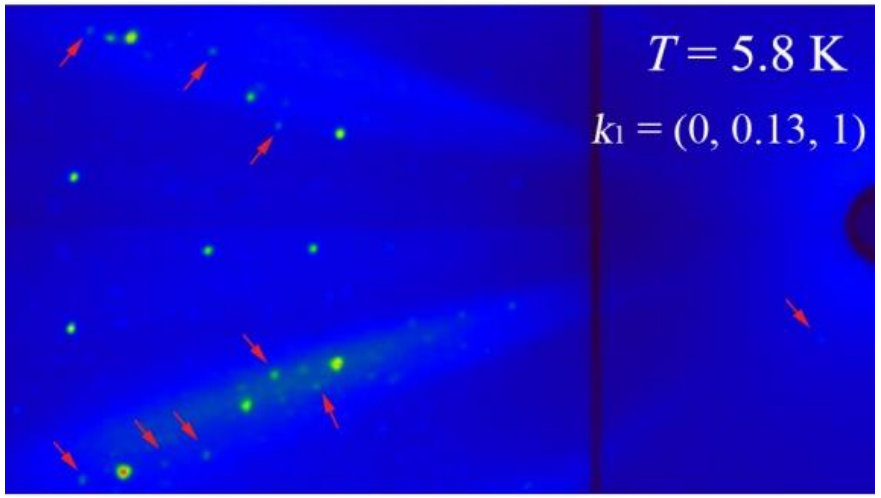
k1,k2,…

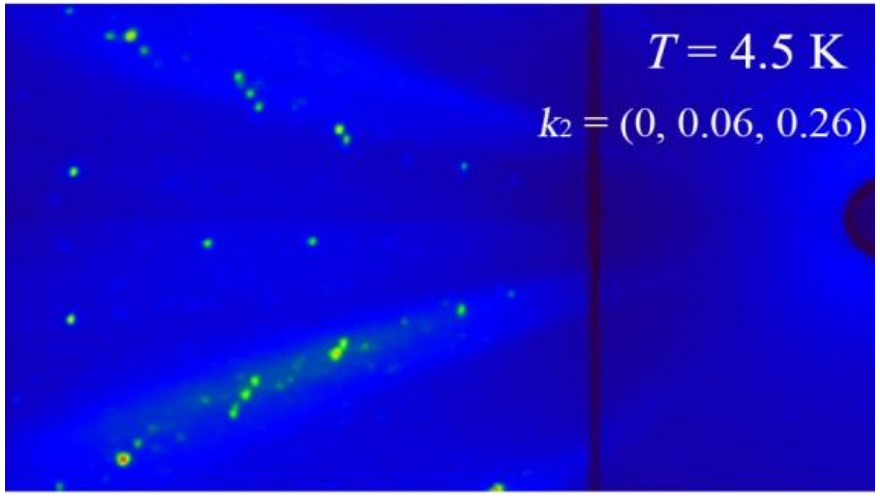


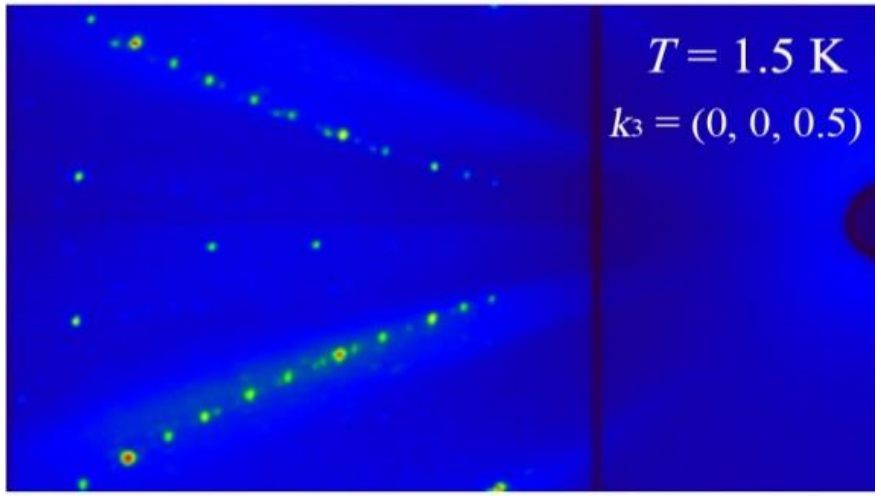
A. Wills, J. Phys. IV France 11 (2001) 133

Magnetic diffraction

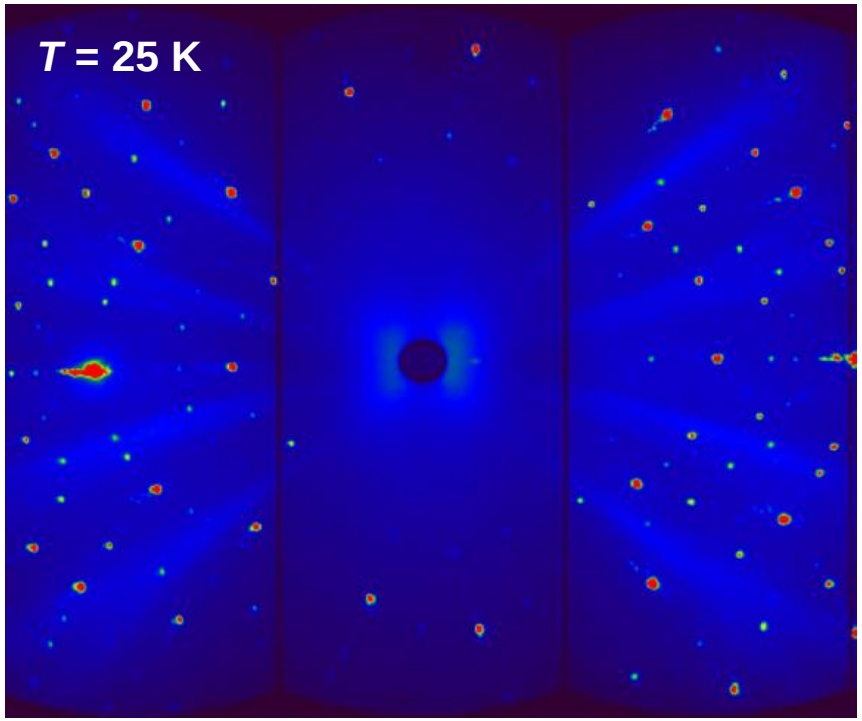


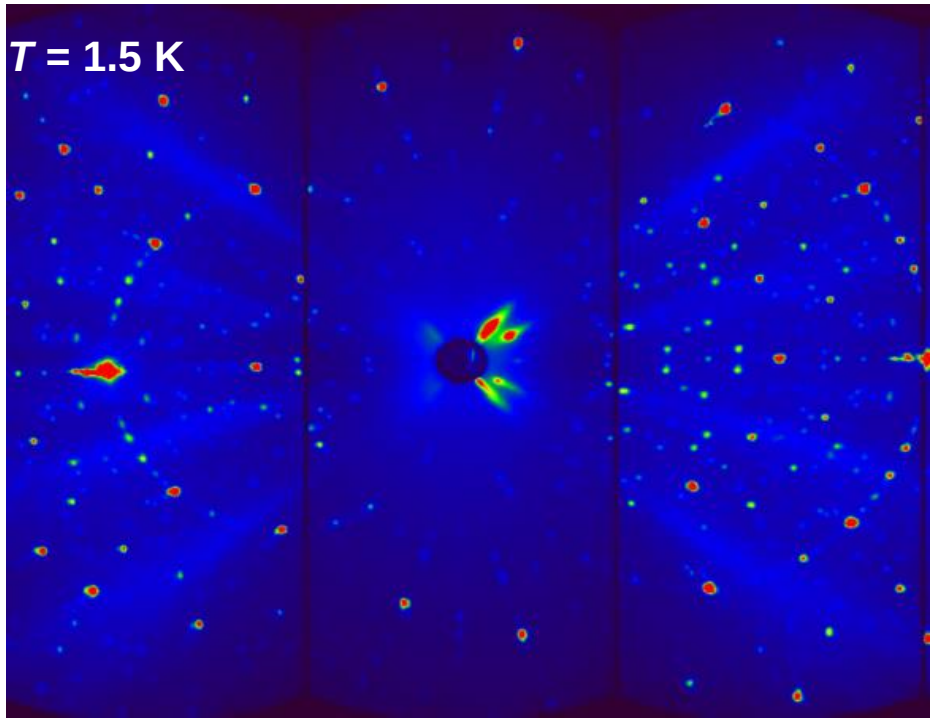






Magnetic diffraction





k_1 = (1/3, 0, 0.9)
k_2 = (2/3, 1/3, 1/2)

Description of magnetic structures

Two main approaches:

- **MSG (or Shubnikov groups)**: extension of the crystallographic SG to include spin (time reversal)
  - The SG determines all constraints: structural and magnetic
- Commensurate and Incommensurate cases (supersymmetry)

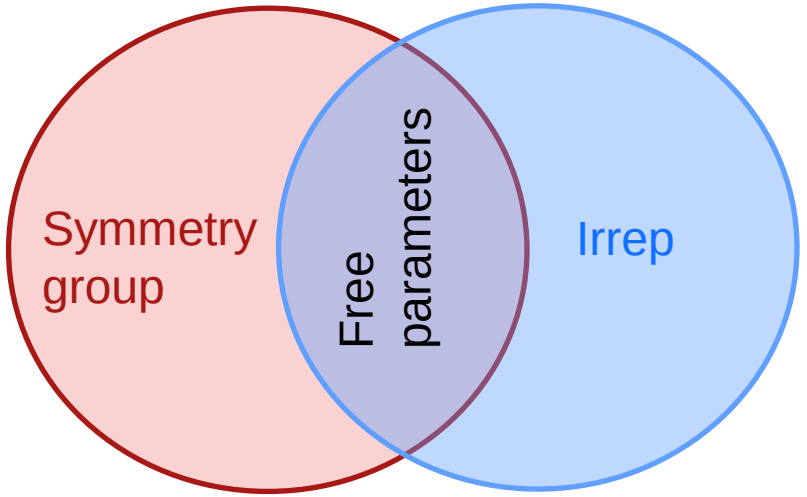
- **RA (irreducible representations, irreps)**
  - General approach that relies on the determination of the basis vectors (projection of the spins in the reference uc) of the irreps of the sg
  - Can be used for any ‘distortion’: spin, vibrations, displacements,…

MSG and MSSG have been standardized, SG operations made available as libraries easily included in many tools, specially for incommensurate structures

Representation analysis

Alternative approach: calculation of Shubnikov groups for the set of possible active *irreps* (**isotropy subgroups of an *irrep***)

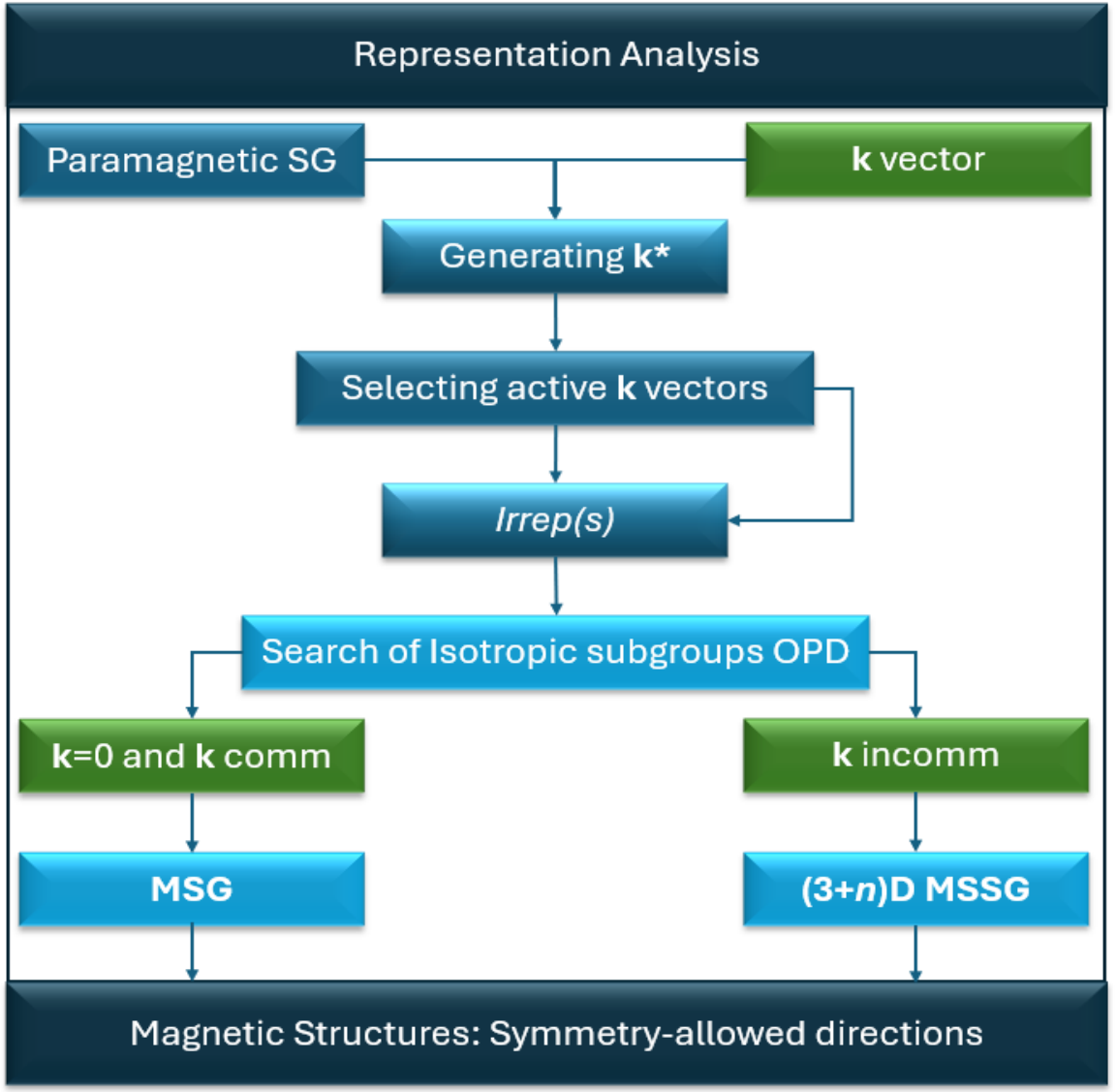
[H. Stokes, D. Hatch, and B. Campbell)]



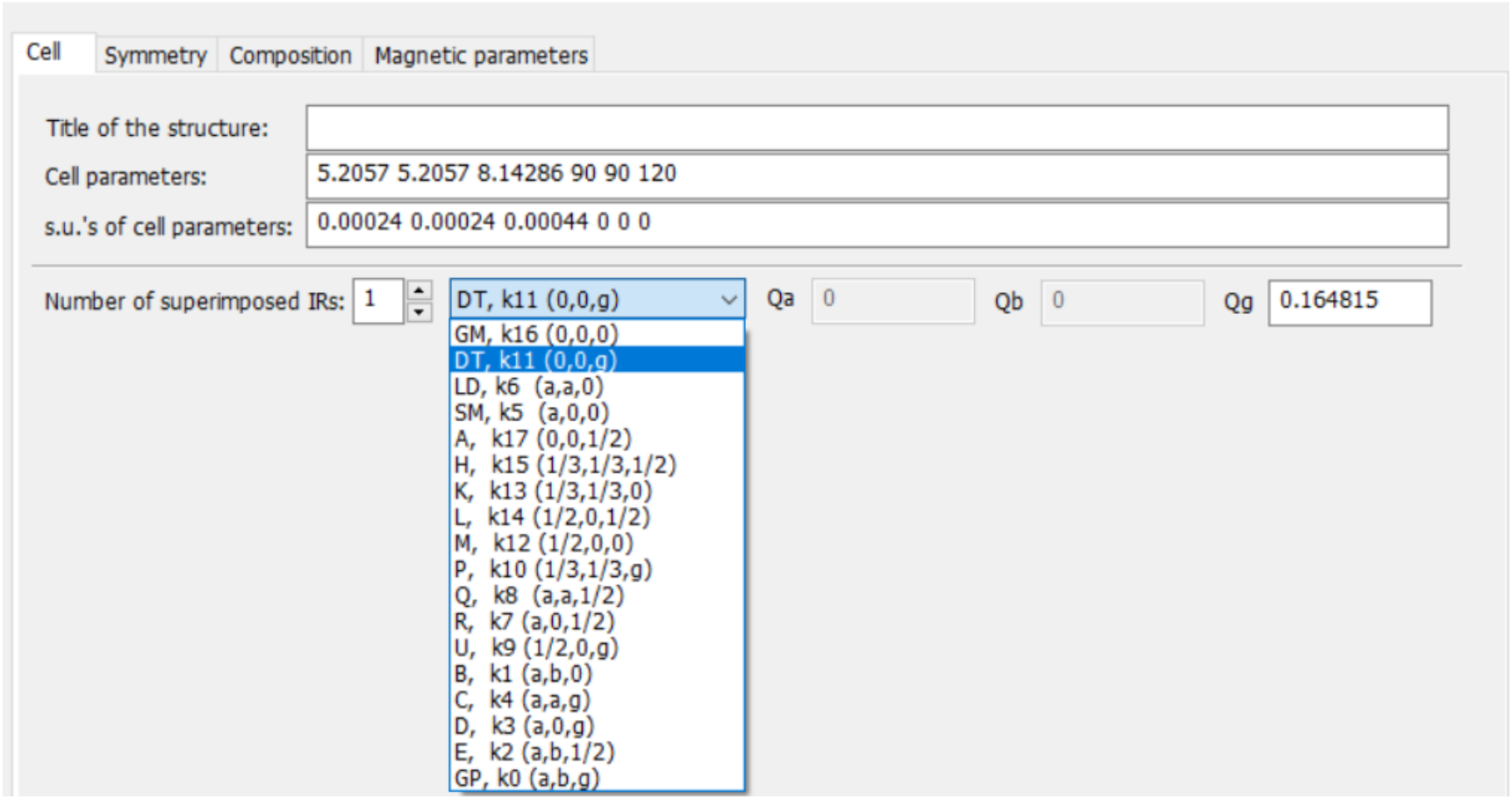
1D *irrep*: a **unique MSG** corresponds to it!

multi-D *irrep*: **several alternative MSG**'s are possible!
(The MSG depends on the way how the spin basis functions are combined!

