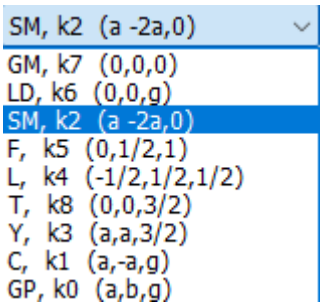
The way the magnetic superspace approach works with modulation (propagation) vectors differs significantly from the traditional approach. Both start with the star of propagation vectors as generated by the parent symmetry operation. For your case, you have collected data with the vector (1/3, 1/3, 0).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



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:

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

Where:

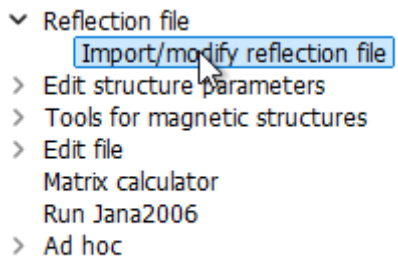
$\mathbf{x}_I = (x_4, x_5, x_6)$ are three internal components in the (3+3) d superspace.

$\boldsymbol{\sigma} = (\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3)$ 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 **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):



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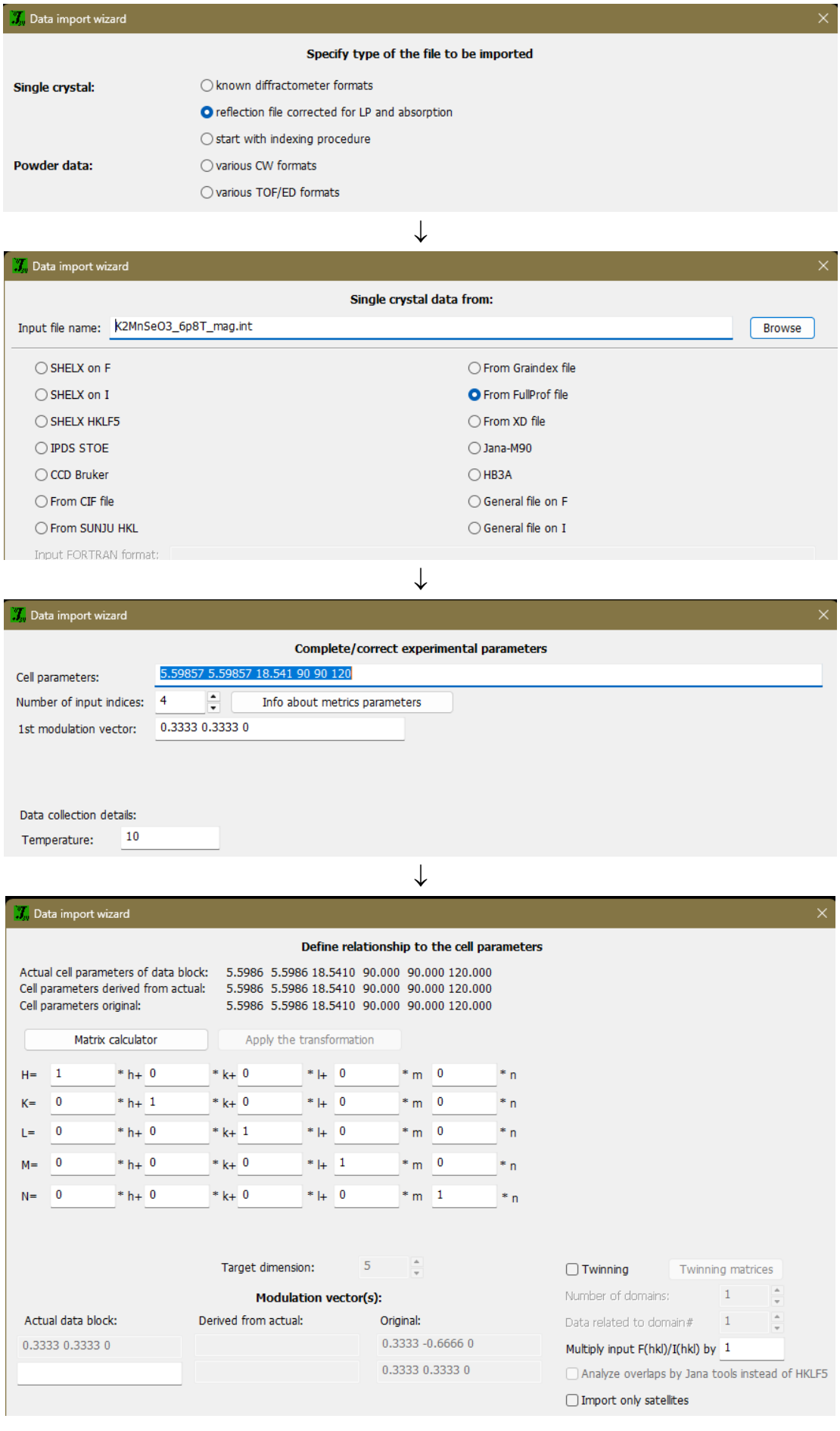
