Example 12.7: $DyMn_6Ge_6$

Last update 6 October 2022

Data	Topic	Level
Neutron powder	Incommensurate magnetic structure	Intermediate

Input data

Data

Neutron powder data measured at 11K on DMC at PSI (Switzerland)

Input files

dymn6ge6.dat (powder profile data)
dymn6ge6_nuclear.cif (nuclear structure)
Equations-circular.txt

Additional information

Chemical formula: $DyMn_6Ge6$
Incommensurate magnetic structure: k=(0,0,0.1651); k=(0,0,0)

Keywords

Import structure from cif, transformation to subgroups, change of origin and chirality

References

J. Rodríguez-Carvajal & F. Bourée, EPJ Web of Conferences 22, 00010 (2012)
P. Schobinger-Papamantellos et al, Journal of Alloys and Compounds, 203 (1994) 243

Highlights

none

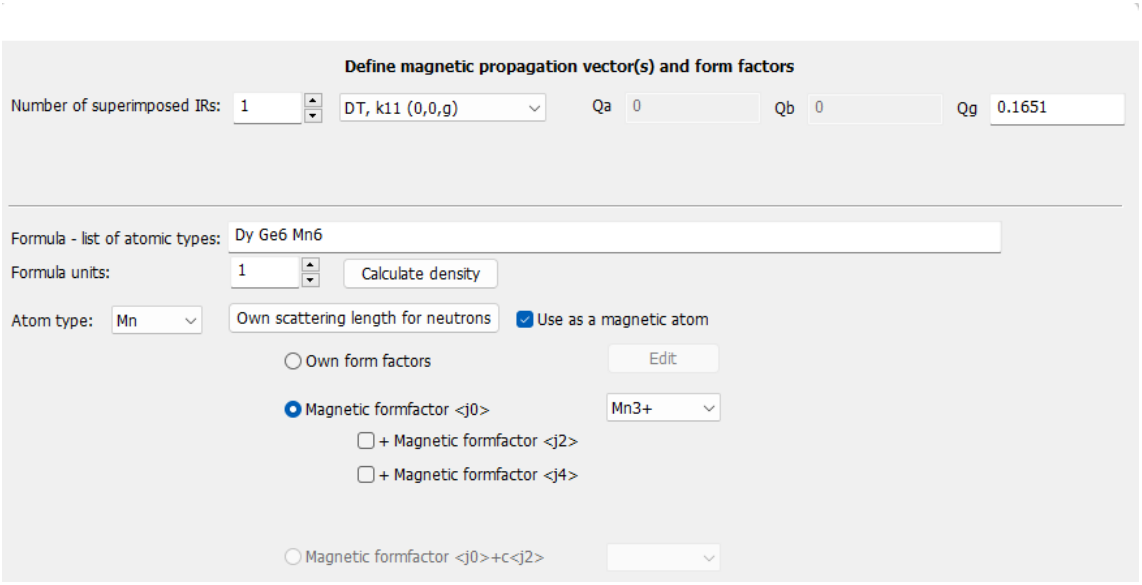
Instructions

1. *Data import*

For details, see Basic tasks
Start Jana2020
In the Main menu bar, use "Structure → New" and open new structure **dymn6ge6** in the directory of Example 12.7
Select "Magnetic parent structure: nuclear model from CIF"; NEXT
In Windows file explorer: select the input file dymn6ge6_nuclear.cif; Open

2. *Define the magnetic propagation vector and form factors*

[On the screen: Define magnetic propagation vector and form factors]
Set the "Number of superimposed IRS:" to '1' and select the propagation magnetic vector to be "DT, k11 (0,0,g)" and fill its value: 0 0 0.1651;
Select atom type Dy; check "Use as a magnetic atom" and "Magnetic formfactor <j0>" Dy3+
Select atom type Mn; check "Use as a magnetic atom" and "Magnetic formfactor <j0>" Mn3+
NEXT; FINISH



3. *Import of the reflection file*

[On the screen: Specify type of the file to be imported]
Select "Various CW format"; NEXT
Check that the name of the input file is "dymn6Ge6.dat" and the format is "PSI format";
Select "Debye-Scherrer method"; NEXT
[On the screen: Complete/correct experimental parameters]
For Wavelength, fill 1.7037; Temperature 11
NEXT; FINISH;OK

4. *Refining of the profile parameters by the le Bail technique*

[On the screen: Information]
NEXT
[On the screen: Powder profile viewer]

Notes

The background is relatively smooth and can be described without introducing a manual background.

In the left toolbar, press the quick button "Edit profile" **or** in the Command tree, expand "Powder" and open "Edit profile"

[On the screen: Powder options]

On the page "Cell", activate the refinement of "a" and "c" parameters and the third component of the modulation vector "q3"

On the page "Profile", keep the starting value of "GW" to 50 and activate its refinement

On the page "Corrections", activate refinement of "shift" parameter and change the number of used Legendre polynomials to 10

OK; YES to save the changes

In the left toolbar, right-click on the quick button "Run refinement", **or** in the Command tree, expand "Refinement" and open "Refinement commands"

On the page "Basic", change the number of cycles to 40

OK; Yes+Start

Notes

Profile R factors :[800/15+1]

GOF~5.7 Rp~4.9 wRp~7.1

R values are visualized at the bottom information line.

Open "Edit profile"

[On the screen: Powder options]

In the page "Profile", activate refinement of "GU" and "GV"

Change the peak-shape function to pseudo-Voigt and activate the refinement of "LX"

OK; YES to save the changes

Press "Run refinement"

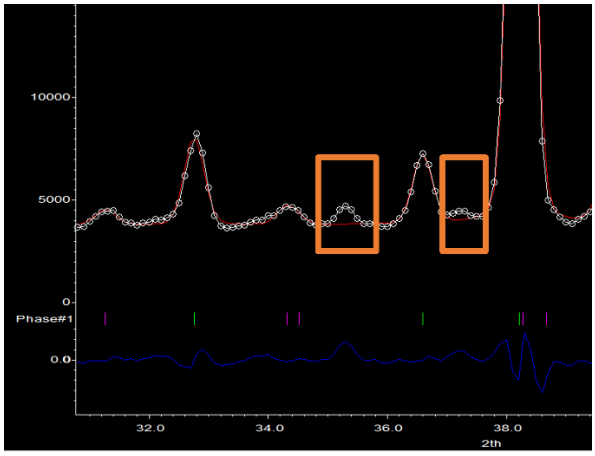
Notes

Profile R factors :[800/18+1]

GOF~3.3 Rp~3.0 wRp~4.1

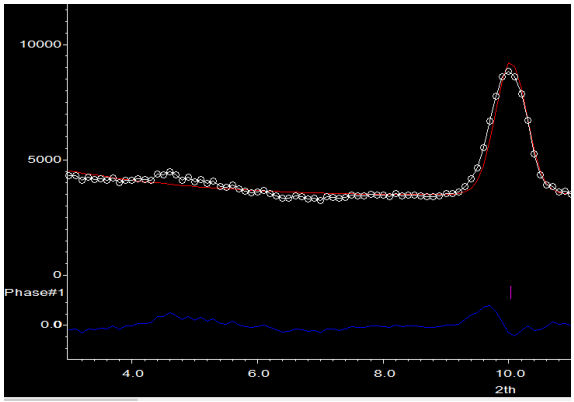
Changes on the calculated profile demonstrate the importance of adding newly introduced parameters.

Zoom the profile to the diffraction angles 2θ from 30 to 45 degs: with the mouse, drag the rectangle with the left button and then click on the rectangle **or** use the 2θ range on the right pane **or** use the mouse wheel



The unfit peaks may correspond to some impurity.

Scroll to the beginning of the powder profile



Around 2θ = 5 deg, an anomaly in the background is observed. No peaks are possible there, we will exclude the region for refinement.

Press "Shrink the profile" to unzoom

Open "Edit profile"

In the page "Corrections"; press the button "Define excluded regions"

"Skip profile from: 0 to 7"; press "Rewrite"

OK; OK; YES

Press "Run refinement"

Notes
Profile R factors :[759/18+1]
GOF~3.3 Rp~2.9 wRp~4.1

Press to close the profile viewer;

Select "Go to the Rietveld refinement"; OK

5. Refinement of the scale for the nuclear structure

[On the screen: Profile viewer]

Notes
All commands to refine only the scale parameter have already been correctly set. You can check it in refinement commands – page Restraints/Constraints.