Representation analysis in Jana2020

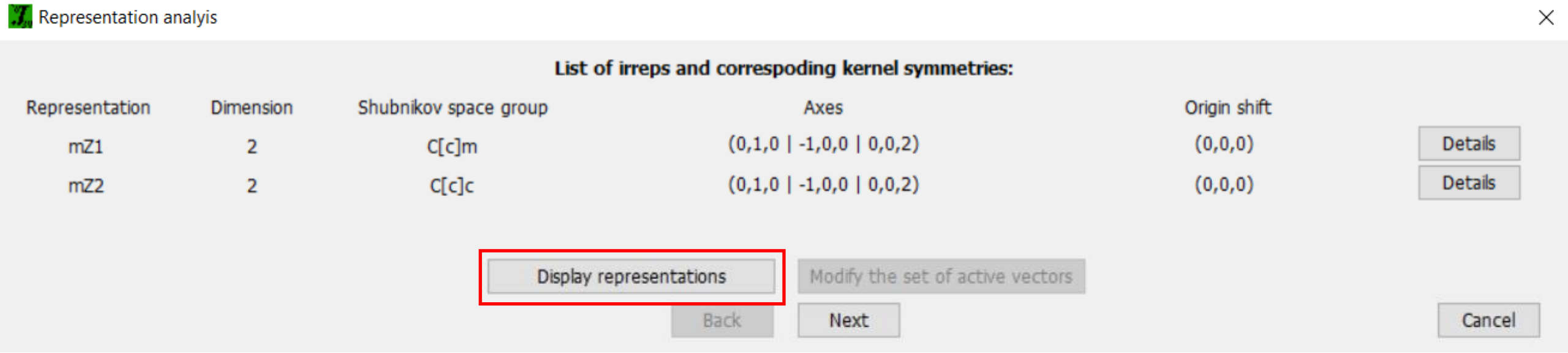


Irrep notations



Representation analysis in Jana2020

Cmcm.1', k= 0 0 1/2



Representation analysis in Jana2020

Cmcm.1’, k= 0 0 1/2

```
List of irreducible representations
structure :


******************
* Structure data *
******************

Centrosymmetric space group: Cmcm  Number : 15

List of centring vectors:

  0.000000  0.000000  0.000000
  0.500000  0.500000  0.000000

Symmetry operators:
```

```
Representation: mZ1  Dimension: 2
---------------------------------

Symmetry operator                          Matrix Character

1:(x,y,z,m)                                |  1  0|     2
                                           |  0  1|

List of irreducible representations
structure :

21[0,0,1]:(-x,-y,z+1/2,m)                  |  0 -1|     0
                                           |  1  0|

2[0,1,0]:(-x,y,-z+1/2,m)                   |  1  0|     0
                                           |  0 -1|

2[1,0,0]:(x,-y,-z,m)                       |  0 -1|     0
                                           | -1  0|

-1:(-x,-y,-z,m)                            |  0 -1|     0
                                           | -1  0|

m[0,0,1]:(x,y,-z+1/2,m)                    |  1  0|     0
                                           |  0 -1|

c[0,1,0]:(x,-y,z+1/2,m)                    |  0 -1|     0
                                           |  1  0|

m[1,0,0]:(-x,y,z,m)                        |  1  0|     2
                                           |  0  1|

1':(x,y,z,-m)                              | -1  0|    -2
                                           |  0 -1|

21'[0,0,1]:(-x,-y,z+1/2,-m)                |  0  1|     0
                                           | -1  0|

2'[0,1,0]:(-x,y,-z+1/2,-m)                 | -1  0|     0
                                           |  0  1|
```

Representation analysis in Jana2020

Cmcm.1’, k= 0 0 1/2

Representation analyis

List of irreps and correspoding kernel symmetries:

Representation	Dimension	Shubnikov space group	Axes	Origin shift	
mZ1	2	C[c]m	(0,1,0 | -1,0,0 | 0,0,2)	(0,0,0)	Details
mZ2	2	C[c]c	(0,1,0 | -1,0,0 | 0,0,2)	(0,0,0)	Details

Representation analysis in Jana2020

Cmcm.1', k= 0 0 1/2

Representation analyis

List of kernels and epikernels:

Shubnikov space group	Axes	Origin shift	Representation	OPD
A[a]mm2	(0,0,2 | 1,0,0 | 0,1,0)	(1/8,0,0)	mZ1	(0,a)
A[a]ma2	(0,0,2 | 1,0,0 | 0,1,0)	(1/8,0,0)	mZ2	(0,a)
C[c]2/m	(0,1,0 | -1,0,0 | 0,0,2)	(0,0,1/4)	mZ1	(a,a)
C[c]2/c	(0,1,0 | -1,0,0 | 0,0,2)	(0,0,0)	mZ2	(a,a)
C[c]m	(0,1,0 | -1,0,0 | 0,0,2)	(0,0,0)	mZ1	(a,b)
C[c]c	(0,1,0 | -1,0,0 | 0,0,2)	(0,0,0)	mZ2	(a,b)

Representation analysis in Jana2020

Pnma.1', k= 0.15858 0 0

Representation analyis

List of irreps and correspoding kernel symmetries:

Representation	Dimension	Shubnikov superspace group	Axes	Origin shift	
mSM1	2	Pmc21.1'(00g)000s	(0,1,0 | 0,0,1 | 1,0,0)	(1/4,1/4,0,0)	Details
mSM2	2	Pmc21.1'(00g)ss0s	(0,1,0 | 0,0,1 | 1,0,0)	(1/4,1/4,0,0)	Details
mSM3	2	Pmc21.1'(00g)0sss	(0,1,0 | 0,0,1 | 1,0,0)	(1/4,1/4,0,0)	Details
mSM4	2	Pmc21.1'(00g)s0ss	(0,1,0 | 0,0,1 | 1,0,0)	(1/4,1/4,0,0)	Details

Representation analysis in Jana2020

Pnma.1’, k= 0.15858 0 0

Representation analyis

List of kernels and epikernels:

Shubnikov superspace	Axes	Origin shift	Representation	OPD
Pnma.1'(a00)000s	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0,0)	mSM1	(a,0)
Pnma.1'(a00)0sss	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0,0)	mSM2	(0,a)
Pnma.1'(a00)00ss	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0,0)	mSM3	(a,0)
Pnma.1'(a00)0s0s	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0,0)	mSM4	(0,a)
Pmc21.1'(00g)000s	(0,1,0 | 0,0,1 | 1,0,0)	(1/4,1/4,0,0)	mSM1	(a,b)
Pmc21.1'(00g)ss0s	(0,1,0 | 0,0,1 | 1,0,0)	(1/4,1/4,0,0)	mSM2	(a,b)
Pmc21.1'(00g)0sss	(0,1,0 | 0,0,1 | 1,0,0)	(1/4,1/4,0,0)	mSM3	(a,b)
Pmc21.1'(00g)s0ss	(0,1,0 | 0,0,1 | 1,0,0)	(1/4,1/4,0,0)	mSM4	(a,b)

Symmetry and magnetic diffraction

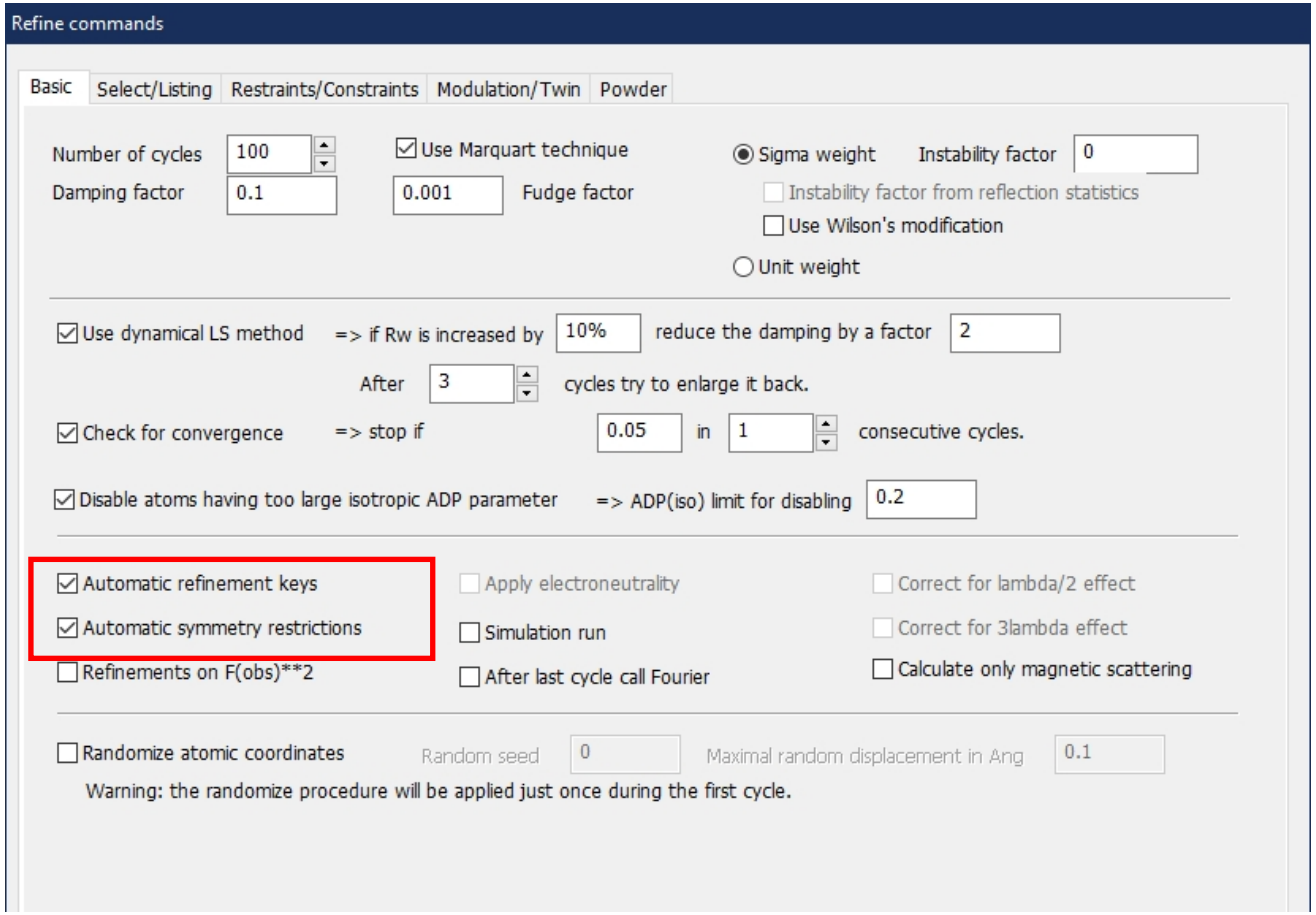
Each **symmetry operation** of the magnetic point group induces **rotation symmetry** (proper or improper) in the magnetic diffraction pattern.

- Magnetic diffraction patterns (upolarized beam) **follow** the Laue symmetry
- There is **no** direct influence of time inversion signal in the diffraction pattern
- The diffraction symmetry **cannot** be used to determine the actual magnetic group!
  - Single crystal data: lowering point group symmetry during the phase transition is usually almost fully “compensated” by creation of equally populated magnetic domains
  - Powder data: reflections which could help are almost completely overlapped

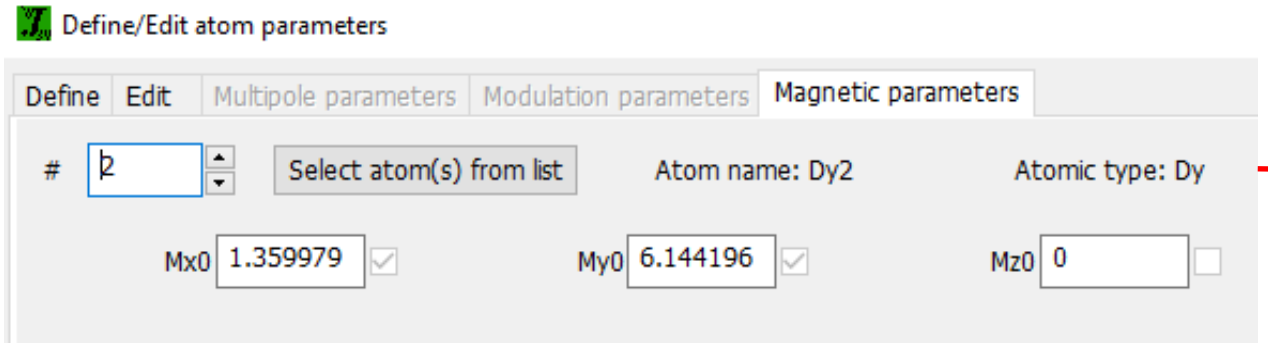
Handling symmetry in Jana2020

- **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
- It supports an interactive **transformation to lower symmetry**
- All **extinction conditions** and **symmetry restrictions** of structural parameters are **derived analytically from symmetry operations and the actual position of the atom**

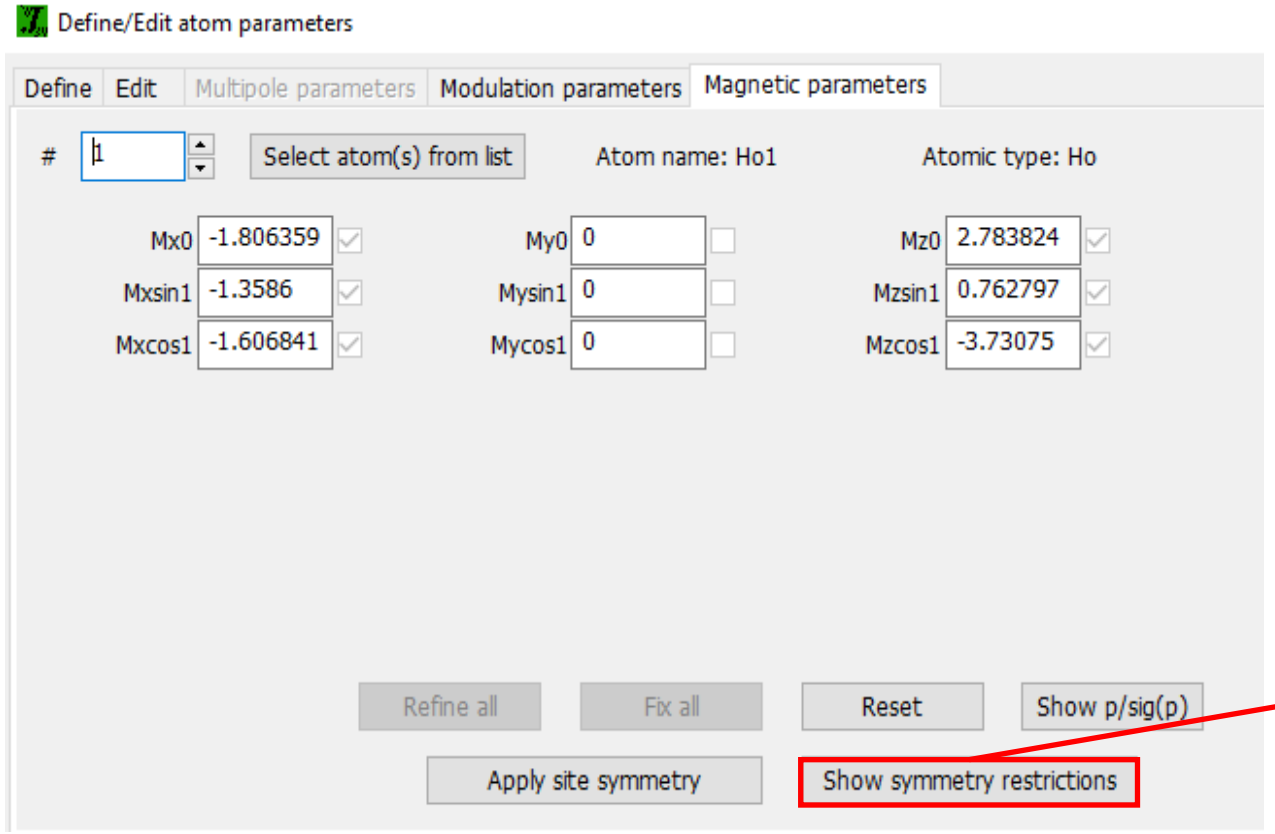
Magnetic option in Jana2020



Magnetic option in Jana2020




```
[Dy1]=0.125
mx0[Dy1]=0
my0[Dy1]=0
```

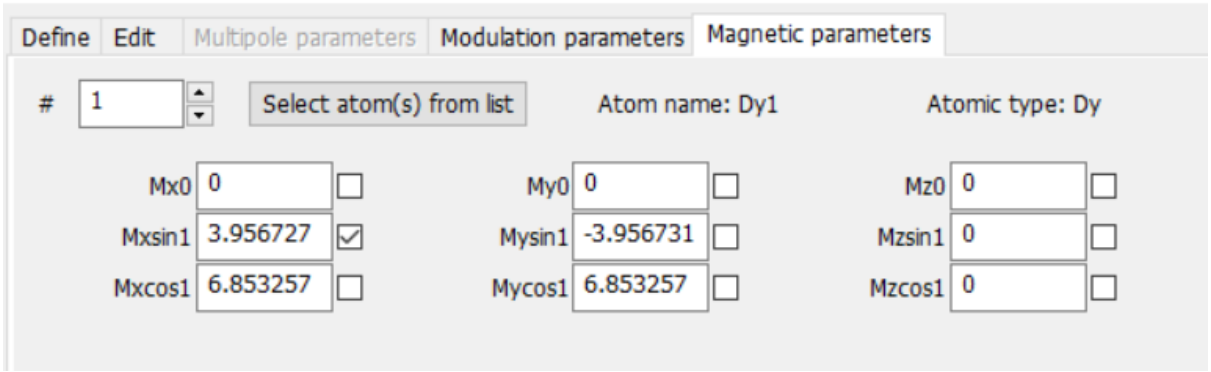



```
y[Ho1]=0.25
my0[Ho1]=0
mysin1[Ho1]=0
mycos1[Ho1]=0
```

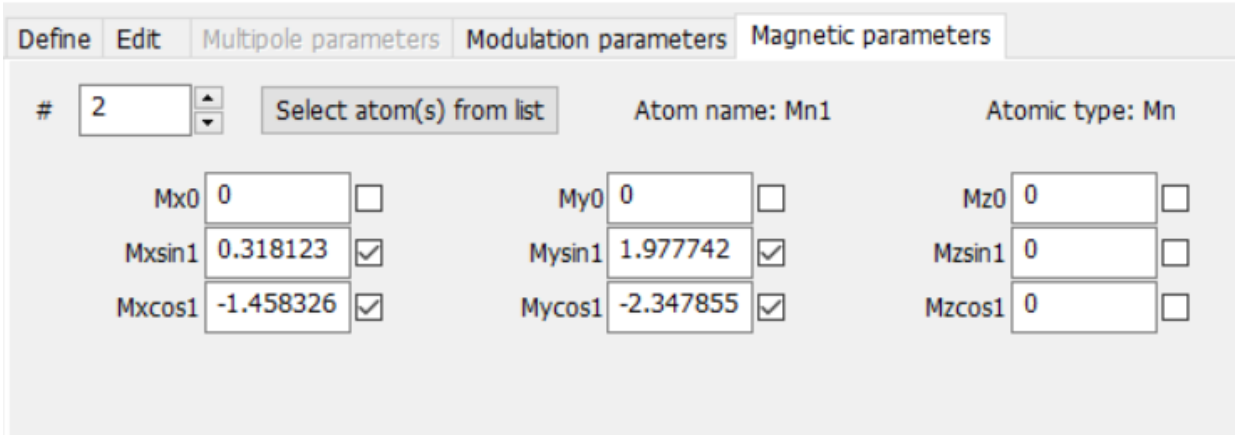
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Magnetic option in Jana2020