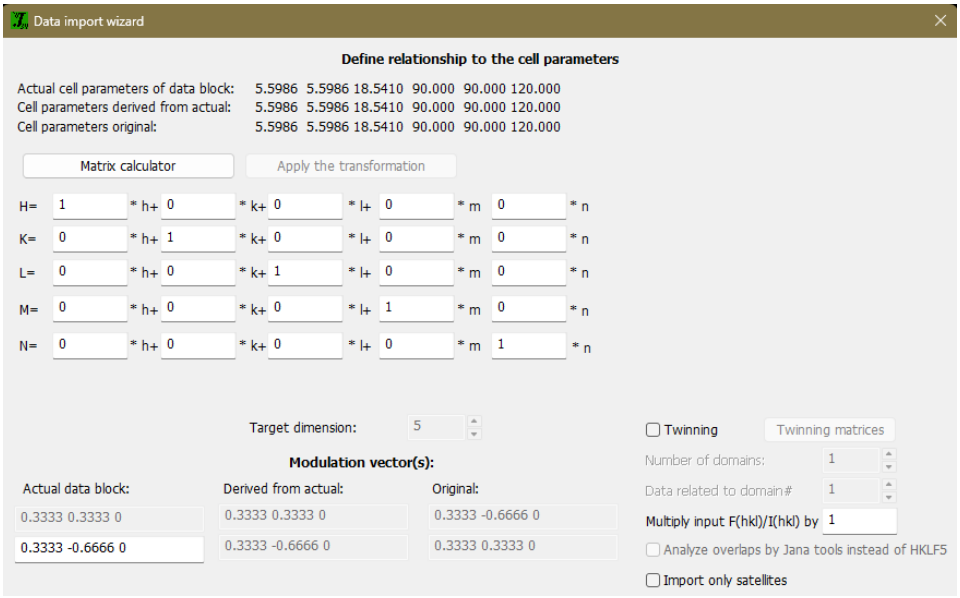
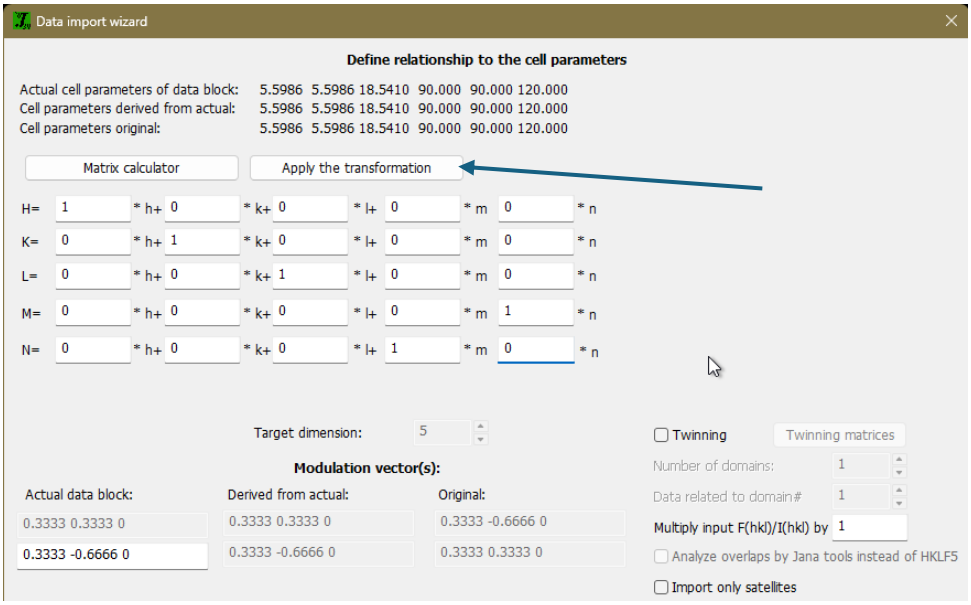

Data import wizard
Specify type of the file to be imported
Single crystal:
known diffractometer formats
reflection file corrected for LP and absorption
start with indexing procedure
Powder data:
various CW formats
various TOF/ED formats
Data import wizard
Single crystal data from:
Input file name:
K2MnSeO3_6p8T_mag.int
Browse
SHELX on F
SHELX on I
SHELX HKLF5
IPDS STOE
CCD Bruker
From CIF file
From SUNJU HKL
From Graindex 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:
5.59857 5.59857 18.541 90 90 120
Number of input indices:
4
Info about metrics parameters
1st modulation vector:
0.3333 0.3333 0
Data collection details:
Temperature:
10
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 -0.6666 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

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.