Right-click on the quick button "Run refinement"

In the page "Restrains/constrains" select "Fixed commands";

Notes
*If the command "fixed all *" is not in the panel, select "All parameters"; write "*" to the Atoms/parameters box; "Rewrite"; OK;*

Run refinement;

Notes
R factors : [36=33+3/1]
R(obs)~7.5 wR2(obs)~9.9 R(all)~11.2 wR2(all)~10.0
Profile R factors :[759/10+1]
GOF~13.0 Rp~11.6 wRp~16.2

Press to close the profile viewer;

Select "Finish the process";

6. Testing different irreps to get the best model

[On the screen: Information]

NEXT

[On the screen: List of irreps and corresponding kernel symmetries]

Notes

This window has an information character. You can see here all irreps leading to magnetic ordering. The "details" buttons provide more information about an individual irrep and its connection to the kernel magnetic symmetry.

Representation	Dimension	Shubnikov superspace group	Axes	Origin shift	
mDT1	2	P6mm.1'(00g)000s	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0,0)	Details
mDT2	2	P6mm.1'(00g)0sss	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0,0)	Details
mDT3	2	P6mm.1'(00g)ss0s	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0,0)	Details
mDT4	2	P6mm.1'(00g)s0ss	(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

NEXT

[On screen: List of kernels and epikernels]

List of kernels and epikernels:

Shubnikov superspace	Axes	Origin shift	Representation	ODP
P6/mmm.1'(00g)0000s	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0,0)	mDT1	(a,0)
P6/mmm.1'(00g)00sss	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0,0)	mDT2	(0,a)
P6/mmm.1'(00g)s0s0s	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0,0)	mDT3	(0,a)
P6/mmm.1'(00g)s00ss	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0,0)	mDT4	(a,0)
P6mm.1'(00g)000s	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0,0)	mDT1	(a,b)
P6mm.1'(00g)0sss	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0,0)	mDT2	(a,b)
P6mm.1'(00g)ss0s	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0,0)	mDT3	(a,b)
P6mm.1'(00g)s0ss	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0,0)	mDT4	(a,b)
P622.1'(00g)t00s	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0,-1/12)	mDT5	(0,a,0,0)
P622.1'(00g)h00s	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0,0)	mDT6	(0,0,0,a)
P6.1'(00g)ts	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0,0)	mDT5	(0,a,0,b)
P6.1'(00g)hs	(1,0,0 | 0,1,0 | 0,0,1)	(0,0,0,0)	mDT6	(0,a,0,b)
Cmmm.1'(00g)ss0s	(-1,0,0 | -1,-2,0 | 0,0,1)	(0,0,0,0)	mDT5	(0,0,a,a)
Cmmm.1'(00g)000s	(-1,0,0 | -1,-2,0 | 0,0,1)	(0,0,0,0)	mDT5	(a,-a,0,0)
Cmmm.1'(00g)s00s	(-1,0,0 | -1,-2,0 | 0,0,1)	(0,0,0,0)	mDT6	(0,0,a,a)
Cmmm.1'(00g)0s0s	(-1,0,0 | -1,-2,0 | 0,0,1)	(0,0,0,0)	mDT6	(a,-a,0,0)
Cmm2.1'(00g)ss0s	(-1,0,0 | -1,-2,0 | 0,0,1)	(0,0,0,0)	mDT5	(a,a,b,b)
Cmm2.1'(00g)000s	(-1,0,0 | -1,-2,0 | 0,0,1)	(0,0,0,0)	mDT5	(a,-a,b,-b)
Cmm2.1'(00g)s0ss	(-1,0,0 | -1,-2,0 | 0,0,1)	(0,0,0,0)	mDT6	(a,a,b,b)
Cmm2.1'(00g)0sss	(-1,0,0 | -1,-2,0 | 0,0,1)	(0,0,0,0)	mDT6	(a,-a,b,-b)
C222.1'(00g)000s	(-1,0,0 | -1,-2,0 | 0,0,1)	(0,0,0,0)	mDT5	(a,b,0,0)
C222.1'(00g)00ss	(-1,0,0 | -1,-2,0 | 0,0,1)	(0,0,0,0)	mDT6	(a,b,0,0)
P2/m.1'(0b0)00s	(0,-1,0 | 0,0,-1 | 1,1,0)	(0,0,0,0)	mDT5	(a,-a,b,b)
P2/m.1'(0b0)s0s	(0,-1,0 | 0,0,-1 | 1,1,0)	(0,0,0,0)	mDT6	(a,-a,b,b)
P2.1'(0b0)0s	(0,-1,0 | 0,0,-1 | 1,1,0)	(0,0,0,0)	mDT5	(a,b,c,d)
P2.1'(0b0)ss	(0,-1,0 | 0,0,-1 | 1,1,0)	(0,0,0,0)	mDT6	(a,b,c,d)

Number of epikernels: 26

Select from above kernels/epikernels one representative of a family of Shubnikov superspace groups for testing.

Back | Next | Cancel

Select the block of hexagonal magnetic superspace groups based on the average space group P6/mmm; NEXT;

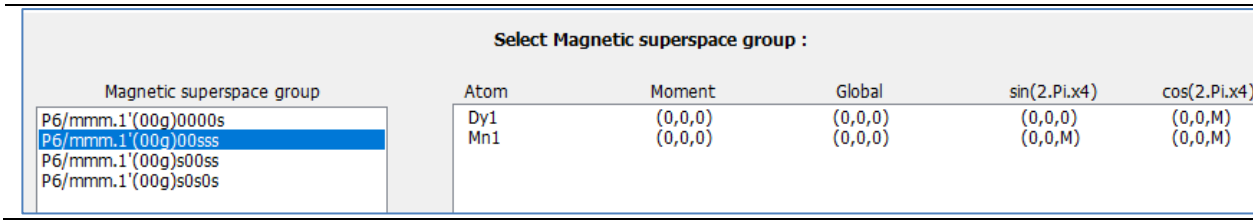
Notes

This will pass all present hexagonal magnetic superspace groups of type P6/mmm to further testing. We assume that both magnetic atoms ***should have a non-zero magnetic moment****.*

[On the screen: Select magnetic space group]

Notes

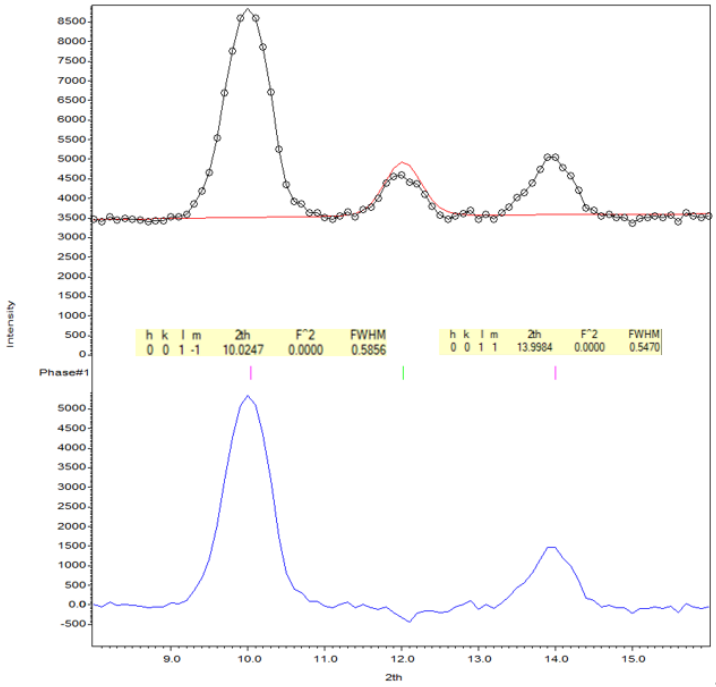
Only the second magnetic superspace group allows for non-zero magnetic moments for Mn and Dy atoms.



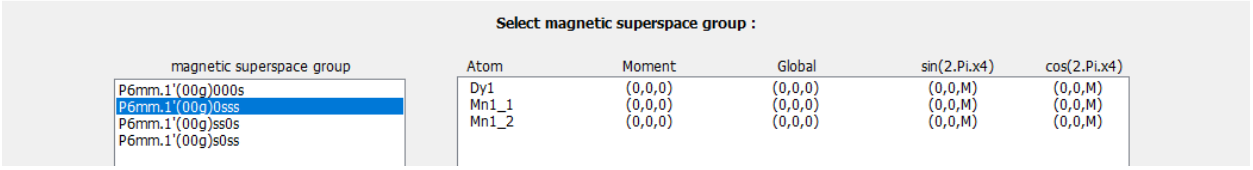
Select the second magnetic superspace group: P6/mmm.1'(00g)00sss
Press "Start profile simulation"
Select 2th(min) and 2th(max) range from 8 to 16 degrees
Press "Fit Y":

Notes

Two dominant magnetic peaks in this region have zero intensity. Therefore, the tested model cannot describe the magnetic ordering correctly. In making such a conclusion, we have to consider that the simulation procedure uses randomly generated magnetic moments and that the result can be affected by an actual random choice. We recommend repeating the simulation when some doubt exists.



