Example 12.10: $MnWO_4$

Last update 19.6.2024

Data	Topic	Level
Neutron single crystal	Commensurate AFM structure	Intermediate

Input data

Data

Single crystal data collected on DEMAND at HFIR, ORNL neutron source at 5 K

Input files

MnWO4_magneticAF4_5K.int (single crystal data from FullProf)
MnWO4_N_5K.cif (nuclear structure)

Additional information

Chemical formula: MnWO4
Antiferromagnetic commensurate: k=(1/2,0,0)

References

F. Ye, S. Chi, J. A. Fernandez-Baca, H. Cao, K.-C. Liang, Y. Wang, B. Lorenz, and C. W. Chu, (2012), Phys. Rev. B 86, 094429.

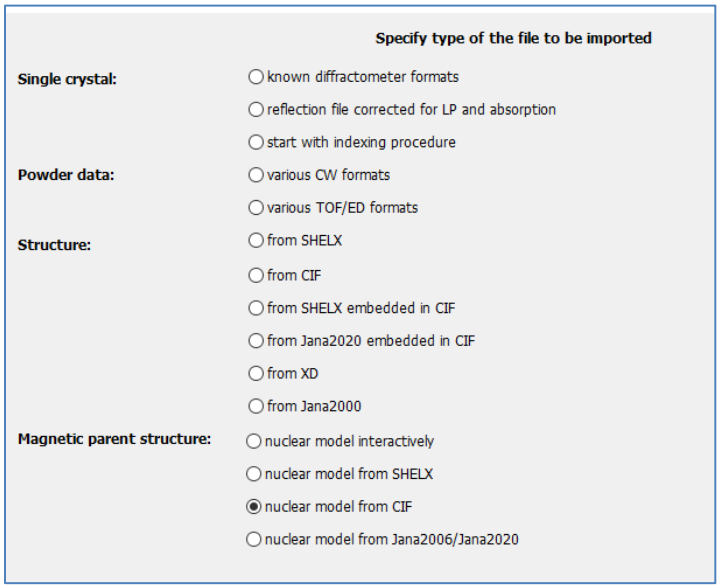
Highlights

In this example, a single crystal data files from FullProf are imported. Correction for $\lambda/2$ is performed, several type IV Shubnikov groups are tested.

Instructions

1. *Data import*

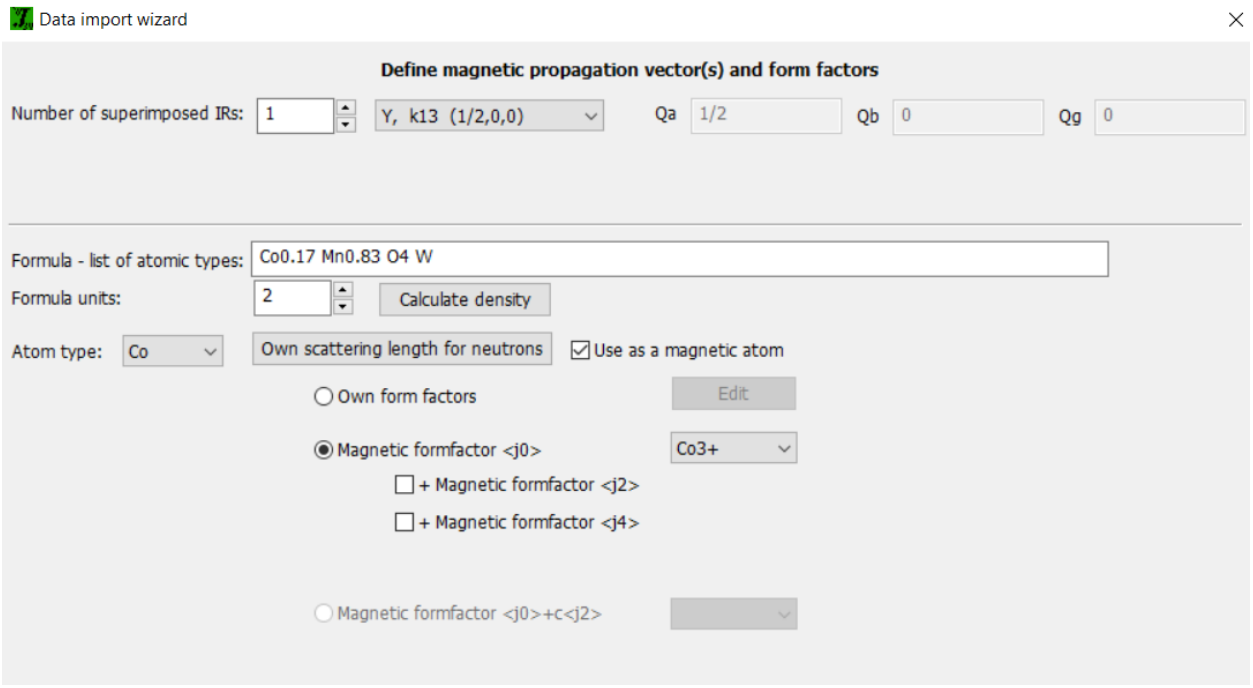
Start Jana2020
In the Main menu bar, use "Structure → New" and open a new structure MnWO4_AF4_5K in the directory of Example 12.10
[On the screen: Specify type of the file to be imported]
Select "Magnetic parent structure: nuclear model from CIF"; NEXT;