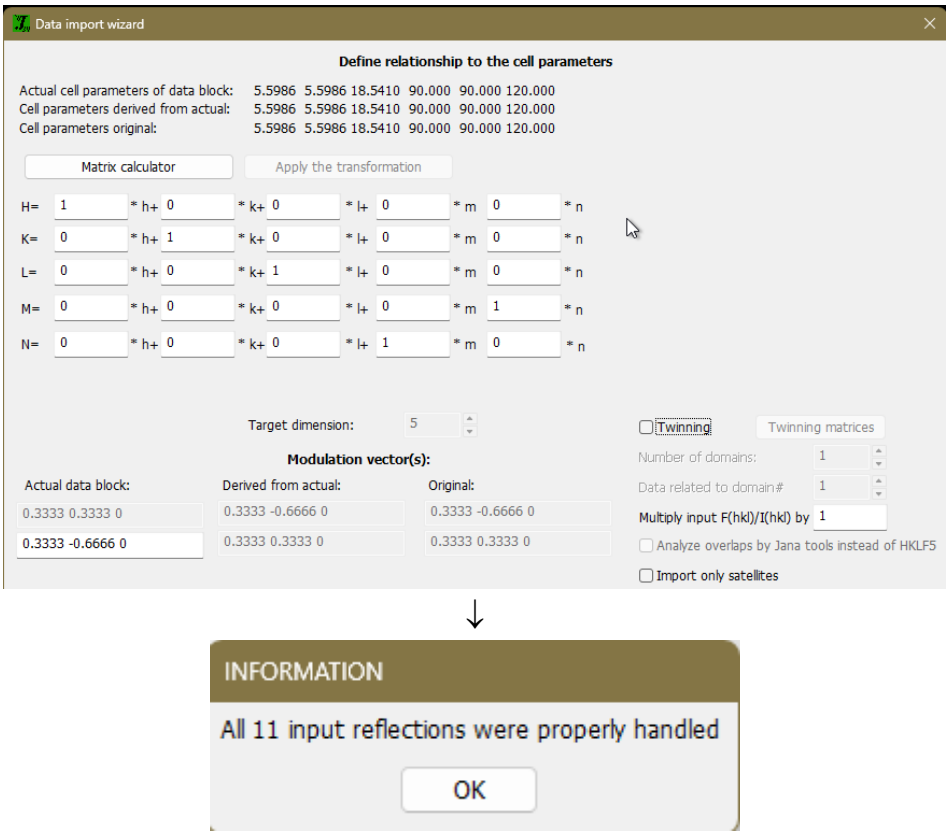
After filling the second vector and pressing the “tab” key:



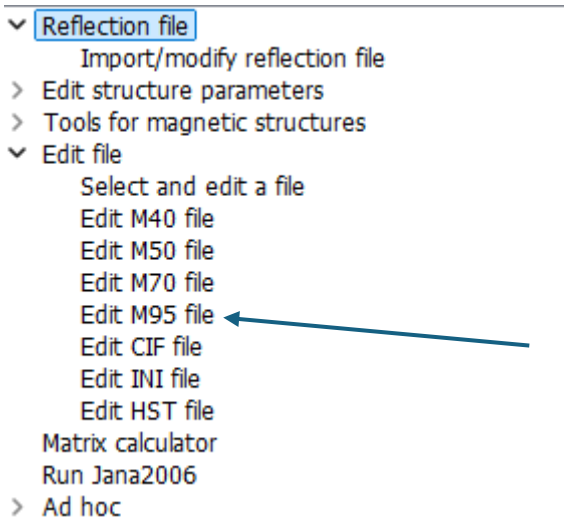
Applying the transformation matrix:



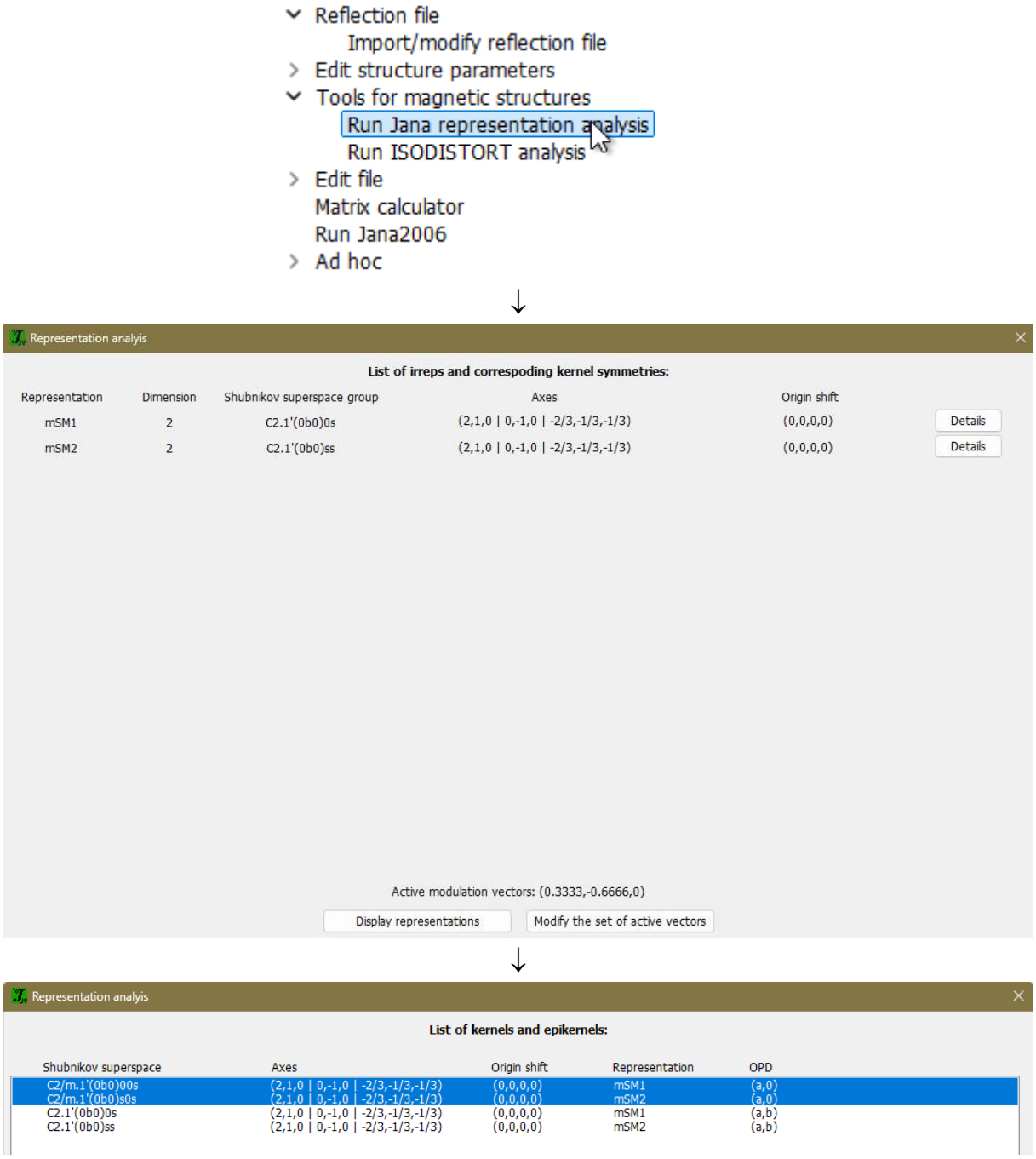
↓



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

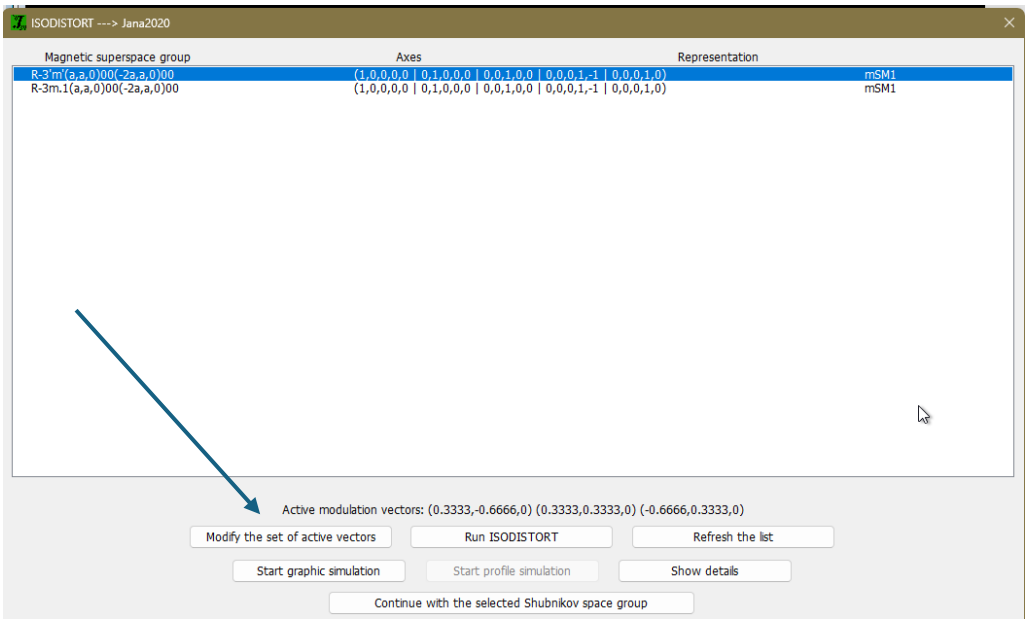


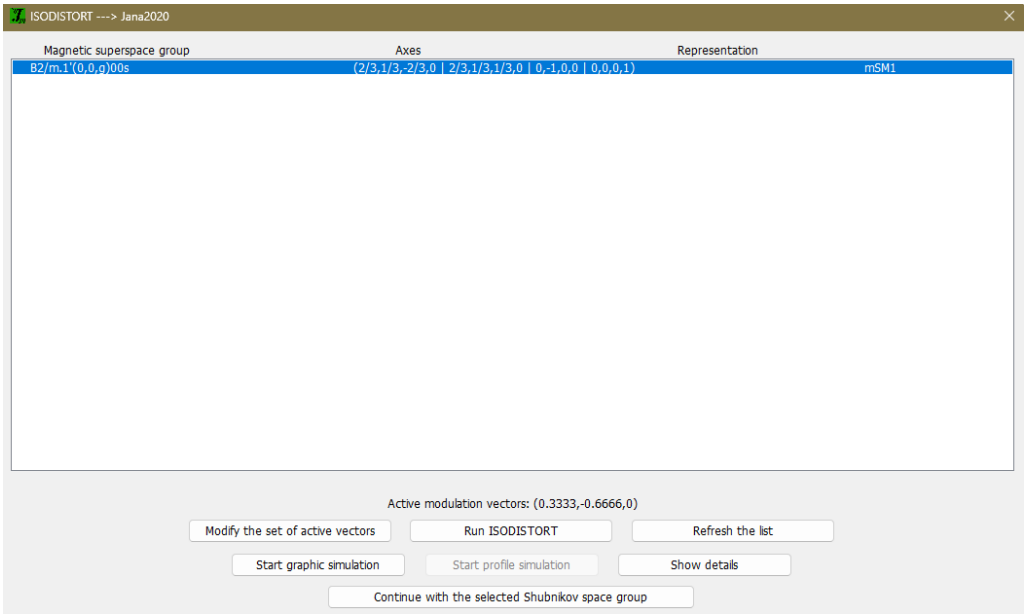
The final refinement reflection file, M90, is created when we select a particular model from the representation analysis, which can be generated either by the Jana procedure or by