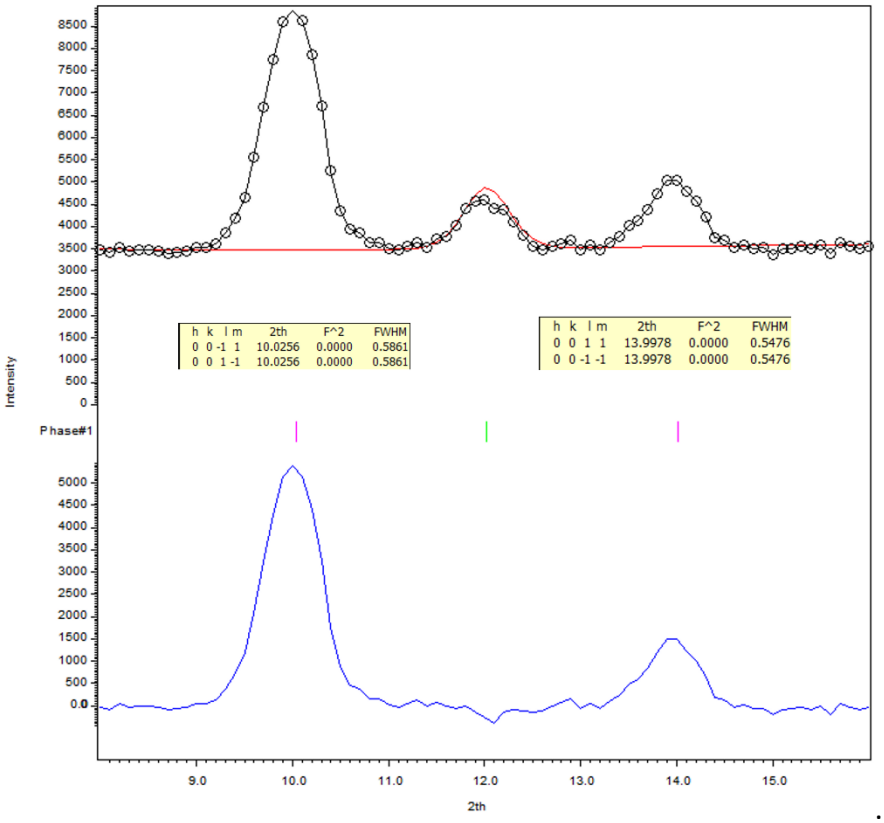
Press ✖ to close the profile viewer;
[On the screen: Select magnetic space group]
Press "Back" and return to the "List of kernels and epikernels"
[On screen: List of kernels and epikernels]
Select the block of hexagonal superspace groups based on P6mm; NEXT;



Select the second magnetic superspace group: P6mm.1'(00g)0sss
Press "Start profile simulation";
Select 2th(min) and 2th(max) range from 8 to 16 degrees,
Press "Fit Y":

Notes

The test in the P6mm subgroup did not change the symmetry restrictions of the magnetic moments, which resulted in the identical result as for P6/mmm.

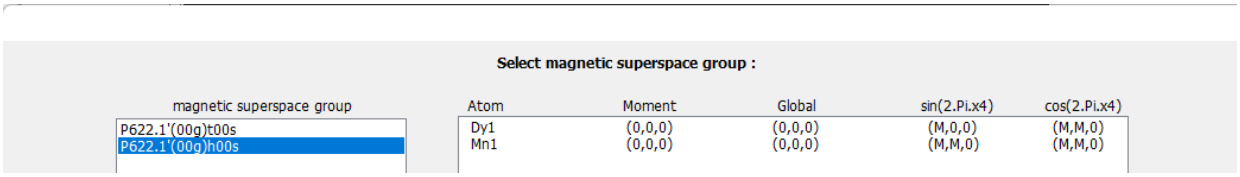


[On screen: List of kernels and epikernels]

Select the block of hexagonal superspace groups based on P622; NEXT;

Notes

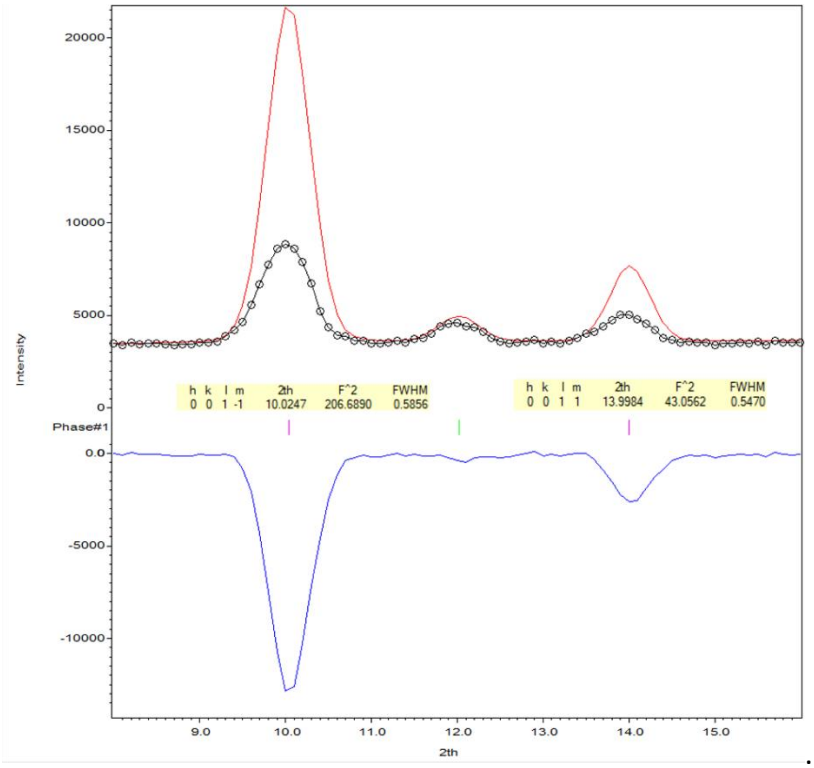
While the first one P622.1’(00g)t00s restricts the magnetic moments of the Dy atom to zero, the second one P622.1’(00g)-h00s allows non-zero magnetic moments for both magnetic atoms.



Select the second magnetic superspace group: P622.1’(00g)h00s
Press “Start profile simulation”;
Select 2th(min) and 2th(max) range from 8 to 16 degrees,
Press “Fit Y”:

Notes

The simulation demonstrates that the intensity of both magnetic peaks in the interval 8-16 degs is non-zero:



Press ✖ to close the profile viewer

7. *Refinement of the magnetic structure in – P622.1’ (00g)h00s*

[On the screen: Select magnetic superspace group]
Select the magnetic superspace group P622.1’ (00g)h00s
Press “Continue with the selected magnetic superspace group”
[On the screen: Select structure name]
Use the default name, i.e. dymn6ge6_01; Save
[On the screen: Basic window of Jana2020]
Right-click on the quick button “Run refinement”
In the page “Constrains/Restrains”, select “Restrictions” and ensure that all atoms are restricted to have identical ADP parameters (“restric * 13”).
In the page “Constrains/Restrains”, select “Fixed commands” and ensure that coordinates of all atoms are fixed (“fixed xyz *”).
In the page “Basic”, check if the “Number of cycles” is set to 100 and the “Damping factor” to 0.1
OK; YES to start the refinement;

Notes

R factors : [114=112+2/7]
R(obs)~5.1 wR2(obs)~6.2 R(all)~5.3 wR2(all)~6.2
R factors for main reflections : [40=40+0]
R(obs)~4.8 wR2(obs)~6.7 R(all)~4.8 wR2(all)~6.7
R factors for satellites +-(1) : [74=72+2]
R(obs)~5.7 wR2(obs)~5.8 R(all)~6.2 wR2(all)~5.9
Profile R factors :[759/10+7]
GOF~5.9 Rp~5.1 wRp~7.3

If your R Value are different just follow the next steps

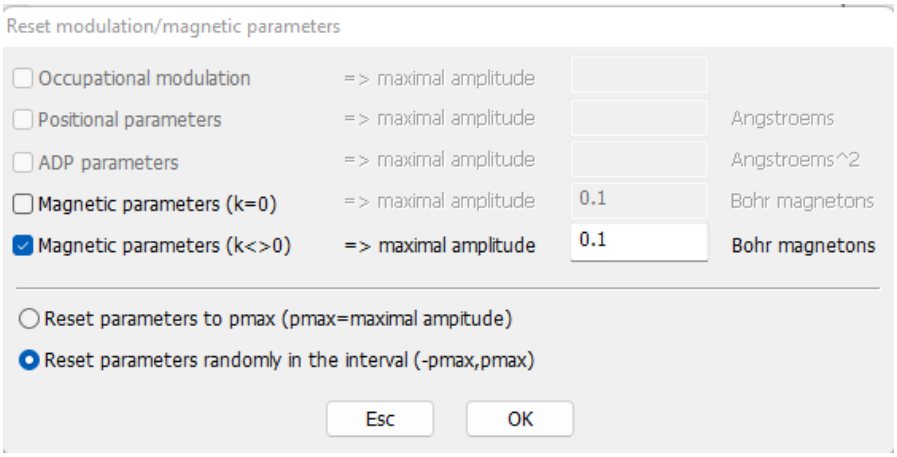
Change focus to “Profile viewer”
Use “Profile viewer” to check the fit of the calculated powder profile

Notes

The starting model uses a random procedure for setting magnetic moments. Therefore, your result can differ from what is written above. Then it would help if you tried what is written in the following paragraph. Otherwise, you can skip repeating the randomized procedure.