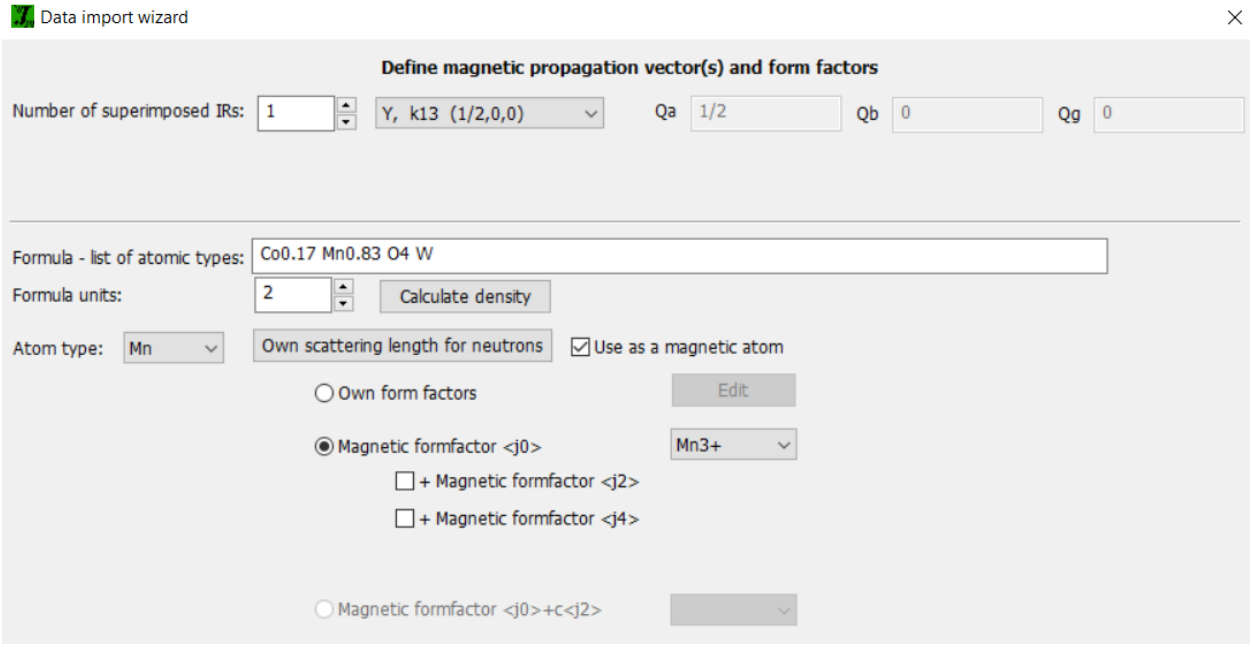
In Windows file explorer: select the input file MnWO4_N_5K.cif; Open

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 "Y, k13 (1/2,0,0)"
Select "Atom type" Co; check "Use as a magnetic atom" and for "Magnetic formfactor <j0>" select "Co3+";



Repeat for Mn and use Mn3+ for its magnetic form factor.

