

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:

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

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:

SHELLX on F  From Graindex file  
 SHELLX on I  From FullProf file  
 SHELLX HKL5  From XD file  
 IPDS STOE  Jana-M90  
 CCD Bruker  HB3A  
 From CIF file  General file on F  
 From SUNJU HKL  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=   
 K=   
 L=   
 M=   
 N=

Target dimension:

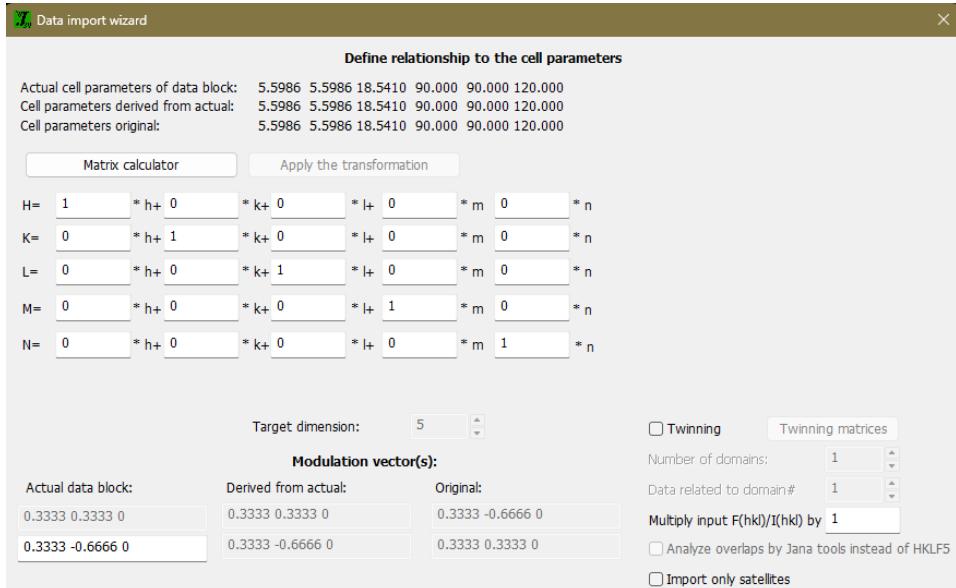
**Modulation vector(s):**

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

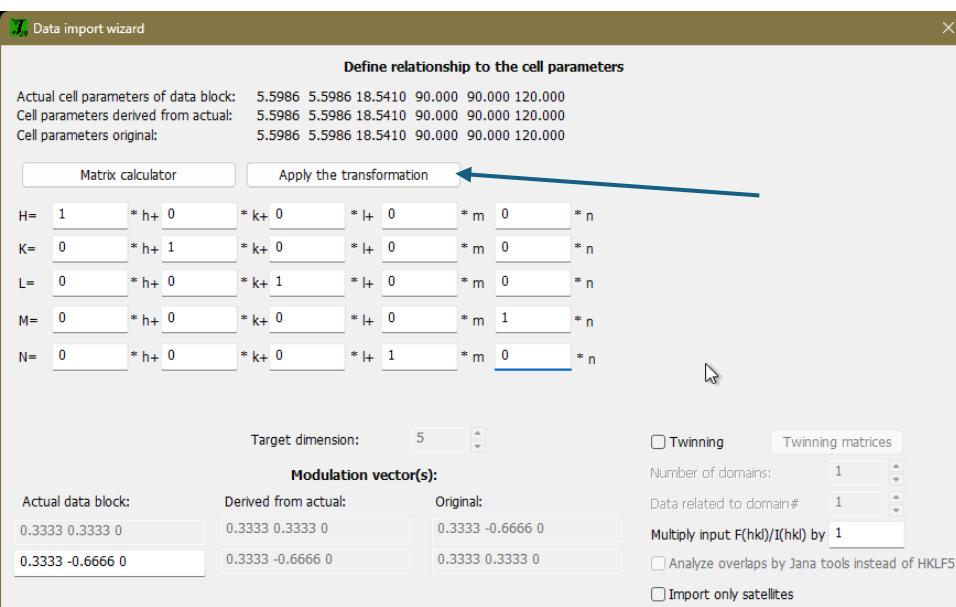
Twinning   
 Number of domains:    
 Data related to domain #:    
 Multiply input F(hkl)/I(hkl) by   
 Analyze overlaps by Jana tools instead of HKL5  
 Import only satellites