Press the quick button “Edit atom”
Select both magnetic atom Dy1 and Mn1 atoms then Press “Action” and “Reset modulation/magnetic parameters.”

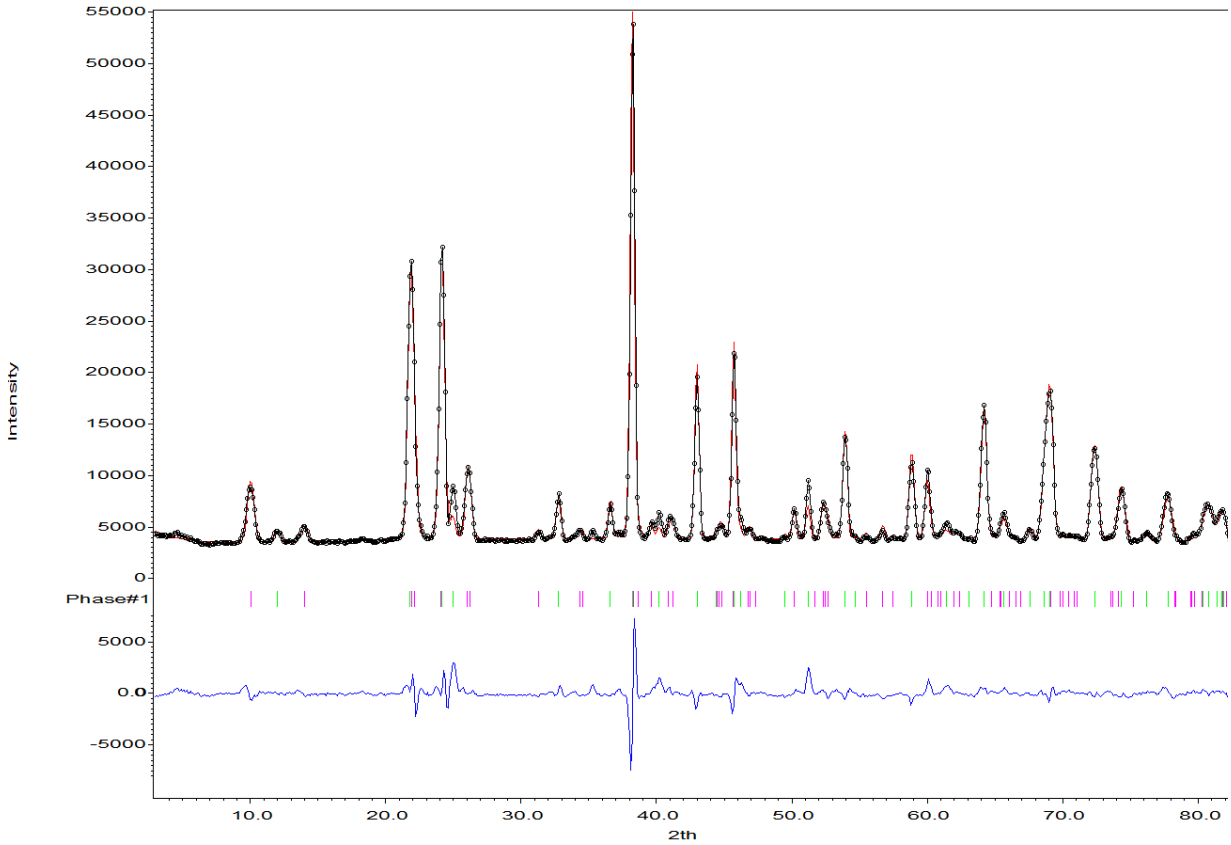
Clear the checkbox “Magnetic parameters (k=0),



OK; OK; YES to save changes
Press “Run refinement”

Notes

You might need to repeat the above procedure several times until the profile fit is as expected.



The fit of some main reflections, e.g. (1 0 1 0) around 25 degrees or (2 -1 0 0) at about 40 degrees, is poor. To exclude some additional nuclear effects, we can allow the refinement of the atomic positions.

Right-click on quick button "Run refinement"
In the page "Constrains/Restrains", Select "Fixed commands" and disable "fixed xyz *";
OK; OK;Yes + start

Notes

Now the atomic coordinates are refined
R factors : [114=113+1/9]
R(obs)~5.1 wR2(obs)~6.3 R(all)~5.1 wR2(all)~6.3
R factors for main reflections : [40=40+0]
R(obs)~4.5 wR2(obs)~6.8 R(all)~4.5 wR2(all)~6.8
R factors for satellites +-(1) : [74=73+1]
R(obs)~6.0 wR2(obs)~5.9 R(all)~6.1 wR2(all)~5.9
Profile R factors :[800/10+9]
GOF~5.7 Rp~5.0 wRp~7.2
The improvement is minimal. Some of the main reflections remain poorly fit with systematically low calculated intensity.
This can lead to the conclusion that an additional magnetic ordering with k=0 is present.

8. Refinement in subgroups allowing k = (0,0,0)

[On the screen: Basic Jana window]

Notes

We test the possibility that magnetic scattering also occurs at main reflections, i.e., an ***additional magnetic ordering with k=(0 0 0)*** *is taking place. In the language of the symmetry group of the phase, this implies lowering its symmetry by dropping the operation {1'|0001/2} associated with the existence of a single primary incommensurate wave vector.*
There are several maximal subgroups without this operation. They can be generated by the Jana tool "Transformations→Go to subgroup structure".

The possible maximal subgroups will then be generated by:

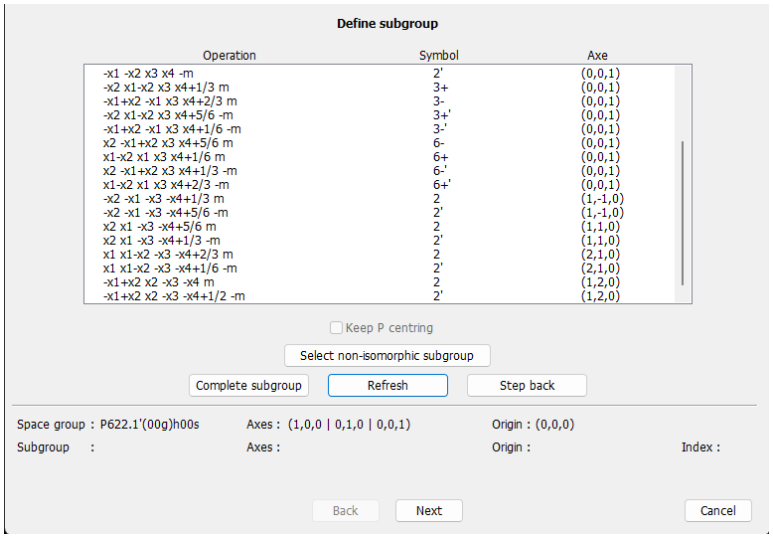
P622(00g) h00
{6+|0 0 0 5/6}: x1-x2, x1, x3, x4+5/6, m in the Jana dialog: Symbol 6+ Axes (0,0,1)
{2_xy| 0 0 0 0}: x2, x1, -x3, -x4, m in the Jana dialog: Symbol 2 Axes (1,1,0)

P6'22'(00g)-t00
{6+'|0 0 0 1/3}: x1-x2, x1, x3, x4+1/3, -m in the Jana dialog: Symbol 6+' Axes (0,0,1)
{2_xy| 0 0 0 0}: x2, x1, -x3, -x4, m in the Jana dialog: Symbol 2 Axes (1,1,0)