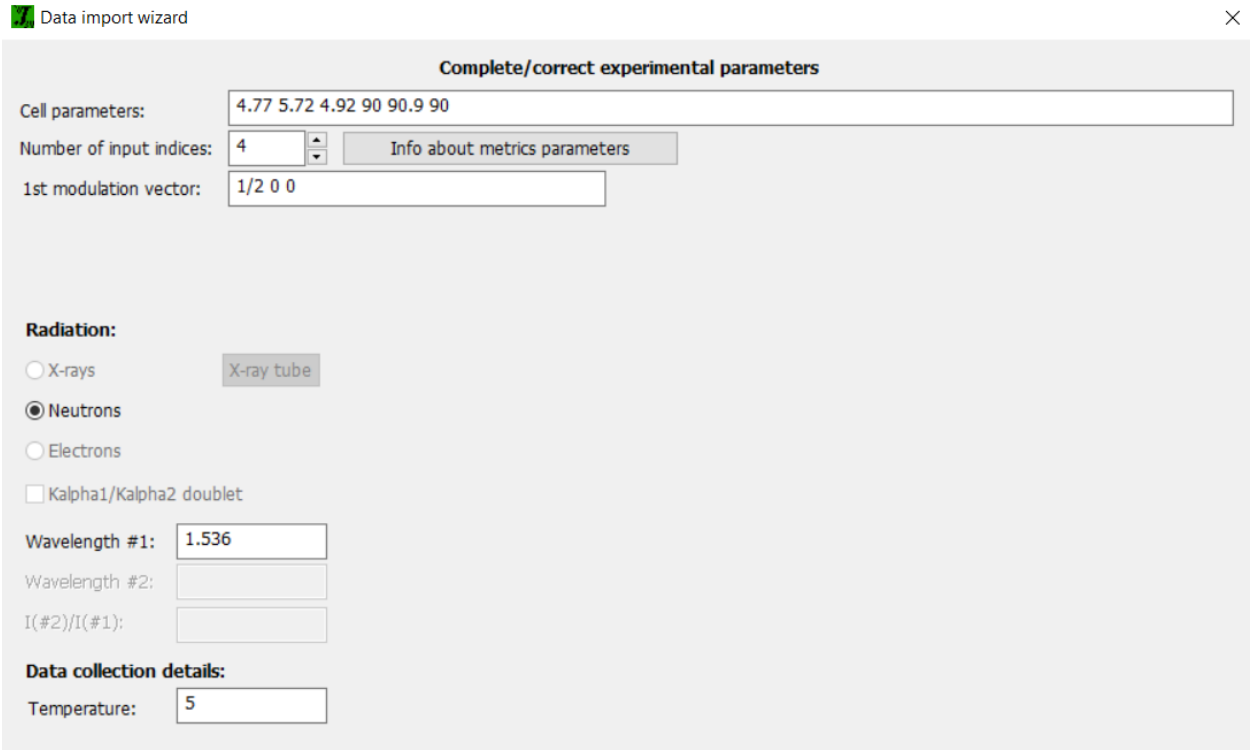


NEXT
[On the screen: Information]
The parent structure is now created.
NEXT

3. *Import of the reflection file*

[On the screen: Specify type of the file to be imported]
Select “Single crystal: Reflection file corrected for LP and absorption”; NEXT
Select the format “From FullProf file”; Check that the name of the input file is “MnWO4_magneticAF4_5K.int ”; NEXT
[On the screen: Complete/correct experimental parameters]

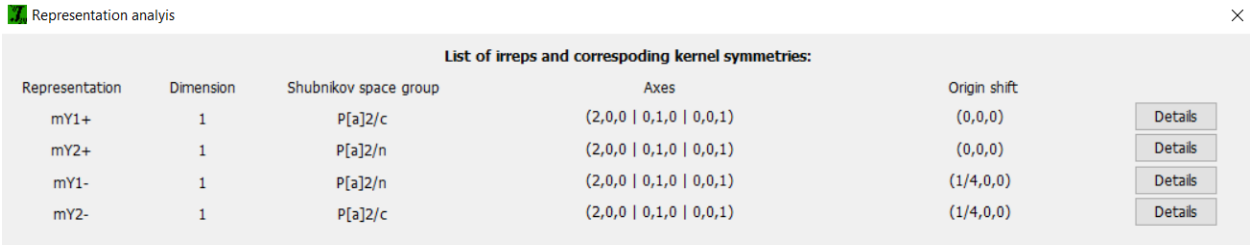
Check that wavelength is 1.536; Temperature is 5 K.



NEXT; NEXT
[On the screen: Data repository]
OK
[On the screen: Information]
FINISH
[On the screen: Data repository]
OK

4. Testing different irreps to get the best model

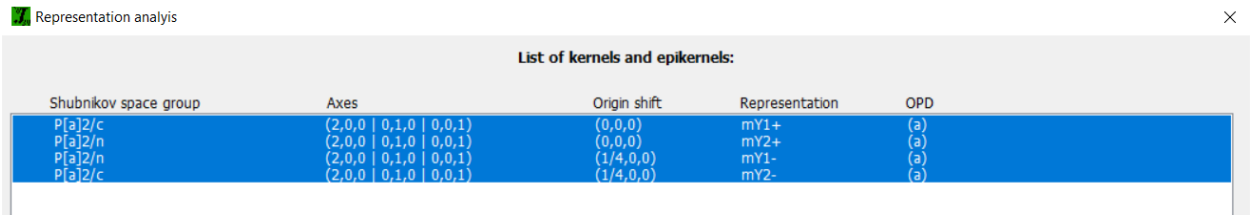
[On the screen: Information]
OK
[On the screen: List of irreps and corresponding kernel symmetries]



Notes

This window has an informative 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.

NEXT
[On screen: List of kernels and epikernels]

