

The way the magnetic superspace approach works with modulation (propagation) vectors differs significantly from the traditional approach. Both start with the star of propagation vectors as generated by the parent symmetry operation. For your case, you have collected data with the vector $(1/3, 1/3, 0)$. For the parent symmetry $R\bar{3}m$, we have the following special k-points:

SM, k2	(a -2a,0)
GM, k7	(0,0,0)
LD, k6	(0,0,g)
SM, k2	(a -2a,0)
F, k5	(0,1/2,1)
L, k4	(-1/2,1/2,1/2)
T, k8	(0,0,3/2)
Y, k3	(a,a,3/2)
C, k1	(a,-a,g)
GP, k0	(a,b,g)

The vector $(1/3, 1/3, 0)$ does not represent an individual special k-point. It can be classified as one vector from the SM star $(a, -2a, 0), (-2a, a, 0), (a, a, 0), (-a, 2a, 0), (2a, -a, 0), (-a, -a, 0)$.

The fact that $a \approx 1/3$ does not mean that the parent symmetry fixes this value. The superspace approach means that we need just three vectors for a full description, just three vectors, e.g., $(a, -2a, 0), (-2a, a, 0), (a, a, 0)$ as the remaining three vectors are

just reversed and automatically included by using the sin/cos terms in the modulation function:

$$\mathbf{M}(\mathbf{x}_I) = \mathbf{M}_0 + \sum_{\mathbf{n}} [\mathbf{M}_{\text{ns}} \sin 2\pi \mathbf{n} \cdot \boldsymbol{\sigma} \cdot \mathbf{x}_I + \mathbf{M}_{\text{nc}} \cos 2\pi \mathbf{n} \cdot \boldsymbol{\sigma} \cdot \mathbf{x}_I]$$

Where:

$\mathbf{x}_I = (x_4, x_5, x_6)$ are three internal components in the (3+3) d superspace.

$\boldsymbol{\sigma} = (\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3)$ is the row composed of three modulation vectors.

$\mathbf{n} = (n_1, n_2, n_3)$ $n_1 > 0$ or $\mathbf{n} = (0, n_2, n_3)$ $n_2 > 0$ or $\mathbf{n} = (0, 0, n_3)$ $n_3 > 0$

The selection of the used harmonics, described by the various coefficients \mathbf{n} , depends on the set of detected satellite reflections.

The fact that in the modulation function we can use any combination of harmonics allows further reduction of the superspace dimension: $-(a, -2a, 0) - (-2a, a, 0) = (a, a, 0)$. Therefore, for your case, we can use a lower dimension (3+2). This is why, during the import procedure, the program makes the first transformation of the indices of the detected satellites into the form (h,k,l,m,n):

- ▼ Reflection file
 - Import/modify reflection file
 - > Edit structure parameters
 - > Tools for magnetic structures
 - > Edit file
 - Matrix calculator
 - Run Jana2006
 - > Ad hoc



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



Data import wizard

Single crystal data from:

Input file name:

- ☐ SHELX on F
- ☐ SHELX on I
- ☐ SHELX HKLF5
- ☐ IPDS STOE
- ☐ CCD Bruker
- ☐ From CIF file
- ☐ From SUNJU HKL
- ☐ From Grindex file
- ☒ From FullProf file
- ☐ From XD file
- ☐ Jana-M90
- ☐ HB3A
- ☐ General file on F
- ☐ General file on I

Input FORTRAN format:



Data import wizard

Complete/correct experimental parameters

Cell parameters:

Number of input indices:

1st modulation vector:

Data collection details:

Temperature:



Data import wizard

Define relationship to the cell parameters

Actual cell parameters of data block: 5.5986 5.5986 18.5410 90.000 90.000 120.000
 Cell parameters derived from actual: 5.5986 5.5986 18.5410 90.000 90.000 120.000
 Cell parameters original: 5.5986 5.5986 18.5410 90.000 90.000 120.000

H= * h+ * k+ * l+ * m * n
 K= * h+ * k+ * l+ * m * n
 L= * h+ * k+ * l+ * m * n
 M= * h+ * k+ * l+ * m * n
 N= * h+ * k+ * l+ * m * n

Target dimension:

Modulation vector(s):

Actual data block:	Derived from actual:	Original:
<input type="text" value="0.3333 0.3333 0"/>	<input type="text"/>	<input type="text" value="0.3333 -0.6666 0"/>
<input type="text"/>	<input type="text"/>	<input type="text" value="0.3333 0.3333 0"/>

☐ Twinning

Number of domains:

Data related to domain#:

Multiply input F(hkl)/I(hkl) by

☐ Analyze overlaps by Jana tools instead of HKLF5

☐ Import only satellites

The independent modulation vectors are generated from the full star belonging to the specific point SM k2. The measured satellite reflections have indices h,k,l,1, with an additional vector of (0.3333, 0.3333, 0). To transform it into a (3+2)d description, we must first formally complete the second modulation vector by (0.3333, -0.6666, 0) and change the order by applying the transformation matrix.