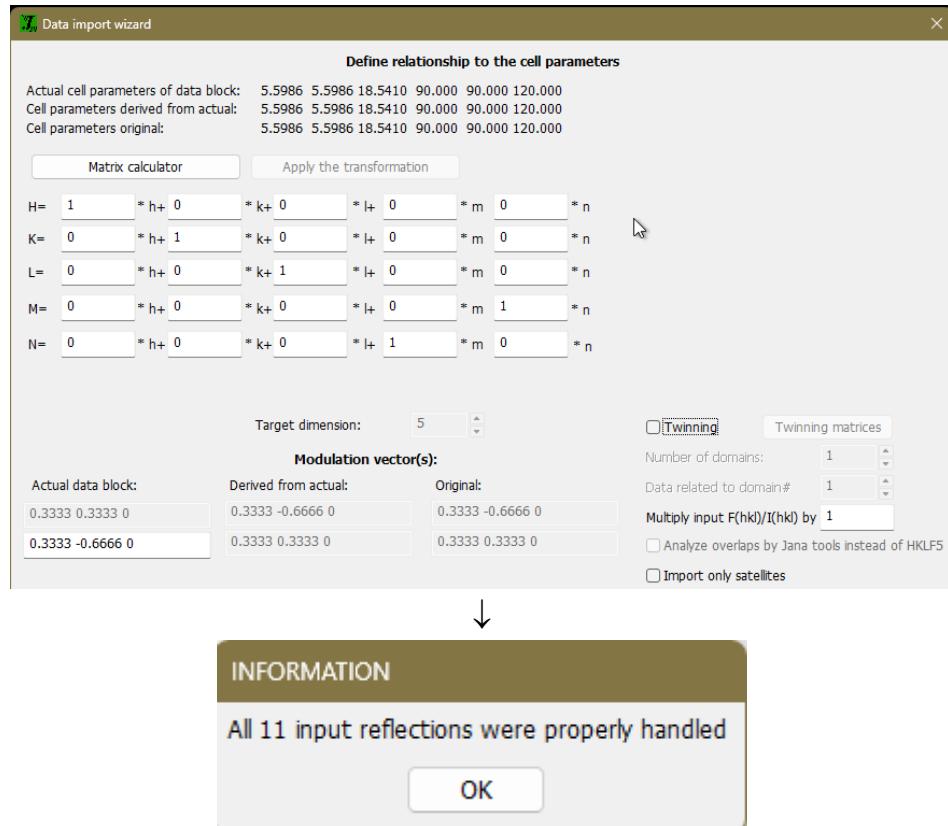
The independent modulation vectors are generated from the full star belonging to the specific point SM k2. The measured satellite reflections have indices  $h, k, l, 1$ , with an additional vector of  $(0.3333, 0.3333, 0)$ . To transform it into a (3+2)d description, we must first formally complete the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

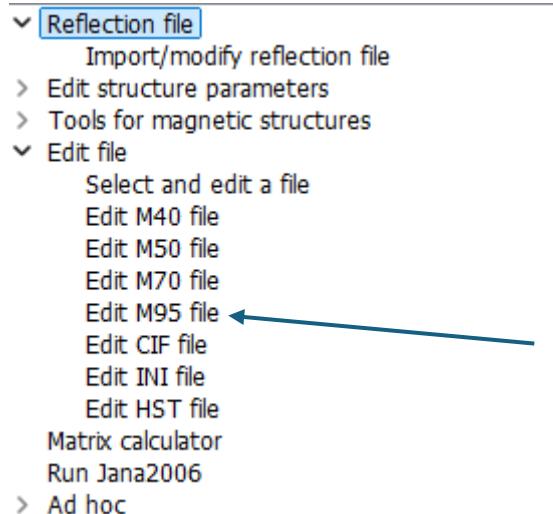


Applying the transformation matrix:





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:

- › 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)
mSM2	2	C2.1'(0b0)ss	(2,1,0   0,-1,0   -2/3,-1/3,-1/3)	(0,0,0,0)

Details      Details

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

[Display representations](#)      [Modify the set of active vectors](#)