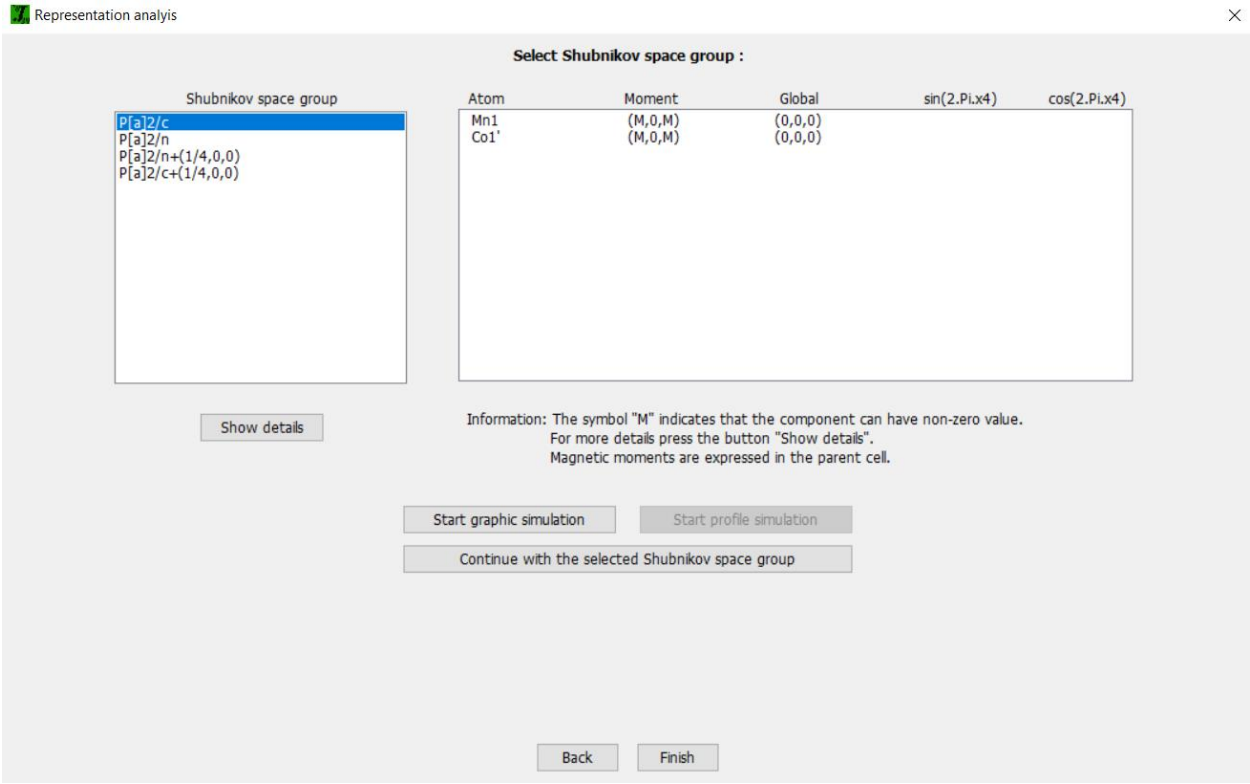


The four monoclinic Shubnikov space groups are selected by default (if not, just click over one of them to select the block); NEXT

Notes

This will pass all the magnetic space groups to further testing.

[On the screen: Select Shubnikov space group]



Notes

For each space group, the components allowed for the magnetic moment of the Co and Mn atoms are indicated in the column 'Moment'. In this case, the y-component is zero, whereas x- and z-components are free.

Select the first Shubnikov group P_a 2/*c* and press "Show details" for a detailed list of relationships between magnetic moments of individual atoms

[On the screen: Details for selected space group structure]

Close the window

Refinement in P_a 2/*c*

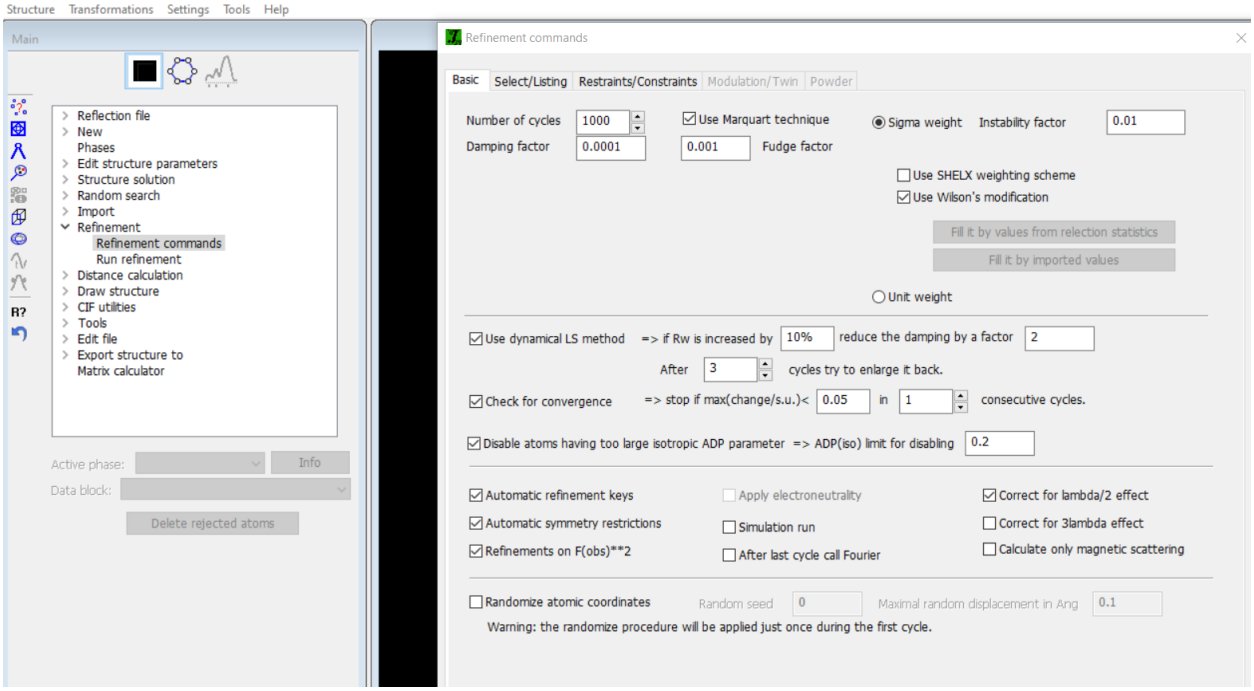
Press 'Continue with the selected Shubnikov space group'

[On the screen: Select structure name]