Define/Edit atom parameters



Define/Edit atom parameters

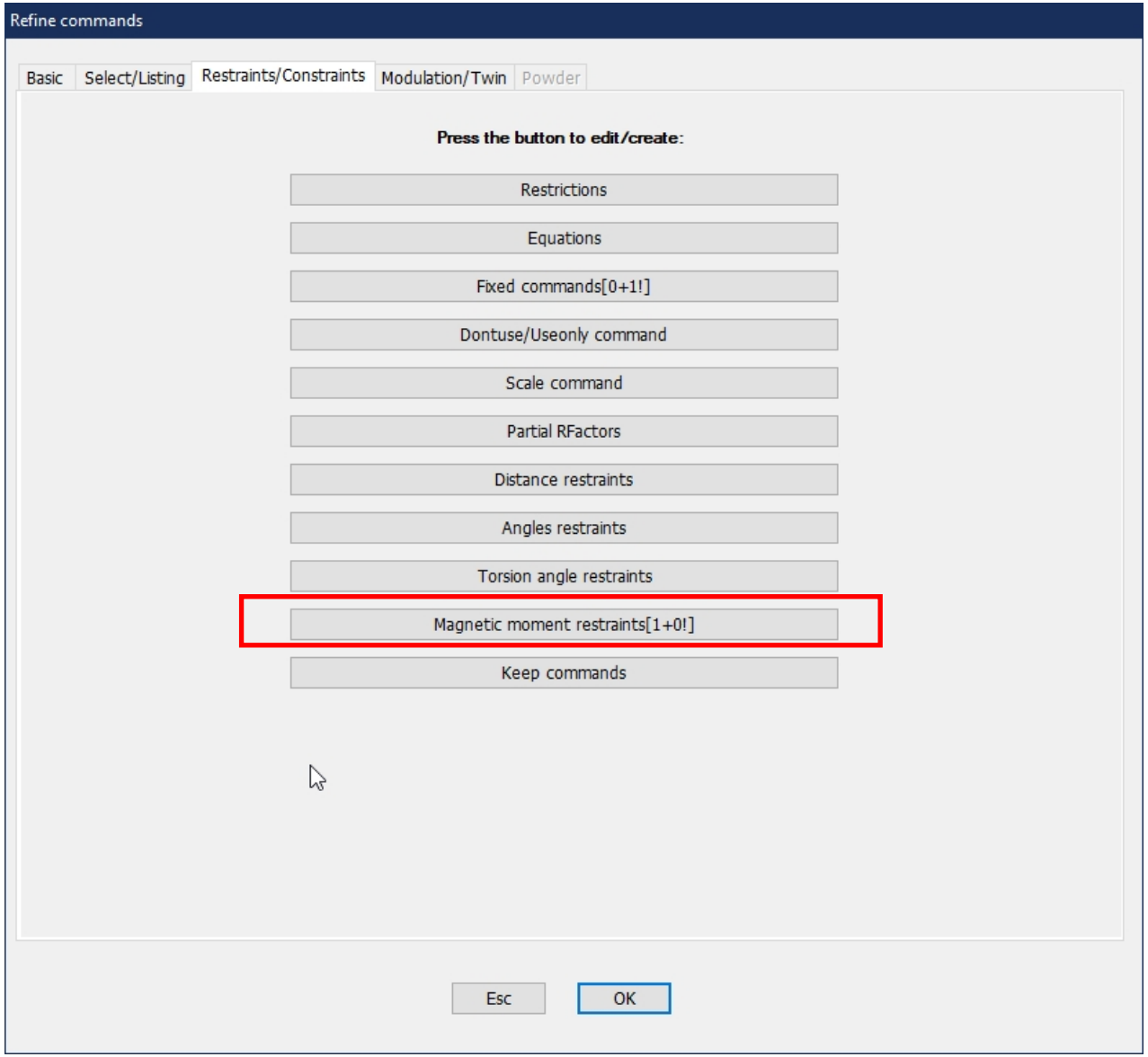


Refinement file

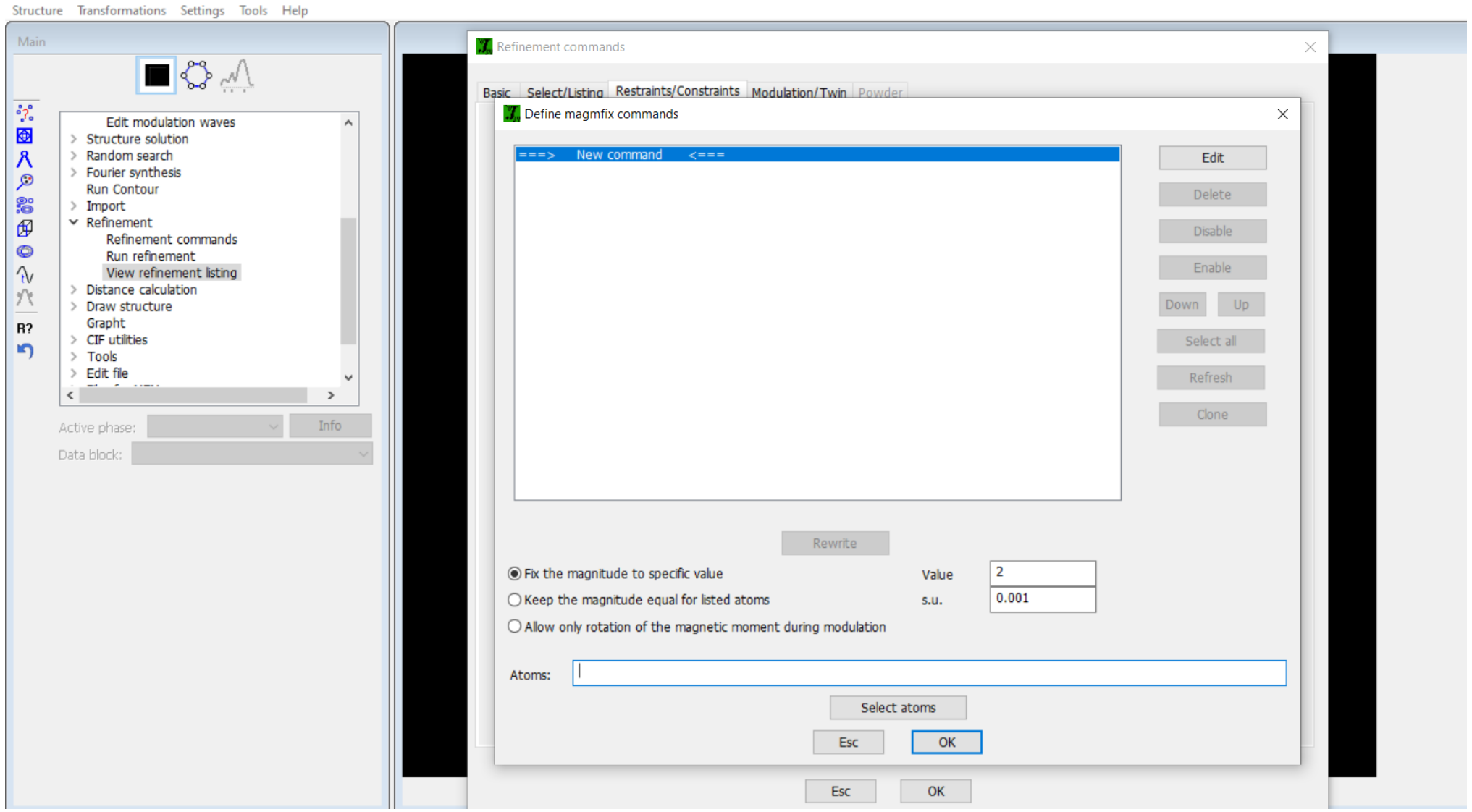
```
y[Dy1]=0
z[Dy1]=0
mx0[Dy1]=0
Refinement program
structure :

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
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

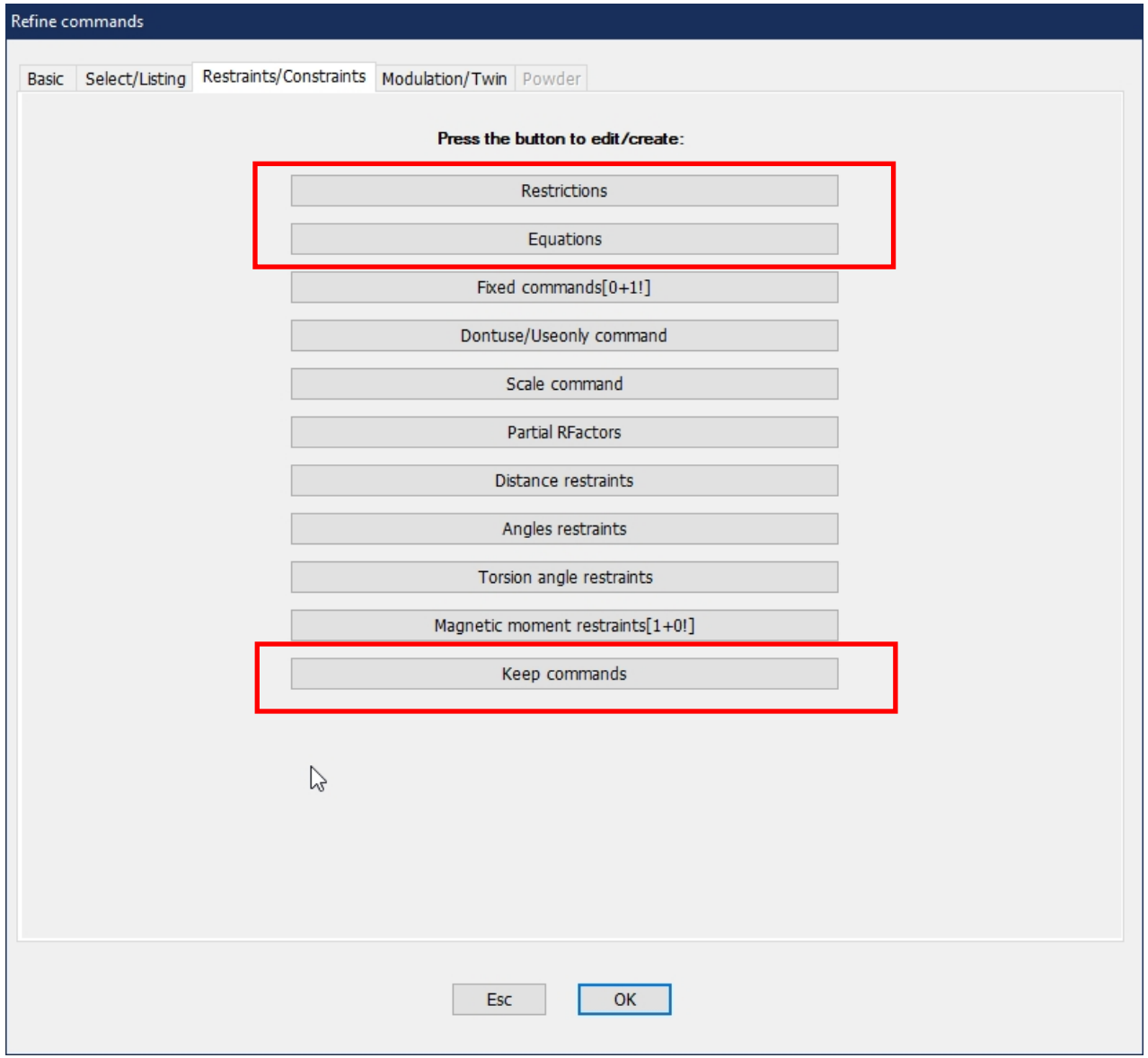
Jana2020


Structure Transformations Settings Tools Help
Main
Edit modulation waves
Structure solution
Random search
Fourier synthesis
Run Contour
Import
Refinement
Refinement commands
Run refinement
View refinement listing
Distance calculation
Draw structure
Grapht
CIF utilities
Tools
Edit file
Active phase:
Info
Data block:
Refinement commands
Basic
Select/Listing
Restraints/Constraints
Modulation/Twin
Powder
Define magmfix commands
===> New command <===
Edit
Delete
Disable
Enable
Down
Up
Select all
Refresh
Clone
Rewrite
Fix the magnitude to specific value
Keep the magnitude equal for listed atoms
Allow only rotation of the magnetic moment during modulation
Value
s.u.
2
0.001
Atoms:
Select atoms
Esc
OK
Esc
OK

Jana2020

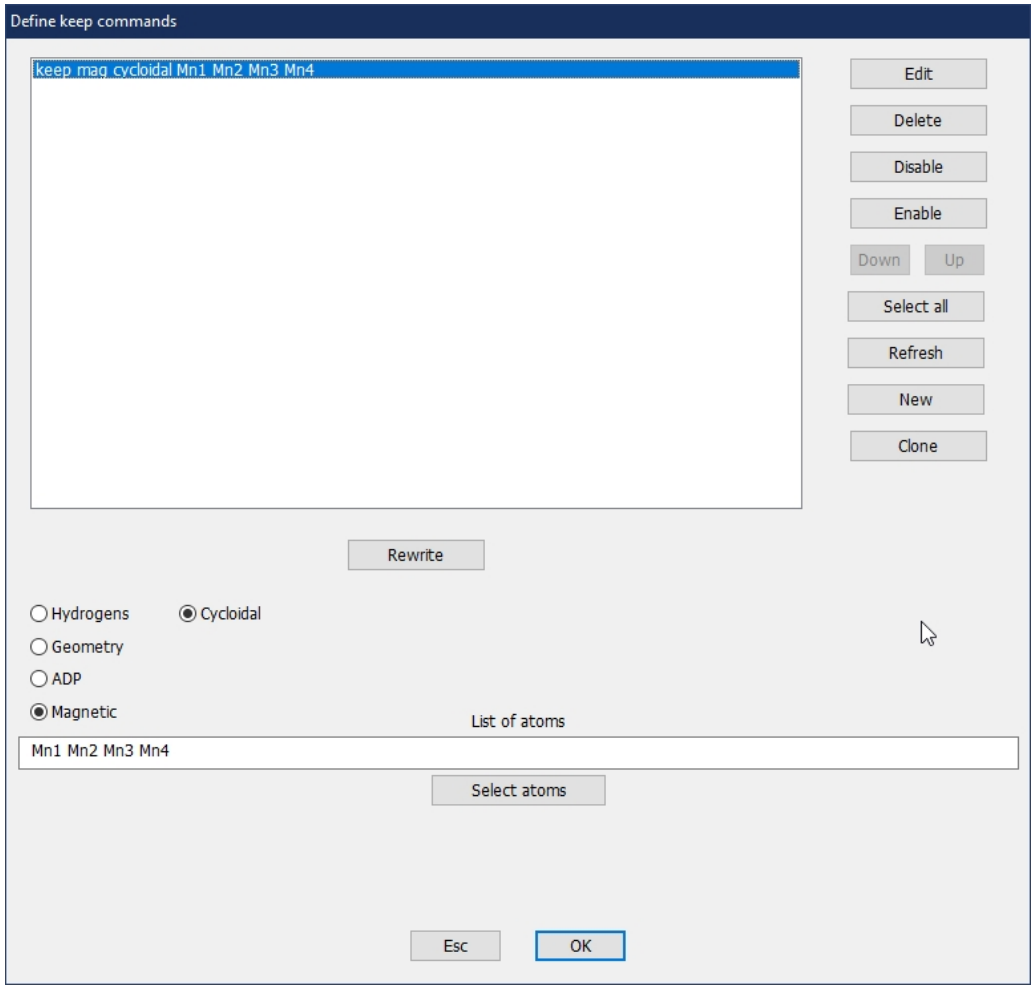
There are three different types of constrains:

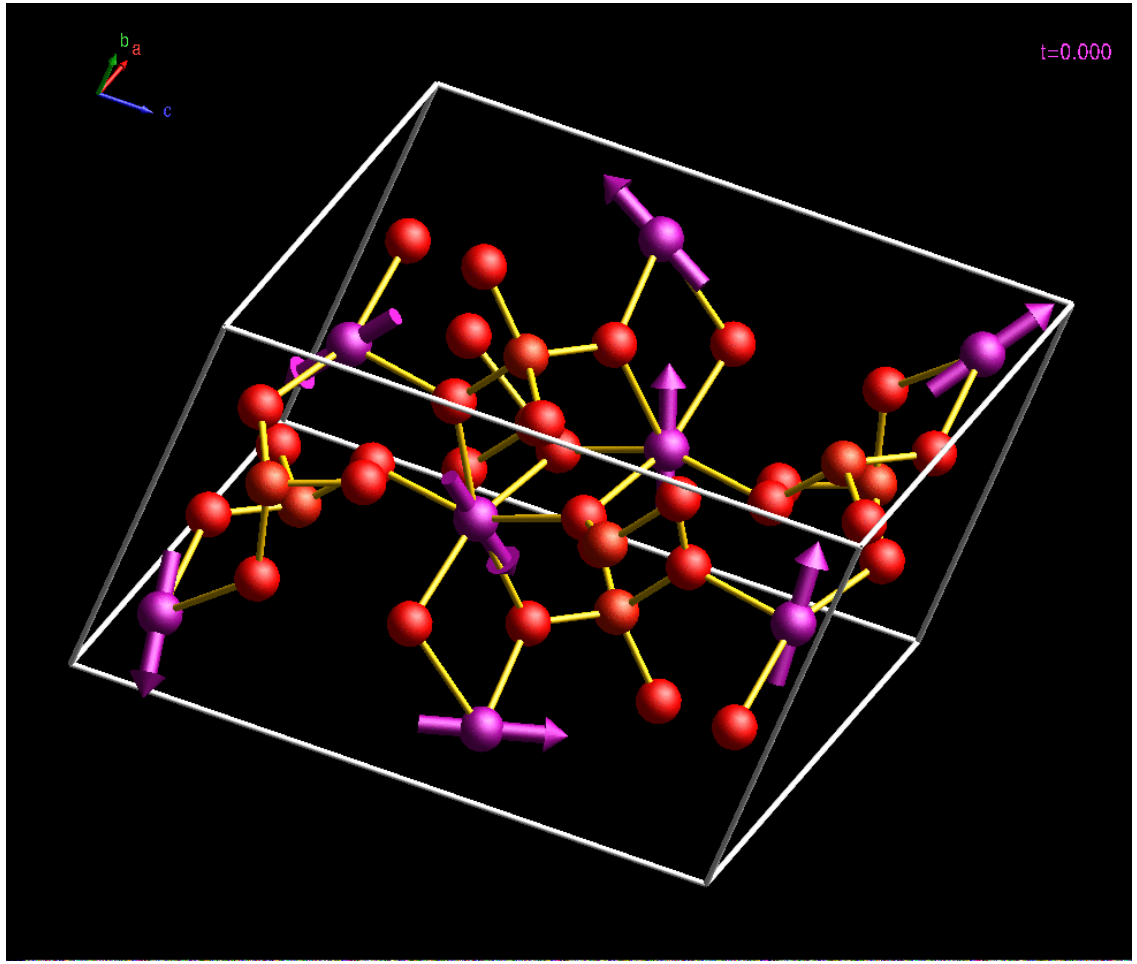
- “restrict” commands: Selected parameters (coordinates, ADP, modulation, **magnetic parameters…**) of two or more atoms can be made identical or related by a local symmetry operation
- “equation” commands: user-defined linear equations containing linear combinations of parameters
- “keep” commands



Jana2020

The command keeps a cycloidal modulation for Mn atoms





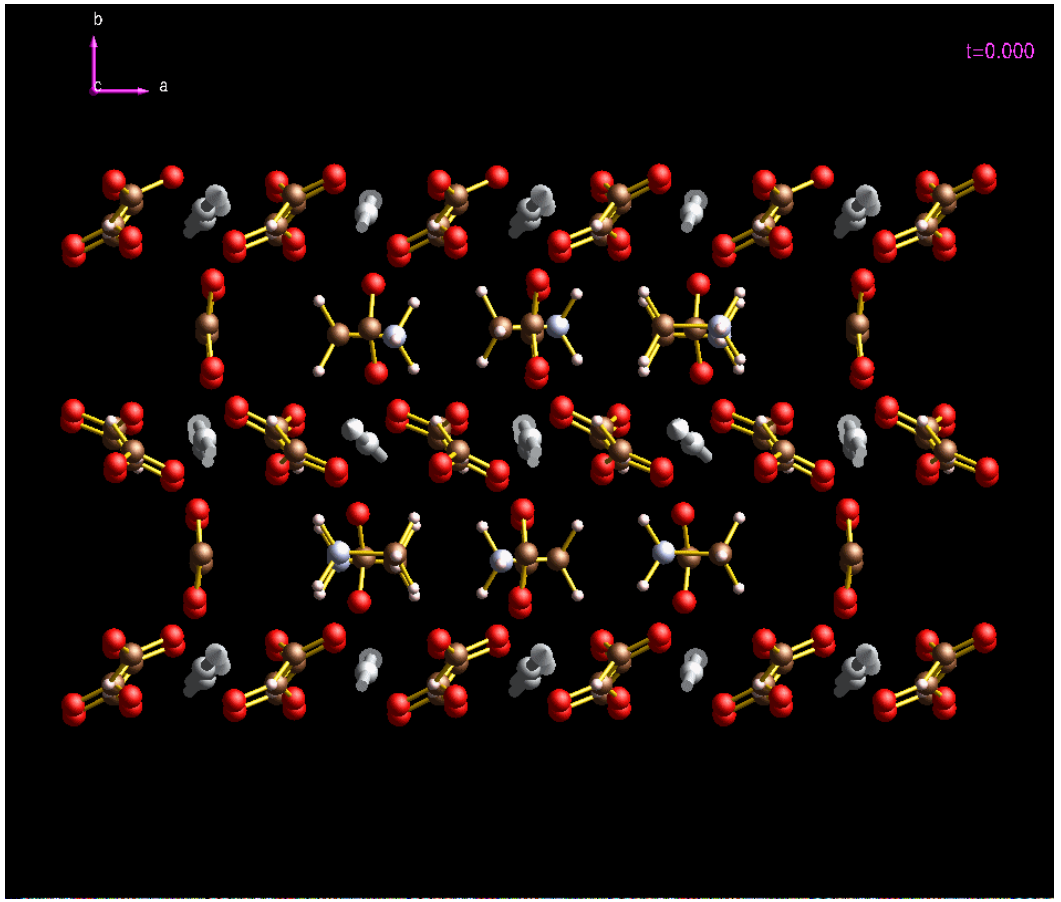
Magnetic option in Jana2020

Magnetic structures

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

+

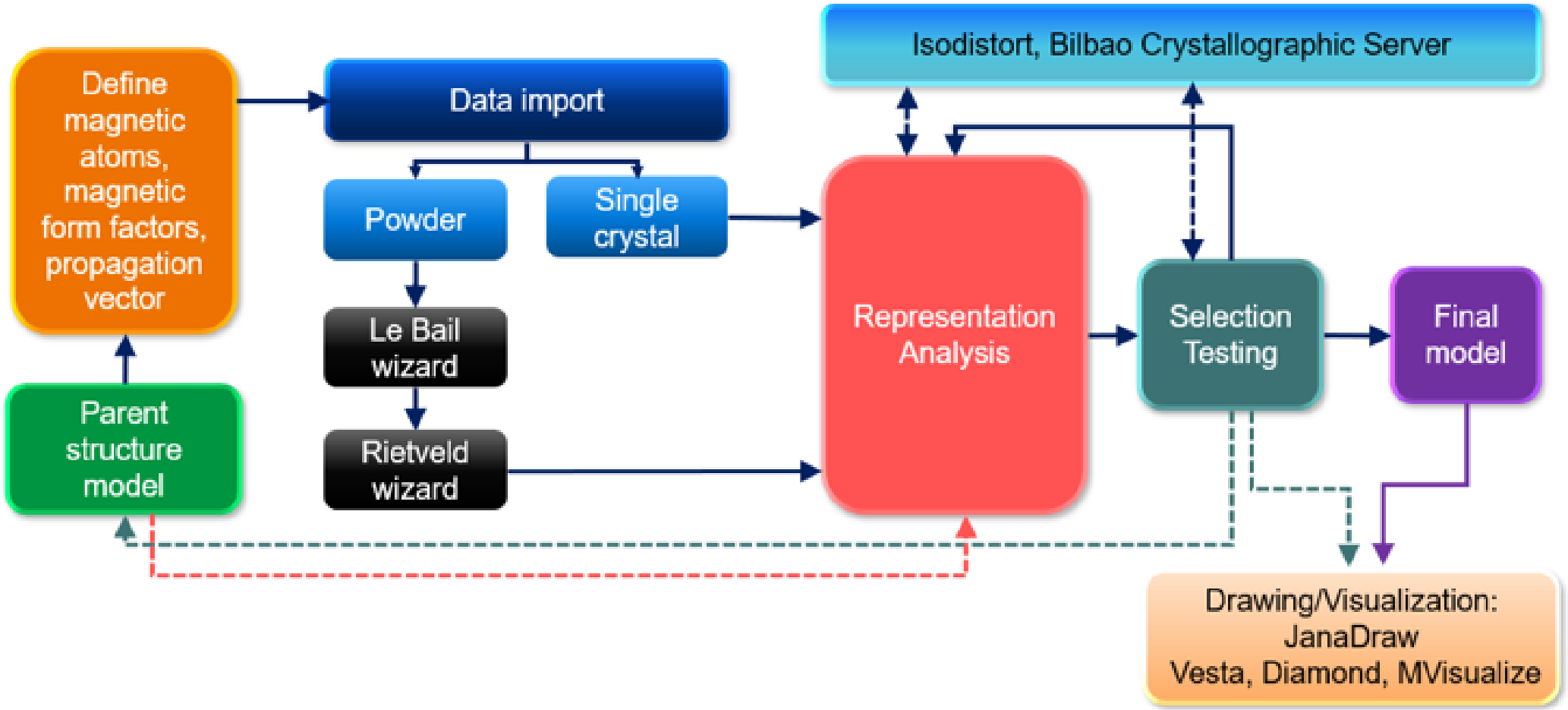
Modulation functions for the atomic parameters



Magnetic option in Jana2020

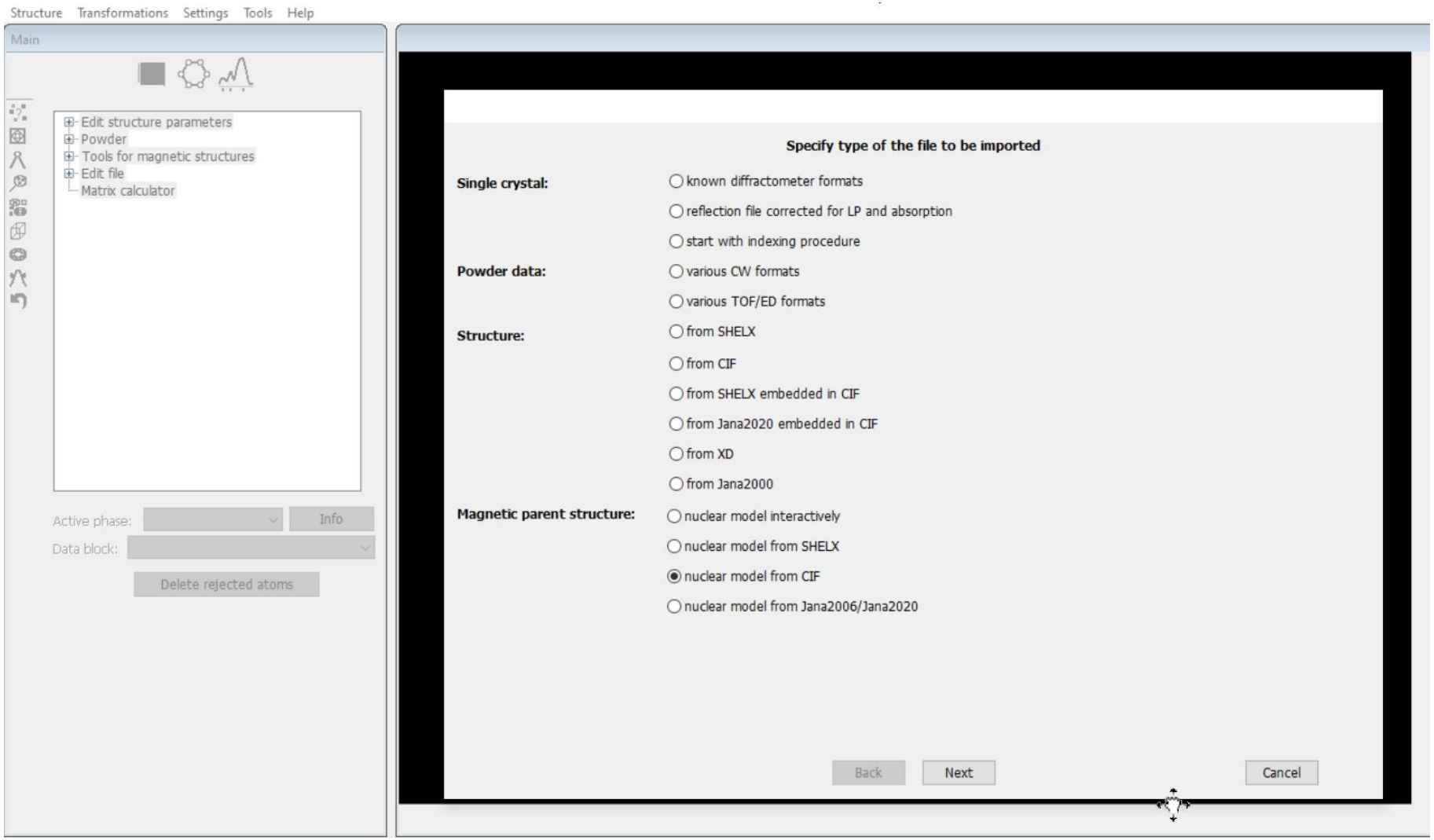
- **Superspace** approach is implemented for modulations:
  - **Structure factors** calculated from **MS(S)G**
  - Systematic **extinctions** and all **symmetry restrictions** are **derived analytically**
- **Mag+nuclear** contributions calculated in **parallel** and combined accordingly
- A wizard creates a "**parent" structure** which is used to test different MS(S)G
- **RA** is performed by a simple tool which calculates **Isotropy subgroups** of active irreps (multi-k incommensurate structures: ISODISTORT)
- For graphic visualization
  - internal drawing program: JanaDraw
  - calls VESTA, Diamond, other programs (cif or mcif)

Magnetic option in Jana2020



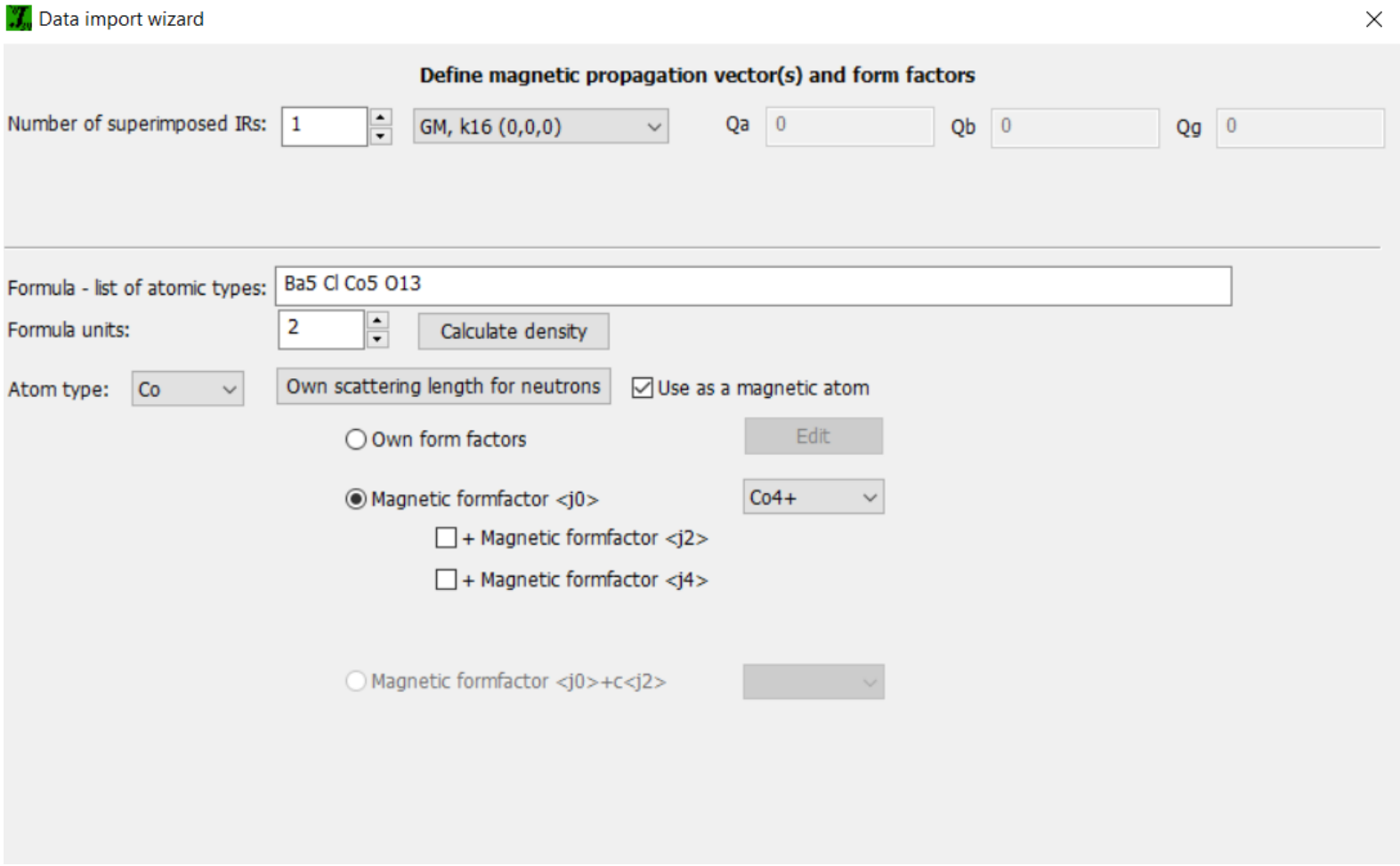
Magnetic option in Jana2020

Importing the parent structure



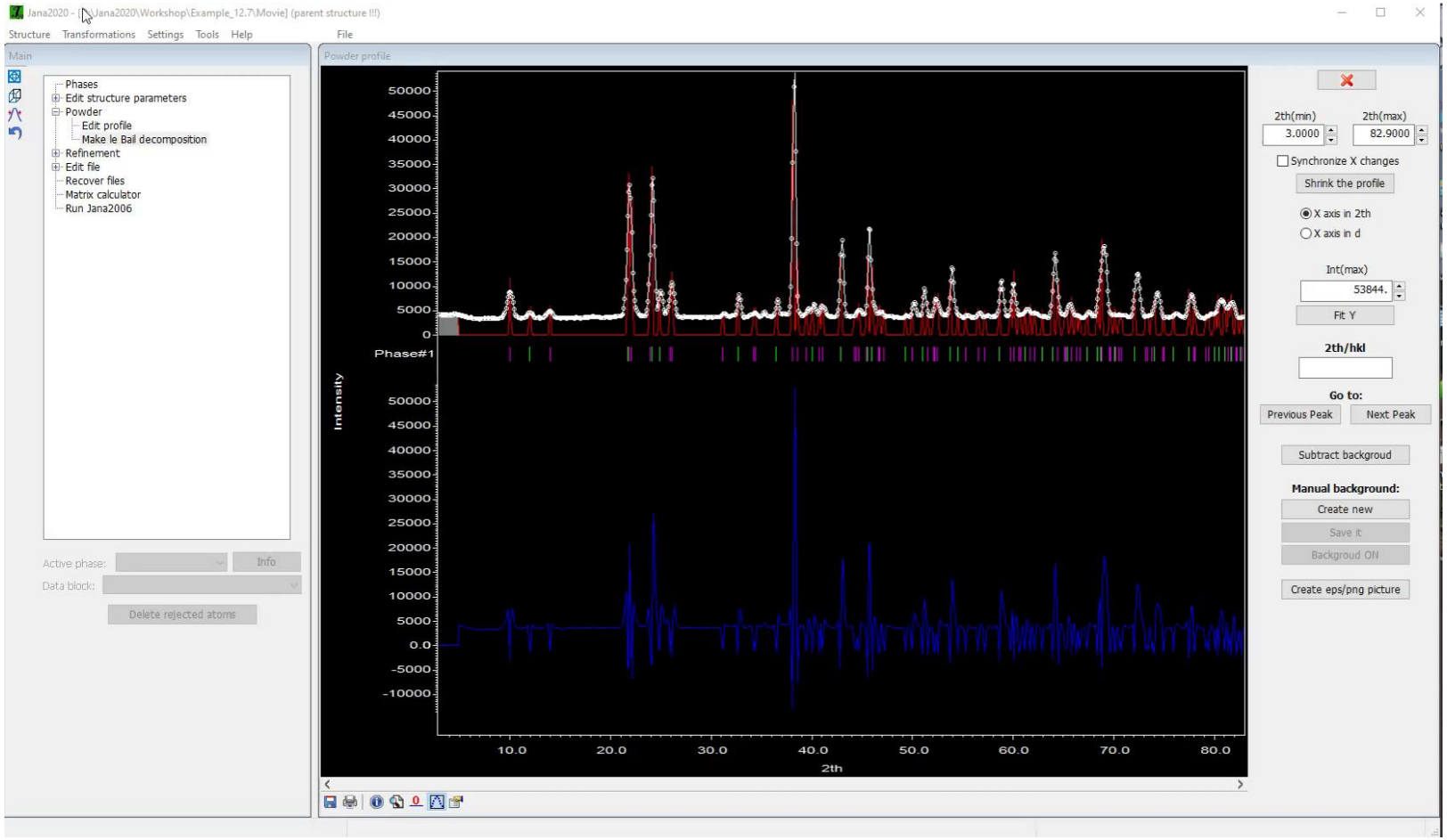