using the ISODISTORT program. However, the current version of Jana2020 allows only models based on one active modulation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



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

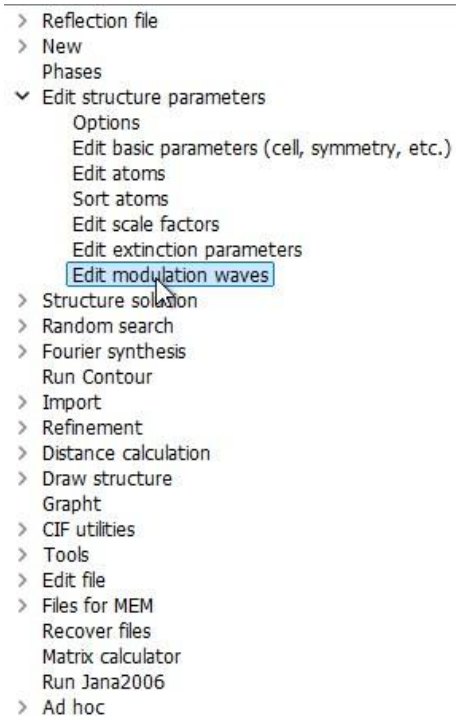
Then you can create in the ISODISTOR the CIF file based on either one or three active vectors:

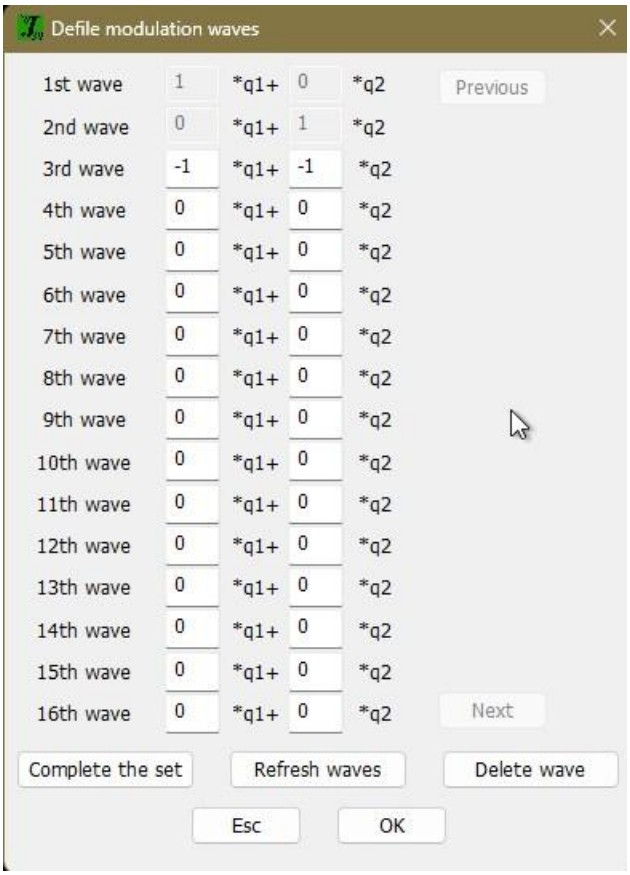




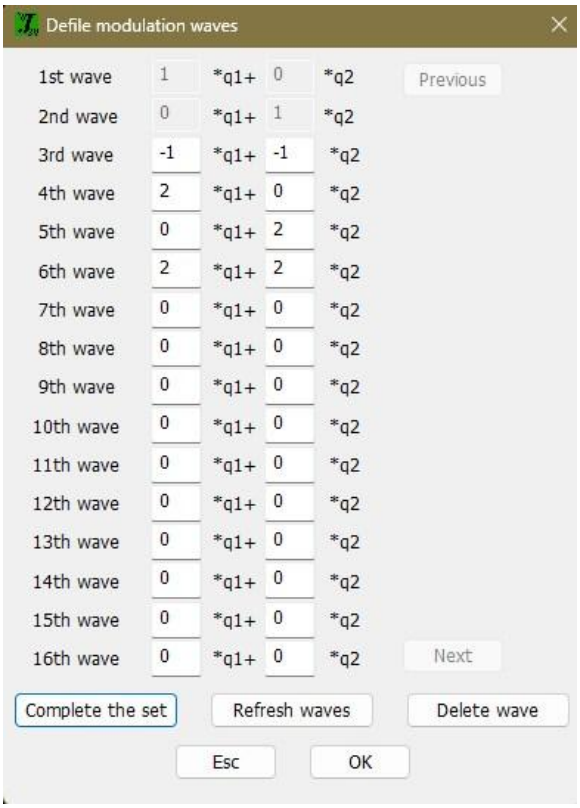
Just a few remarks:

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:

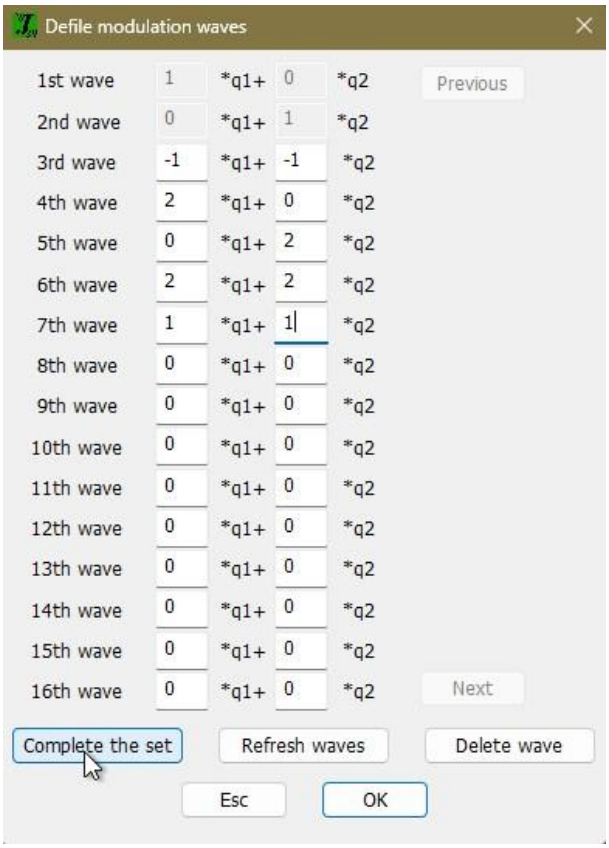




Add the modulation wave (2,0) and press the button “Complete the set”:

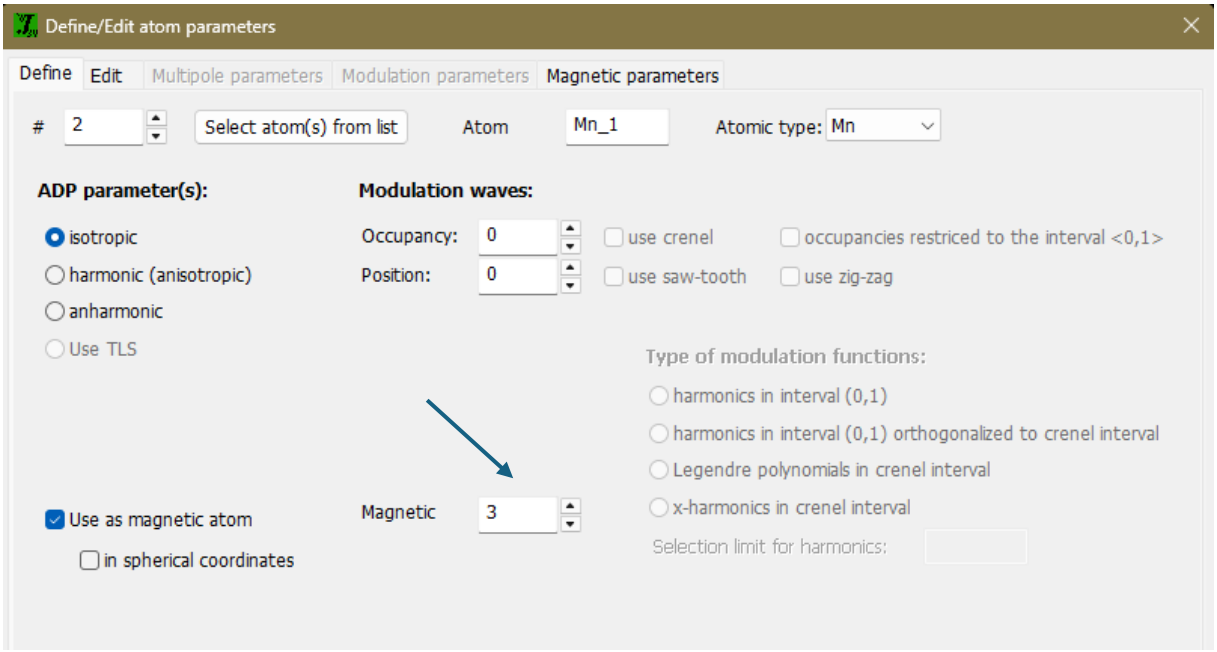


Add the modulation wave (1,1) and press the button “Complete the set”:

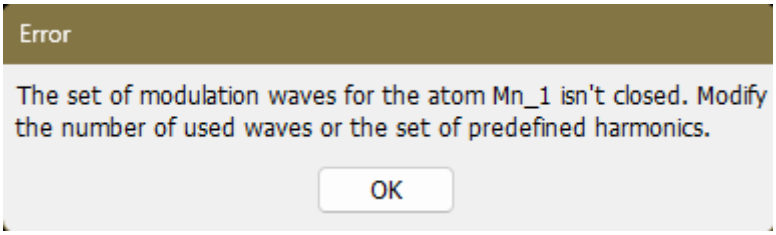


The wave (1,1) doesn’t generate the symmetry-related ones.