After filling the second vector and pressing the “tab” key:

Data import wizard

Define relationship to the cell parameters

Actual cell parameters of data block: 5.5986 5.5986 18.5410 90.000 90.000 120.000
 Cell parameters derived from actual: 5.5986 5.5986 18.5410 90.000 90.000 120.000
 Cell parameters original: 5.5986 5.5986 18.5410 90.000 90.000 120.000

Matrix calculator Apply the transformation

H= 1 * h+ 0 * k+ 0 * l+ 0 * m 0 * n
 K= 0 * h+ 1 * k+ 0 * l+ 0 * m 0 * n
 L= 0 * h+ 0 * k+ 1 * l+ 0 * m 0 * n
 M= 0 * h+ 0 * k+ 0 * l+ 1 * m 0 * n
 N= 0 * h+ 0 * k+ 0 * l+ 0 * m 1 * n

Target dimension: 5

Modulation vector(s):

Actual data block:	Derived from actual:	Original:
0.3333 0.3333 0	0.3333 0.3333 0	0.3333 -0.6666 0
0.3333 -0.6666 0	0.3333 -0.6666 0	0.3333 0.3333 0

☐ Twinning Twinning matrices

Number of domains: 1
 Data related to domain#: 1
 Multiply input F(hkl)/I(hkl) by 1

☐ Analyze overlaps by Jana tools instead of HKLF5
☐ Import only satellites

Applying the transformation matrix:

Data import wizard

Define relationship to the cell parameters

Actual cell parameters of data block: 5.5986 5.5986 18.5410 90.000 90.000 120.000
 Cell parameters derived from actual: 5.5986 5.5986 18.5410 90.000 90.000 120.000
 Cell parameters original: 5.5986 5.5986 18.5410 90.000 90.000 120.000

Matrix calculator Apply the transformation

H= 1 * h+ 0 * k+ 0 * l+ 0 * m 0 * n
 K= 0 * h+ 1 * k+ 0 * l+ 0 * m 0 * n
 L= 0 * h+ 0 * k+ 1 * l+ 0 * m 0 * n
 M= 0 * h+ 0 * k+ 0 * l+ 0 * m 1 * n
 N= 0 * h+ 0 * k+ 0 * l+ 1 * m 0 * n

Target dimension: 5

Modulation vector(s):

Actual data block:	Derived from actual:	Original:
0.3333 0.3333 0	0.3333 0.3333 0	0.3333 -0.6666 0
0.3333 -0.6666 0	0.3333 -0.6666 0	0.3333 0.3333 0

☐ Twinning Twinning matrices

Number of domains: 1
 Data related to domain#: 1
 Multiply input F(hkl)/I(hkl) by 1

☐ Analyze overlaps by Jana tools instead of HKLF5
☐ Import only satellites

Data import wizard

Define relationship to the cell parameters

Actual cell parameters of data block: 5.5986 5.5986 18.5410 90.000 90.000 120.000
 Cell parameters derived from actual: 5.5986 5.5986 18.5410 90.000 90.000 120.000
 Cell parameters original: 5.5986 5.5986 18.5410 90.000 90.000 120.000

H= 1 * h+ 0 * k+ 0 * l+ 0 * m 0 * n
 K= 0 * h+ 1 * k+ 0 * l+ 0 * m 0 * n
 L= 0 * h+ 0 * k+ 1 * l+ 0 * m 0 * n
 M= 0 * h+ 0 * k+ 0 * l+ 0 * m 1 * n
 N= 0 * h+ 0 * k+ 0 * l+ 1 * m 0 * n