Magnetic option in Jana2020

Defining propagation vectors and magnetic atoms



Magnetic option in Jana2020

Le Bail and Rietveld refinements

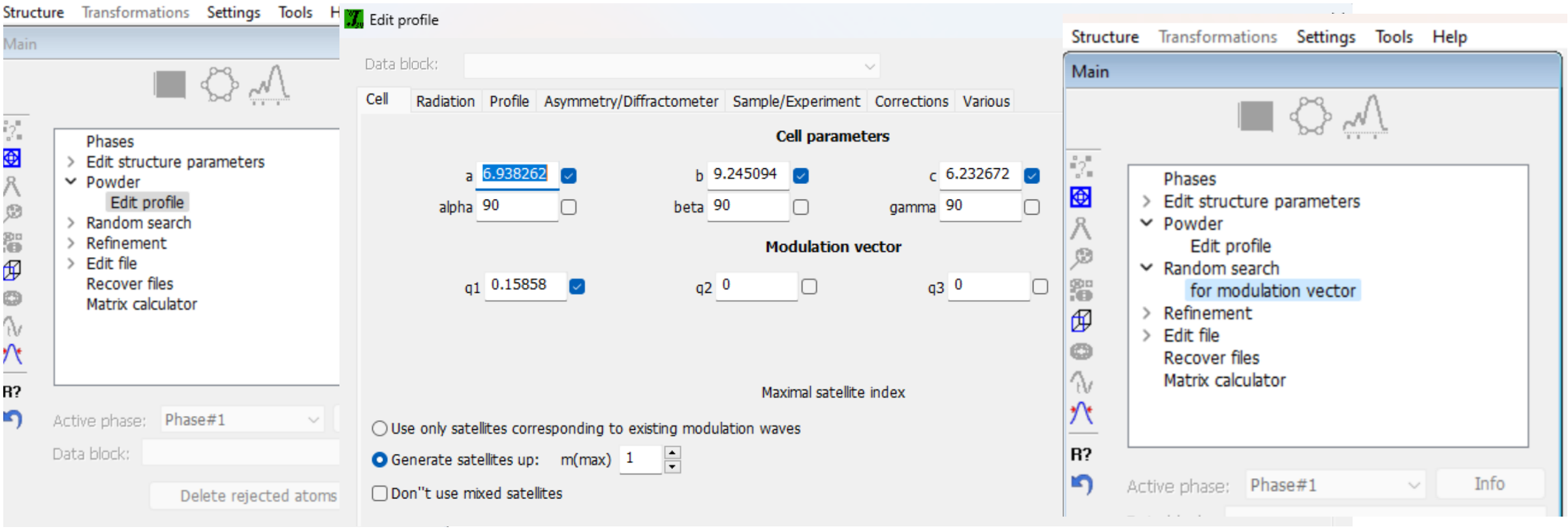


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Magnetic option in Jana2020

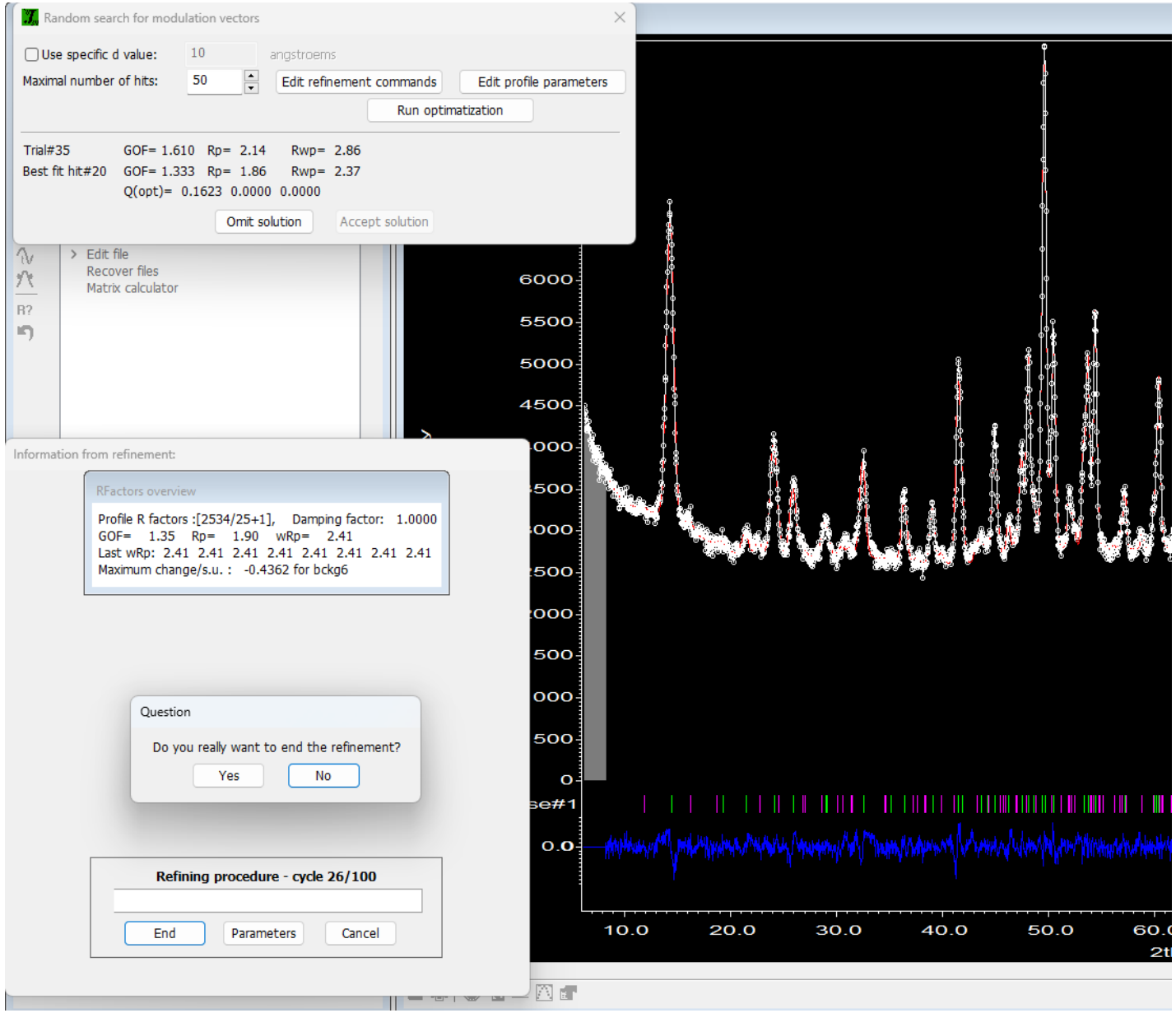
K-search (powder data): Accessible from the parent structure

Edit profile → change **k** → Random search for modulation vector



Magnetic option in Jana2020

K-search (powder data):



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Representation analysis in Jana2020

Jana2020: limited to **one** modulation vector

More vectors: ISODISTORT



stokes.byu.edu/iso/isotropy.php

ISOTROPY Software Suite

Harold T. Stokes, Dorian M. Hatch, and Branton J. Campbell, Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84606, USA, branton_campbell@byu.edu

Description: The ISOTROPY software suite is a collection of software which applies group theoretical methods to the analysis of phase transitions in crystalline solids.

How to cite: To cite a tool from the ISOTROPY Software Suite, see the citation instructions on the tool's individual home page. To cite the entire suite, use the following:
H. T. Stokes, D. M. Hatch, and B. J. Campbell, ISOTROPY Software Suite, iso.byu.edu.

References and Resources

Isotropy subgroups and distortions

- **ISODISTORT**: Explore and visualize distortions of crystalline structures. Possible distortions include atomic displacements, atomic ordering, strain, and magnetic moments.
- **ISOSUBGROUP**: Interactive program using user-friendly interface to list isotropy subgroups.
- **ISOTROPY**: Interactive program using command lines to explore isotropy subgroups and their associated distortions.
- **ISOTILT**: **NEW!** Interactive program for detecting cooperative rigid-unit modes (RUMs) in framework materials.
- **SMODES**: Find the displacement modes in a crystal which brings the dynamical matrix to block-diagonal form, with the smallest possible blocks.
- **FROZSL**: Calculate phonon frequencies and displacement modes using the method of frozen phonons.
- **ISOVIZ**: Stand-alone utility for viewing interactive distortions created by ISODISTORT (installers only, alpha version).

Space groups and irreducible representations

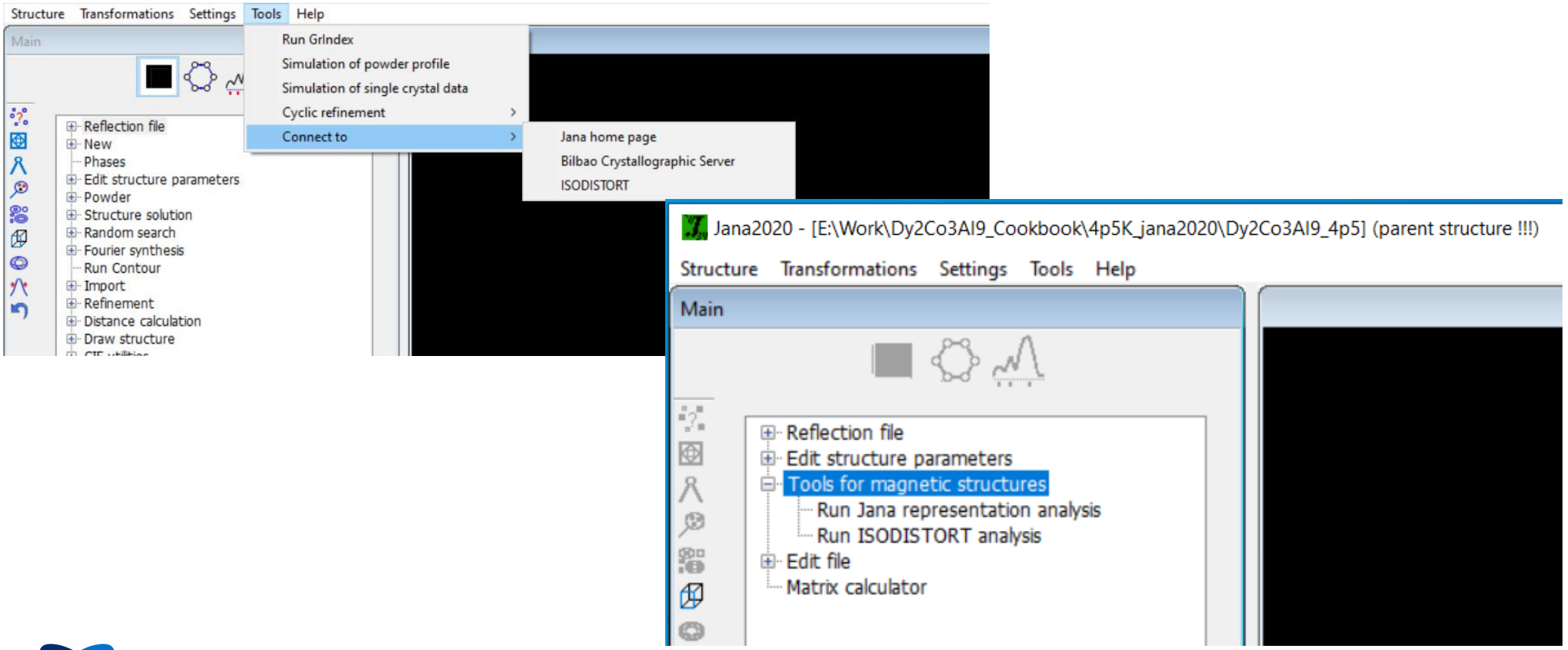
- **ISOCIF**: Create or modify CIF files.
- **FINDSYM**: Identify the space group of a crystal, given the positions of the atoms in a unit cell.
- **ISOSPACEGROUP**: **NEW!** Tables of crystallographic space groups: nonmagnetic and magnetic 3-dimensional space groups and (3+d)-dimensional superspace groups.
- **ISO-IR**: Tables of Irreducible Representations. The 2011 version of IR matrices.