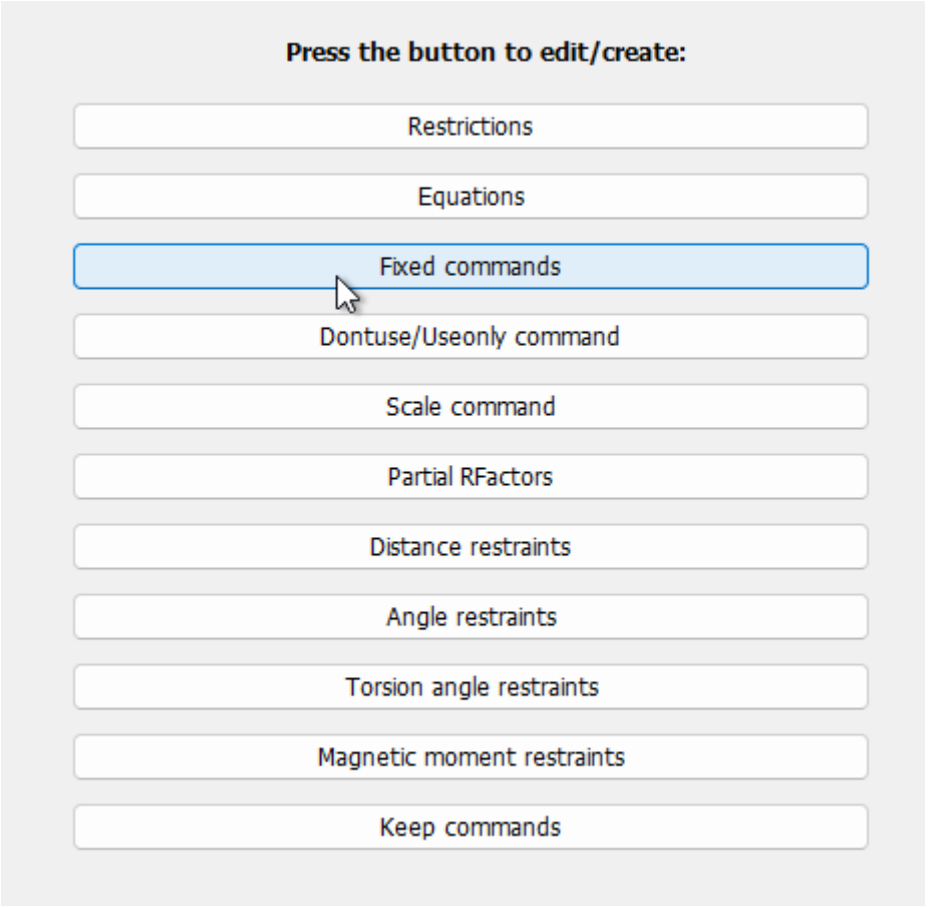
Then, for the introduction of modulation waves for individual atoms, we must use for the above example 3, 6, or 7 waves:

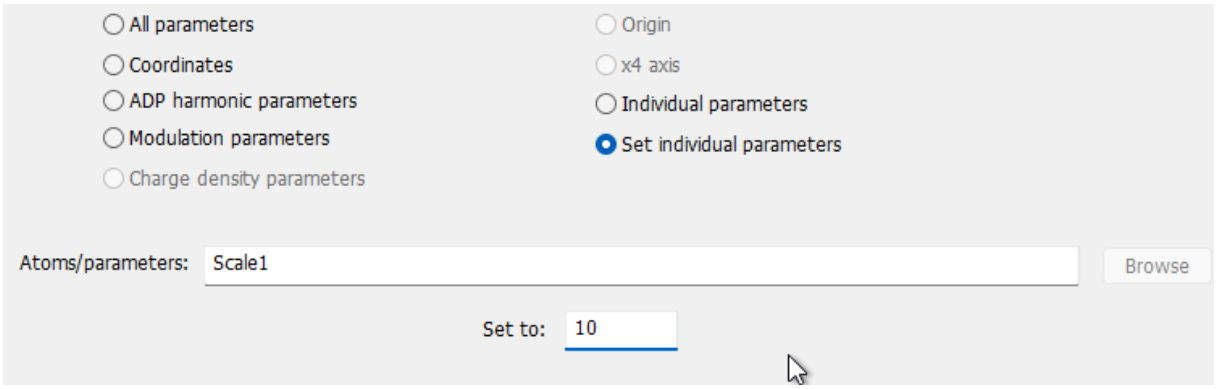


Otherwise, the refinement program will complain about using the set, which is symmetrically closed:



3. 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