Use the default name i.e. MnWO4_AF4_5K_01; Save

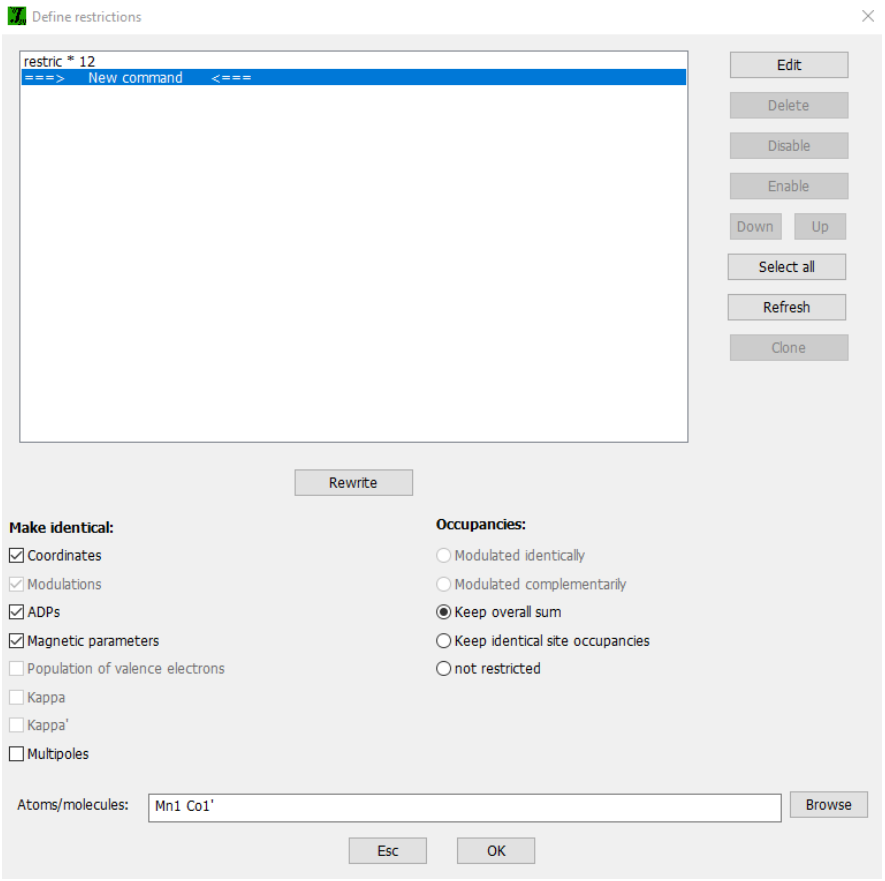
Notes
The test runs under the new job name in a new window to keep the parent structure unchanged. The Jana window with the parent structure remains open.

[On the screen: Basic window of Jana2020]
In the Command tree, expand “Refinement” and open “Refinement commands”
[On the screen: Refinement commands]
On the basic page, increase the number of cycles to 1000 and the damping factor to 0.0001.
Activate “correct for lambda/2 effect”;

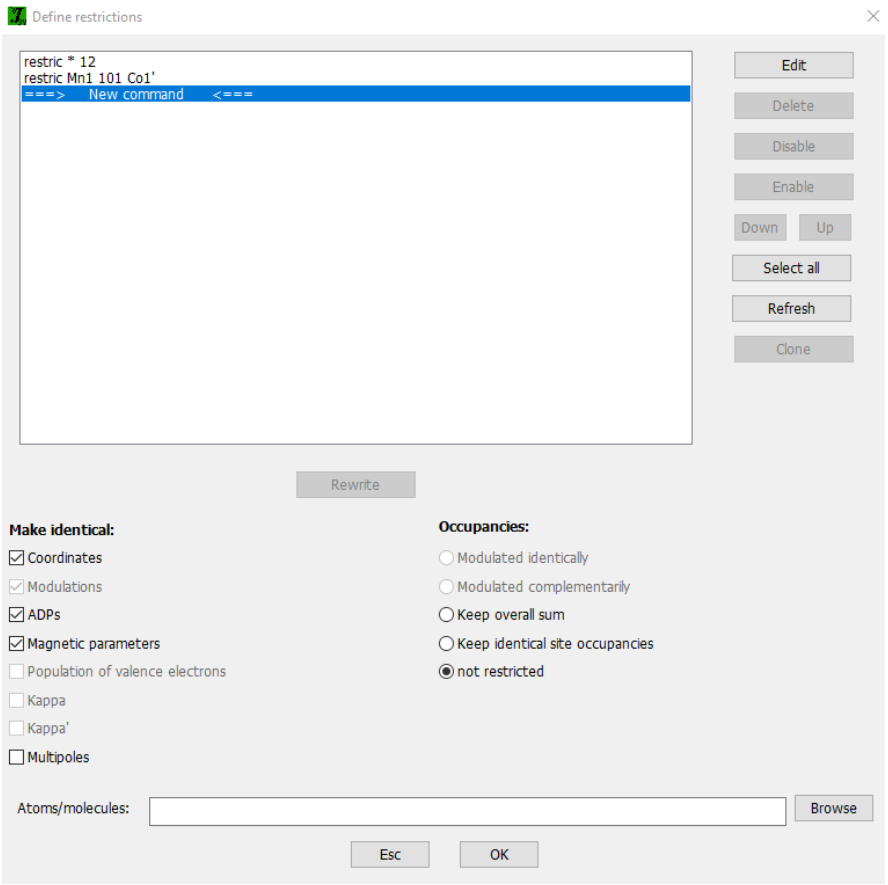


Notes
The atoms Mn1 and Co1’ occupy the same position, and therefore, we must restrict their parameters

On the page “Restrains/Constraints”, select “Restrictions”, focus on the “New command” line.
Select make identical coordinates, ADP parameters, and magnetic parameters
For occupancies, select “Keep overall sum”
In the box “Atoms/molecules” write “Mn1 Co1’”



Press “Rewrite”

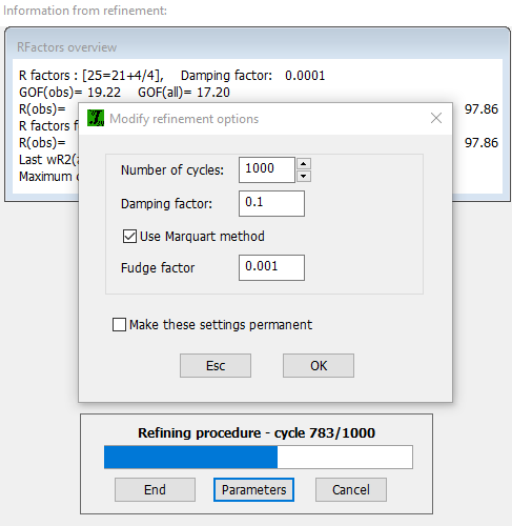


OK

On the page “Restrains/Constraints”, select “Fixed commands” and ensure that all atomic positions are fixed in their current values (“fixed xyz *”). OK; OK; YES+START

Notes
After several cycles, when the refinement converges, you can modify the damping parameters:

On the “R-factors overview”, press “Parameters”
[On the screen: Modify refinement options]
Change the “Damping factor” to 0.1



OK

Notes
R factors : [25=21+4/5] *GOF(obs)~17.0 GOF(all)~15.2* *R(obs)~55.7 wR2(obs)~83.7 R(all)~60.8 wR2(all)~84.6* *R factors for magnetic reflections : [25=21+4]* *R(obs)~55.7 wR2(obs)~83.7 R(all)~60.8 wR2(all)~84.6* *Now we shall test the remaining Shubnikov apce groups on the list.*

Close the window of the structure MnWO4_AF4_5K_01. YES to the question “Do you want to quit Jana2020?”
[On the screen: (Parent structure) Select Shubnikov space group:]

Refinement in P_a 2/*n*

Select the second Shubnikov group P_a 2/*n*. Press “Continue with the selected Shubnikov space group”.
[On the screen: Select structure name]
Use the default name i.e. MnWO4_AF4_5K_02; Save
[On the screen: Basic window of Jana2020]
Repeat the same procedure as for the previous space group.

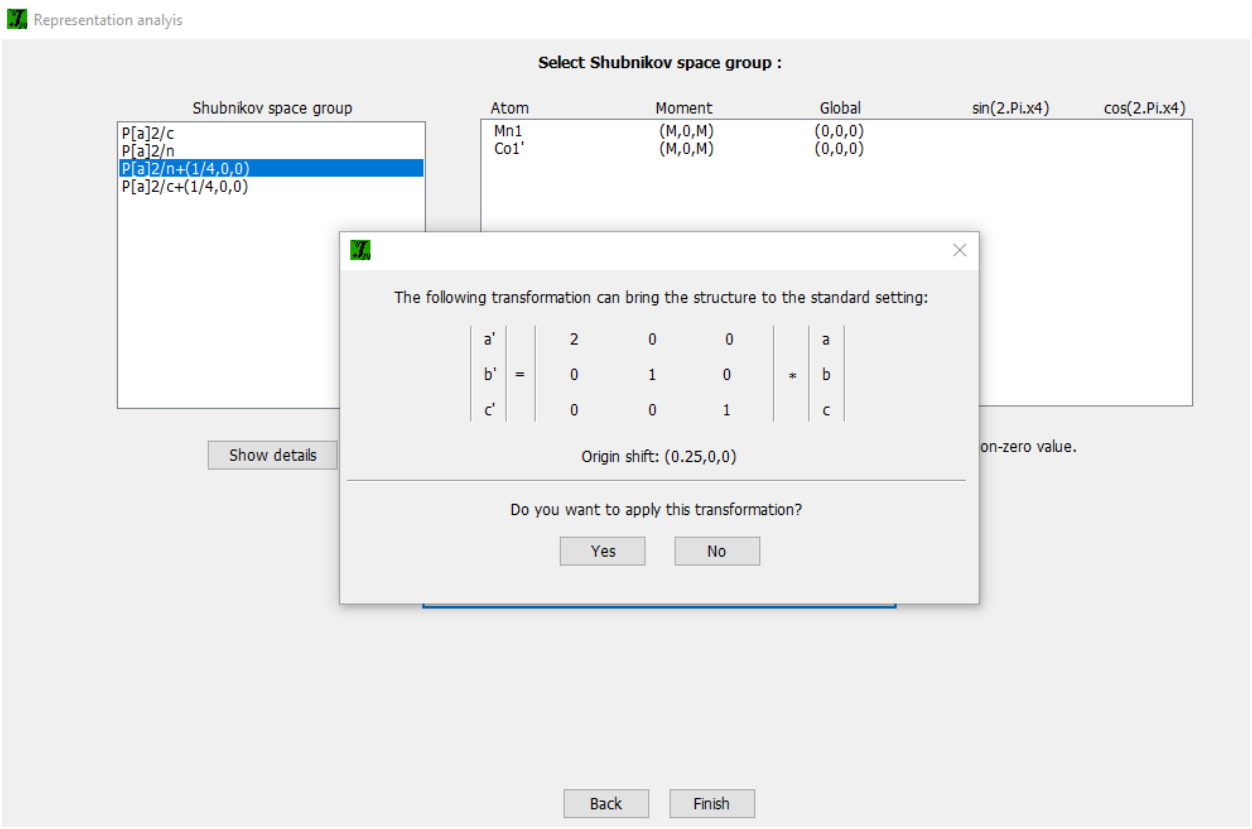
Notes
R factors : [25=21+4/4] *GOF(obs)~16.9 GOF(all)~15.8* *R(obs)~62.3 wR2(obs)~85.5 R(all)~69.1 wR2(all)~89.2* *R factors for magnetic reflections : [25=21+4]* *R(obs)~62.3 wR2(obs)~85.5 R(all)~69.1 wR2(all)~89.2*

Close the window of the structure MnWO4_AF4_5K_02. YES to the question "Do you want to quit Jana2020?"
[On the screen: (Parent structure) Select Shubnikov space group:]

Refinement in P_a 2/*n* +(1/4,0,0)

Select the third Shubnikov group P_a 2/*n* +(1/4,0,0). Press "Continue with the selected Shubnikov space group".
[On the screen: Select structure name]
Use the default name i.e. MnWO4_AF4_5K_03; Save

Notes
For the space groups with origin shift, the program offers a transformation to the standard setting. While the matrix doubling the a-cell parameter is always applied (BNS notation), the origin shift is optional. Skipping this point will keep the atoms in all models at the same positions.



NO to the question "Do you want to apply this transformation?"

[On the screen: Basic window of Jana2020]

Repeat the same procedure as for the previous space groups.

Notes
R factors : [25=21+4/5]
GOF(obs)~1.7 GOF(all)~1.6
R(obs)~3.7 wR2(obs)~9.1 R(all)~4.6 wR2(all)~9.4
R factors for magnetic reflections : [25=21+4]
R(obs)~3.7 wR2(obs)~9.1 R(all)~4.6 wR2(all)~9.4

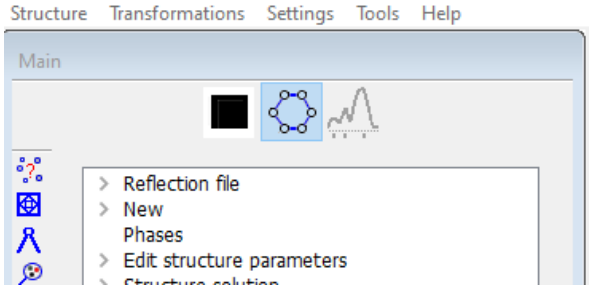
Close the window of the structure MnWO4_AF4_5K_03. YES to the question "Do you want to quit Jana2020?"
[On the screen: (Parent structure) Select Shubnikov space group:]

Refinement in P_a 2/*c* +(1/4,0,0)

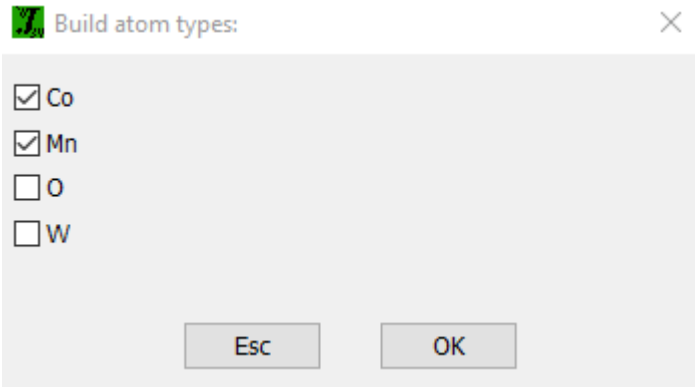
Select the fourth Shubnikov group P_a 2/*c* +(1/4,0,0). Press 'Continue with the selected Shubnikov space group'
[On the screen: Select structure name]
Use the default name i.e. MnWO4_AF4_5K_04; Save
NO to the question "Do you want to apply this transformation?"
[On the screen: Basic window of Jana2020]
Repeat the same procedure as for the previous space groups.

Notes
R factors : [25=21+4/4]
GOF(obs)~14.7 GOF(all)~13.2
R(obs)~49.5 wR2(obs)~75.2 R(all)~53.4 wR2(all)~75.7
R factors for magnetic reflections : [25=21+4]
R(obs)~49.5 wR2(obs)~75.2 R(all)~53.4 wR2(all)~75.7
Clearly the best group is P_a 2/n +(1/4,0,0).