- **ISO-KOV**: **NEW!** Mapping of the irreducible representations of Kovalev onto those of Cracknell, Davies, Miller and Love.
- **ISO-MAG**: Tables of magnetic space groups, both in human-readable and computer-readable forms.

Superspace Groups

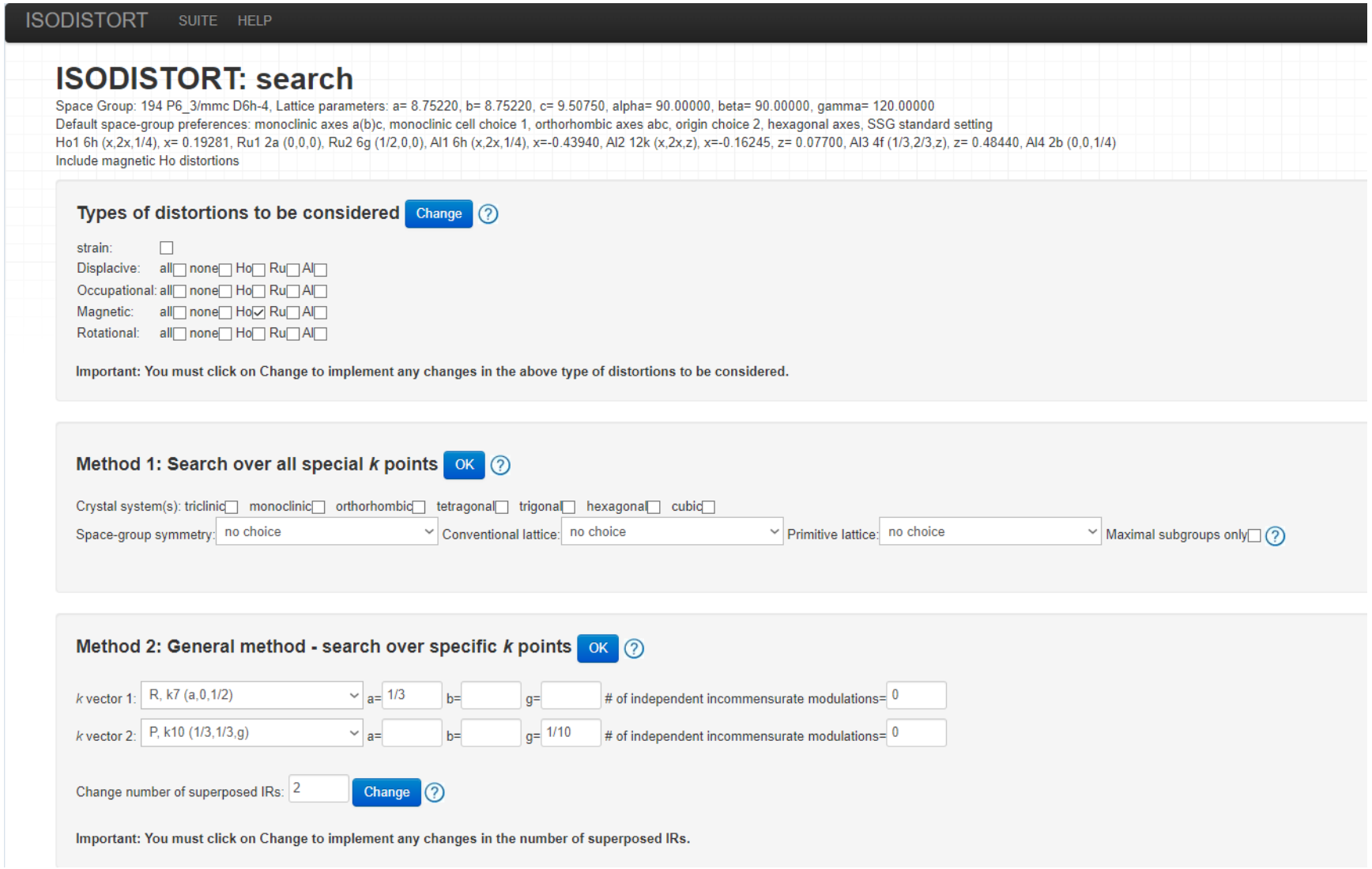
- **ISO(3+d)D**: (3+d)-Dimensional Superspace Groups for d=1,2,3
- **ISO(3+1)D**: Isotropy Subgroups for Incommensurately Modulated Distortions in Crystalline Solids: A Complete List for One-Dimensional Modulations
- **FINDSSG**: Identify the superspace group symmetry given a list of symmetry operators.
- **TRANSFORMSSG**: Transform a superspace group to a new setting.

Magnetic option in Jana2020

ISODISTORT



Magnetic option in Jana2020



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Magnetic option in Jana2020

ISODISTORT SUITE HELP

ISODISTORT: distortion

Space Group: 194 P6_3/mmc D6h-4, Lattice parameters: a= 8.75220, b= 8.75220, c= 9.50750, alpha= 90.00000, beta= 90.00000, gamma= 120.00000
Default space-group preferences: monoclinic axes a(b)c, monoclinic cell choice 1, orthorhombic axes abc, origin choice 2, hexagonal axes, SSG standard setting
Ho1 6h (x,2x,1/4), x= 0.19281, Ru1 2a (0,0,0), Ru2 6g (1/2,0,0), Al1 6h (x,2x,1/4), x=-0.43940, Al2 12k (x,2x,z), x=-0.16245, z= 0.07700, Al3 4f (1/3,2/3,z), z= 0.48440, Al4 2b (0,0,1/4)
Include magnetic Ho distortions
k point: R, k7 (a,0,1/2), a=1/3
IR: mR1R3, mk7t1t4
k point: P, k10 (1/3,1/3,g), g=1/10
IR: mP3, mk10t3
C7(1)C8(1) (a,-a,b,b;b,-b,-a,-a;0,0,0,0|c,-c,d,d;-c,c,d,d) 15.90 C2/c.1'_c[C2/m], basis={(3,-3,0),(3,3,0),(0,0,10)}, origin=(0,0,0), s=90, i=540, k-active= (1/3,0,1/2),(0,1/3,1/2);(1/3,1/3,1/10),(2/3,2/3,1/10)
Lattice parameters of undistorted supercell: a=45.47777, b=26.25660, c=95.07500, alpha=90.00000, beta=90.00000, gamma=90.00000

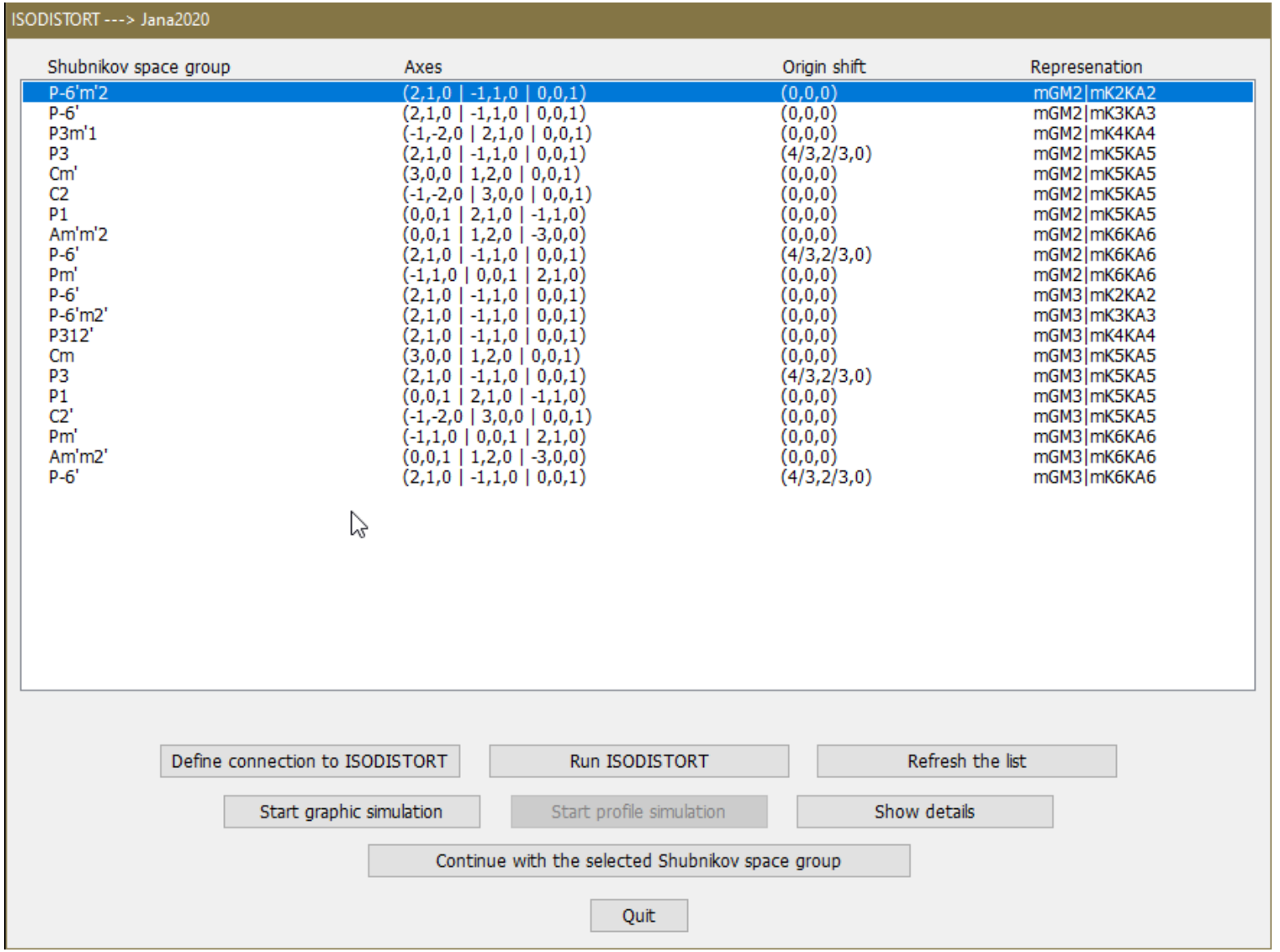
○ Save interactive distortion ○ Save interactive diffractio ◉ CIF file ○ Distortion file ○ Domains ○ Primary order parameters ○ Modes details ○ Complete modes details ○ TOPAS.STR ○ FULLPROF.pcr ○ IR matrices ○ Subgroup tree OK

Warning: mode-amplitude input fields are not provided when the number of modes (210) is greater than 200

P6_3/mmc[1/3,0,1/2]mR1R3 (a,-a,b,b;b,-b,-a,-a;0,0,0,0) 15.90 C2/c.1'_c[C2/m], basis={(3,-3,0),(3,3,0),(0,0,2)}, origin=(0,0,0), s=18, i=108, k-active= (1/3,0,1/2),(0,1/3,1/2)
0 [Ho1:h:mag]B2(a)
0 [Ho1:h:mag]B2(b)
0 [Ho1:h:mag]A2(a)
0 [Ho1:h:mag]A2(b)
0 [Ho1:h:mag]B1_1(a)
0 [Ho1:h:mag]B1_1(b)
0 [Ho1:h:mag]B1_2(a)
0 [Ho1:h:mag]B1_2(b)

P6_3/mmc[1/3,1/3,1/10]mP3 (a,-a,b,b;-a,a,b,b) 15.90 C2/c.1'_c[C2/m], basis={(1,-1,0),(3,3,0),(0,0,10)}, origin=(0,0,0), s=30, i=180, k-active= (1/3,1/3,1/10),(2/3,2/3,1/10)