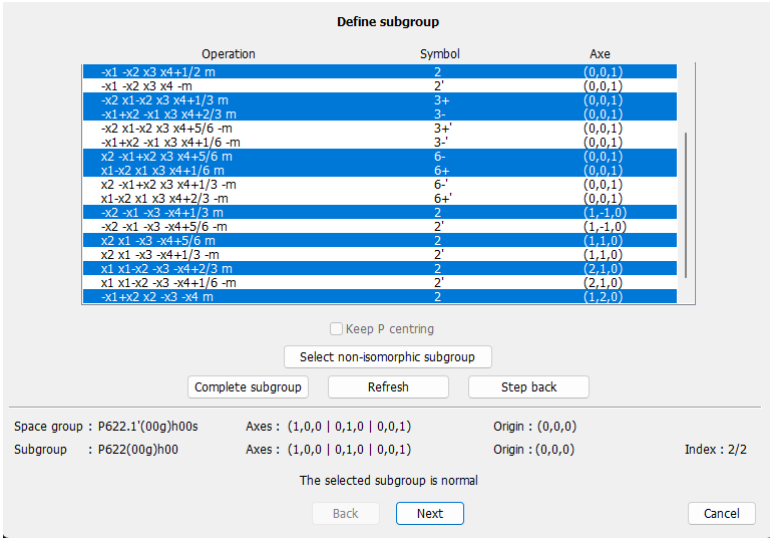
P62'2'(00g)h00
{6+|0 0 0 5/6}: x1-x2, x1, x3, x4+5/6, m in the Jana dialog: Symbol 6+ Axes (0,0,1)
{2'_xy| 0 0 0 1/2}: x2, x1, -x3, -x4+1/2, -m in the Jana dialog: Symbol 2' Axes (1,1,0)

P6'2'2(00g)-t00
{6+'|0 0 0 1/3}: x1-x2, x1, x3, x4+1/3, -m in the Jana dialog: Symbol 6+' Axes (0,0,1)
{2'_xy| 0 0 0 1/2}: x2, x1, -x3, -x4+1/2, -m in the Jana dialog: Symbol 2' Axes (1,1,0)

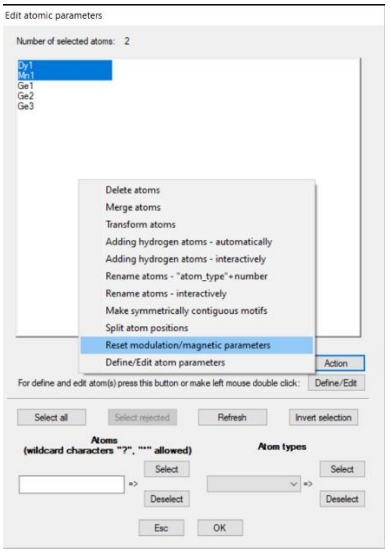
In the Main menu bar, use Transformations → Go to a subgroup;
Press the "Refresh" button and select the generators:
x1-x2 x1 x3 x4+5/6 m Symbol 6+ Axes (0,0,1)
x2 x1 -x3 -x4 m Symbol 2 Axes (1,1,0)



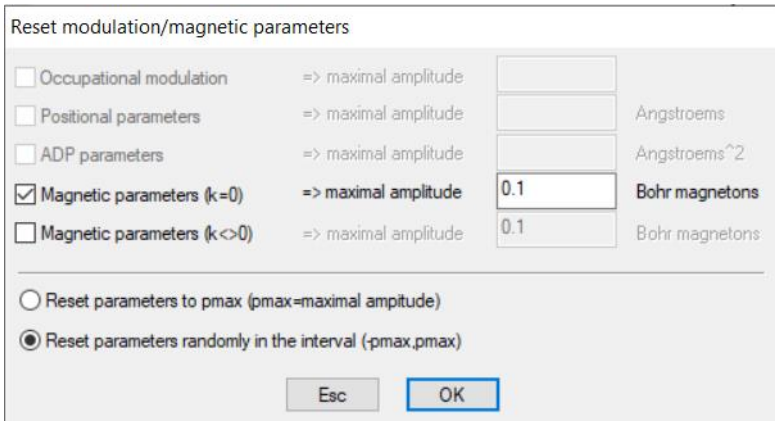
Press the button "Complete subgroup"



NEXT;
Select the radio button “Use automatic procedure for selection of coset representatives”
NEXT
[On the screen: Specify the output structure]
Type “dymn6ge6_01_subgroup_1”
NEXT; FINISH;
YES to continue with the new structure
[On the screen: Basic window]
In the left toolbar, press the quick button “Edit Atoms” **or** in the Command tree, expand “Edit structure parameters”, and open “Edit Atoms”
Select atoms Dy1 and Mn1;
Press the button “Action” or make the right mouse click
Select “Reset modulation/magnetic parameters”



Clear the checkbox “Magnetic parameters k<>0”
Choose “Reset parameters randomly in the interval (-pmax,pmax)



OK; OK;
YES to rewrite files
Press "Run Refinement"
Change focus to "Profile viewer"; Select 2th(min) and 2th(max) range from 20 to 45 degrees,

Notes

R factors : [114=113+1/8]
R(obs)~4.8 wR2(obs)~6.0 R(all)~4.8 wR2(all)~6.0
R factors for main reflections : [40=40+0]
R(obs)~4.3 wR2(obs)~6.4 R(all)~4.3 wR2(all)~6.4
R factors for satellites +-(1) : [74=73+1]
R(obs)~5.5 wR2(obs)~5.6 R(all)~5.6 wR2(all)~5.6
Profile R factors :[759/10+8]
GOF~5.5 Rp~4.8 wRp~6.8

[On the screen: Basic window]
In the Main menu bar, use "Structure → History" and return to the structure in P622.1' (00g) h00s (filename **dymn6ge6_01**)
In the Main menu bar, use "Transformations → Go to a subgroup" and test the second subgroup
Repeat the procedure for **all** remaining subgroups

Notes

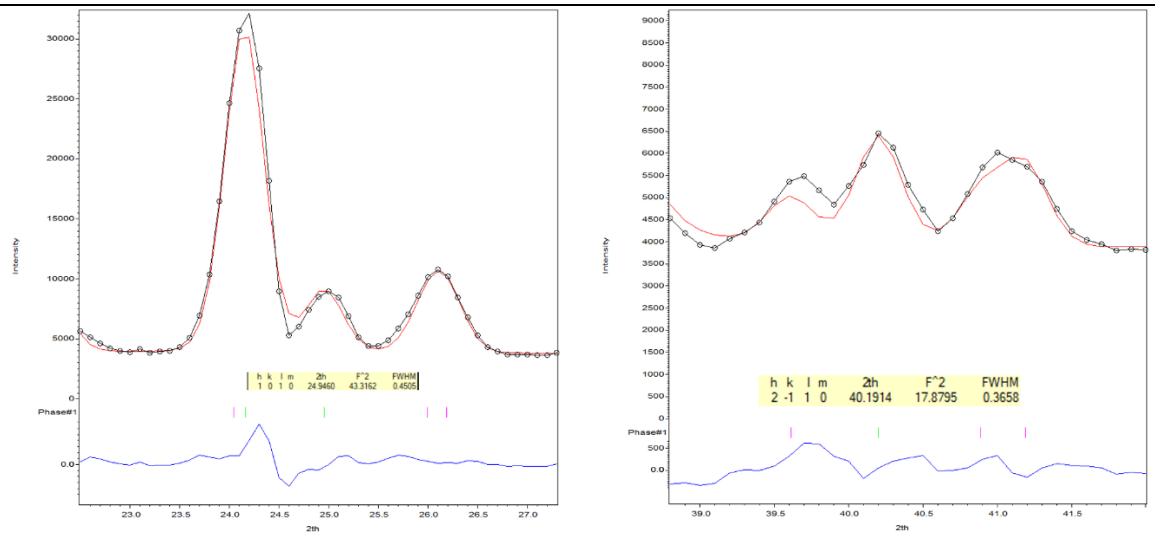
P622(00g) h00 (*subgroup_1)*
Rp=4.8%, R(obs)=4.8%,4.3%,5.5% for all, nuclear and magnetic reflections, respectively.

***P6'22'(00g)-t00** (subgroup_2)*
Rp=4.7%, R(obs)=4.5%,4.0%,5.5% for all, nuclear and magnetic reflections, respectively.

***P62'2'(00g)h00** (subgroup_3)*
Rp=4.2%, R(obs)=3.0%,2.3%,4.1% for all, nuclear and magnetic reflections, respectively.