Target dimension: 5

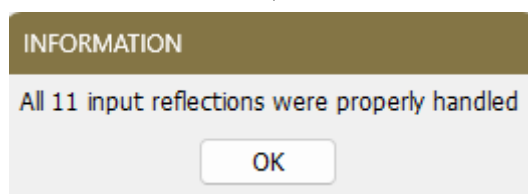
☐ **Twinning**

Number of domains: 1
 Data related to domain# 1
 Multiply input F(hkl)/I(hkl) by 1

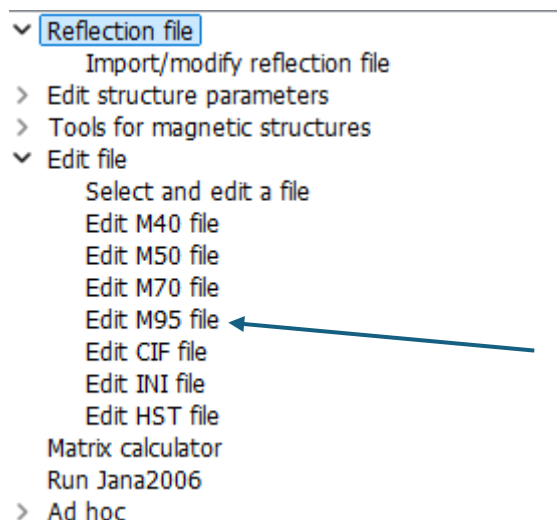
☐ Analyze overlaps by Jana tools instead of HKLF5
☐ Import only satellites

Modulation vector(s):

Actual data block:	Derived from actual:	Original:
0.3333 0.3333 0	0.3333 -0.6666 0	0.3333 -0.6666 0
0.3333 -0.6666 0	0.3333 0.3333 0	0.3333 0.3333 0



After importing all data sets, the program creates the file M95, which contains all the collected reflections:



The final refinement reflection file, M90, is created when we select a particular model from the representation analysis, which can be generated either by the Jana procedure or by using the ISODISTORT program. However, the current version of Jana2020 allows only models based on one active modulation vector:

- ✓ Reflection file
 - Import/modify reflection file
- > Edit structure parameters
- ✓ Tools for magnetic structures
 - Run Jana representation analysis
 - Run ISODISTORT analysis
- > Edit file
 - Matrix calculator
 - Run Jana2006
- > Ad hoc



Representation analysis

List of irreps and corresponding kernel symmetries:

Representation	Dimension	Shubnikov superspace group	Axes	Origin shift	
mSM1	2	C2.1'(0b0)0s	(2,1,0 0,-1,0 -2/3,-1/3,-1/3)	(0,0,0,0)	Details
mSM2	2	C2.1'(0b0)ss	(2,1,0 0,-1,0 -2/3,-1/3,-1/3)	(0,0,0,0)	Details

Active modulation vectors: (0.3333,-0.6666,0)