0 [Ho1:h:mag]B2_1(a)
0 [Ho1:h:mag]B2_1(b)
0 [Ho1:h:mag]B2_2(a)
0 [Ho1:h:mag]B2_2(b)
0 [Ho1:h:mag]A2_1(a)
0 [Ho1:h:mag]A2_1(b)
0 [Ho1:h:mag]A2_2(a)
0 [Ho1:h:mag]A2_2(b)
0 [Ho1:h:mag]B1_1(a)
0 [Ho1:h:mag]B1_1(b)
0 [Ho1:h:mag]B1_2(a)
0 [Ho1:h:mag]B1_2(b)

Magnetic option in Jana2020



Magnetic option in Jana2020

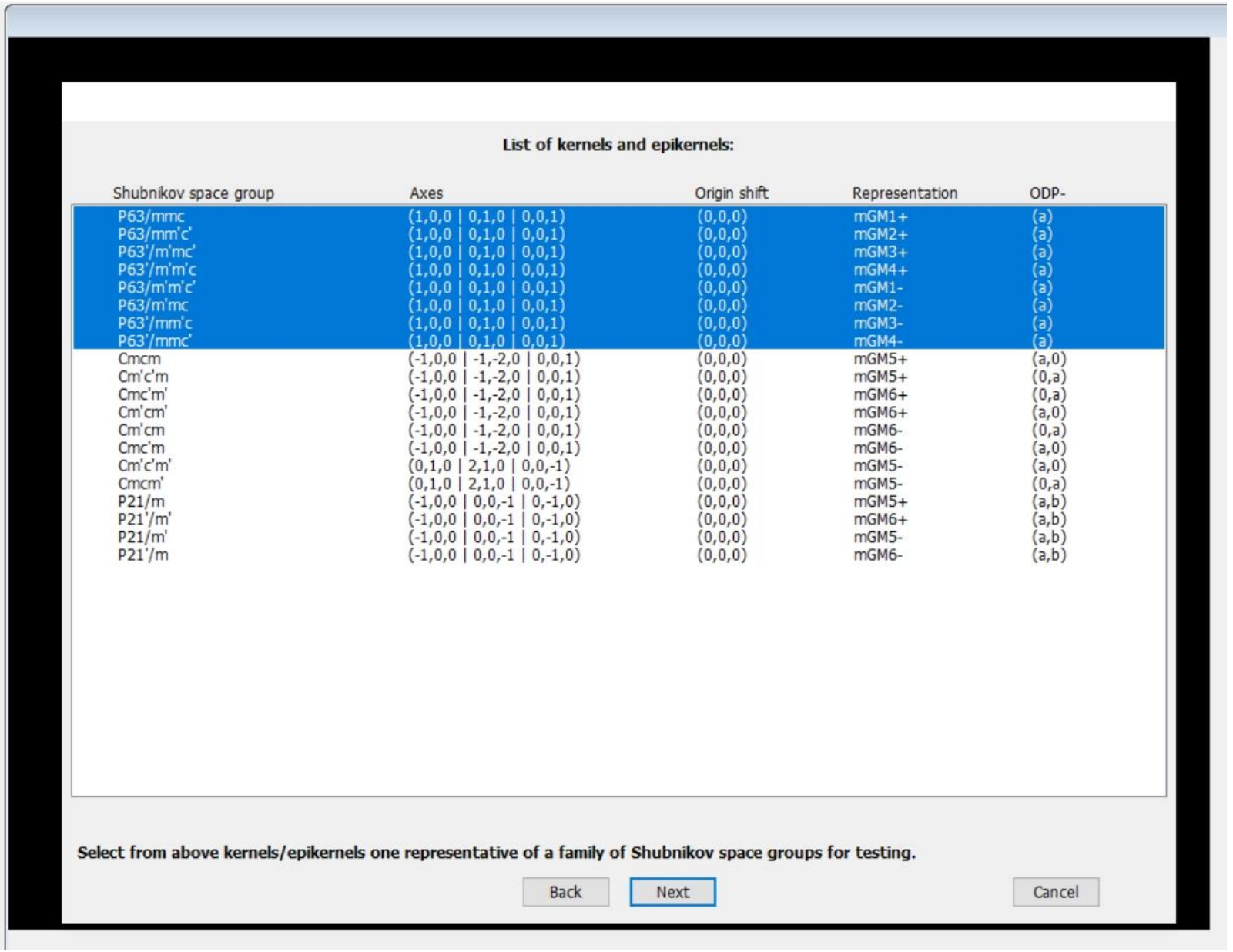
Representation Analysis

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

Magnetic option in Jana2020

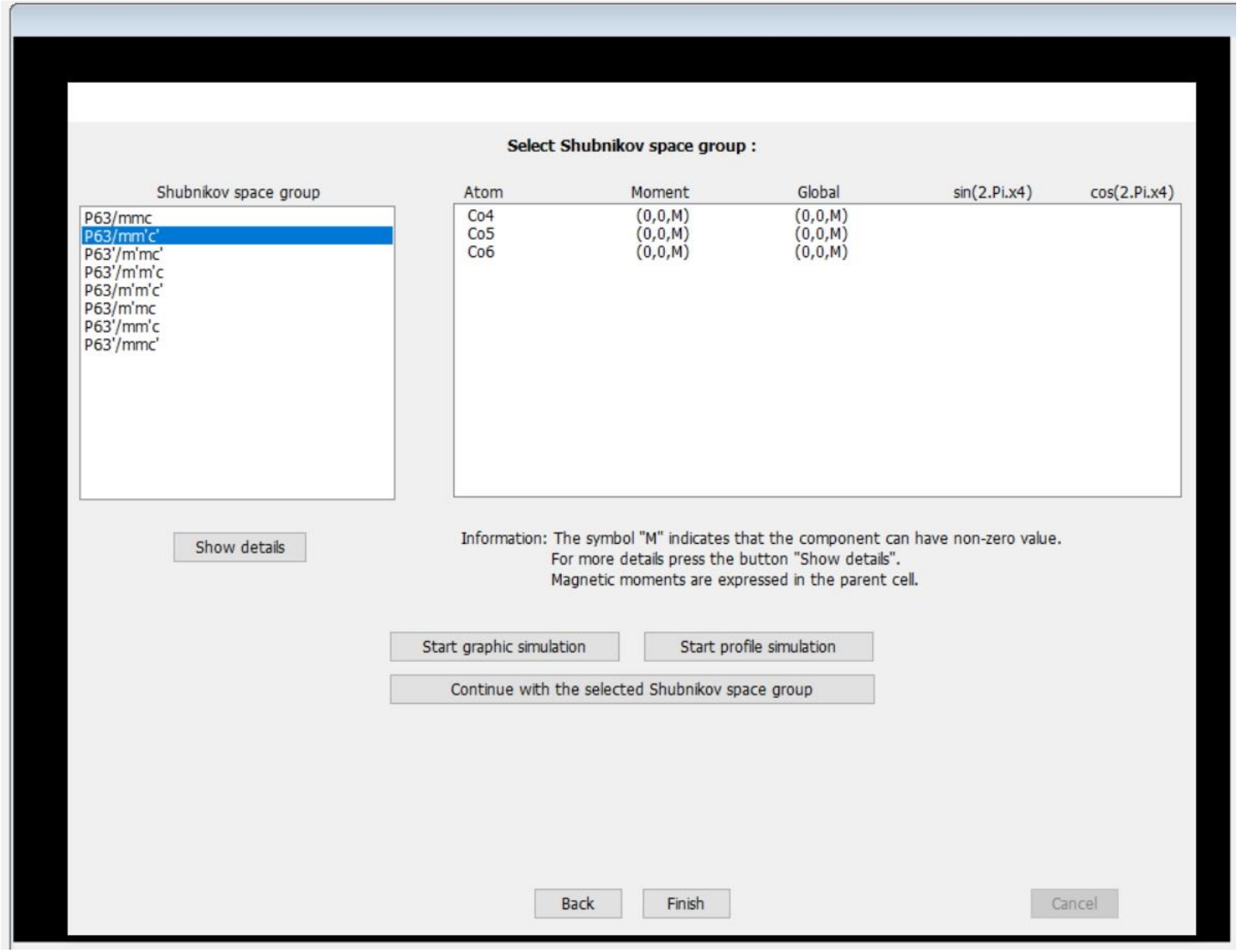
List of kernels and epikernels (isotropy subgroups)



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Magnetic option in Jana2020

Testing a kernel/epikernel ‘family’



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List of irreps and correspoding kernel symmetries:

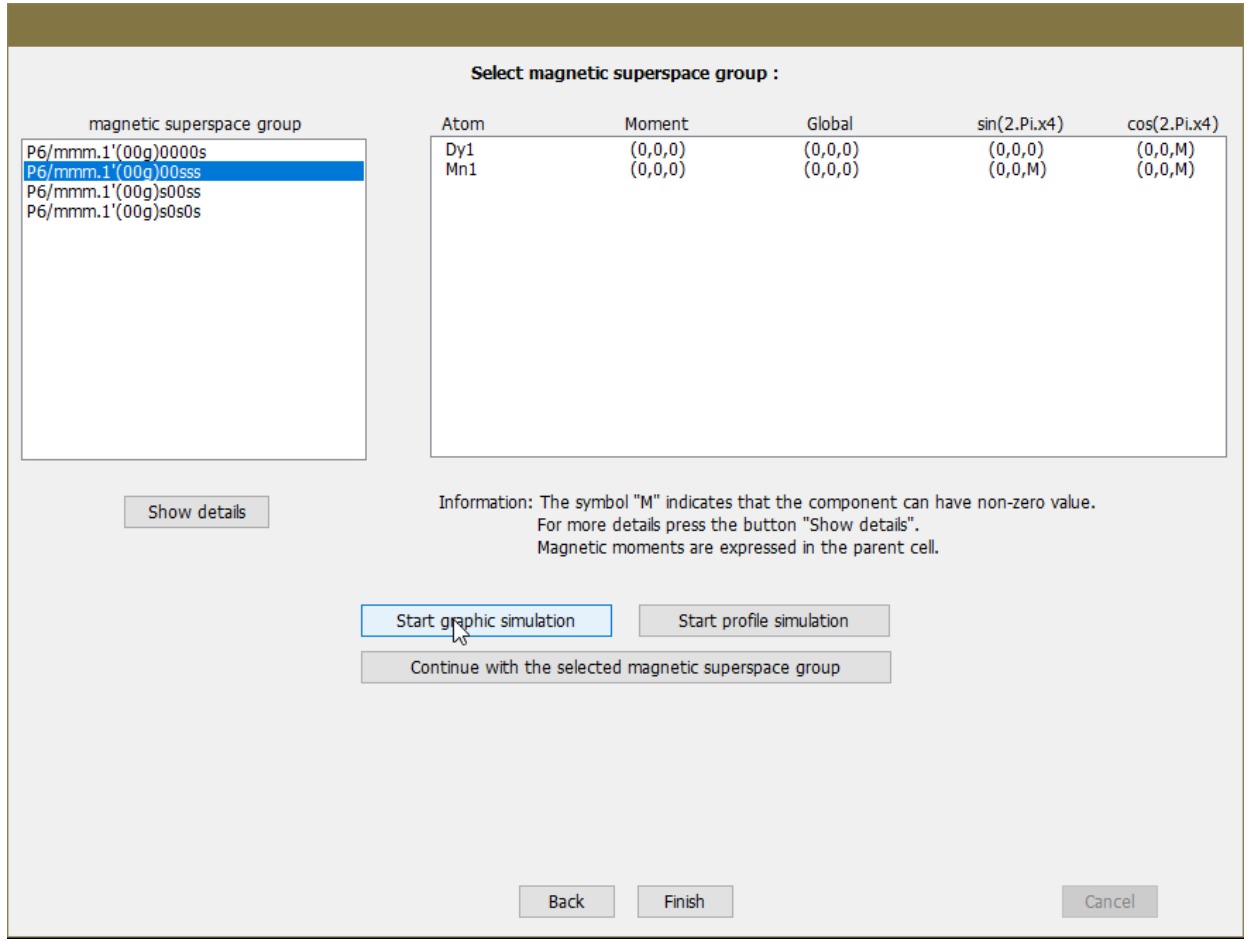
Representation	Dimension	Shubnikov superspace group	Axes	Origin shift	
mDT1	2	P6/mmm.1'(00g)0000s	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0,0)	Details
mDT2	2	P6/mmm.1'(00g)00sss	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0,0)	Details
mDT3	2	P6/mmm.1'(00g)s00ss	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0,0)	Details
mDT4	2	P6/mmm.1'(00g)s0s0s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

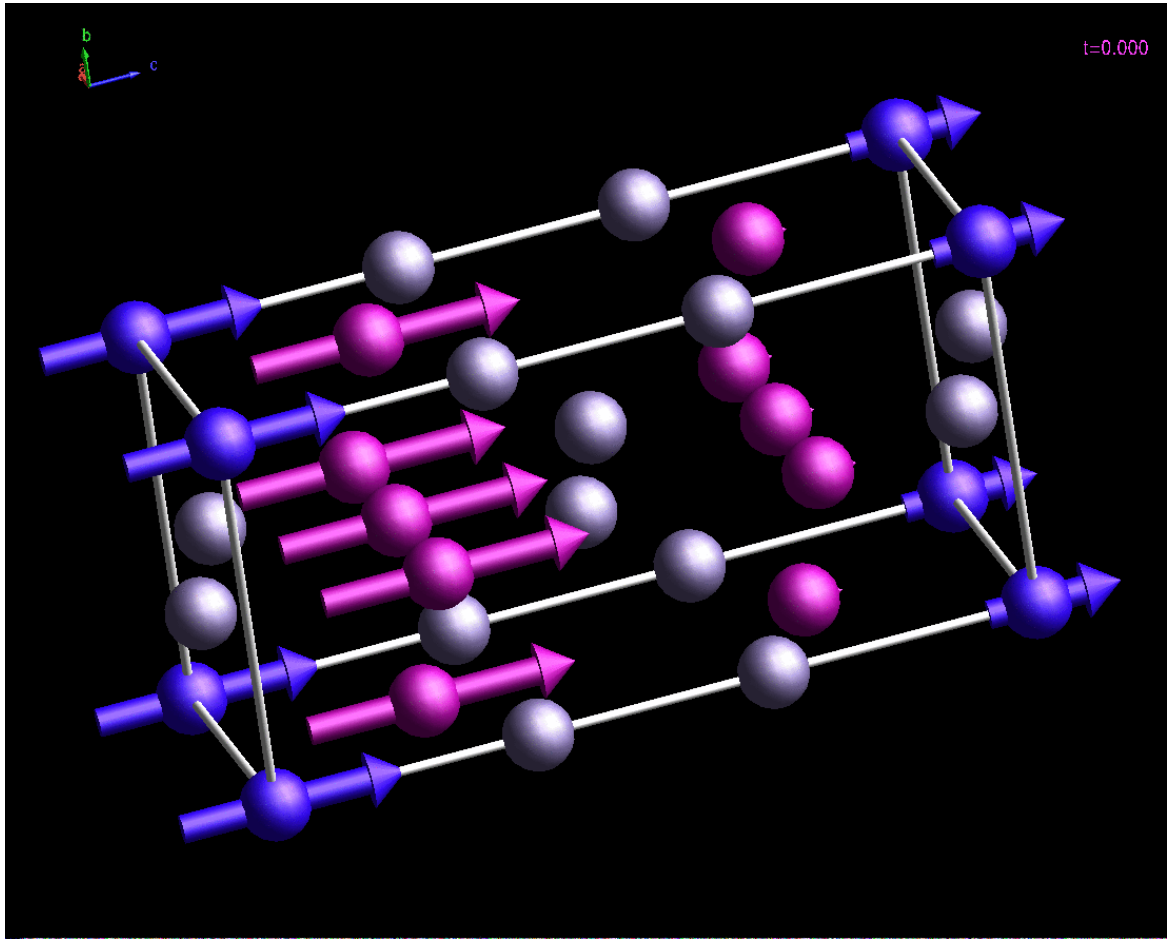
Select Magnetic superspace group :

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

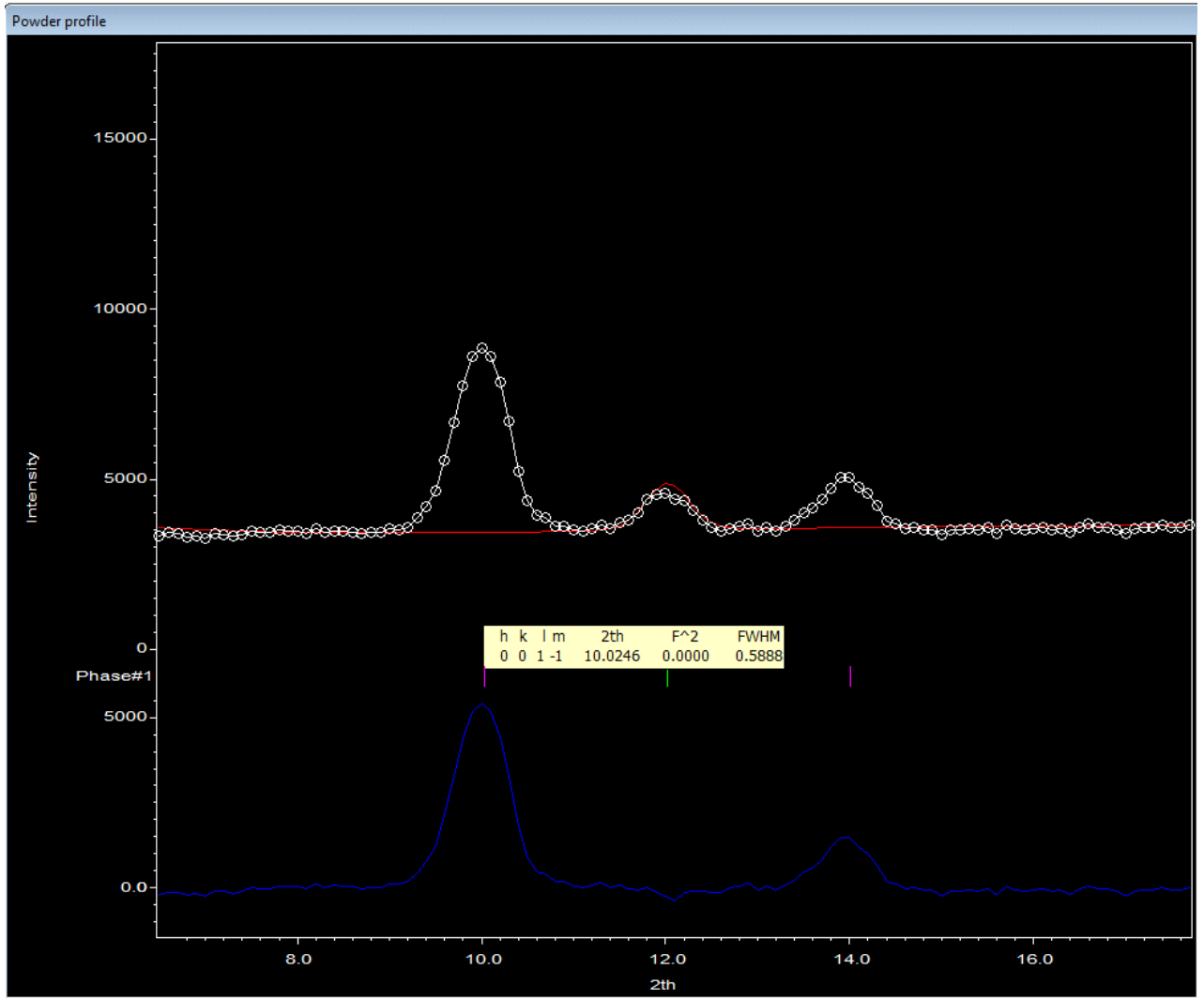
Atom	Moment	Global	sin(2.Pi.x4)	cos(2.Pi.x4)
Dy1	(0,0,0)	(0,0,0)	(M,M,0)	(M,M,0)
Mn1	(0,0,0)	(0,0,0)	(M,M,0)	(M,M,0)

Magnetic option in Jana2020



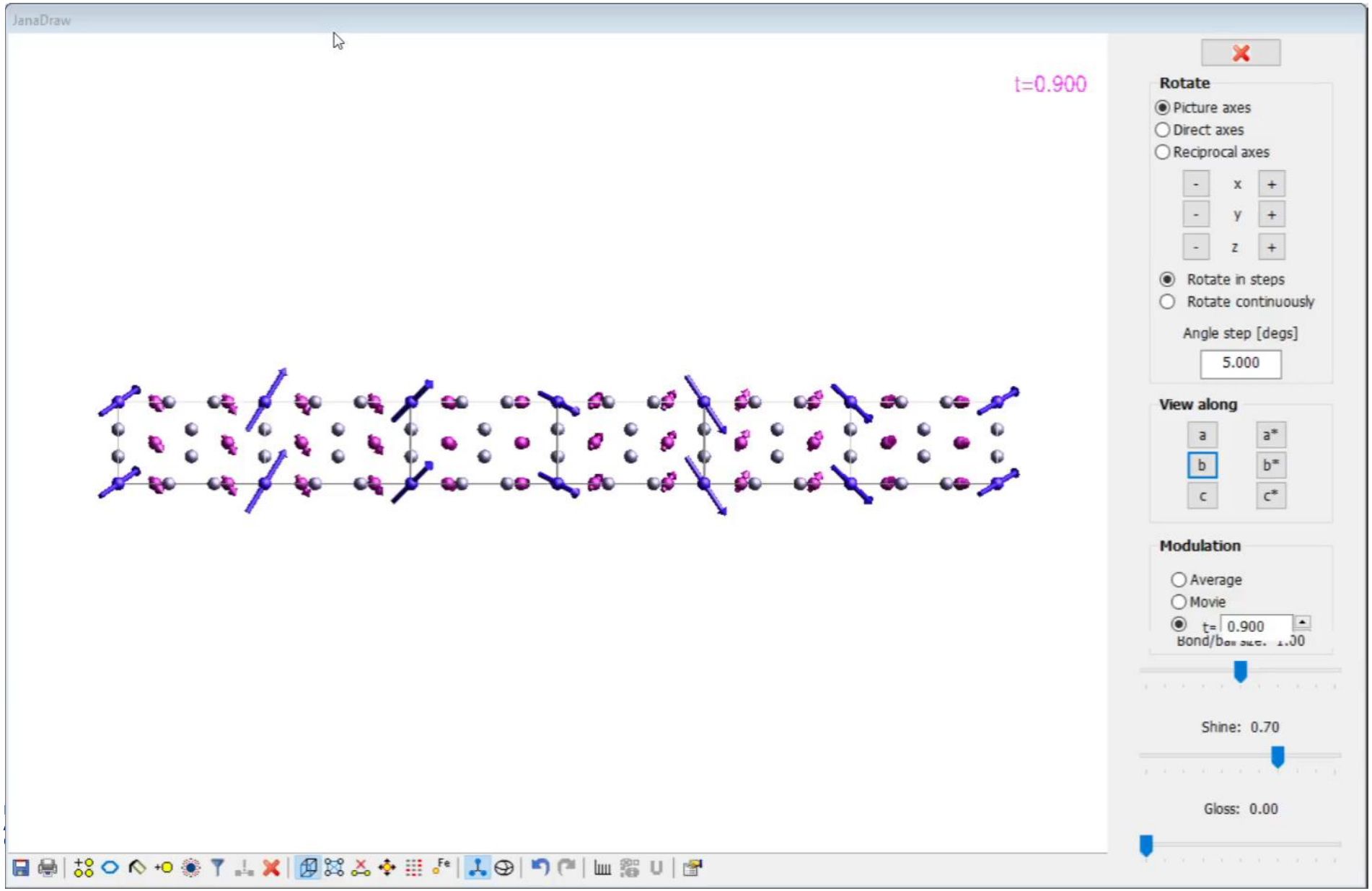


Magnetic option in Jana2020



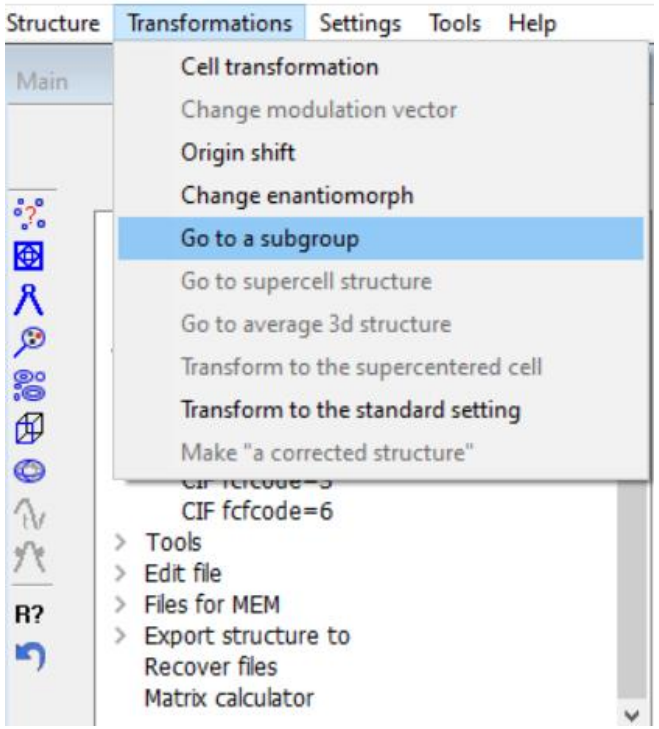
Magnetic option in Jana2020

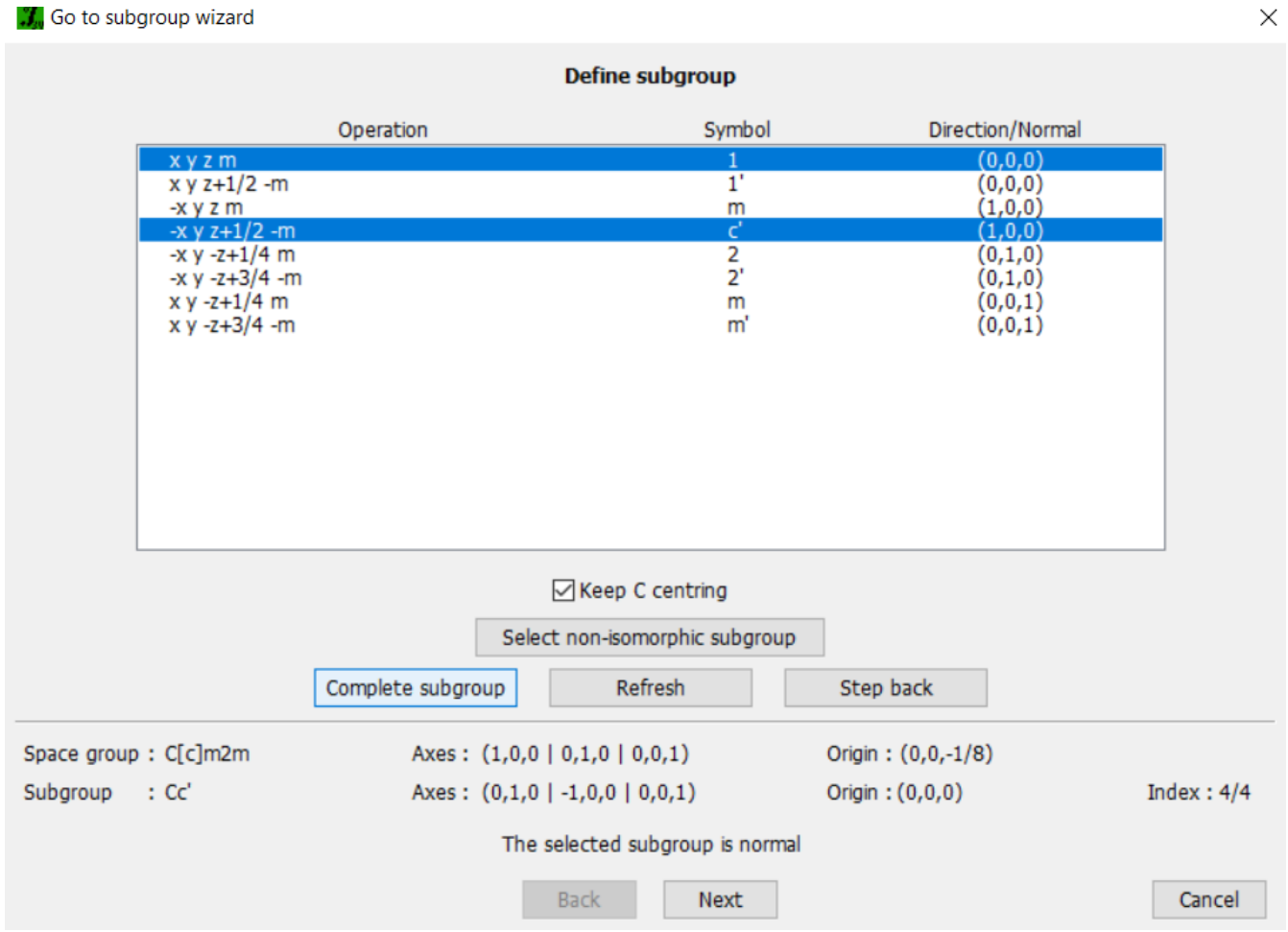
JanaDraw



Magnetic option in Jana2020

Group-Subgroup transformation





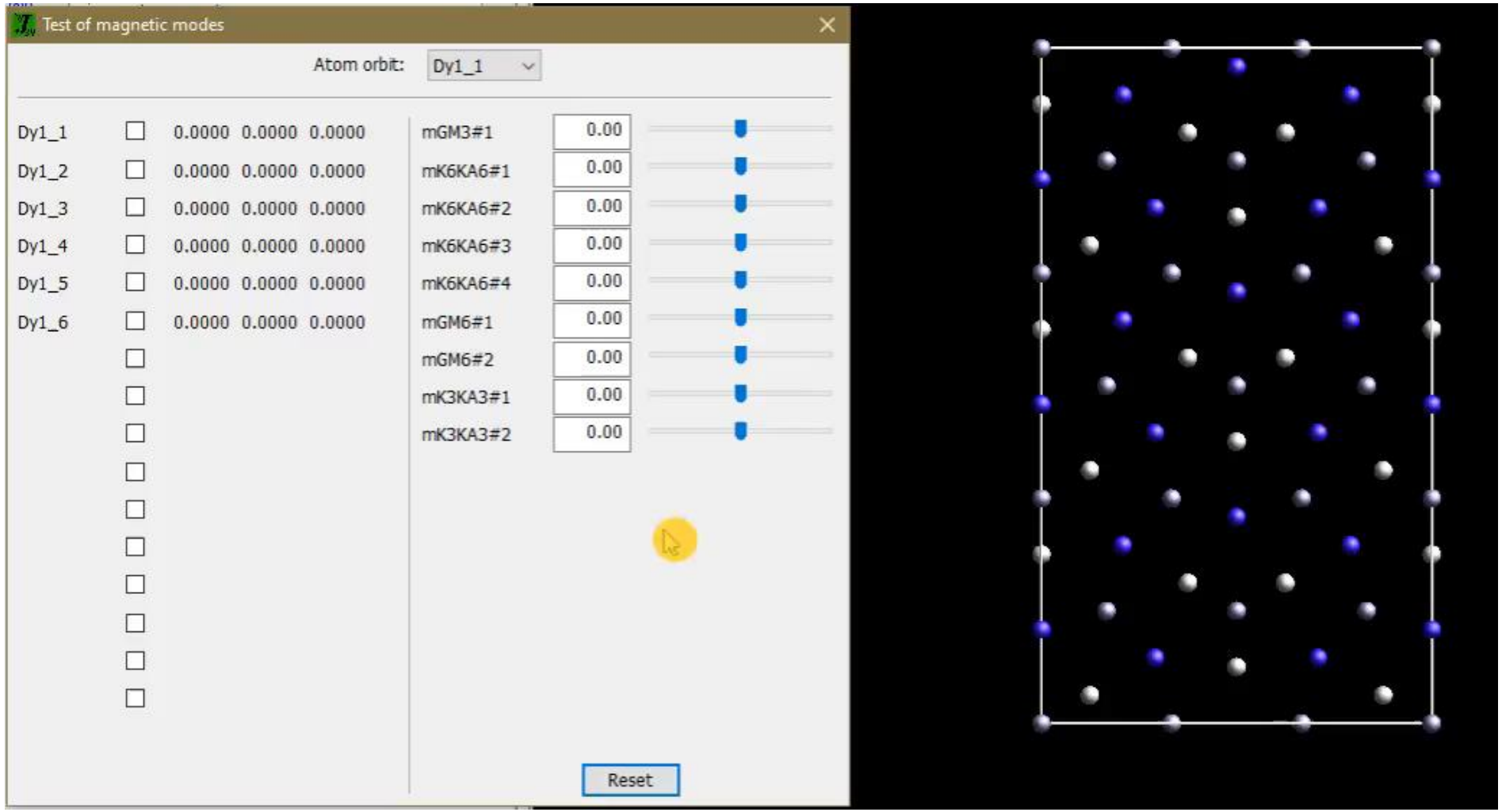
Magnetic option in Jana2020

Group-Subgroup transformation



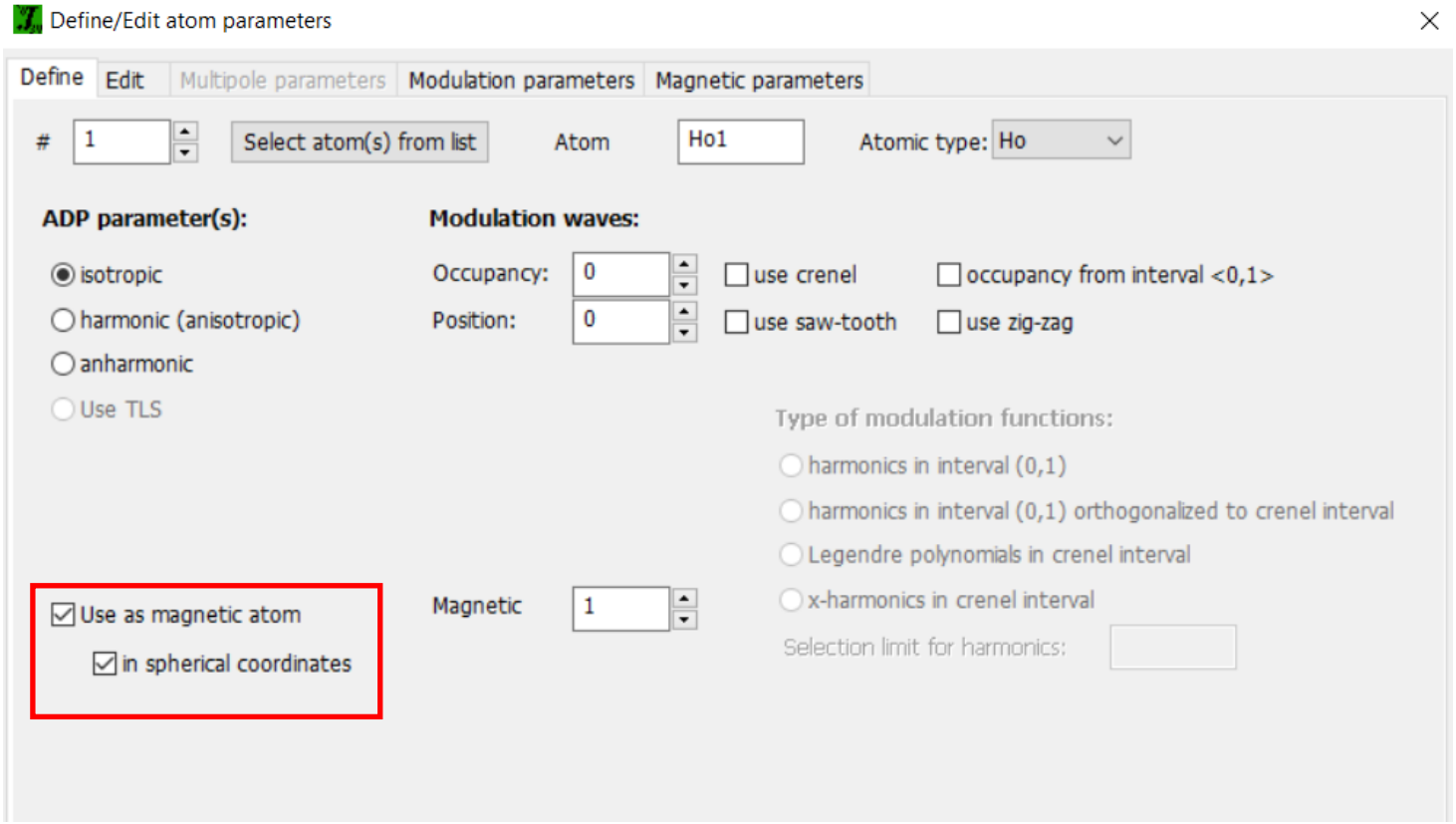
Describing/reporting magnetic structures:

Mode Analysis



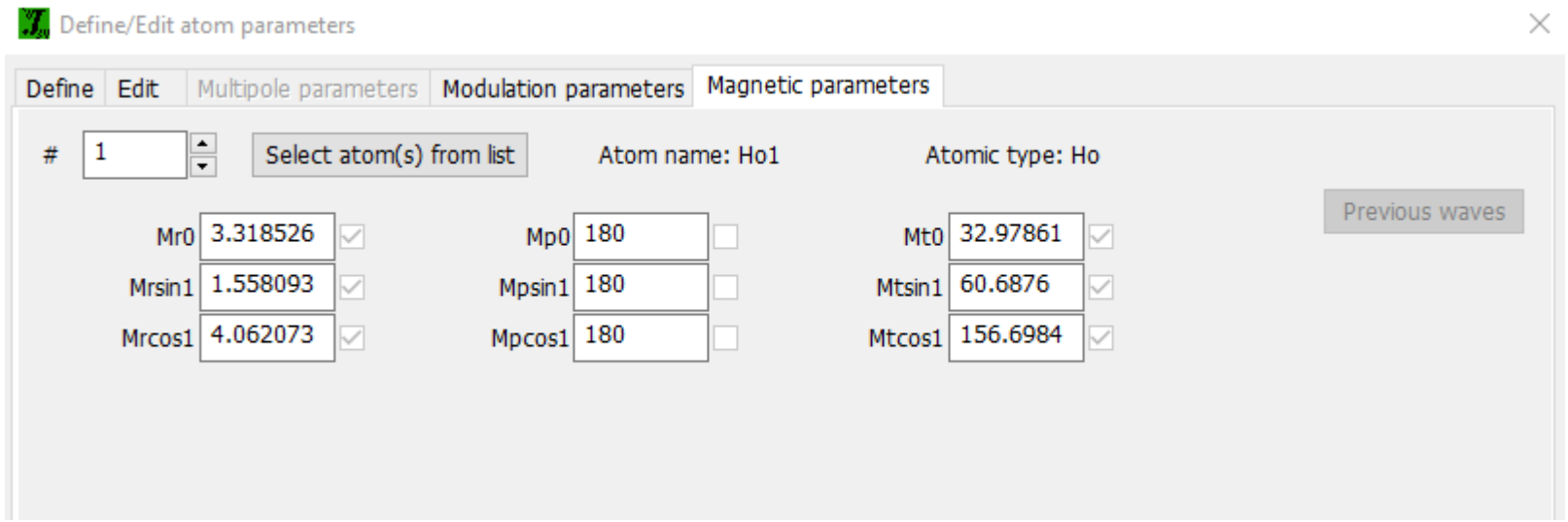
Describing/reporting magnetic structures:

Spherical coordinates



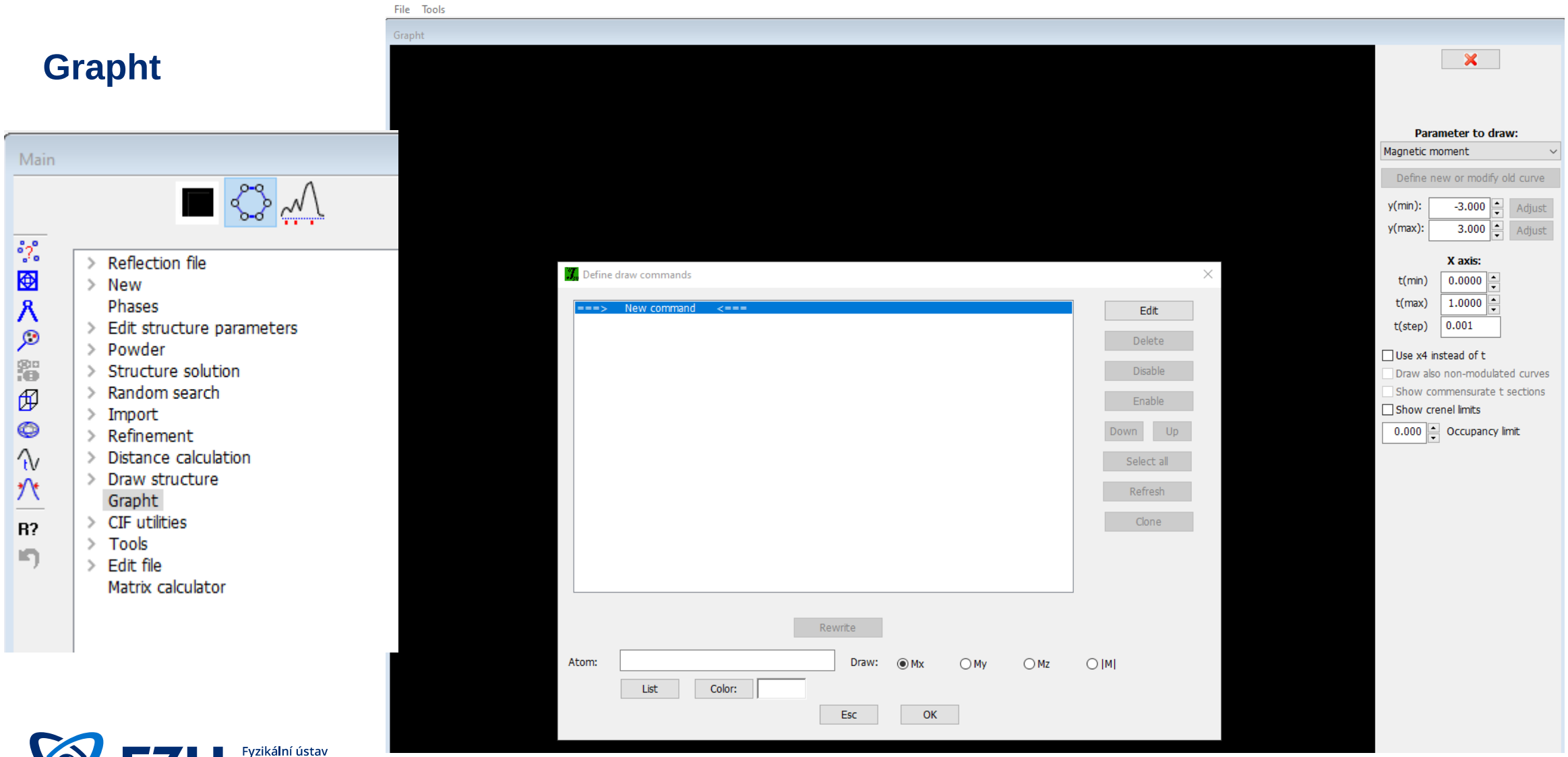
Describing/reporting magnetic structures:

Spherical coordinates



Describing/reporting magnetic structures:

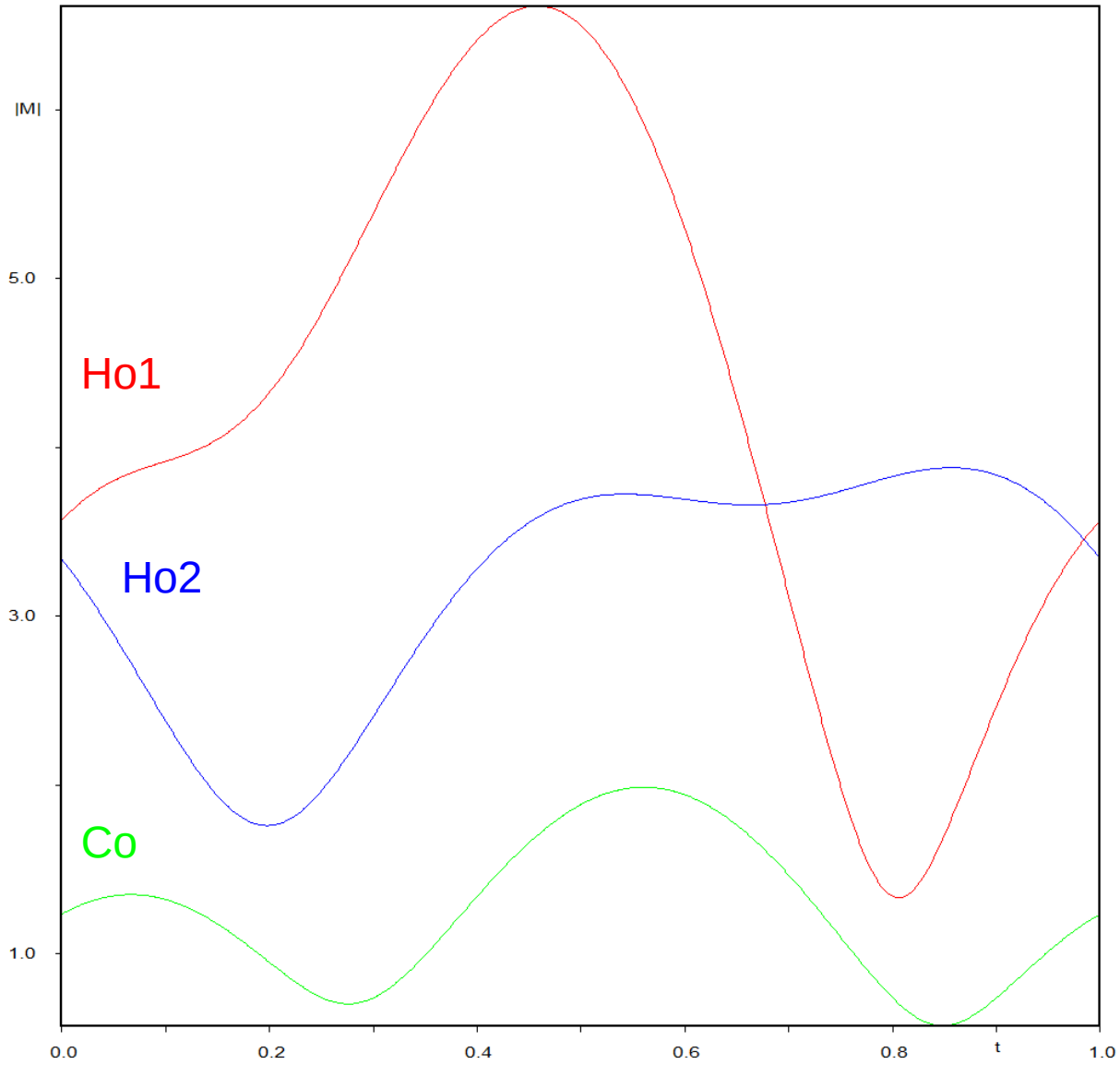
Grapht



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Describing/reporting magnetic structures:

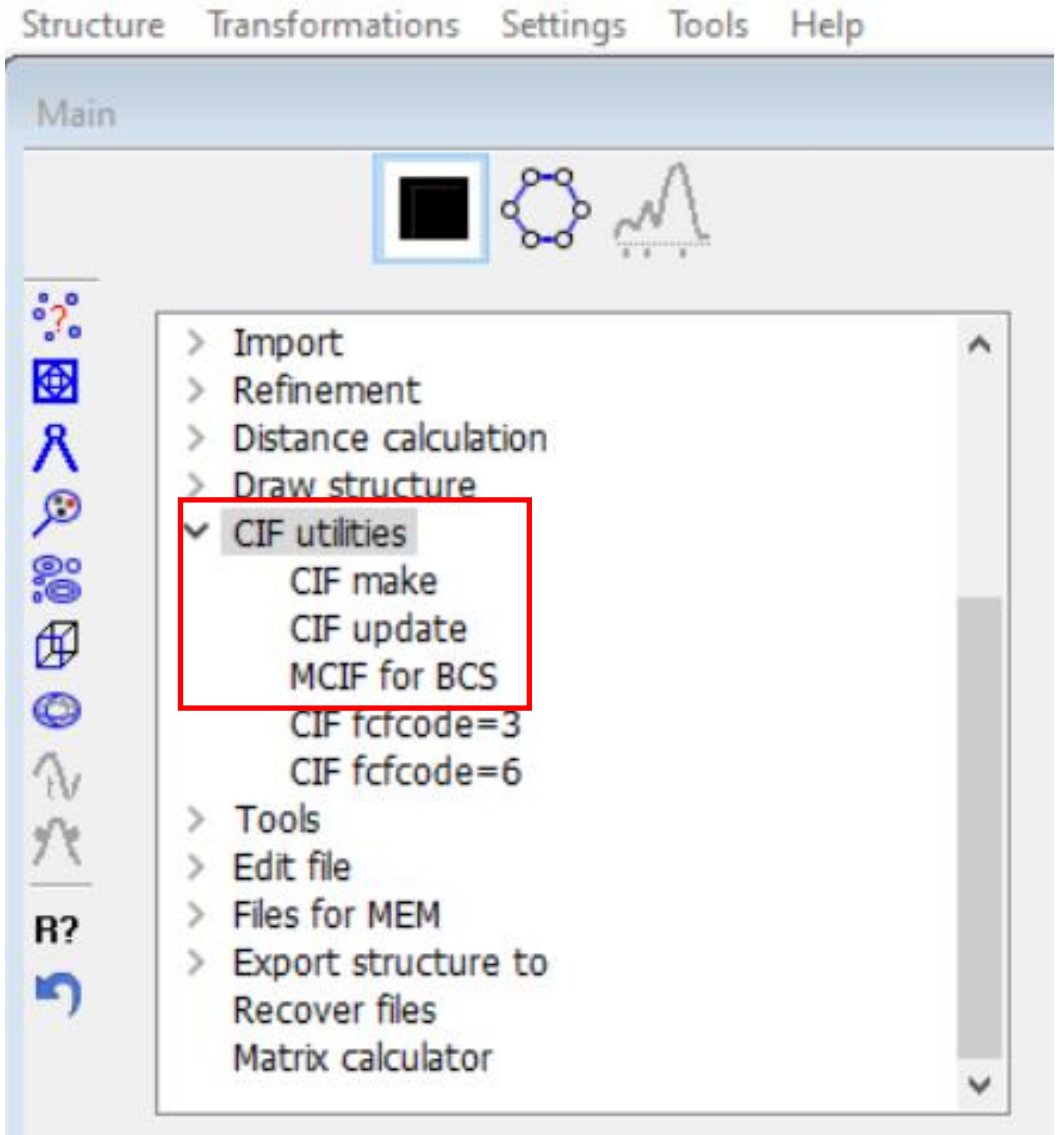
Grapht



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Describing/reporting magnetic structures:

Producing (m)CIF's



Submit to MAGNDATA!

Describing/reporting magnetic structures