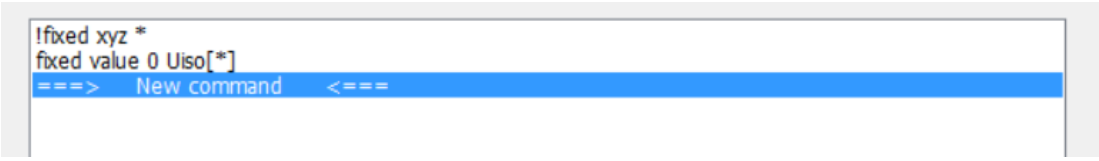
***P6'2'2(00g)-t00** (subgroup_4)*
Rp=4.8%, R(obs)=4.8%,4.4%,5.6% for all, nuclear and magnetic reflections, respectively.

One of the symmetries clearly fits the data better: P62'2'(00g) h00. We can observe that the strong misfit of some of the main reflections has disappeared.



The final common Uiso is still negative, but its absolute value is minimal.

In the Main menu bar, use Structure → History to return to the structure in dymn6ge6_01_subgroup_3 (the one corresponding to P62'2'(00g) h00)
Right-click on the quick button "Run refinement"
In the page "Restraints /Constraints", use the button "Fixed commands"
Focus on the "New command" line
Select "Set individual parameters"; For "Set to", use zero
For "Atoms/parameters" textbox, write "Uiso[*]"
Press Rewrite

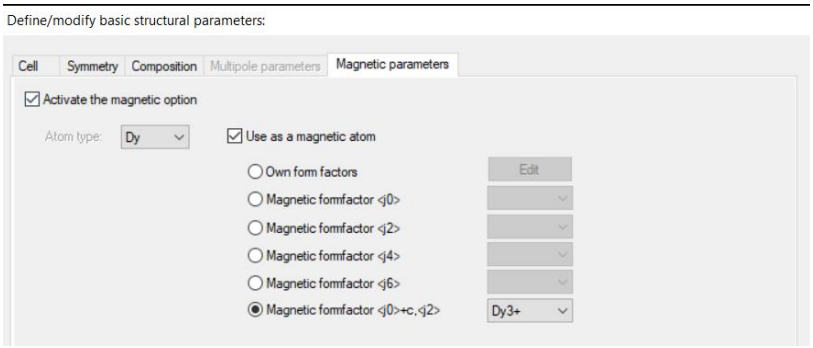


OK; OK; Press Button "Yes+start"

Notes

R factors : [114=113+1/8]
R(obs)~3.5 wR2(obs)~3.9 R(all)~3.5 wR2(all)~3.9
R factors for main reflections : [40=40+0]
R(obs)~3.0 wR2(obs)~3.1 R(all)~3.0 wR2(all)~3.1
R factors for satellites +-(1) : [74=73+1]
R(obs)~4.3 wR2(obs)~4.4 R(all)~4.3 wR2(all)~4.4
Profile R factors :[759/10+8]
GOF~4.7 Rp~4.2 wRp~5.9
There is no warning about negative ADP as Uiso of all atoms is set to zero

Open "Edit basic parameters (cell, symmetry, …)"
On the page "Magnetic parameters", Change the magnetic form factor for Dy to <j0>+c<j2> and Dy3+

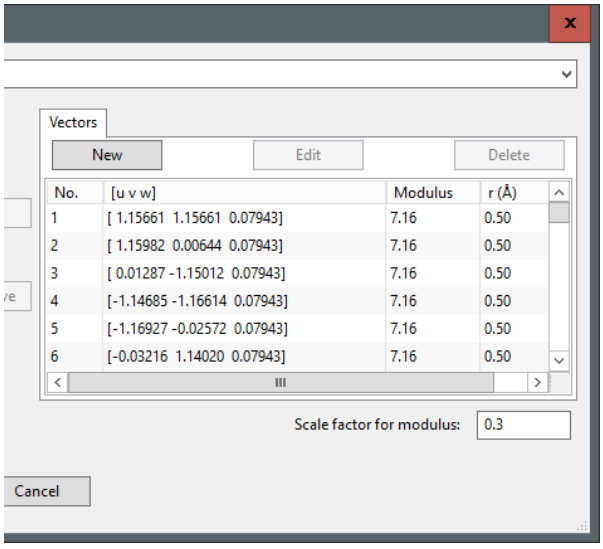


OK; YES to save changes
Press “Run Refinement”

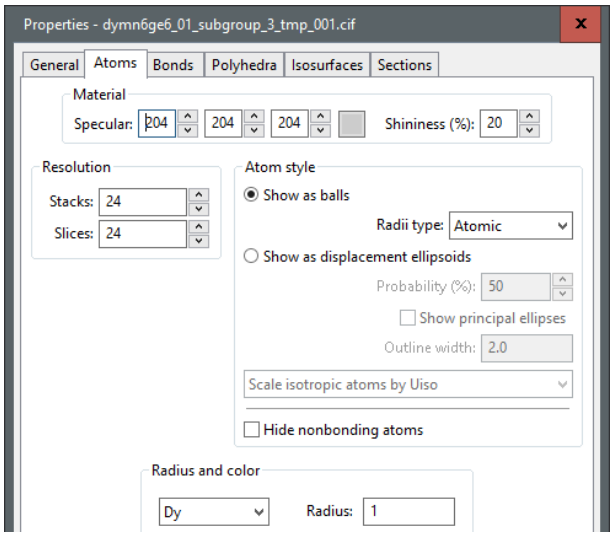
Notes
R factors : [114=114+0/8]
R(obs)~3.0 wR2(obs)~3.5 R(all)~3.0 wR2(all)~3.5
R factors for main reflections : [40=40+0]
R(obs)~2.6 wR2(obs)~2.8 R(all)~2.6 wR2(all)~2.8
R factors for satellites +-(1) : [74=74+0]
R(obs)~3.7 wR2(obs)~4.0 R(all)~3.7 wR2(all)~4.0
Profile R factors :[759/10+8]
GOF~4.7 Rp~4.2 wRp~5.8

9. *Visualization of the refined model with VESTA*

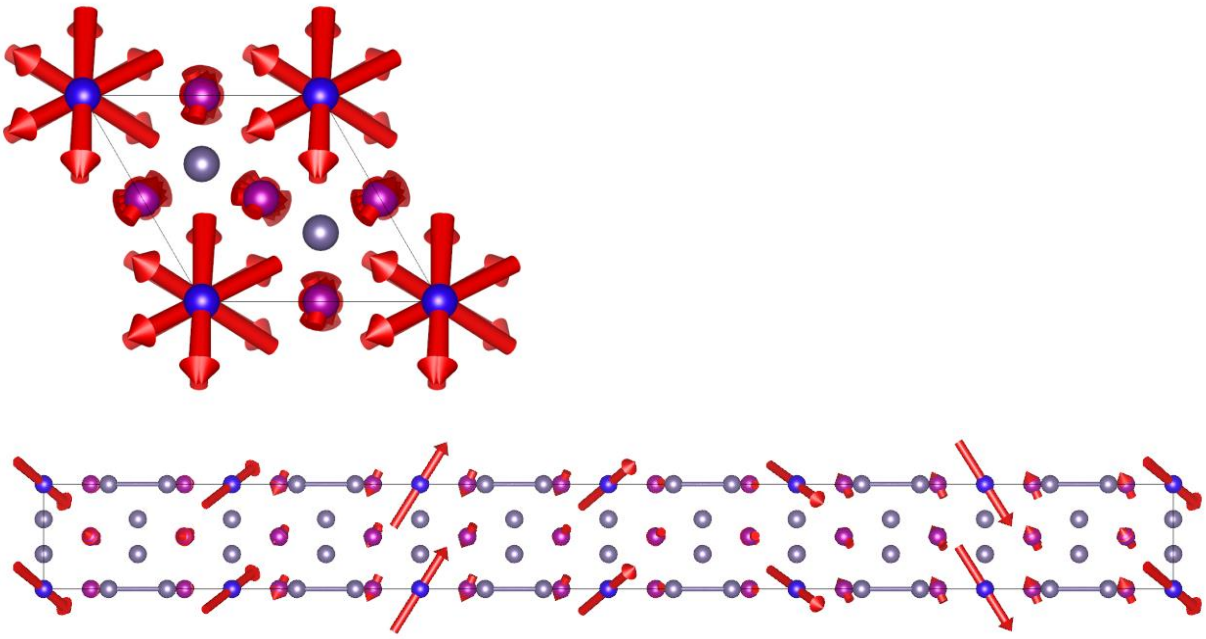
In the Command tree, expand “Draw structure” and open “Vesta”
Select “Draw approximant structure”; x from 0 to 1; y from 0 to 1; z from 0 to 6 (c* component of the propagation vector is close to 1/6)
Press “Draw- Jana waits for end” or “Draw - Jana continues”
[On the screen: Vesta]
Select “Edit→Vectors” and modify “Scale factor for modulus” to 0.3; OK