Display representations Modify the set of active vectors



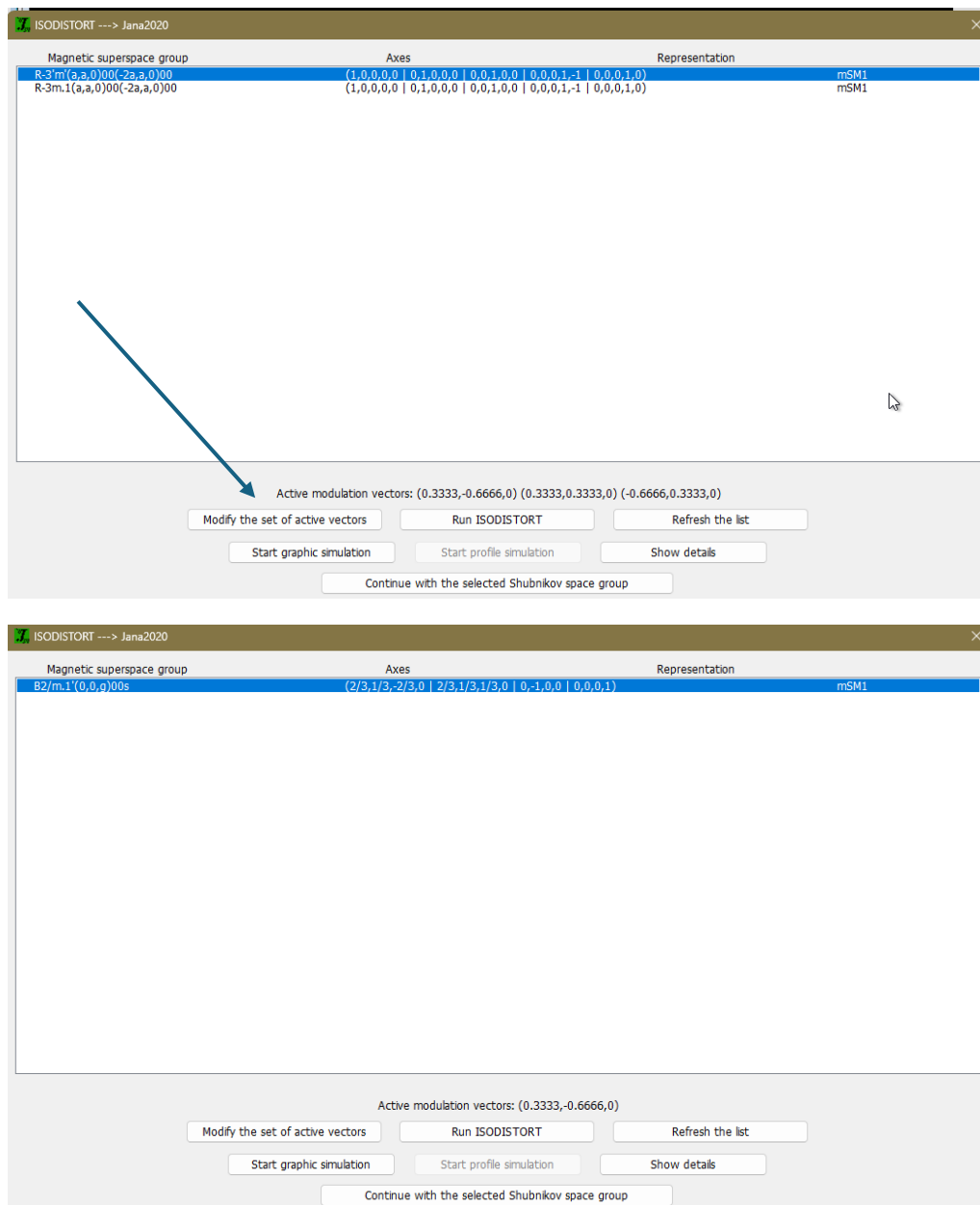
Representation analysis

List of kernels and epikernels:

Shubnikov superspace	Axes	Origin shift	Representation	OPD
C2/m.1'(0b0)00s	(2,1,0 0,-1,0 -2/3,-1/3,-1/3)	(0,0,0,0)	mSM1	(a,0)
C2/m.1'(0b0)s0s	(2,1,0 0,-1,0 -2/3,-1/3,-1/3)	(0,0,0,0)	mSM2	(a,0)
C2.1'(0b0)0s	(2,1,0 0,-1,0 -2/3,-1/3,-1/3)	(0,0,0,0)	mSM1	(a,b)
C2.1'(0b0)ss	(2,1,0 0,-1,0 -2/3,-1/3,-1/3)	(0,0,0,0)	mSM2	(a,b)

The ISODISTORT can be started from the Jana2020 program, as described in Example 12.6 of our cookbook.

Then you can create in the ISODISTOR the CIF file based on either one or three active vectors:



Just a few remarks:

1. The selection of more active vectors calls for higher dimensionality, (3+2)d, and the possibility of using higher magnetic superspace groups. Fewer modulation vectors result in lower symmetry and the existence of more independently diffracting domains. However, for both, we should detect geometrically similar diffraction patterns.
2. In the case of using (3+2)s magnetic superspace groups, we can always use harmonic functions to make a closed set which can be defined in the following dialog:

- > 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 modulation waves
- > Structure solution
- > Random search
- > Fourier synthesis
- Run Contour
- > Import
- > Refinement
- > Distance calculation
- > Draw structure
- Graph
- > CIF utilities
- > Tools
- > Edit file
- > Files for MEM
 - Recover files
 - Matrix calculator
 - Run Jana2006
- > Ad hoc



Defile modulation waves

1st wave	1	*q1+	0	*q2	Previous
2nd wave	0	*q1+	1	*q2	
3rd wave	-1	*q1+	-1	*q2	
4th wave	0	*q1+	0	*q2	
5th wave	0	*q1+	0	*q2	
6th wave	0	*q1+	0	*q2	
7th wave	0	*q1+	0	*q2	
8th wave	0	*q1+	0	*q2	
9th wave	0	*q1+	0	*q2	
10th wave	0	*q1+	0	*q2	
11th wave	0	*q1+	0	*q2	
12th wave	0	*q1+	0	*q2	
13th wave	0	*q1+	0	*q2	
14th wave	0	*q1+	0	*q2	
15th wave	0	*q1+	0	*q2	
16th wave	0	*q1+	0	*q2	