Recommendation and good practice: full description of the structure in Supplemental material and/or submission of the mCIF

	$Dy_2Co_3Al_9$ (MAGNDATA #1.267) (BNS setting)		$Dy_2Co_3Al_9$ (OG setting)	
MSG symbol	A_amm2		$A_{2a}mm2$	
MSG number	38.192		38.6.270	
Transformation to standard setting of MSG	(**c**,**a**,**b**;0,0,-1/8)		(**c**,**a**,**b**;0,0,-1/4)	
Magnetic point group	*mm21'* (**c**,**a**,**b**) *or m2m1'*		*mm21'* (**c**,**a**,**b**) *or m2m1'*	
Unit cell parameters (Å)	a=12.72390 α=90º b=7.45860 β =90º c=18.59880 γ =90º		a=12.72390 α=90º b=7.45860 β =90º c=9.2994 γ =90º	
MSG symmetry operations	x,y,z,+1 -x,y,-z+3/4,+1 -x,y,z,+1 x,y,-z+3/4,+1	{1|0,0,0} {2_{010}|0,0,¾} {m_{100}|0,0,0} {m_{001}|0,0,¾}	x,y,z,+1 -x,y,-z+1/2,-1 -x,y,z,+1 x,y,-z+1/2,-1	{1|0,0,0} {$2'_{010}$|0,0,½} {m_{100}|0,0,0} {m'_{001}|0,0,½}
MSG symmetry centering operations	x,y,z,+1 x+1/2,y+1/2,z,+1 x,y,z+1/2,-1 x+1/2,y+1/2,z+1/2,-1	{1|0,0,0} {1|½,½,0} {1'|0,0,½} {1'|½,½,½ }	x,y,z x+1/2,y+1/2,z	{1|0,0,0} {1|½,½,0}
OG wavevector k_OG	------		(0,0,1/2)	
Positions of magnetic atoms	Dy1_1 Dy 0.33940 0.33290 0.12500 Dy1_2 Dy 0.66060 0.66710 0.37500		Dy1_1 Dy 0.33940 0.33290 0.250 Dy1_2 Dy 0.66060 0.66710 0.750	
Positions of non-magnetic atoms	Co1 Co 0.32880 0.00000 0.00000 Co2 Co 0.00000 0.00000 0.00000 Al1_1 Al 0.00000 0.1249 0.125 Al1_2 Al 0.00000 0.8751 0.375		Co1 Co 0.32880 0.00000 0.00000 Co2 Co 0.00000 0.00000 0.00000 Al1_1 Al 0.00000 0.12490 0.250 Al1_2 Al 0.00000 0.87510 0.750	

Description of a commensurate/incommensurate magnetic structure using its MSG/MSSG

	Al2_1 Al 0.1079 0.4459 0.125 Al2_2 Al 0.8921 0.5541 0.375 Al3_1 Al 0.0000 0.3322 0.2714 Al3_2 Al 0.00000 0.6678 0.5214 Al4_1 Al 0.1686 0.3330 0.03585 Al4_2 Al 0.8314 0.6670 0.28585	Al2_1 Al 0.10790 0.44590 0.250 Al2_2 Al 0.89210 0.55410 0.750 Al3_1 Al 0.00000 0.33220 0.5428 Al3_2 Al 0.00000 0.66780 0.0428 Al4_1 Al 0.16860 0.33300 0.0717 Al4_2 Al 0.83140 0.66700 0.5717
Magnetic moments (μ_B) of magnetic atoms, their symmetry constraints and moment magnitudes (μ_B)	Dy1_1 1.34(2) 8.35(2) 0.0 (mx,my,0) 8.46(2) Dy1_2 0.0 0.0 1.38(1) (0,0,mz) 1.38(1)	Dy1_1 1.34(2) 8.35(2) 0.0 (mx,my,0) 8.46(2) Dy1_2 0.0 0.0 1.38(1) (0,0,mz) 1.38(1)

Describing/reporting magnetic structures



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ISSN 2052-5206

Guidelines for communicating commensurate magnetic structures. A report of the International Union of Crystallography Commission on Magnetic Structures

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This article is part of a focused issue on Magnetic Structures.

Keywords: IUCr Commission on Magnetic Structures; magnetic structures; magnetic space groups; representation analysis; magnetic CIF; guidelines.