Press the button “Properties…”; Go to the page “Atoms”
Modify “Radius” for each atom to be equal to 1; OK



[On Vesta basic windows]



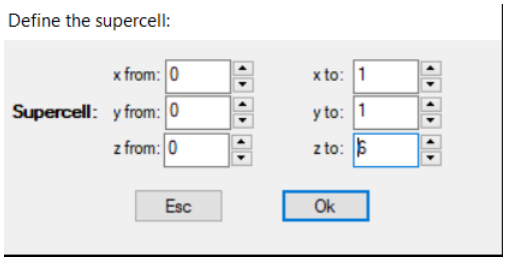
10. *Visualization of the refined model with JanaDraw*

[On the screen: Basic window]

Change focus to “JanaDraw”

In the Main menu bar, use “Build → Fill → Supercell”

Select supercell x from 0 to 1, y from 0 to 1 and z from 0 to 6; OK

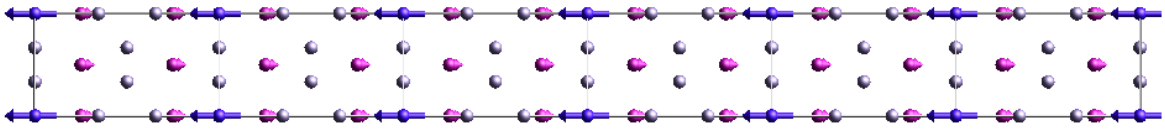


In the right pane, select view along “b”; for “Modulation”, select “Average”

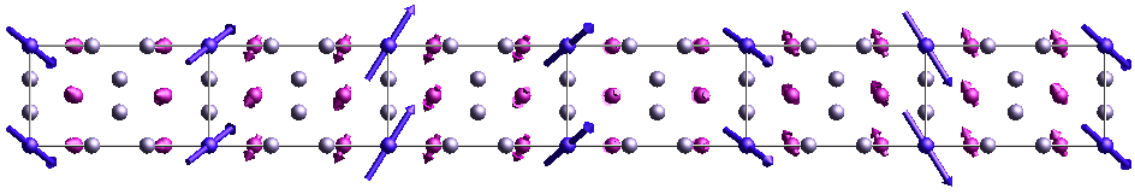
Adjust the figure by the button and remove bonds between atoms

Start “Options” and select Bohr to angstrom ratio 0.5; OK

Average structure:



In the right pane, “Modulation”, select “t=0”
Modulated structure for t=0:



11. Transformation to the standard setting as used in MAGNDATA

Notes
The structure has been already included in the database “MAGNDATA” in Bilbao Crystallographic Server, and you can get the originally published results as follows

Press to close JanaDraw
[On the screen: Basic window]
In the Main menu bar, use “Tools → Connect to → Bilbao Crystallographic Server”
Select “Magnetic Symmetry and Applications → MAGNDATA”; Enter the label of the structure “1.1.10”; Submit
Scroll down and click the link “View symmetry operations”
Compare the displayed symmetry operations with the ones in Jana2020 (see “Edit basic parameters”, page “Symmetry”

Notes

Reference: Rodriguez-Carvajal, J et al., *EPJ Web of Conferences* (2012) **22** 00010
DOI: 10.1051/epjconf/20122200010
Atomic positions from: ICSD #57229

Parent space group (paramagnetic phase): P6/mmm (#191)
Propagation vector: k1 (0.000000, 0.000000, 0.1651)

Lattice parameters of the basic unit cell:
5.2081 5.2081 8.1522 90 90 120
Transformation from parent structure: (**a**,**b**,**c**;0,0,0)
[View matrix form]

Magnetic Superspace Group: P62'2'(00γ)h00
[View symmetry operations]

Magnetic Point Group: 62'2' (24.4.90)
[View symmetry operations]
Symmetry-adapted form of material tensors via MTENSOR

Average positions, magnetic moments and magnetic modulations of symmetry independent atoms:
From now on, magnetic atoms are in boldface and colored in red. Magnetic moments are expressed in units of μB

[Show only magnetic atoms]
[Show all the atoms]

Average atomic positions and magnetic moments of symmetry independent atoms

Label	Atom type	x	y	z	Multiplicity	Symmetry constraints on M	M_{0x}	M_{0y}	M_{0z}	|M|
Dy1	Dy	0	0	0	1	0,0,m_z	0.0	0.0	3.932	3.93
Mn1	Mn	0.5	0	0.2510	6	0,0,m_z	0.0	0.0	-1.149	1.15

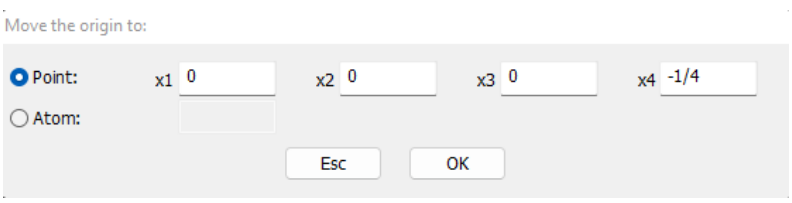
Magnetic moment modulation parameters of symmetry independent atoms

Wave vector 1

Atom	Magnetic moment Fourier Cos coeffs						Magnetic moment Fourier Sin coeffs					
	Symmetry constraints			Numerical values			Symmetry constraints			Numerical values		
	x	y	z	x	y	z	x	y	z	x	y	z
Dy1	√3$M_x$sin1	0	0	6.195546	0.0	0.0	$M_x$sin1	2$M_x$sin1	0	3.577	7.154	0.0
Mn1	$M_x$cos1	$M_y$cos1	0	-1.877	-0.206	0.0	$M_x$sin1	$M_y$sin1	0	-0.846	-2.049	0.0

N	(x,y,z)	Seitz notation
1	x1,x2,x3,x4,+1	{ 1 | 0 }
2	-x2,x1-x2,x3,x4+1/3,+1	{ 3^+_{001} | 0 0 0 1/3 }
3	-x1+x2,-x1,x3,x4+2/3,+1	{ 3^-_{001} | 0 0 0 2/3 }
4	-x1,-x2,x3,x4+1/2,+1	{ 2_{001} | 0 0 0 1/2 }
5	x2,-x1+x2,x3,x4+5/6,+1	{ 6^-_{001} | 0 0 0 5/6 }
6	x1-x2,x1,x3,x4+1/6,+1	{ 6^+_{001} | 0 0 0 1/6 }
7	x2,x1,-x3,-x4+5/6,-1	{ $2'_{110}$ | 0 0 0 5/6 }
8	x1-x2,-x2,-x3,-x4+1/2,-1	{ $2'_{100}$ | 0 0 0 1/2 }
9	-x1,-x1+x2,-x3,-x4+1/6,-1	{ $2'_{010}$ | 0 0 0 1/6 }
10	-x2,-x1,-x3,-x4+1/3,-1	{ $2'_{1\text{-}10}$ | 0 0 0 1/3 }
11	-x1+x2,x2,-x3,-x4,-1	{ $2'_{120}$ | 0 }
12	x1,x1-x2,-x3,-x4+2/3,-1	{ $2'_{210}$ | 0 0 0 2/3 }

Open “Edit basic parameters (cell, symmetry, …)”; go to the page “Symmetry”
Compare symmetry operations
Our result is the same as the one used in MAGNDATA (SSG P62’2’(00g)h00). However, origin is shifted by 1/4 in x4.
Press ESC
“Transformations → Origin shift”
Use shift to the point 0 0 0 -1/4