Next

Complete the set Refresh waves Delete wave

Esc OK

Add the modulation wave (2,0) and press the button “Complete the set”:

Defile modulation waves

1st wave	1	*q1+	0	*q2
2nd wave	0	*q1+	1	*q2
3rd wave	-1	*q1+	-1	*q2
4th wave	2	*q1+	0	*q2
5th wave	0	*q1+	2	*q2
6th wave	2	*q1+	2	*q2
7th wave	0	*q1+	0	*q2
8th wave	0	*q1+	0	*q2
9th wave	0	*q1+	0	*q2
10th wave	0	*q1+	0	*q2
11th wave	0	*q1+	0	*q2
12th wave	0	*q1+	0	*q2
13th wave	0	*q1+	0	*q2
14th wave	0	*q1+	0	*q2
15th wave	0	*q1+	0	*q2
16th wave	0	*q1+	0	*q2

Previous

Next

Complete the set Refresh waves Delete wave

Esc OK

Add the modulation wave (1,1) and press the button “Complete the set”:

Defile modulation waves

1st wave	1	*q1+	0	*q2
2nd wave	0	*q1+	1	*q2
3rd wave	-1	*q1+	-1	*q2
4th wave	2	*q1+	0	*q2
5th wave	0	*q1+	2	*q2
6th wave	2	*q1+	2	*q2
7th wave	1	*q1+	1	*q2
8th wave	0	*q1+	0	*q2
9th wave	0	*q1+	0	*q2
10th wave	0	*q1+	0	*q2
11th wave	0	*q1+	0	*q2
12th wave	0	*q1+	0	*q2
13th wave	0	*q1+	0	*q2
14th wave	0	*q1+	0	*q2
15th wave	0	*q1+	0	*q2
16th wave	0	*q1+	0	*q2

Previous

Next

Complete the set Refresh waves Delete wave

Esc OK

The wave (1,1) doesn't generate the symmetry-related ones.

Then, for the introduction of modulation waves for individual atoms, we must use for the above example 3, 6, or 7 waves:

Define/Edit atom parameters

Define Edit Multipole parameters Modulation parameters **Magnetic parameters**

2 Select atom(s) from list Atom Mn_1 Atomic type: Mn

ADP parameter(s):

☒ isotropic
☐ harmonic (anisotropic)
☐ anharmonic
☐ Use TLS

☒ Use as magnetic atom
☐ in spherical coordinates

Modulation waves:

Occupancy: 0 ☐ use crenel ☐ occupancies restricted to the interval <0,1>
Position: 0 ☐ use saw-tooth ☐ use zig-zag

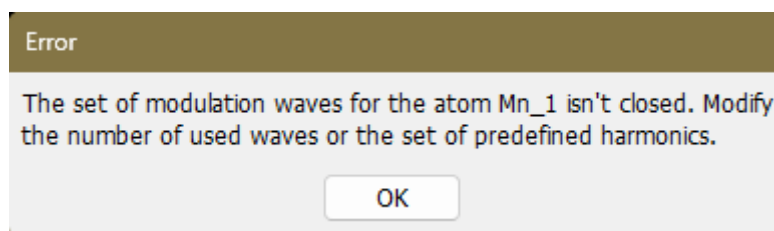
Type of modulation functions:

☐ 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:

Magnetic 3

Otherwise, the refinement program will complain about using the set, which is symmetrically closed:



- I am not sure if you also measured main reflections. If not, you must adjust the scale factor to avoid a singularity.

Press the button to edit/create:

Restrictions

Equations

Fixed commands

Dontuse/Useonly command

Scale command

Partial RFactors

Distance restraints

Angle restraints

Torsion angle restraints

Magnetic moment restraints

Keep commands



☐ All parameters

☐ Coordinates

☐ ADP harmonic parameters

☐ Modulation parameters

☐ Charge density parameters

☐ Origin

☐ x4 axis

☐ Individual parameters

☒ Set individual parameters

Atoms/parameters: Scale1

Browse

Set to: 10