Volume 80 | **Part 4** | August 2024 | Pages 219-234
https://doi.org/10.1107/S2052520624004268
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Jana2020 – magnetic option

research papers

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ISSN 2052-5206

Analysis of magnetic structures in *JANA2020*

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Received 14 May 2024
Accepted 17 August 2024

Edited by V. Garlea, Oak Ridge National Laboratory, USA

This article is part of a focused issue on Magnetic Structures.

Keywords: magnetism; superspace; modulations; crystallography.

JANA2020 is a program developed for the solution and refinement of regular, twinned, modulated, and composite crystal structures. In addition, *JANA2020* also includes a magnetic option for solving magnetic structures from powder and single-crystal neutron diffraction data. This tool uses magnetic space and superspace symmetry to describe commensurate and incommensurate magnetic structures. The basics of the underlying formulation of magnetic structure factors and the use of magnetic symmetry for handling modulated and non-modulated magnetic structures are presented here, together with the general features of the magnetic tool. Examples of structures solved in the magnetic option of *JANA2020* are given to illustrate the operation and capabilities of the program.

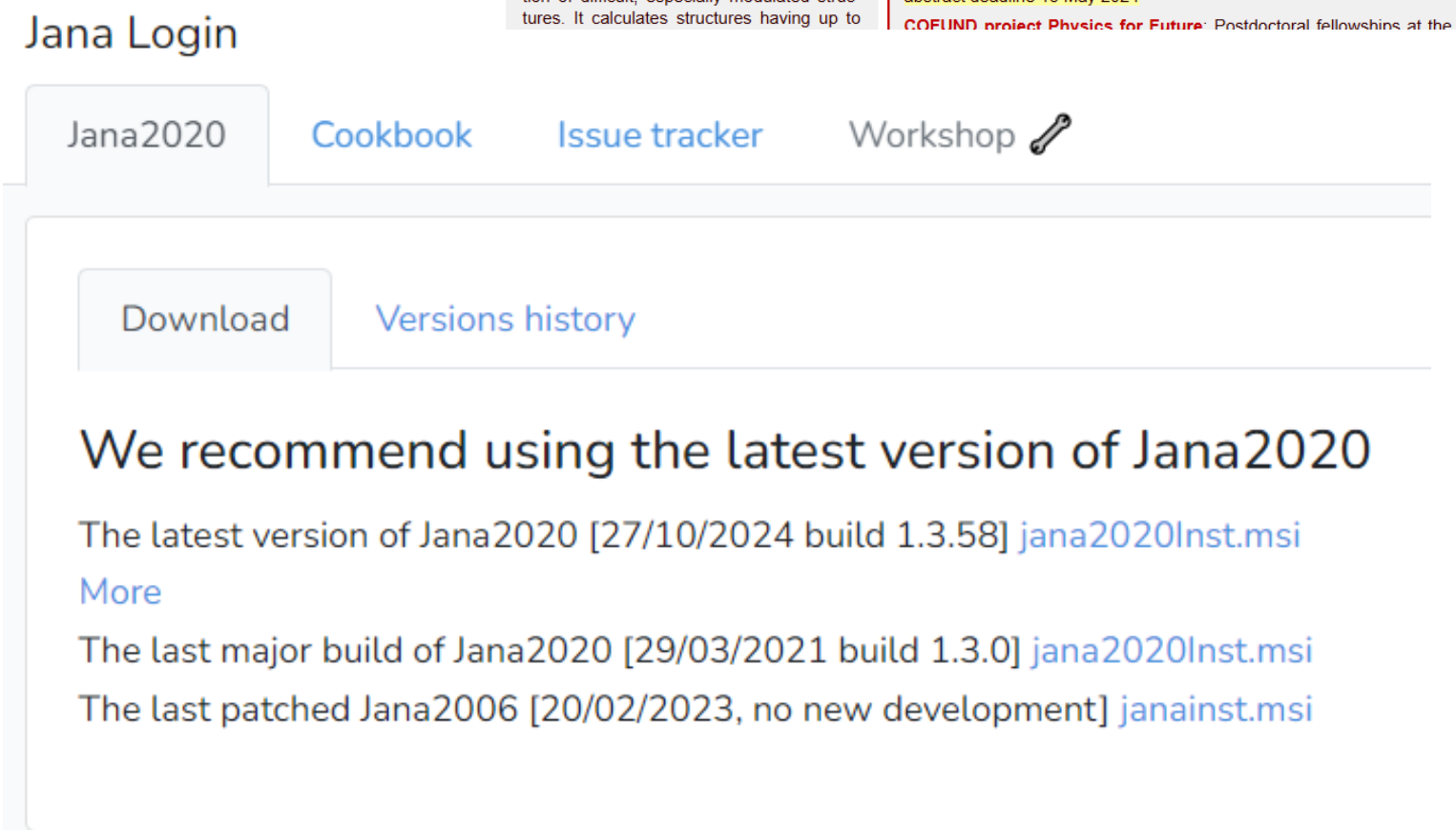
Volume 80 | **Part 5** | October 2024 | Pages 409-423
https://doi.org/10.1107/S2052520624008163

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Jana2020

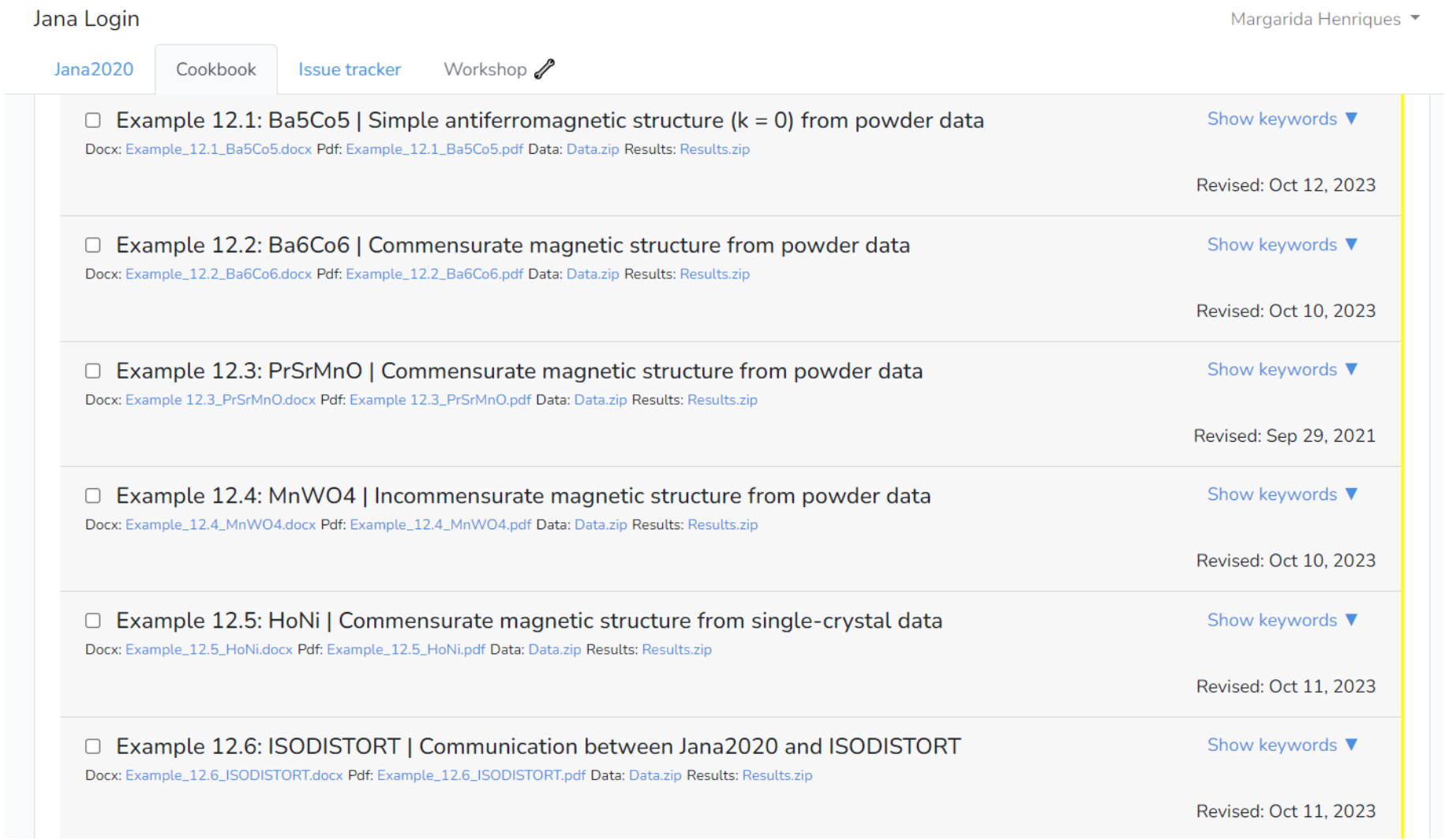
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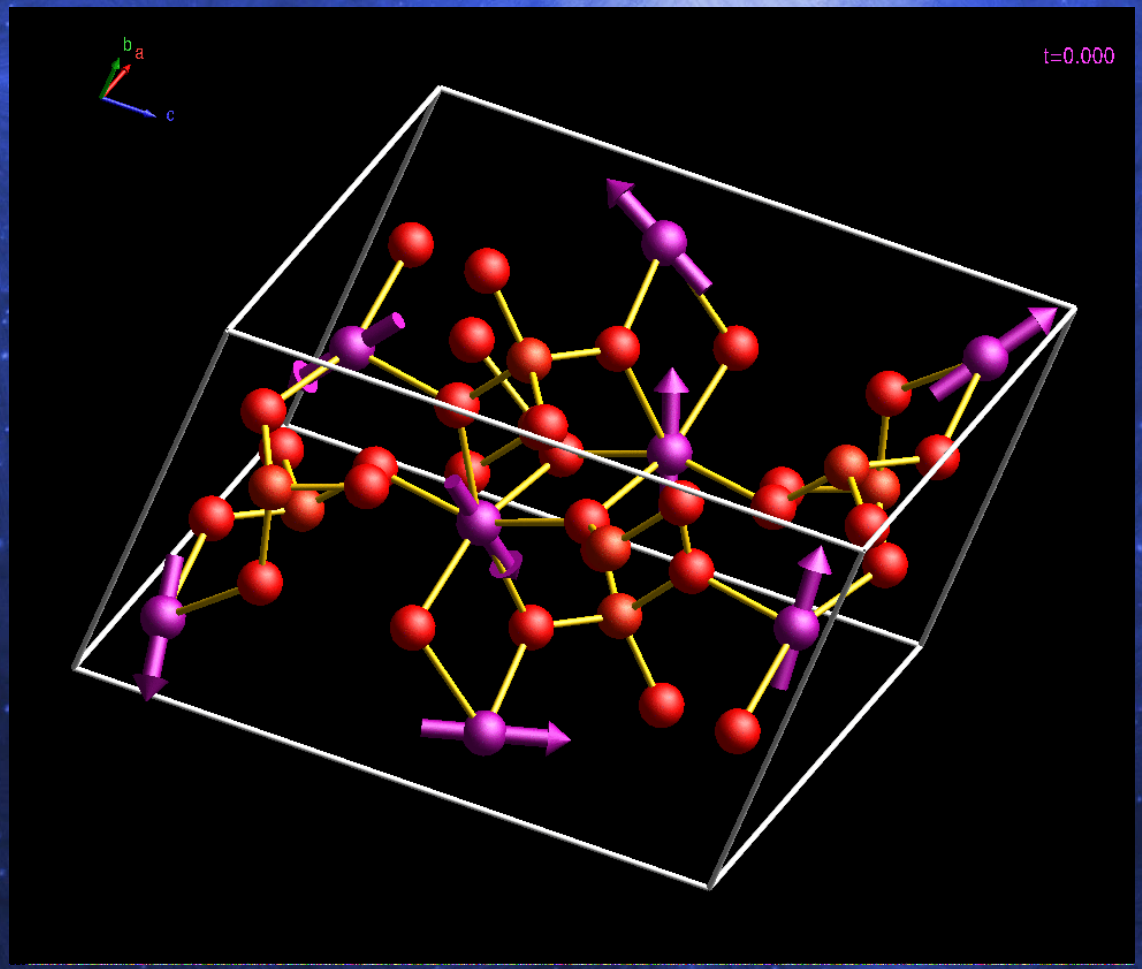


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Jana2020


Jana Login
Margarida Henriques
Jana2020
Cookbook
Issue tracker
Workshop
Example 12.1: Ba5Co5 | Simple antiferromagnetic structure (k = 0) from powder data
Show keywords
Docx: Example_12.1_Ba5Co5.docx Pdf: Example_12.1_Ba5Co5.pdf Data: Data.zip Results: Results.zip
Revised: Oct 12, 2023
Example 12.2: Ba6Co6 | Commensurate magnetic structure from powder data
Show keywords
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Revised: Oct 10, 2023
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: Sep 29, 2021
Example 12.4: MnWO4 | Incommensurate magnetic structure from powder data
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Example 12.5: HoNi | Commensurate magnetic structure from single-crystal data
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Example 12.6: ISODISTORT | Communication between Jana2020 and ISODISTORT
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Thank you!



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