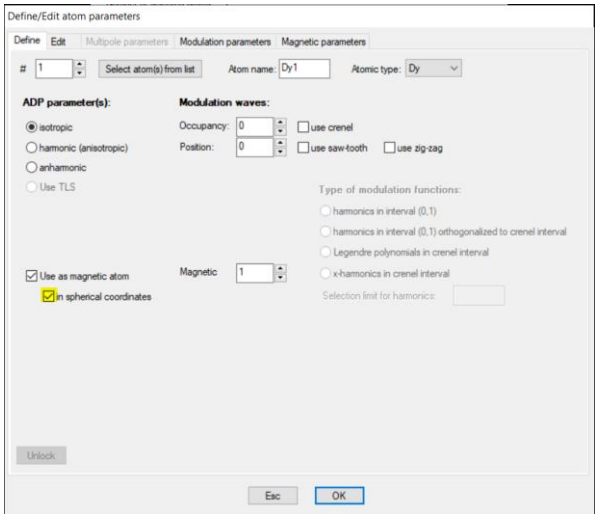
Press OK and rewrite the old structure

Press “R?” to check that R values are still the same

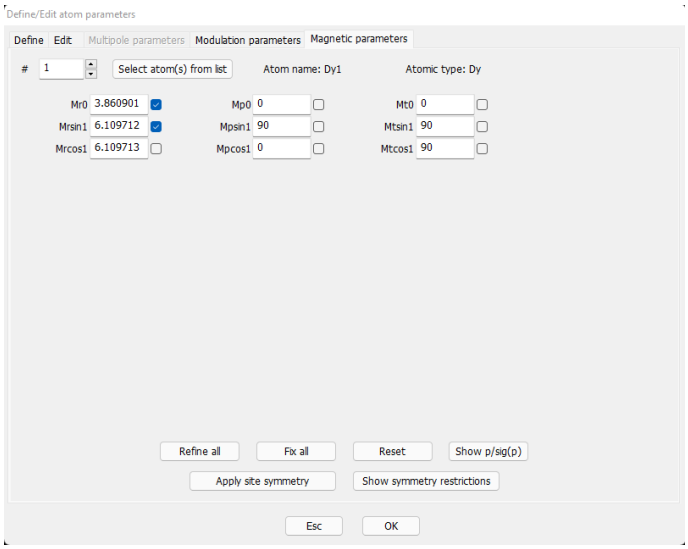
Use of the option of spherical coordinates

Notes
This will allow constraining the spin of Mn to have a circular modulation. However, symmetry restrictions of spherical coordinates are not linear. Therefore, they cannot be set automatically.

[On the screen: Basic window]
In the Main menu bar, use “Structure → Make backup”; Use e.g. “dymn6ge6_01_subgroup_3_final”
[On the screen: Basic window]
Open “Edit atoms”
[On the screen: Select atoms to be used]
Double click on the atom Dy1;
Activate the option “in spherical coordinates”



Go to the page “Magnetic parameters”

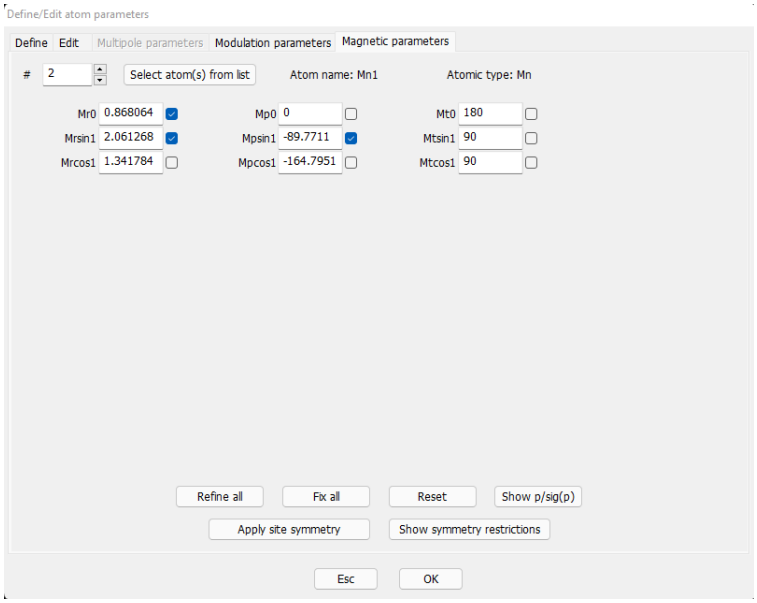


Activate the refinement keys as indicated in the above figure; OK;

Notes
For k=0, the spin has only Mr0-amplitude as a free parameter. Both angles φ=Mp0 and ϑ=Mt0 are fixed by symmetry.

For the modulation wave, the only free parameter is the amplitude of the modulation Mrsin1, as due to the site symmetry of Dy1 Mrcos1=Mrsin1, and all angular components are fixed. It means that the symmetry fully induces circular modulation.

Double click on the atom Mn1
Activate option “in spherical coordinates”;
Go to the page “Magnetic parameters”



Activate the refinement keys as indicated in the above figure

Notes

For Mn1, the spin has only Mr0-amplitude as a free parameter. Both angles φ=Mp0 and ϑ=Mt0 are fixed by symmetry.
For the modulation wave, Mrcos1≠Mrsin1 and only the inclination angle is fixed by the site symmetry. In order to force a circular modulation, the constraints must be used: Mrcos1=Mrsin1, Mpcos1=Mpsin1-90.
These equations are satisfied only roughly in the previous refined model.

OK; OK; YES to rewrite files;
Right-click on the quick button “Run refinement”
In the page “Restraints/Constraints”, click on the button “Equations”;
Define the equations mentioned above

Notes

Mp0[Dy1]=0
Mrcos1[Dy1]=Mrsin1[Dy1]
Mpsin1[Dy1]=90
Mpcos1[Dy1]=0
Mtsin1[Dy1]=90
Mtcos1[Dy1]=90
Mp0[Mn1]=0
Mt0[Mn1]=180
Mrcos1[Mn1]=Mrsin1[Mn1]
Mpcos1[Mn1]= Mpsin1[Mn1]-90
Mtsin1[Mn1]=90
Mtcos1[Mn1]=90
You can do either one by one or you can use the pre-prepared file “Equations-circular.txt”.
For the latter method:

Press the button “Edit” and use the copy-paste method from the file “Equations-circular.txt

OK; OK; Yes+start

Notes

R factors : [114=114+0/8]
R(obs)~3.0 wR2(obs)~3.5 R(all)~3.0 wR2(all)~3.5
R factors for main reflections : [40=40+0]
R(obs)~2.6 wR2(obs)~2.8 R(all)~2.6 wR2(all)~2.8
R factors for satellites +-(1) : [74=74+0]
R(obs)~3.7 wR2(obs)~4.0 R(all)~3.7 wR2(all)~4.0
Profile R factors :[759/10+8]
GOF~4.7 Rp~4.2 wRp~5.8

Notes

After transforming from spherical to crystallographic coordinates

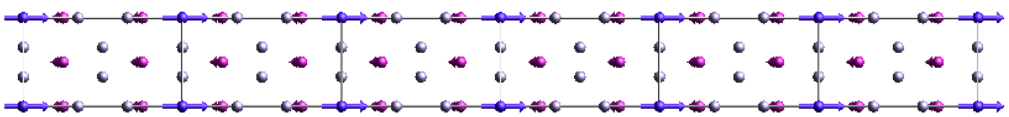
Profile R factors: [759/10+8],
GOF≈ 4.8 Rp ≈ 4.2 wRp≈ 5.9

		M_{0x}	M_{0y}	M_{0z}	|M|
Dy1	MAGNDATA	0.0	0.0	3.93	3.93
	Jana	0.0	0.0	3.96(11)	3.96(11)
Mn1	MAGNDATA	0.0	0.0	-1.15	1.15
	Jana	0.0	0.0	-1.00(8)	1.00(8)

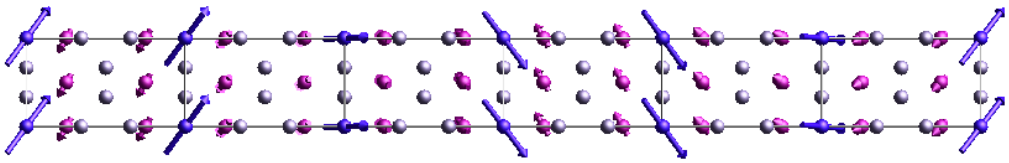
		cos			Sin		
		M_x	M_y	M_z	M_x	M_y	M_z
Dy1	MAGNDATA	6.20	0.0	0.0	3.58	7.15	0.0
	Jana	6.18	0.0	0.0	3.57(5)	7.13	0.0
Mn1	MAGNDATA	-1.88	-0.21	0.0	-0.85	-2.05	0.0
	Jana	-1.88(10)	-0.20(9)	0.0	-0.86(9)	-2.06(8)	0.0

12. Visualization of the refined model with JanaDraw

[On the screen: Basic window]
Press “JanaDraw”
In the Main menu bar, use Build→Fill→Supercell
Select supercell x from 0 to 1, y from 0 to 1 and z from 0 to 6;
In the right pane, select view along “b”;
Adjust the figure by the button ;
Start “Options” and select Bohr to angstrom ratio 0.5; OK
Release the button „Draw bonds“
Average structure:



Structure for t=0:



In the right pane, select view along “c”;
Adjust the figure by the button ;
In the right pane, select Movie
For “Number of steps”, type 200
OK
ESC