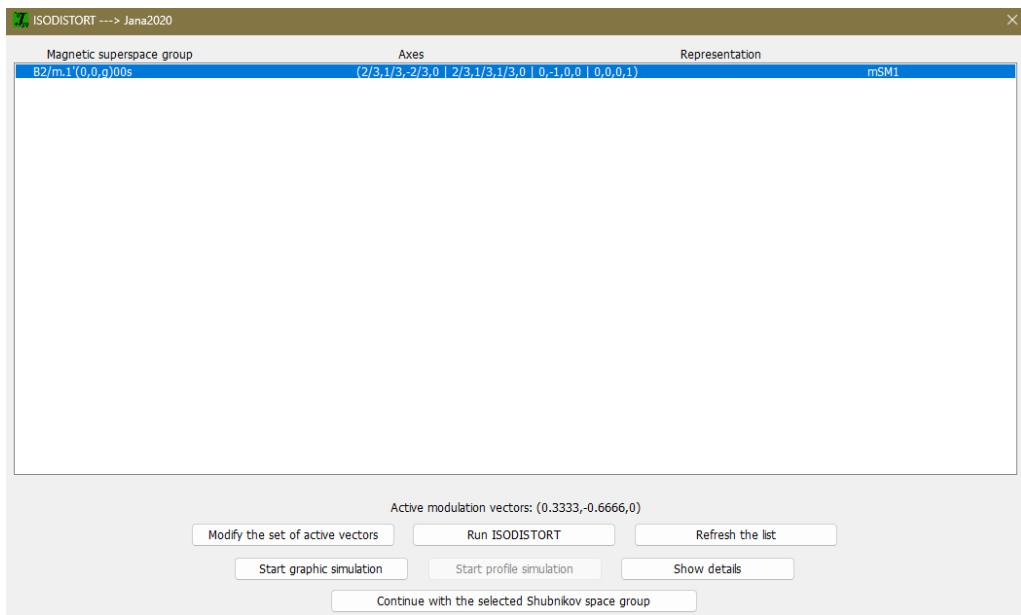
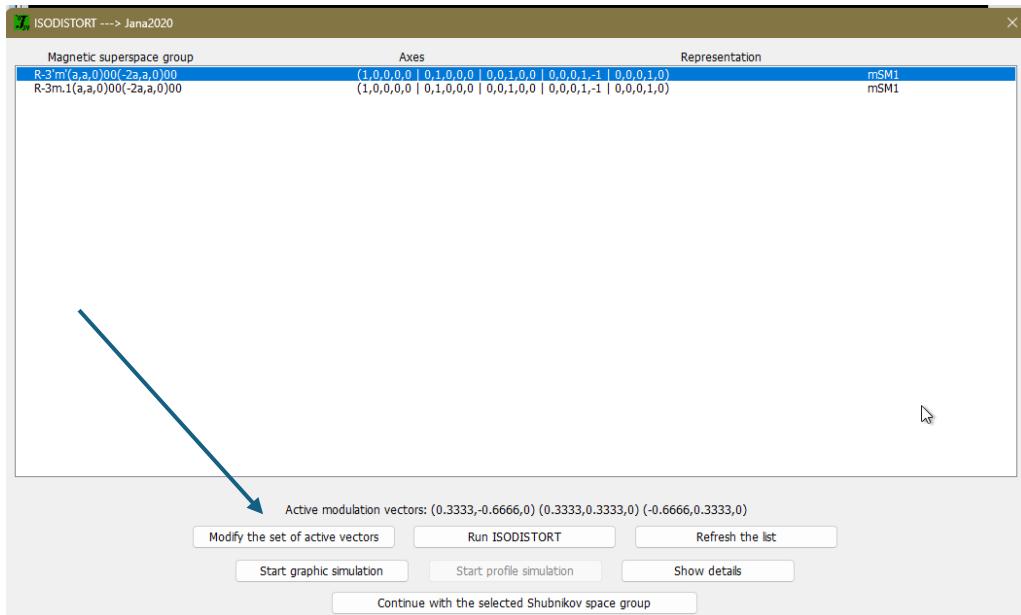
**Representation analysis**

**List of kernels and epikernels:**

Shubnikov superspace	Axes	Origin shift	Representation	OPD
C2/m.1'(0b0)0s	(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 ISODISTORT 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”:

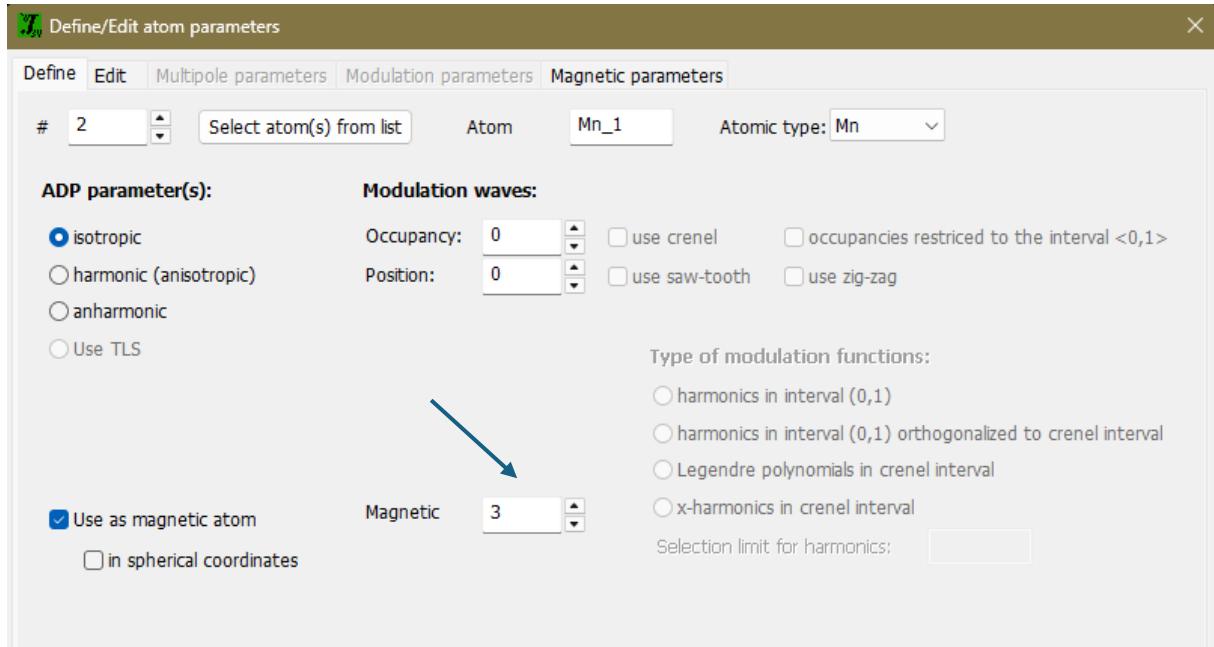
Defile modulation waves					X
1st wave	1	*q1+	0	*q2	Previous
2nd wave	0	*q1+	1	*q2	
3rd wave	-1	*q1+	-1	*q2	
4th wave	2	*q1+	0	*q2	
5th wave	0	*q1+	2	*q2	
6th wave	2	*q1+	2	*q2	
7th wave	0	*q1+	0	*q2	
8th wave	0	*q1+	0	*q2	
9th wave	0	*q1+	0	*q2	
10th wave	0	*q1+	0	*q2	
11th wave	0	*q1+	0	*q2	
12th wave	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	Next
<input type="button" value="Complete the set"/> <input type="button" value="Refresh waves"/> <input type="button" value="Delete wave"/>					
<input type="button" value="Esc"/> <input type="button" value="OK"/>					

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

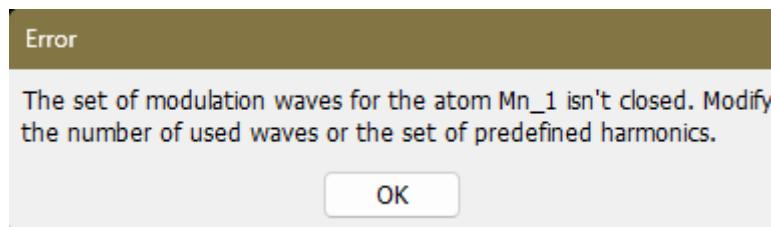
Defile modulation waves					X
1st wave	1	*q1+	0	*q2	Previous
2nd wave	0	*q1+	1	*q2	
3rd wave	-1	*q1+	-1	*q2	
4th wave	2	*q1+	0	*q2	
5th wave	0	*q1+	2	*q2	
6th wave	2	*q1+	2	*q2	
7th wave	1	*q1+	1	*q2	
8th wave	0	*q1+	0	*q2	
9th wave	0	*q1+	0	*q2	
10th wave	0	*q1+	0	*q2	
11th wave	0	*q1+	0	*q2	
12th wave	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	Next
<input type="button" value="Complete the set"/> <input type="button" value="Refresh waves"/> <input type="button" value="Delete wave"/>					
<input type="button" value="Esc"/> <input type="button" value="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:



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:

Set to:

