

Tutorial: DyFeWO₆

Nuclear and Magnetic Structures refinement using symmetry modes.

DyFeWO₆

Powder data collected at ILL on the high-resolution diffractometer D2B with $\lambda = 1.59446$ Å.

The space group is S.G. = $Pna2_1$, the cell parameters are $a \approx 10.9714$ Å, $b \approx 5.1831$ Å and $c \approx 7.3365$ Å.

The T_N is around 18K.

The crystal structure of this compound was unknown; however, this could be derived from the CaTa₂O₆ using “subgroupgraph” and “transtru” programs from BCS. However, this is not the aim of this tutorial. In the input file you can find the data collected on the paramagnetic phase, just in case you want to try to solve the nuclear structure.

The initial structural parameters could be obtained from the input CIF file.

This compound contains a single Dy and Fe atom, both ions located at the 4a Wyckoff position of $Pna2_1$.

A detailed explanation of symmetry and magnetic structures concerned with this example can be consulted on PHYSICAL REVIEW B95, 224416 (2017).

Input files:

DyFeWO6-30K.dat

DyFeWO6-3p5K.dat

The format of the data corresponds to $Ins = 10$ in FullProf.

$\mu_R = 1.35$

$U, V, W = 0.051646, -0.158272, 0.157798$

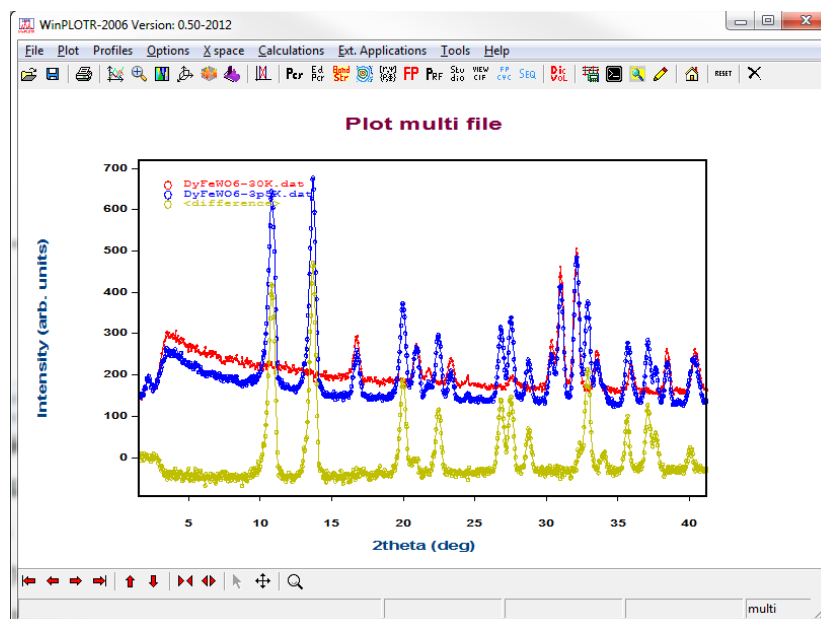
$S_L = 0.07964$ $D_L = 0.00000$

DyFeWO6-30K.cif

The standard magnetic structures determination using neutron powder diffraction (NPD) data consists on the following steps:

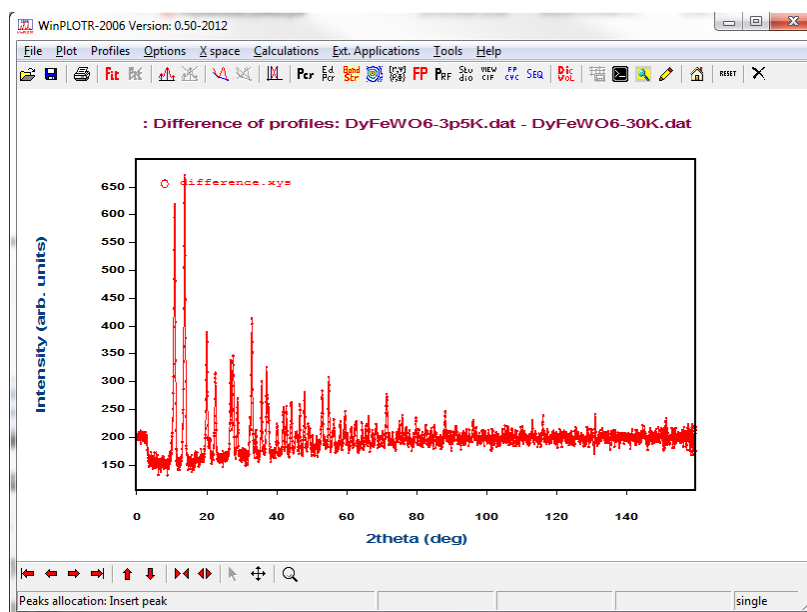
- 1) Plot the NPD patterns above and below the order temperature.
- 2) Refine the crystal structure using the collected data; and get all the relevant structural and profile parameters.
- 3) Normally additional magnetic peaks appear in the low temperature diffraction pattern (below the order temperature). Index the new reflection to determine the propagation vector. K-SEARCH program included in the FullProf suite can be used.

- 4) Determine the possible irreducible representations of the propagation vector group. The program Baslreps could be used to get the basis vectors of the irreducible representations (*irreps*) of the propagation vector group (G_k). The Shubnikov group and the appropriate magnetic symmetry operators, or, alternatively, the basis vectors of the *irreps* could be used to refine the experimental data.
 - 5) Alternatively simulated annealing refinement can also be done (no information about the magnetic symmetry is needed)
 - 6) Refine against the data the different models and check the output files to discard incompatibilities or inconsistencies.
- 1) **Create a working directory; do not use space or special characters in the path.**
 - a. Copy in this folder all the data files.
 - 2) **Create an initial PCR file from the CIF file (see LaMnO₃ example for details).**
 - 3) **Modify the PCR file according to the current example.**
 - a. Change the JOB, instrument, wavelength, background, scale, UVW, etc...
 - 4) **Determine the magnetic propagation vector.**
 - a. Here we can use the paramagnetic PCR file to compare the calculated pattern with that of 3.5K experimental pattern in order to detect the magnetic reflections or, alternatively, as we have both patterns (in the ordered and in the paramagnetic phase) we can do the difference to isolate the magnetic contribution.



- b. The difference pattern can be saved clicking on "Save data as > xy/xys data file (*xys)". We have to add an offset (the B parameter on the dialog box) in order to get positives

- values of the intensity in the full range of 2theta (you should put B = -200 because it corresponds to the subtraction of a linear background). Before doing that, click on Profile > Show and unclick on the 3.5 and 30K pattern, to save only the difference.
- c. Click on reset, and open the difference pattern.



- d. The shift and changes in intensity of some relatively high 2theta reflections suggest two effects: slight change of cell parameters or the crystal structure presents a slight distortion, probably related with the occurrence of the long-range magnetic order (magneto-structural coupling). In order to determine the propagation vector we are going to focus on the four strongest low angle reflections on the different pattern.
- e. Zoom in the region of interest, and click on Calculations > Peak detection > Enable.
- f. Click on Calculations > Peak detection > Insert Peak Insert a new peak into each reflection. You can zoom in/out with the left/right mouse button.
- g. Click on Calculations > Peak detection > Save Peaks > K-search program and run the program. The program suggests a short list of candidates:

```

C:\windows\system32\cmd.exe
=> Special k-vector solutions found?
=> List of the best 10 solutions for 4 satellites

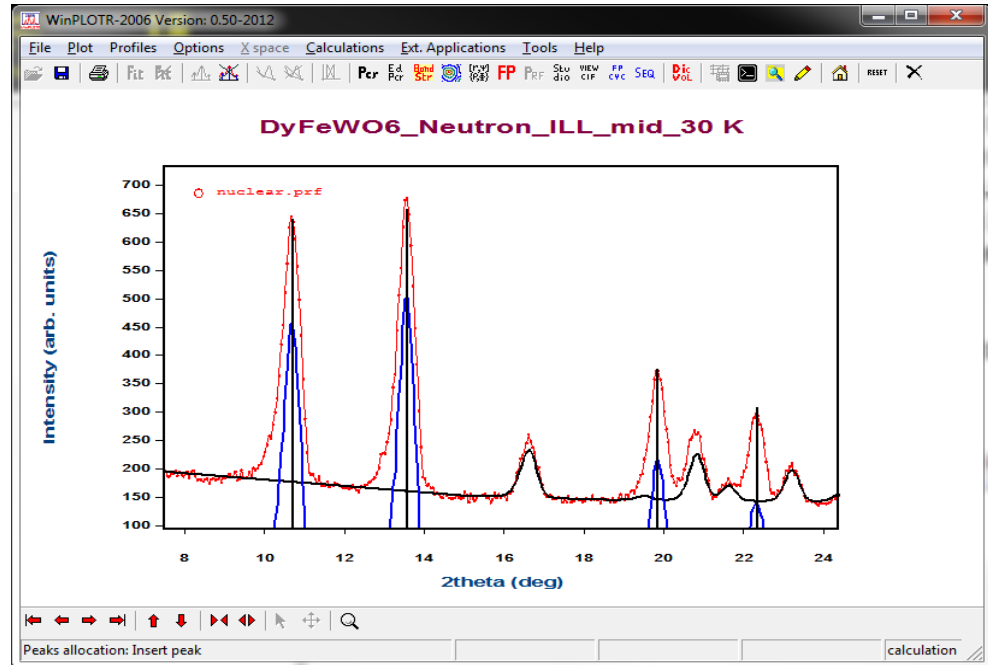
  Kx      Ky      Kz      R-factor
0.000000  0.000000  0.125000  1.019738
0.000000  0.500000  0.500000  1.739029
0.250000  0.250000  0.250000  2.932171
0.250000  0.000000  0.250000  3.622235
0.333330  0.333330  0.333330  3.644988
0.000000  0.125000  0.125000  4.702662

=> A probable solution is the special kvector ks =< 0.0000 0.0000 0.1250>
=> The corresponding R-factor is: 1.0197

      Total CPU-Time
      CPU-seconds: 0.00
      CPU-minutes: 0.00
      CPU-hours  : 0.00

```

- h. The first two solutions have a quite similar R-factor, we have to test each of these propagation vectors adding a second phase in LeBail mode and check the fit.
- i. Although this method can give good results, it deserves to be noted that neither the cell parameter nor the zero has been taken into account in the positions of the selected peaks. So we recommend use a protocol similar to that shown on $\text{Ho}_2\text{BaNiO}_5$ example. Apply the structural model of the paramagnetic phase to fit the pattern collected at 3.5 K and refine only the scale factor, cell parameters and the zero-shift. Once the refinement is done you can select the magnetic reflections (now corrected from zero-shift) and search the possible propagation vectors.



- j. After running the k-search program using the same four reflections, the list of solution is shown here below:

```

C:\windows\system32\cmd.exe

Solution:      5 k =< 0.1250 0.2500 0.1250> R-F:   5.1232
=> Special k-vector solutions found!

=> List of the best 10 solutions for 4 satellites

      Kx      Ky      Kz      R-factor
0.000000  0.500000  0.500000  2.032817
0.000000  0.000000  0.125000  4.212438
0.333333  0.333333  0.333333  4.247099
0.250000  0.250000  0.250000  4.343046
0.125000  0.250000  0.125000  5.123182

=> A probable solution is the special kvector ks =< 0.0000 0.5000 0.5000>
=> The corresponding R-factor is:      2.0328

      Total CPU-Time
      CPU-seconds:      0.00
      CPU-minutes:      0.00
      CPU-hours   :      0.00
  
```

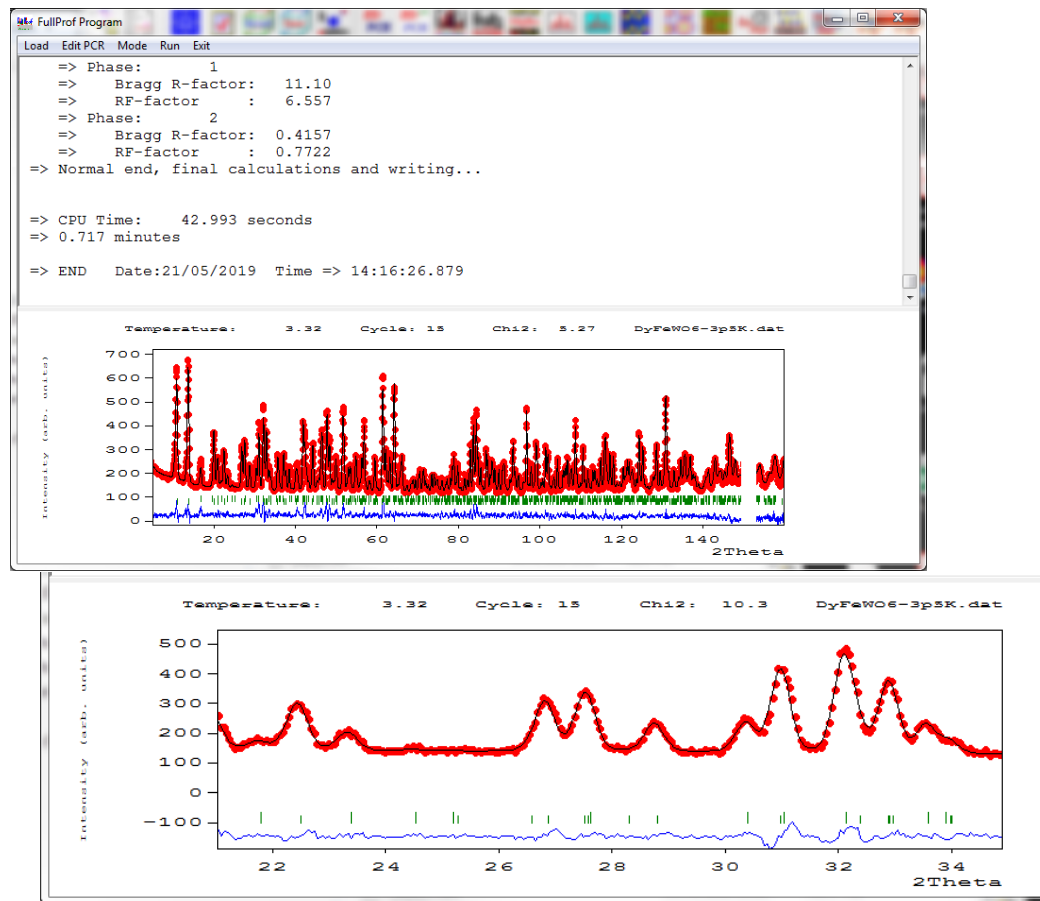
- k. Now there is a clear difference between the first and the other solutions. As in the previous case, we can add a second phase to our nuclear PCR file to check the two most probable solutions. However, from the R-factor the solution $\mathbf{k} = (0, \frac{1}{2}, \frac{1}{2})$ seems to be the most reliable.

5) **Adding a second phase to fit the magnetic reflections (follow $\text{Ho}_2\text{BaNiO}_5$ Example).**

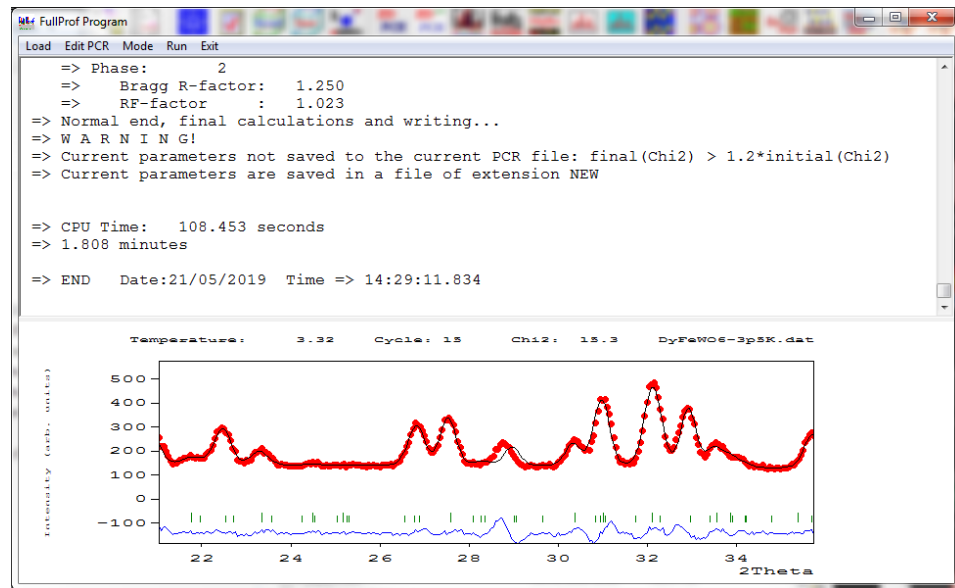
- a. Use EdPCR to add a second phase as profile matching mode. Include the instrument and the sample part as in phase 1, add a propagation vector and remember to select: "Satellite reflections are generated automatically from Space group symbol".

Here below we plot the results after some cycles of refinements.

$\mathbf{k} = (0, \frac{1}{2}, \frac{1}{2})$:



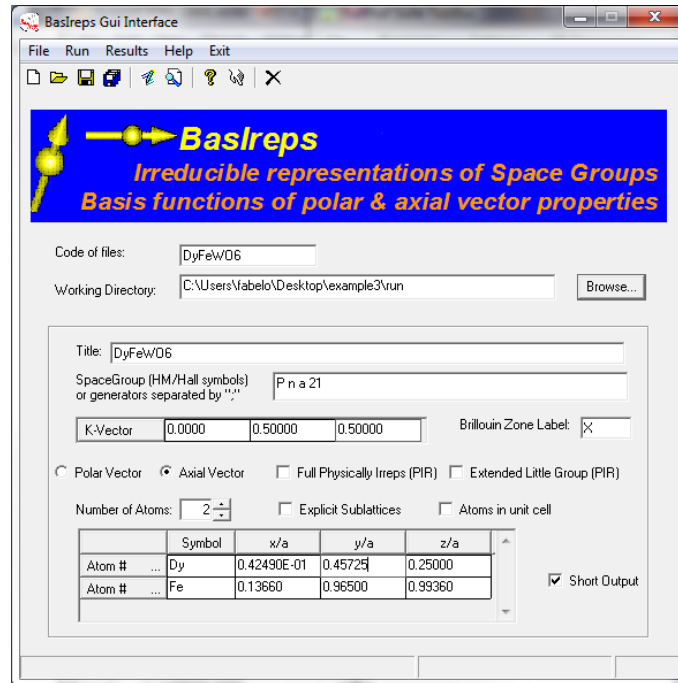
$\mathbf{k} = (0, 0, 1/8)$:



Although there is no so much difference between these two propagation vectors, from the zoom in the 22-32 2θ -zone, we can observe that for the case of $\mathbf{k} = (0, 0, 1/8)$, there is a prominent reflection that is not well fitted. Therefore, we can conclude than the propagation vector is $\mathbf{k} = (0, \frac{1}{2}, \frac{1}{2})$.

6) Calculation of Irreducible representations.

- For a first exploration of the Irreps of this system, we are going to use the Baslreps program. However, as the primary objective of this tutorial is to carry out nuclear and magnetic structure refinement using symmetry modes; in a second step we will use the ISOTROPY Software Suite, and in particular, ISODISTORT, to prepare a PCR file compatible with FullProf.
- Open Baslreps, and fill all the boxes according with the know information.



- c. Open the output file (*.bsr) and check the list of irreducible representation. In this case there is only one Irreps of dimension two. Moreover, it is complex and for obtaining real moments, one has to use real matrices that can be obtained by checking the PIR box. This is done in Baslreps by reading the database of Campbell *et al.* [J. Appl. Crystallogr.39, 607(2006)].

```

=====
Writing of Irreps matrices in symbolic form: Module:Phase (fractions of 2pi)
Numeric values of symbols a,b,c,d, ... are given at the end of the table
=====

```

```

In this section the translations associated to Seitz symbols are simplified as
1/2 1/3 2/3 1/4 3/4 1/6 5/6 1/8 3/8 5/8 7/8
p q r s t u v w x y z

```

```

|
The rotational part of Seitz symbols contains information about the orientation as
defined in Kovalev. The international symbols may be truncated (for format reasons) in
the table below. The complete international symbols can be found in the previous list.
Symmetry elements are reduced to the standard form (positive translations < 1)
The matrices of Irreps have been multiplied by the appropriate phase factor

```

```

-----
Irreps      Symmetry operators ->
v           1           2 (0,0,1/2) 0,0,z      a x,1/4,z      n (0,1/2,1/2) 1/4,y,
v           {1|000}      {2_00z|00p}      {m_x0z|pp0}      {m_0yz|ppp}
v           Symm( 1)      Symm( 2)          Symm( 3)          Symm( 4)
-----

IRrep( 1):   1           0           i           0           0           1           0           -i
              0           1           0          -i           1           0           i           0

```

- d. In order to carry out this symmetry analysis in a simpler way, determining the possible Shubnikov groups, we are going to use the “k-subgroupsmag” program from the BCS (http://www.cryst.ehu.es/cgi-bin/cryst/programs/subgrmag1_k.pl). Fill the space group information, the propagation vector and the Wyckoff position of the magnetic atoms and click on submit.

Space group of the paramagnetic phase: Pna2₁ (No. 33)

Set of chosen propagation wave-vectors

$k_1=(0,0,5,0,5)$

☐ Include the subgroups compatible with intermediate cells.
(It is not applied when only the maximal subgroups are calculated)

Wyckoff positions of the magnetic atoms
4a (x,y,z)

☐ Optional: Show only subgroups that can be the result of a Landau-type transition (single irrep order parameter).

Optional: refine further the subgroups of the output giving a set of irreps

Choose the irreps

Optional: possible limitations of the subgroup list
(Check only one option on the left and the specific value on the right)

☒ Lowest space group to consider
☐ Lowest point group to consider
☐ Lowest crystal system to consider
☐ Only maximal subgroups

choose it: 1.1

Optional: further limitations considering physical properties of the point groups

☐ Only centrosymmetric / non-centrosymmetric groups
☐ Only polar / non-polar groups

all
all

☒ List of subgroups
☐ Graph of subgroups

- e. The program provide us the three only possible groups compatible with the previous information, C_{2c} (No. 9.41), P_{2c} (No. 7.27) and P_{S1} (No. 1.3). From here we can create the mcif file and refine the magnetic structures using the Shubnikov formulation as described in the previous exercises. However, this is not the objective of this exercise so we invite you to refine the different magnetic models by yourself if you have time after finishing the proposed exercise.

| N | Group Symbol | Transformation matrix | Group-Subgroup Index | Other members of the Conjugacy Class | irreps | Magnetic structure models (MAGMODELIZE) |
|---|---------------------|---|----------------------|--|---|---|
| 1 | C_{2c} (No. 9.41) | $\begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 2 & 0 & -1/4 \\ 2 & 0 & 0 & 0 \end{pmatrix}$ | 4=2x2 | <input type="button" value="Conjugacy Class"/> | <input type="button" value="Get irreps"/> | <input checked="" type="checkbox"/> |
| 2 | P_{2c} (No. 7.27) | $\begin{pmatrix} 0 & -1 & 0 & 1/4 \\ 0 & 0 & -1 & 0 \\ 2 & 0 & 1 & 0 \end{pmatrix}$ | 4=2x2 | <input type="button" value="Conjugacy Class"/> | <input type="button" value="Get irreps"/> | <input checked="" type="checkbox"/> |
| 3 | P_{S1} (No. 1.3) | $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -1 & 2 & 0 \end{pmatrix}$ | 8=2x4 | <input type="button" value="Conjugacy Class"/> | <input type="button" value="Get irreps"/> | <input checked="" type="checkbox"/> |

☒ Include structure data of the parent phase

Submit selected subgroups to MAGMODELIZE:

**Hint: Submit many subgroups to MAGMODELIZE, when the 'include structure' option is selected, may take too long*

7) Create a PCR file using ISOTROPY SOFTWARE SUITE.

- a. Open ISOTROPY software suite on the web page and click on ISODISTORT. Here we can upload the CIF file and CLICK on OK.

(<https://stokes.byu.edu/iso/isotropy.php>)

In the first box, "Types of distortions to be considered" include the displacive distortions for all the atoms (Dy, Fe, W and O). In the occupation distortion, we do not need to add

any atom. The magnetics correspond only to Dy and Fe, the magnetic atoms. After that we have to CLICK on Change.

We are going to use the “Method 2: General method - search over specific k points”, here we have to specify the k -point, in this particular case that labelled T, K23, which corresponds to the propagation vector $\mathbf{k} = (0, \frac{1}{2}, \frac{1}{2})$. After that, we click on OK.

ISODISTORT: search

Space Group: 33 Pna2₁ C2v-9, Lattice parameters: a=10.97235, b=5.18323, c=7.33724, alpha=90.00000, beta=90.00000, gamma=90.00000
 Default space-group preferences: monoclinic axes a(b)c, monoclinic cell choice 1, orthorhombic axes abc, origin choice 2, hexagonal axes, SSG standard setting
 Dy 4a (x,y,z), x=0.04249, y=0.45725, z=0.25000, Fe 4a (x,y,z), x=0.13660, y=-0.03500, z=-0.00640, W 4a (x,y,z), x=0.35220, y=0.45370, z=0.00890, O1 4a (x,y,z), x=-0.02760, y=-0.23340, z=0.04410, O2 4a (x,y,z), z=-0.06590, O5 4a (x,y,z), x=0.14370, y=0.06010, z=0.25740, O6 4a (x,y,z), x=0.11990, y=-0.17080, z=-0.25290
 Include displacive ALL, magnetic Dy Fe distortions

Types of distortions to be considered [Change](#) [?](#)

strain: ☐
 Displacive: all ☐ none ☐ Dy ☒ Fe ☒ W ☒ O ☒
 Occupational: all ☐ none ☐ Dy ☐ Fe ☐ W ☐ O ☐
 Magnetic: all ☐ none ☐ Dy ☒ Fe ☒ W ☐ O ☐
 Rotational: all ☐ none ☐ Dy ☐ Fe ☐ W ☐ O ☐

Important: You must click on Change to implement any changes in the above type of distortions to be considered.

Method 1: Search over all special k points [OK](#) [?](#)

Crystal system(s): triclinic ☐ monoclinic ☐ orthorhombic ☐ tetragonal ☐ trigonal ☐ hexagonal ☐ cubic ☐
 Space-group symmetry: no choice ☐ Conventional lattice: no choice ☐ Primitive lattice: no choice ☐ Maximal subgroups only [?](#)

Method 2: General method - search over specific k points [OK](#) [?](#)

Specify k point: T, k23 (0, 1/2, 1/2) a= b= g= # of independent incommensurate modulations=

Change number of superposed IRs: [Change](#) [?](#)

Important: You must click on Change to implement any changes in the number of superposed IRs.

- b. ISODISTORT gives a list with three possible solutions; the first one is the 9.41 C_{ac}, which corresponds to C_{ac} (No. 9.41). The other two correspond to P_{ac} (No. 7.27) and P_s1 (No. 1.3), which is in complete agreement with the symmetry analysis done by using the BCS.

ISODISTORT: order parameter direction

Space Group: 33 Pna2₁ C2v-9, Lattice parameters: a=10.97235, b=5.18323, c=7.33724, alpha=90.00000, beta=90.00000, gamma=90.00000
 Default space-group preferences: monoclinic axes a(b)c, monoclinic cell choice 1, orthorhombic axes abc, origin choice 2, hexagonal axes, SSG standard setting
 Dy 4a (x,y,z), x=0.04249, y=0.45725, z=0.25000, Fe 4a (x,y,z), x=0.13660, y=-0.03500, z=-0.00640, W 4a (x,y,z), x=0.35220, y=0.45370, z=0.00890, O1 4a (x,y,z), x=-0.02760, y=-0.23340, z=0.04410, O2 4a (x,y,z), z=-0.06590, O5 4a (x,y,z), x=0.14370, y=0.06010, z=0.25740, O6 4a (x,y,z), x=0.11990, y=-0.17080, z=-0.25290
 Include displacive ALL, magnetic Dy Fe distortions
 k point: T, k23 (0, 1/2, 1/2)
 IR: mT1, mk23t1

Finish selecting the distortion mode by choosing an order parameter direction [?](#)

- ☒ P1 (a,0) 9.41 C_{ac}, basis={ (0,0,2), (0,-2,0), (1,0,0) }, origin=(0,-3/4,3/4), s=2, i=4, k-active= (0, 1/2, 1/2)
☐ P3 (a,a) 7.27 P_{ac}, basis={ (0,2,0), (-1,0,0), (0,-1,1) }, origin=(-1/4,0,0), s=2, i=4, k-active= (0, 1/2, 1/2)
☐ C1 (a,b) 1.3 P_s1, basis={ (0,1,1), (-1,0,0), (0,0,2) }, origin=(0,0,0), s=2, i=8, k-active= (0, 1/2, 1/2)

[OK](#)

- c. We select the first solution and CLICK on OK. The program give us a long output including all the modes, with all the values fixed to zero. ISODISTORT allow us save this output in different formats that allow us to understand better the physics behind a

particular problem. For the purposes of this tutorial, we CLICK on the FULLPROF.pcr, in order to generate a PCR file with the most important information to run FullProf using the symmetry mode refinements. CLICK on OK, and save the generated file in the working folder.

- d. Open the file with your favourite text editor. This file is a template, therefore should be modified according to your experimental data. Here below you have a list of the parameters that can be modified. Unfortunately, the EDPCR program is not able to handle this format of PCR. Therefore, we need to modify the PCR file by hand.
- e. First change the JOB from 3 (calculation) to 1 (neutron refinement). After that the wavelength from 1.227200 to 1.594460 and add the muR (1.35). The number of refinement cycles can be increased from 1 to 15 (NCY). The excluded regions can be modified according to the experimental data. Two regions from 0 to 5 and from 149.5 to 153 can be used. The first region is to avoid the direct beam influence while the second one is to exclude a peak from the low temperature sample environment.
- f. In the template, the background is included as a six coefficient polynomial function, but it could be changed to the Linear Interpolation mode, as in the previous examples, or using the Chebychev Polynomial.

Example of Chebychev background:

```
!Job Npr Nph Nba Nex Nsc Nor Dum Iwg Ilo Ias Res Ste Nre Cry Uni Cor Opt Aut
  1   7   2  -5   2   0   1   1   0   0   1   0   0   0   0   0   0   0   1
.
.
.
.
! Zero      Code      SyCos      Code      SySin      Code      Lambda      Code MORE ->Patt# 1
0.04561     0.0      0.04353     191.0     0.05861     701.0     0.000000     0.00  0

! Background coefficients/codes for Pattern# 1 (Chebychev polynomials, up to 24 coefficients)
0.000 0.000 0.000 0.000 0.000 0.000 0.000 ! Coefficient
0.00 0.00 0.00 0.00 0.00 0.00 0.00 ! Refinement code
0.000 0.000 0.000 0.000 0.000 0.000 0.000 ! Coefficient
0.00 0.00 0.00 0.00 0.00 0.00 0.00 ! Refinement code
0.000 0.000 0.000 0.000 0.000 0.000 0.000 ! Coefficient
0.00 0.00 0.00 0.00 0.00 0.00 0.00 ! Refinement code
0.000 0.000 0.000 0.000 0.000 0.000 0.000 ! Coefficient
0.00 0.00 0.00 0.00 0.00 0.00 0.00 ! Refinement code
```

NB: Between 12 and 18 coefficients are enough to reproduce a standard background.

- g. In the next step, we can refine the Scale, and add the instrumental resolution parameters. These parameters can be obtained from the PCR obtained in the point 5 of this tutorial. Finally, we can refine the SyCos and the SySin, to correct the sample position.

Here below you have the initial PCR file after adding all the missing information:

```
COMM AMPLIMODES for FullProf
! Current global Chi2 (Bragg contrib.) = 2.493
! Files => DAT-file: DyFeWO6-3p5K.dat, PCR-file: fullprof
!Job Npr Nba Nex Nsc Nor Dum Iwg Ilo Ias Res Ste Nre Cry Uni Cor Opt Aut
  1   7   1  35   2   0   0   0   0   0   0   0   0   0   0   0   0   0   1
!
!Ipr Ppl Ioc Mat Pcr Ls1 Ls2 Ls3 NLI Prf Ins Rpa Sym Hkl Fou Sho Ana
  0   0   1   0   1   0   4   0   0   3  10   0   0   0   0   0   0   0
!
! Lambda1 Lambda2 Ratio Bkpos Wdt Cthm muR AsyLim Rpolarz 2nd-muR -> Patt# 1
1.594460 1.594460 0.00000 90.000 20.0000 0.0000 1.3500 180.00 0.0000 0.0000
!
!NCY Eps R_at R_an R_pr R_gl Thmin Step Thmax PSD Sent0
15 0.10 1.00 1.00 1.00 1.00 0.0000 0.050018 159.9500 0.000 0.000
!
!2Theta/TOF/E(Kev) Background for Pattern# 1
```

```

3.5235      259.2666      0.00 ! Background included as Linear Interpolation
4.7544      235.6365      0.00
6.2749      203.2665      0.00
7.5058      191.6020      0.00
12.5018     163.3146      0.00
15.1808     147.1508      0.00
18.4269     145.1437      0.00
25.5399     136.3910      0.00
29.5707     135.1979      0.00
34.9450     124.8652      0.00
39.4499     128.6702      0.00
50.9099     121.8150      0.00
60.6052     114.1386      0.00
67.3144     115.7318      0.00
75.4707     112.1017      0.00
80.9960     112.0342      0.00
86.1266     112.3232      0.00
89.2691     114.2595      0.00
91.7784     113.4069      0.00
99.9163     115.7983      0.00
103.1037    118.1137      0.00
109.6141    118.2810      0.00
112.4624    117.4060      0.00
114.7003    121.4133      0.00
115.7176    119.4538      0.00
123.8306    119.0084      0.00
126.8798    120.9113      0.00
132.7985    119.5897      0.00
134.0146    118.9380      0.00
139.6898    121.5258      0.00
142.3923    125.5318      0.00
148.8782    129.7946      0.00
153.2021    165.3936      0.00
155.0938    149.2822      0.00
159.5529    160.5602      0.00

!
! Excluded regions (LowT HighT) for Pattern# 1
0.00      5.00
149.50    153.00

!
!
51      !Number of refined parameters
!
! Zero      Code      SyCos      Code      SySin      Code      Lambda      Code MORE ->Patt# 1
0.07485    51.0      0.03395    461.0     0.03738    471.0     0.000000      0.00 0
!-----
! Data for PHASE number: 1 ==> Current R_Bragg for Pattern# 1: 4.28
!-----
AMPLIMODES for FullProf      FIX xyz ! The nuclear structure should be fixed and only the ! amplitudes
are refinables. The crystal structure described below correspond with the parent.
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth      ATZ      Nvk Npr More
18 0 0 0.0 0.0 1.0 -6 0 2 0 66      31884.371 0 7 0 !code to symmetry modes
!
C_ac number: 9.41 <--Magnetic Space Group Symbol (BNS symbol and number)
Transform to standard: a,b,c;0,0,0 <--Basis transformation from alt setting to standard BNS
Parent space group: Pna2_1 IT_number: 33 <--Nonmagnetic Parent Group
Transform from Parent: 2c,-2b,a;0,-3/4,3/4 <--Basis transformation from parent to current setting
!
!Atom      Typ      Mag Vek      X      Y      Z      Biso      Occ      N_type      Spc/Fftype /Line
below:Codes
!      Rx      Ry      Rz      Ix      Iy      Iz      MagPh / Line below:Codes
!      beta11    beta22    beta33    beta12    beta13    beta23 / Line below:Codes
Dy_1      JDY3      1 0      0.75000    0.39637    0.04249    0.50000    4.00000    1 1
          0.00      0.00      0.00      0.00      0.00      0.00      0.00
          0.00000    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 <-MagPar
          0.00      0.00      0.00      0.00      0.00      0.00      0.00
Dy_2      JDY3      1 0      0.00000    0.35363    0.95751    0.50000    4.00000    1 1
          0.00      0.00      0.00      0.00      0.00      0.00      0.00
          0.00000    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 <-MagPar
          0.00      0.00      0.00      0.00      0.00      0.00      0.00
Fe_1      MFE3      1 0      0.62180    0.14250    0.13660    0.50000    4.00000    1 2
          0.00      0.00      0.00      0.00      0.00      0.00      0.00
          0.00000    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000 <-MagPar
          0.00      0.00      0.00      0.00      0.00      0.00      0.00

```

| | | | | | | | | | | |
|------|---------|---------|---------|---------|---------|---------|---------|---------|----------|---|
| Fe_2 | MFE3 | 1 | 0 | 0.87180 | 0.10750 | 0.86340 | 0.50000 | 4.00000 | 1 | 2 |
| | | | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | |
| | 0.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 | <-MagPar | |
| | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | |
| W_1 | W | 0 | 0 | 0.62945 | 0.39815 | 0.35220 | 0.50000 | 4.00000 | 0 | 3 |
| | | | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | |
| W_2 | W | 0 | 0 | 0.87945 | 0.35185 | 0.64780 | 0.50000 | 4.00000 | 0 | 3 |
| | | | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | |
| O1_1 | O | 0 | 0 | 0.64705 | 0.24170 | 0.97240 | 0.50000 | 4.00000 | 0 | 4 |
| | | | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | |
| O1_2 | O | 0 | 0 | 0.89705 | 0.00830 | 0.02760 | 0.50000 | 4.00000 | 0 | 4 |
| | | | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | |
| O2_1 | O | 0 | 0 | 0.60590 | 0.49700 | 0.52310 | 0.50000 | 4.00000 | 0 | 4 |
| | | | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | |
| O2_2 | O | 0 | 0 | 0.85590 | 0.25300 | 0.47690 | 0.50000 | 4.00000 | 0 | 4 |
| | | | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | |
| O3_1 | O | 0 | 0 | 0.65655 | 0.31895 | 0.21400 | 0.50000 | 4.00000 | 0 | 4 |
| | | | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | |
| O3_2 | O | 0 | 0 | 0.90655 | 0.43105 | 0.78600 | 0.50000 | 4.00000 | 0 | 4 |
| | | | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | |
| O4_1 | O | 0 | 0 | 0.59205 | 0.06055 | 0.29340 | 0.50000 | 4.00000 | 0 | 4 |
| | | | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | |
| O4_2 | O | 0 | 0 | 0.84205 | 0.18945 | 0.70660 | 0.50000 | 4.00000 | 0 | 4 |
| | | | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | |
| O5_1 | O | 0 | 0 | 0.75370 | 0.09495 | 0.14370 | 0.50000 | 4.00000 | 0 | 4 |
| | | | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | |
| O5_2 | O | 0 | 0 | 0.00370 | 0.15505 | 0.85630 | 0.50000 | 4.00000 | 0 | 4 |
| | | | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | |
| O6_1 | O | 0 | 0 | 0.49855 | 0.21040 | 0.11990 | 0.50000 | 4.00000 | 0 | 4 |
| | | | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | |
| O6_2 | O | 0 | 0 | 0.74855 | 0.03960 | 0.88010 | 0.50000 | 4.00000 | 0 | 4 |
| | | | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | |

! Polarisation Vectors of Symmetry Modes for each atom

V_MODES 108

! displacive structural modes

| ! Nm | Atm | Irrep | Vx | Vy | Vz | Coeff |
|------|------|-------|----------|-----------|-----------|----------|
| 1 | Dy_1 | GM1 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 1 | Dy_2 | GM1 | 0.000000 | 0.000000 | -0.032200 | 1.000000 |
| 2 | Dy_1 | GM1 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 2 | Dy_2 | GM1 | 0.000000 | 0.034100 | 0.000000 | 1.000000 |
| 3 | Dy_1 | GM1 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 3 | Dy_2 | GM1 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 4 | Fe_1 | GM1 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 4 | Fe_2 | GM1 | 0.000000 | 0.000000 | -0.032200 | 1.000000 |
| 5 | Fe_1 | GM1 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 5 | Fe_2 | GM1 | 0.000000 | 0.034100 | 0.000000 | 1.000000 |
| 6 | Fe_1 | GM1 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 6 | Fe_2 | GM1 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 7 | W_1 | GM1 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 7 | W_2 | GM1 | 0.000000 | 0.000000 | -0.032200 | 1.000000 |
| 8 | W_1 | GM1 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 8 | W_2 | GM1 | 0.000000 | 0.034100 | 0.000000 | 1.000000 |
| 9 | W_1 | GM1 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 9 | W_2 | GM1 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 10 | O1_1 | GM1 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 10 | O1_2 | GM1 | 0.000000 | 0.000000 | -0.032200 | 1.000000 |
| 11 | O1_1 | GM1 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 11 | O1_2 | GM1 | 0.000000 | 0.034100 | 0.000000 | 1.000000 |
| 12 | O1_1 | GM1 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 12 | O1_2 | GM1 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 13 | O2_1 | GM1 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 13 | O2_2 | GM1 | 0.000000 | 0.000000 | -0.032200 | 1.000000 |
| 14 | O2_1 | GM1 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 14 | O2_2 | GM1 | 0.000000 | 0.034100 | 0.000000 | 1.000000 |
| 15 | O2_1 | GM1 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 15 | O2_2 | GM1 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 16 | O3_1 | GM1 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 16 | O3_2 | GM1 | 0.000000 | 0.000000 | -0.032200 | 1.000000 |
| 17 | O3_1 | GM1 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 17 | O3_2 | GM1 | 0.000000 | 0.034100 | 0.000000 | 1.000000 |
| 18 | O3_1 | GM1 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 18 | O3_2 | GM1 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 19 | O4_1 | GM1 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 19 | O4_2 | GM1 | 0.000000 | 0.000000 | -0.032200 | 1.000000 |
| 20 | O4_1 | GM1 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 20 | O4_2 | GM1 | 0.000000 | 0.034100 | 0.000000 | 1.000000 |

| | | | | | | |
|----|------|-----|-----------|-----------|-----------|----------|
| 21 | O4_1 | GM1 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 21 | O4_2 | GM1 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 22 | O5_1 | GM1 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 22 | O5_2 | GM1 | 0.000000 | 0.000000 | -0.032200 | 1.000000 |
| 23 | O5_1 | GM1 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 23 | O5_2 | GM1 | 0.000000 | 0.034100 | 0.000000 | 1.000000 |
| 24 | O5_1 | GM1 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 24 | O5_2 | GM1 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 25 | O6_1 | GM1 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 25 | O6_2 | GM1 | 0.000000 | 0.000000 | -0.032200 | 1.000000 |
| 26 | O6_1 | GM1 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 26 | O6_2 | GM1 | 0.000000 | 0.034100 | 0.000000 | 1.000000 |
| 27 | O6_1 | GM1 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 27 | O6_2 | GM1 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 28 | Dy_1 | GM4 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 28 | Dy_2 | GM4 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 29 | Dy_1 | GM4 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 29 | Dy_2 | GM4 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 30 | Dy_1 | GM4 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 30 | Dy_2 | GM4 | -0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 31 | Fe_1 | GM4 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 31 | Fe_2 | GM4 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 32 | Fe_1 | GM4 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 32 | Fe_2 | GM4 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 33 | Fe_1 | GM4 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 33 | Fe_2 | GM4 | -0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 34 | W_1 | GM4 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 34 | W_2 | GM4 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 35 | W_1 | GM4 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 35 | W_2 | GM4 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 36 | W_1 | GM4 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 36 | W_2 | GM4 | -0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 37 | O1_1 | GM4 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 37 | O1_2 | GM4 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 38 | O1_1 | GM4 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 38 | O1_2 | GM4 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 39 | O1_1 | GM4 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 39 | O1_2 | GM4 | -0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 40 | O2_1 | GM4 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 40 | O2_2 | GM4 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 41 | O2_1 | GM4 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 41 | O2_2 | GM4 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 42 | O2_1 | GM4 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 42 | O2_2 | GM4 | -0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 43 | O3_1 | GM4 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 43 | O3_2 | GM4 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 44 | O3_1 | GM4 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 44 | O3_2 | GM4 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 45 | O3_1 | GM4 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 45 | O3_2 | GM4 | -0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 46 | O4_1 | GM4 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 46 | O4_2 | GM4 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 47 | O4_1 | GM4 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 47 | O4_2 | GM4 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 48 | O4_1 | GM4 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 48 | O4_2 | GM4 | -0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 49 | O5_1 | GM4 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 49 | O5_2 | GM4 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 50 | O5_1 | GM4 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 50 | O5_2 | GM4 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 51 | O5_1 | GM4 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 51 | O5_2 | GM4 | -0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 52 | O6_1 | GM4 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 52 | O6_2 | GM4 | 0.000000 | 0.000000 | 0.032200 | 1.000000 |
| 53 | O6_1 | GM4 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 53 | O6_2 | GM4 | 0.000000 | -0.034100 | 0.000000 | 1.000000 |
| 54 | O6_1 | GM4 | 0.024100 | 0.000000 | 0.000000 | 1.000000 |
| 54 | O6_2 | GM4 | -0.024100 | 0.000000 | 0.000000 | 1.000000 |

! Basis Vectors of Magnetic Symmetry Modes for each atom

M_MODES 24 ! magnetic modes

| ! Nm | Atom | Irrrep | Mx | My | Mz | Coeff |
|------|------|--------|----------|----------|-----------|----------|
| 1 | Dy_1 | mT1 | 0.000000 | 0.000000 | 0.045600 | 1.000000 |
| 1 | Dy_2 | mT1 | 0.000000 | 0.000000 | 0.000000 | 1.000000 |
| 2 | Dy_1 | mT1 | 0.000000 | 0.000000 | 0.000000 | 1.000000 |
| 2 | Dy_2 | mT1 | 0.000000 | 0.000000 | -0.045600 | 1.000000 |

| | | | | | | |
|----|------|-----|-----------|-----------|-----------|----------|
| 3 | Dy_1 | mT1 | 0.000000 | -0.048200 | 0.000000 | 1.000000 |
| 3 | Dy_2 | mT1 | 0.000000 | 0.000000 | 0.000000 | 1.000000 |
| 4 | Dy_1 | mT1 | 0.000000 | 0.000000 | 0.000000 | 1.000000 |
| 4 | Dy_2 | mT1 | 0.000000 | 0.048200 | 0.000000 | 1.000000 |
| 5 | Dy_1 | mT1 | 0.034100 | 0.000000 | 0.000000 | 1.000000 |
| 5 | Dy_2 | mT1 | 0.000000 | 0.000000 | 0.000000 | 1.000000 |
| 6 | Dy_1 | mT1 | 0.000000 | 0.000000 | 0.000000 | 1.000000 |
| 6 | Dy_2 | mT1 | 0.034100 | 0.000000 | 0.000000 | 1.000000 |
| 7 | Fe_1 | mT1 | 0.000000 | 0.000000 | -0.045600 | 1.000000 |
| 7 | Fe_2 | mT1 | 0.000000 | 0.000000 | 0.000000 | 1.000000 |
| 8 | Fe_1 | mT1 | 0.000000 | 0.000000 | 0.000000 | 1.000000 |
| 8 | Fe_2 | mT1 | 0.000000 | 0.000000 | -0.045600 | 1.000000 |
| 9 | Fe_1 | mT1 | 0.000000 | 0.048200 | 0.000000 | 1.000000 |
| 9 | Fe_2 | mT1 | 0.000000 | 0.000000 | 0.000000 | 1.000000 |
| 10 | Fe_1 | mT1 | 0.000000 | 0.000000 | 0.000000 | 1.000000 |
| 10 | Fe_2 | mT1 | 0.000000 | 0.048200 | 0.000000 | 1.000000 |
| 11 | Fe_1 | mT1 | -0.034100 | 0.000000 | 0.000000 | 1.000000 |
| 11 | Fe_2 | mT1 | 0.000000 | 0.000000 | 0.000000 | 1.000000 |
| 12 | Fe_1 | mT1 | 0.000000 | 0.000000 | 0.000000 | 1.000000 |
| 12 | Fe_2 | mT1 | 0.034100 | 0.000000 | 0.000000 | 1.000000 |

! Amplitudes of Symmetry Modes

A MODES 54 2

Max_Amplitude 0.2500

| | | | |
|---------|-----------|------------|-------------------------------------|
| A1_GM1 | 0.000000 | 0.000000 | ! Amplitude and refinement code for |
| A2_GM1 | 0.000000 | 0.000000 | ! Displacive structural modes |
| A3_GM1 | 0.000000 | 0.000000 | |
| A4_GM1 | 0.000000 | 0.000000 | |
| A5_GM1 | 0.000000 | 0.000000 | |
| A6_GM1 | 0.000000 | 0.000000 | |
| A7_GM1 | 0.000000 | 0.000000 | |
| A8_GM1 | 0.000000 | 0.000000 | |
| A9_GM1 | 0.000000 | 0.000000 | |
| A10_GM1 | 0.000000 | 0.000000 | |
| A11_GM1 | 0.000000 | 0.000000 | |
| A12_GM1 | 0.035692 | 31.000000 | |
| A13_GM1 | 0.000000 | 0.000000 | |
| A14_GM1 | 0.000000 | 0.000000 | |
| A15_GM1 | 0.000000 | 0.000000 | |
| A16_GM1 | 0.000000 | 0.000000 | |
| A17_GM1 | 0.000000 | 0.000000 | |
| A18_GM1 | 0.000000 | 0.000000 | |
| A19_GM1 | 0.000000 | 0.000000 | |
| A20_GM1 | 0.000000 | 0.000000 | |
| A21_GM1 | 0.000000 | 0.000000 | |
| A22_GM1 | 0.000000 | 0.000000 | |
| A23_GM1 | 0.000000 | 0.000000 | |
| A24_GM1 | 0.000000 | 0.000000 | |
| A25_GM1 | 0.000000 | 0.000000 | |
| A26_GM1 | 0.000000 | 0.000000 | |
| A27_GM1 | 0.000000 | 0.000000 | |
| A28_GM4 | 0.000000 | 0.000000 | |
| A29_GM4 | 0.000000 | 0.000000 | |
| A30_GM4 | -0.047903 | 481.000000 | |
| A31_GM4 | 0.000000 | 0.000000 | |
| A32_GM4 | 0.000000 | 0.000000 | |
| A33_GM4 | 0.000000 | 0.000000 | |
| A34_GM4 | 0.000000 | 0.000000 | |
| A35_GM4 | 0.000000 | 0.000000 | |
| A36_GM4 | 0.000000 | 0.000000 | |
| A37_GM4 | -0.250000 | 441.000000 | |
| A38_GM4 | 0.000000 | 0.000000 | |
| A39_GM4 | 0.000000 | 0.000000 | |
| A40_GM4 | 0.000000 | 0.000000 | |
| A41_GM4 | 0.000000 | 0.000000 | |
| A42_GM4 | -0.155794 | 511.000000 | |
| A43_GM4 | 0.000000 | 0.000000 | |
| A44_GM4 | -0.166548 | 501.000000 | |
| A45_GM4 | 0.000000 | 0.000000 | |
| A46_GM4 | 0.000000 | 0.000000 | |
| A47_GM4 | 0.000000 | 0.000000 | |
| A48_GM4 | 0.000000 | 0.000000 | |
| A49_GM4 | 0.000000 | 0.000000 | |
| A50_GM4 | 0.085814 | 491.000000 | |
| A51_GM4 | 0.000000 | 0.000000 | |
| A52_GM4 | 0.000000 | 0.000000 | |

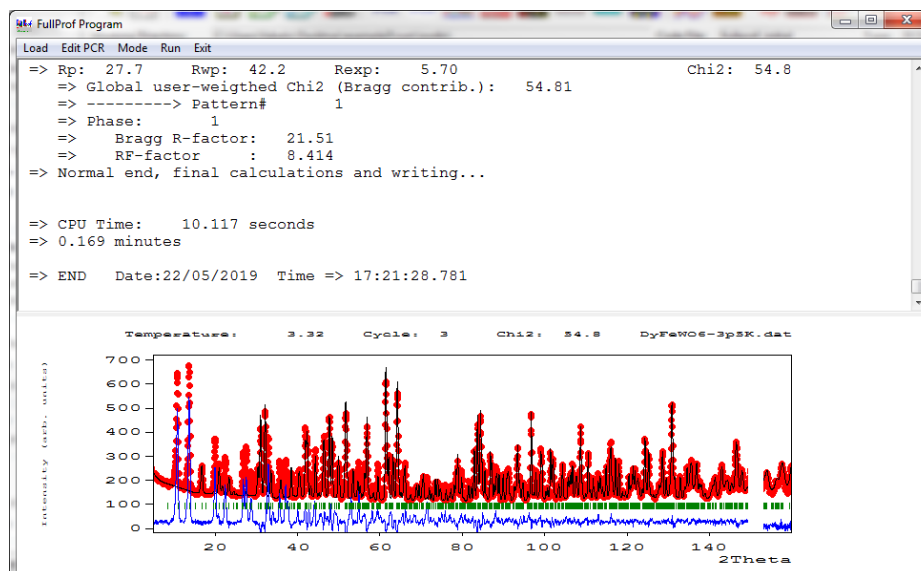
```

A53_GM4          0.000000      0.000000
A54_GM4          0.000000      0.000000
! Amplitudes of Magnetic Symmetry Modes
MA_MODES 12
A55_mT1          0.000000      0.000000 ! Amplitude and refinement code
A56_mT1          0.000000      0.000000 ! for magnetic modes
A57_mT1          10.415851      41.000000
A58_mT1          12.023539      61.000000
A59_mT1          10.101987      71.000000
A60_mT1          11.477082      81.000000
A61_mT1          -5.755133      91.000000
A62_mT1          0.909696      101.000000
A63_mT1          -3.628206      111.000000
A64_mT1          10.661194      121.000000
A65_mT1          4.538995      21.000000
A66_mT1          -1.525731      451.000000
!-----> Profile Parameters for Pattern # 1
! Scale      Shape1      Bov      Str1      Str2      Str3      Strain-Model
0.16842E-02  0.000000  0.31628  0.000000  0.000000  0.000000  0
11.000000  0.000  431.000  0.000  0.000  0.000
! U      V      W      X      Y      GauSiz      LorSiz      Size-Model
0.051646  -0.158272  0.157798  0.000000  0.061586  0.000000  0.000000  0
0.000  0.000  0.000  0.000  0.000  0.000  0.000
! a      b      c      alpha      beta      gamma      #Cell Info
14.674476  10.366457  10.972347  90.000000  90.000000  90.000000  #box -0.15 1.15 -0.15 1.15 -0.15
1.15
0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
! Pref1      Pref2      Asy1      Asy2      Asy3      Asy4      S_L      D_L
0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.07964  0.000000
0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
! 2Th1/TOF1      2Th2/TOF2      Pattern to plot
5.000  159.950  1

```

8) Refinement of the low temperature phase.

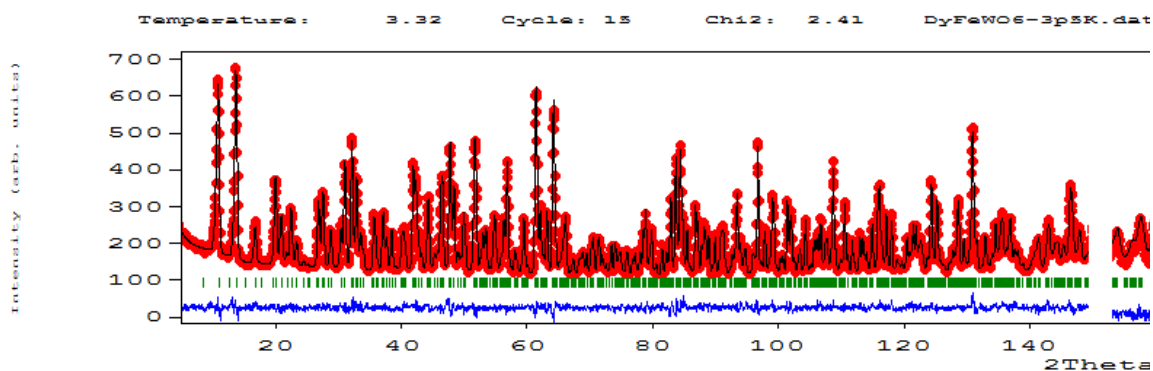
- Open in the FullProf toolbar the previously created PCR file. NB: change the name of the PCR file.
This PCR file will be used to refine the model against the data collected at 3.5K; so, be sure that both files are in the same folder.
- In the first cycle of refinement be sure that all the parameters are fixed with the exception of the SCALE factor and the ZERO-shift. Run FullProf until getting convergence. After that, refine the CELL parameters and BOV in order to refine with a unique term all the thermal parameters. Another alternative is to refine the individual Bs using the same code for each chemical element.
- After this initial refinement, we can start to refine the amplitudes of the modes. As you can see from the plot, the low angle reflections are not fitted while those at high angle are better fitted. This feature suggests us that the magnetic modes are the most important. So we should start refining these modes.



- d. In the Amplitudes of the magnetic symmetry modes, we can change all the refinement codes from 0 to 1. In order to avoid problems we should add an initial value to each amplitude. In this case we put all the amplitudes equal to 3, although in the summary file these amplitudes will be transformed to μ_B , here are in “non-intuitive” units.

! Amplitudes of Magnetic Symmetry Modes

| MA_MODES | 12 | | |
|----------|----------|----------|--|
| A55_mT1 | 3.000000 | 1.000000 | |
| A56_mT1 | 3.000000 | 1.000000 | |
| A57_mT1 | 3.000000 | 1.000000 | |
| A58_mT1 | 3.000000 | 1.000000 | |
| A59_mT1 | 3.000000 | 1.000000 | |
| A60_mT1 | 3.000000 | 1.000000 | |
| A61_mT1 | 3.000000 | 1.000000 | |
| A62_mT1 | 3.000000 | 1.000000 | |
| A63_mT1 | 3.000000 | 1.000000 | |
| A64_mT1 | 3.000000 | 1.000000 | |
| A65_mT1 | 3.000000 | 1.000000 | |
| A66_mT1 | 3.000000 | 1.000000 | |



- e. Check the summary file (*.sum) to see if there are some warnings. For the moment there are some potential problematic modes highlighted on red in the table below. We can leave them like that and check the values after including the displacive modes.

```

=> Amplitudes of magnetic symmetry modes ==>

```

| Name | Value | Sigma |
|---------|-----------|----------|
| A55_mT1 | 0.558410 | 0.712920 |
| A56_mT1 | -0.759550 | 0.626660 |

| | | |
|---------|-----------|----------|
| A57_mT1 | 10.889650 | 0.677645 |
| A58_mT1 | 11.706916 | 0.420681 |
| A59_mT1 | 10.287498 | 0.312696 |
| A60_mT1 | 11.135660 | 0.434455 |
| A61_mT1 | -5.886064 | 0.353433 |
| A62_mT1 | -0.325774 | 1.110964 |
| A63_mT1 | -4.315520 | 0.617593 |
| A64_mT1 | 9.834519 | 0.941061 |
| A65_mT1 | 5.379397 | 0.796410 |
| A66_mT1 | -1.178067 | 0.380822 |

- f. Now we can include the Amplitude of the displative symmetry modes. In order to avoid problems of convergence, we change all the amplitudes to 0.05 and refine all the amplitudes related with Gamma(1).
Check the sum file and nullify those modes proposed by the program as well as those which have big standard deviations.

=> Amplitudes of symmetry modes ==>

| Name | Value | Sigma |
|---------|-----------|---|
| A1_GM1 | 0.004645 | 0.002960 => Amplitude candidate to be nullified |
| A2_GM1 | 0.006684 | 0.003100 |
| A3_GM1 | 0.153309 | 9.230680 |
| A4_GM1 | 0.021700 | 0.008471 |
| A5_GM1 | 0.008253 | 0.010684 => Amplitude candidate to be nullified |
| A6_GM1 | 0.183470 | 9.230597 |
| A7_GM1 | -0.006048 | 0.016388 => Amplitude candidate to be nullified |
| A8_GM1 | 0.014202 | 0.022321 => Amplitude candidate to be nullified |
| A9_GM1 | 0.127757 | 9.230561 |
| A10_GM1 | -0.003955 | 0.019100 => Amplitude candidate to be nullified |
| A11_GM1 | 0.014684 | 0.017824 => Amplitude candidate to be nullified |
| A12_GM1 | 0.191758 | 9.230714 |
| A13_GM1 | -0.055625 | 0.018316 |
| A14_GM1 | -0.050619 | 0.019760 |
| A15_GM1 | 0.137820 | 9.230705 |
| A16_GM1 | -0.001258 | 0.017752 => Amplitude candidate to be nullified |
| A17_GM1 | 0.055428 | 0.020108 |
| A18_GM1 | 0.127362 | 9.230668 |
| A19_GM1 | 0.053864 | 0.017687 |
| A20_GM1 | -0.060089 | 0.020092 |
| A21_GM1 | 0.128416 | 9.230683 |
| A22_GM1 | -0.008777 | 0.008017 => Amplitude candidate to be nullified |
| A23_GM1 | -0.014779 | 0.009080 => Amplitude candidate to be nullified |
| A24_GM1 | 0.180291 | 9.230721 |
| A25_GM1 | -0.006382 | 0.008397 => Amplitude candidate to be nullified |
| A26_GM1 | -0.013008 | 0.009063 => Amplitude candidate to be nullified |

- g. We can do the same with those amplitude modes relate with Gamma(2). This procedure is a bit tricky and you should proceed with care checking always the SUM file.
- h. Although this procedure can provide you good refinements, sometimes we need to apply constrains into the magnetic sites.

| Atom | Mx | sMx | My | sMy | Mz | sMz | M | sM |
|------|---------|--------|---------|--------|---------|--------|--------|--------|
| Dy_1 | 5.0871 | 0.1511 | -5.3177 | 0.2826 | 0.0000 | 0.0000 | 7.3591 | 0.0291 |
| Dy_2 | 5.7860 | 0.1675 | 6.0235 | 0.1891 | 0.0000 | 0.0000 | 8.3523 | 0.0215 |
| Fe_1 | -2.2519 | 0.2662 | -1.7154 | 0.2667 | 2.9216 | 0.1798 | 4.0681 | 0.0355 |
| Fe_2 | -0.8325 | 0.1897 | 5.4354 | 0.3470 | -0.6450 | 0.4776 | 5.5365 | 0.0564 |

In this case, the value of the Fe_2 atom is slightly above to the ideal value. We can try to constraint the modulus of the magnetic moment of both Fe atoms and both Dy atoms to be equal. However, working with amplitudes there is not a simple relation to constraint the magnetic moments.

In order to apply these kind of constraints, the most effective procedure is to fix all the magnetic amplitudes to zero and refine the magnetic moment using spherical coordinated. We can use this option directly on the parent structural description section.

| !Atom | Typ | Mag Vek | X | Y | Z | Biso | Occ | N_type | Spc/Fftype |
|-------------------|------|---------|---------|---------|---------|---------|---------|--------------------|------------|
| /Line below:Codes | | | | | | | | | |
| ! | Rx | Ry | Rz | Ix | Iy | Iz | MagPh | / Line below:Codes | |
| Dy_1 | JDY3 | 1 0 | 0.75000 | 0.39637 | 0.04249 | 0.50000 | 4.00000 | 1 | 1 |
| | | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | |
| | | | 7.00000 | 3.00000 | 3.00000 | 0.00000 | 0.00000 | 2.00000 | <-MagPar |
| | | | 541.00 | 1.00 | 1.00 | 0.00 | 0.00 | 0.00 | |
| Dy_2 | JDY3 | 1 0 | 0.00000 | 0.35363 | 0.95751 | 0.50000 | 4.00000 | 1 | 1 |
| | | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | |
| | | | 7.00000 | 3.00000 | 3.00000 | 0.00000 | 0.00000 | 2.00000 | <-MagPar |
| | | | 541.00 | 1.00 | 1.00 | 0.00 | 0.00 | 0.00 | |
| Fe_1 | MFE3 | 1 0 | 0.62180 | 0.14250 | 0.13660 | 0.50000 | 4.00000 | 1 | 2 |
| | | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | |
| | | | 5.00000 | 3.00000 | 3.00000 | 0.00000 | 0.00000 | 2.00000 | <-MagPar |
| | | | 551.00 | 1.00 | 1.00 | 0.00 | 0.00 | 0.00 | |
| Fe_2 | MFE3 | 1 0 | 0.87180 | 0.10750 | 0.86340 | 0.50000 | 4.00000 | 1 | 2 |
| | | | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | | |
| | | | 5.00000 | 3.00000 | 3.00000 | 0.00000 | 0.00000 | 2.00000 | <-MagPar |
| | | | 551.00 | 1.00 | 1.00 | 0.00 | 0.00 | 0.00 | |

We need to add the green 2 to use spherical coordinated.

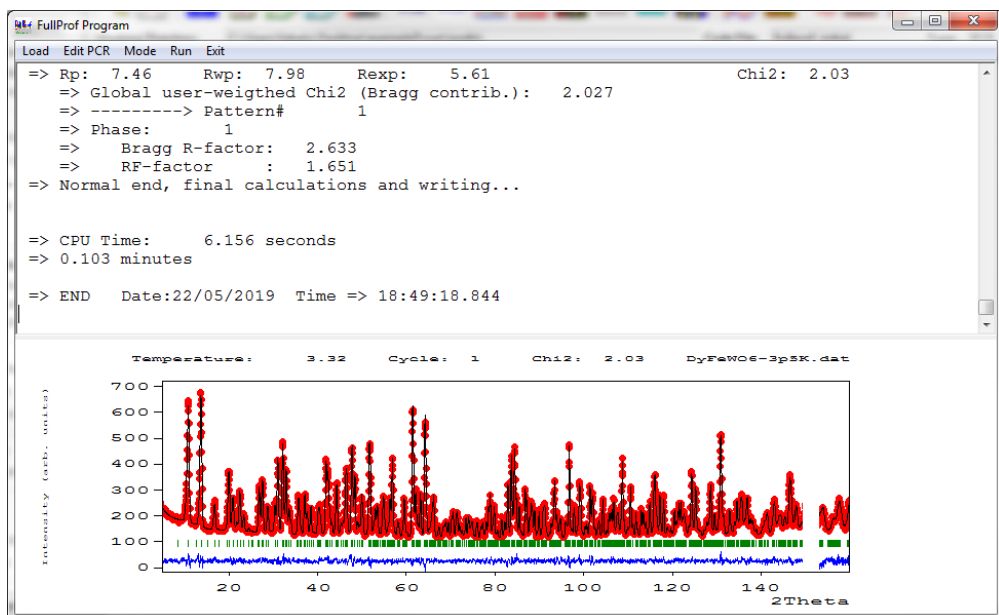
The red numbers are the magnetic moment modulus, with the same refinement code for both Dy and Fe sites.

The blue numbers are Phi and Theta angles, respectively. We have add some initial values to avoid refinement problems.

NB: In the first refinement cycle fix all the refinement codes from the nuclear amplitudes to zero. After convergence, you can start to refine the amplitudes, checking always on the SUM file that all is consistent.

- i. After including the constraint, the magnetic moments of both sites are completely reasonable with values that are in good agreement with those previously reported in the bibliography.

| Name | Mom | sMo | Phi | sPhi | Tet | sTet |
|------|----------------|-------------------|------------------|------|-----|------|
| Dy_1 | 7.840 (0.043) | -47.448 (1.125) | 88.905 (2.446) | | | |
| Dy_2 | 7.840 (0.043) | 226.801 (0.883) | -87.494 (2.166) | | | |
| Fe_1 | 4.717 (0.092) | 34.479 (4.598) | -48.785 (1.694) | | | |
| Fe_2 | 4.717 (0.092) | -260.792 (2.148) | 92.811 (5.613) | | | |

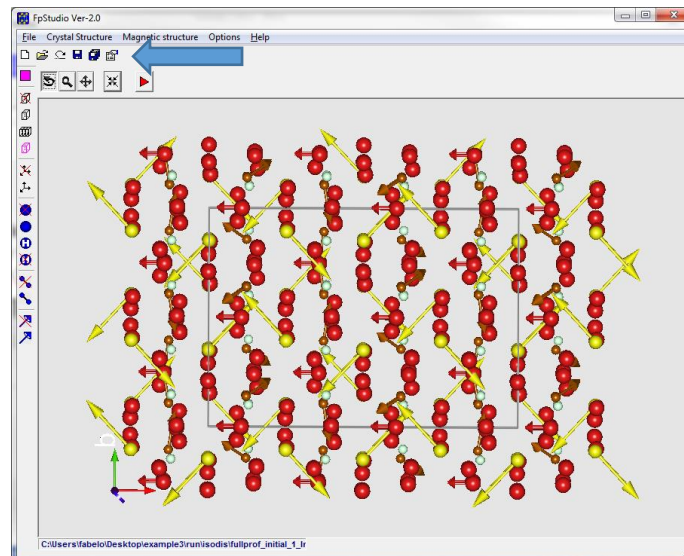


You can refine the model using the other two magnetic space-groups but remember that the symmetry is much low and the number of modes is much higher.

9) **Plot the results.**

- a. After running FullProf several output files are automatically created to help the user visualizing the results. This output files are divided on two different groups, those that are compatible with FpStudio and those with VESTA.
- b. The output files for FpStudio are:
 - 1) Filename.fst (information about the full nuclear and magnetic structure)
 - 2) Filename_GM1.fst (High symmetry structure but now the amplitudes of the refined modes for Gamma(1) are plotted as arrows)
 - 3) Filename_GM2.fst (High symmetry structure but now the amplitudes of the refined modes for Gamma(2) are plotted as arrows)

NB: The scale factor for amplitudes and magnetic moments are the same, however both parameters are quite different. Therefore, if you want to plot both in the same picture, you should change by hand the scale factor of one of them to obtain similar values.



```

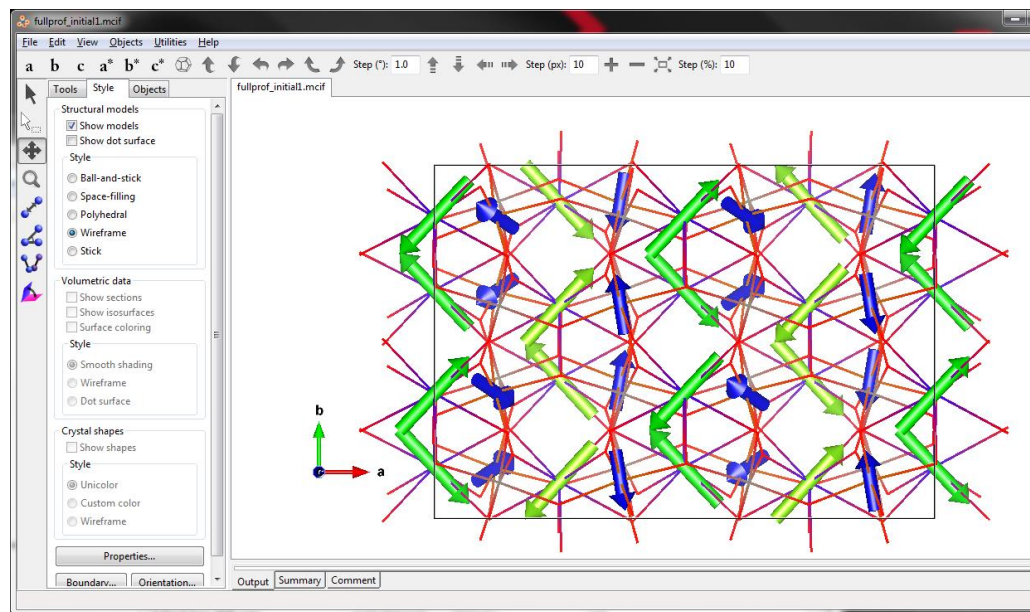
SYMM x+1/2,-y,z+1/2
MSYM u,-v,w, 0.0
MSYM u,-v,w, 0.0
MATOM Dy_1 Dy 0.75000 0.39637 0.04249 Scale 2.3017
SKP 1 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
SKP 1 2 0.91802 -1.00000 0.02594 0.00000 0.00000 0.00000
MATOM Dy_2 Dy 0.00000 0.35363 0.95751 Scale 2.3017
SKP 1 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
SKP 1 2 0.92853 0.98881 0.05935 0.00000 0.00000 0.00000
MATOM Fe_1 Fe 0.62180 0.14250 0.13660 Scale 2.3017
SKP 1 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
SKP 1 2 -0.50654 -0.34787 0.53823 0.00000 0.00000 0.00000
MATOM Fe_2 Fe 0.87180 0.10750 0.86340 Scale 2.3017
SKP 1 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
SKP 1 2 -0.13057 0.80538 -0.04005 0.00000 0.00000 0.00000
MATOM W_1 W 0.62945 0.39815 0.35220 Scale 13.3017
SKP 1 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
SKP 1 2 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
MATOM W_2 W 0.87945 0.35185 0.64780 Scale 13.3017
SKP 1 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
SKP 1 2 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
MATOM O1_1 O 0.64705 0.24170 0.97240 Scale 13.3017
SKP 1 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
SKP 1 2 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
MATOM O1_2 O 0.89705 0.00830 0.02760 Scale 13.3017
SKP 1 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
SKP 1 2 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
MATOM O2_1 O 0.60590 0.49700 0.52310 Scale 13.3017

```

There are two SKP lines, the first one corresponds to the amplitude vectors and the second one correspond to the magnetic contribution.

c. The output files for VESTA are:

1) Filename.mcif (information about nuclear and magnetic structure)



2) Filename_Irrep_GM1.vesta (High symmetry structure but now the amplitudes of the refined modes for Gamma(1) are plotted as arrows)

3) Filename_Irrep_GM2.vesta (High symmetry structure but now the amplitudes of the refined modes for Gamma(2) are plotted as arrows)

NB: As in the previous case, the scale factor for amplitudes and magnetic moments are the same, however both parameters are quite different. Therefore, to adapt the size of both amplitudes you can click on “edit > vectors” on VESTA and modify the

Scale or each individual vector clicking on Edit. Other parameters as the arrow colour is also modifiable from this menu.

The image shows the VESTA software interface. The main window displays a 3D crystal structure with various vectors plotted. The left sidebar contains settings for structural models, style, volumetric data, and crystal shapes. The bottom panel shows the 'Vectors' dialog box, which is used to manage the displayed vectors.

Crystallographic Sites

| No. | Label | x | y | z | Vector |
|-----|-------|---------|---------|---------|--------|
| 1 | Dy_1 | 0.75000 | 0.39637 | 0.04249 | 1, 2 |
| 2 | Dy_2 | 0.00000 | 0.35363 | 0.95751 | 3, 4 |
| 3 | Fe_1 | 0.62180 | 0.14250 | 0.13660 | 5, 6 |
| 4 | Fe_2 | 0.87180 | 0.10750 | 0.86340 | 7, 8 |
| 5 | W_1 | 0.62945 | 0.39815 | 0.35220 | 9 |
| 6 | W_2 | 0.87945 | 0.35185 | 0.64780 | 10 |
| 7 | O1_1 | 0.64705 | 0.24170 | 0.97240 | 11 |
| 8 | O1_2 | 0.89705 | 0.00830 | 0.02760 | 12 |
| 9 | O2_1 | 0.60590 | 0.49700 | 0.52310 | 13 |
| 10 | O2_2 | 0.85590 | 0.25300 | 0.47690 | 14 |
| 11 | O3_1 | 0.65655 | 0.31895 | 0.21400 | 15 |
| 12 | O3_2 | 0.90655 | 0.43105 | 0.78600 | 16 |
| 13 | O4_1 | 0.59205 | 0.06055 | 0.29340 | 17 |
| 14 | O4_2 | 0.84205 | 0.18945 | 0.70660 | 18 |
| 15 | O5_1 | 0.75370 | 0.09495 | 0.14370 | 19 |
| 16 | O5_2 | 0.00370 | 0.15505 | 0.85630 | 20 |
| 17 | O6_1 | 0.49855 | 0.21040 | 0.11990 | 21 |
| 18 | O6_2 | 0.74855 | 0.03960 | 0.88010 | 22 |

Vectors

| No. | [u v w] | Modulus | r (Å) |
|-----|-----------------------------|---------|-------|
| 3 | [0.00000 0.00000 0.00000] | 0.00 | 0.30 |
| 4 | [0.06326 0.09536 0.00541] | 1.36 | 0.40 |
| 5 | [0.00000 0.00000 0.00000] | 0.00 | 0.30 |
| 6 | [-0.03451 -0.03355 0.04904] | 0.82 | 0.40 |
| 7 | [0.00000 0.00000 0.00000] | 0.00 | 0.30 |
| 8 | [-0.00890 0.07767 -0.00365] | 0.82 | 0.40 |
| 9 | [0.00000 0.00000 0.00000] | 0.00 | 0.30 |
| 10 | [0.00000 0.00000 0.00000] | 0.00 | 0.30 |
| 11 | [0.00000 0.00000 0.09491] | 1.04 | 0.30 |
| 12 | [0.00000 0.00000 0.09491] | 1.04 | 0.30 |
| 13 | [0.04246 0.00000 0.00000] | 0.62 | 0.30 |
| 14 | [-0.04246 0.00000 0.00000] | 0.62 | 0.30 |
| 15 | [0.00000 0.00000 0.00000] | 0.00 | 0.30 |
| 16 | [0.00000 0.00000 0.00000] | 0.00 | 0.30 |
| 17 | [0.00000 0.00000 -0.03833] | 0.42 | 0.30 |
| 18 | [0.00000 0.00000 -0.03833] | 0.42 | 0.30 |
| 19 | [0.00000 0.00000 0.00000] | 0.00 | 0.30 |
| 20 | [0.00000 0.00000 0.00000] | 0.00 | 0.30 |
| 21 | [0.00000 0.00000 0.02858] | 0.31 | 0.30 |
| 22 | [0.00000 0.00000 0.02858] | 0.31 | 0.30 |

Scale factor for modulus: 1.15208