On the main menu, Go to "Structure"→ History and choose MnWO4_AF4_5K_03; OK
Change the focus to JanaDraw in the icon



[On the screen: JanaDraw window]
On the lower menu panel choose  to fill the unit cell. Then on the upper menu select "Build" → "Filter" → "Filter atomic types"
[On the screen: Build atomic types]
Deselect O and W



OK

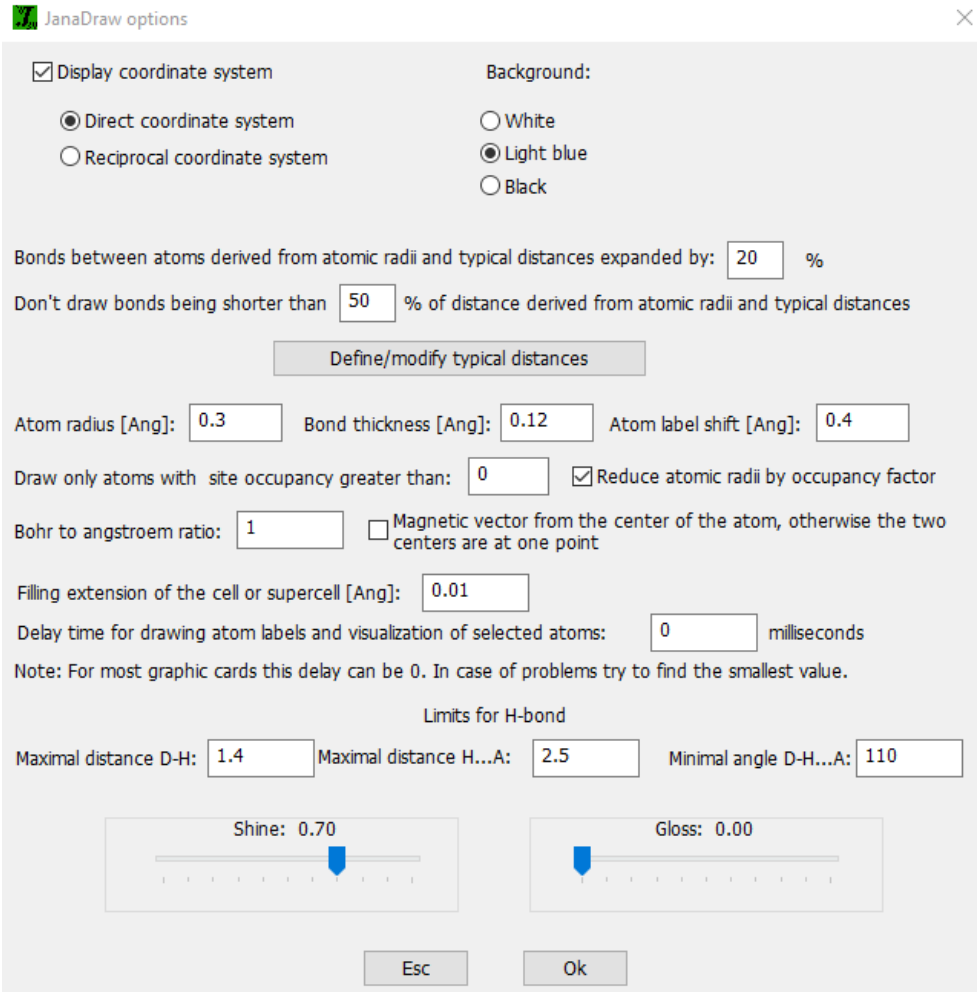
On the menu “Build” → “Fill” → “Supercell”

[On the screen: Define the supercell]

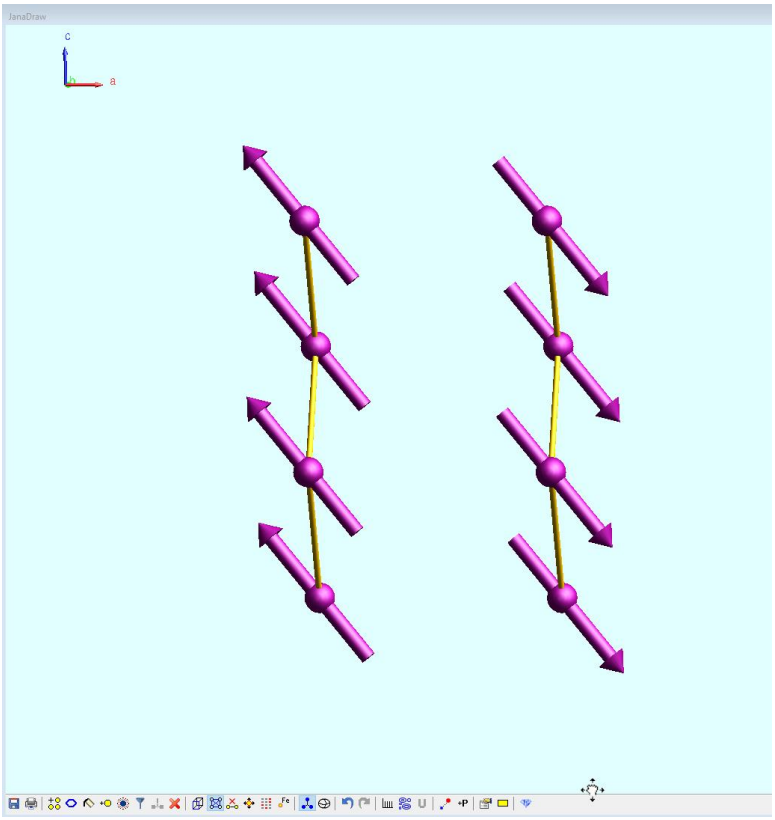
Write “z to:” 2; OK

On the lower menu panel deselect  to hide the unit cell lines the unit cell.

Go to  ; Change “Bonds between atoms derived from atomic radii and typical distances expanded by:” to 20%



OK; choose view along a and slightly rotate the structure, by dragging it with the mouse or by rotate the y axis on the right menu;



Notes
This is the best model refined in P_a 2/n +(1/4,0,0) for MnWO4.