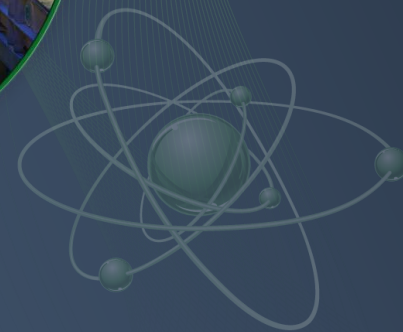


Incommensurate magnetic structure of DyMn_6Ge_6 determined using Fullprof

Stuart Calder

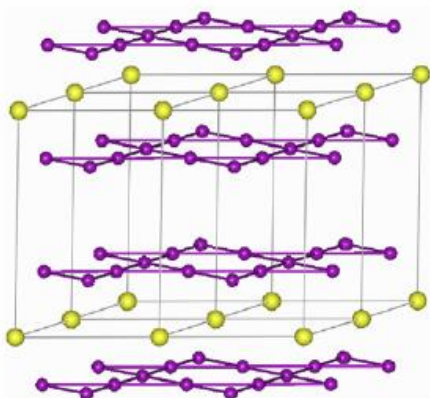
Oak Ridge National Laboratory,
High Flux Isotope Reactor (HFIR)



Magnetic phase diagram of DyMn₆Ge₆

P. Schobinger-Papamantellos et al, Journal of Alloys and Compounds, 203 (1994) 243-250

Atom	X	Y	Z	Wyk
Dy	0	0	0	1b
Mn	1/2	0	0.2504	6i
Ge	1/3	2/3	0	2d
Ge	1/3	2/3	1/2	2c
Ge	0	0	0.345	2e



The compound DyMn₆Ge₆ crystallizes in the hexagonal HfFe₆Ge₆-type structure (*P6₃/mmm*). It orders antiferromagnetically at $T_N=420$ K but there is a second magnetic phase transition near 100 K. Neutron diffraction has shown that the high temperature magnetic structure is a triple flat spiral consisting of ferromagnetic Dy layers and ferromagnetic Mn layers coupled antiparallely in a three-layer sequence Mn(+), Dy(-), Mn(+). The moment direction is perpendicular to [001] but the direction in the basal plane changes by a constant angle $\phi_s=2\pi q_z$ on going from one unit cell to another. The wavevector length of the incommensurate structure is temperature dependent and equal to $q_z=0.184$ at 293 K, which corresponds to $\phi_s=66^\circ$. Below $T_i=100$ K the wavevector length remains constant ($q_z=0.163$) and the magnetic structure is an incommensurate triple-cone structure in which both the Dy and Mn sublattices have a ferromagnetic component along the *c* axis. These components are antiparallel and lead to a net moment in the *c* direction of 2.0(5) μ_B per formula unit. The magnetic isotherm at 4.2 K, studied in fields up to 35 T, suggests that below 22 T the cone angle (55° for $B=0$) gradually decreases. Above 22 T the magnetic isotherm shows a linear behaviour characteristic of bending of the antiparallel rare earth and 3d sublattice moments towards each other. The intersublattice coupling constant derived from the high field slope of the isotherm equals $J_{Dy-Mn}/k = -9.1$ K.

- Hexagonal *P6₃/mmm* $a=b=5.21\text{\AA}$, $c=8.15\text{\AA}$
- Kagome layers of Mn (magenta). Dy atoms (yellow) at origin of unit cell (grey boxes).
- Two magnetic transitions: $T_N=420$ K and $T_N=100$ K.
- Exercise will refine 11 K data using an incommensurate propagation vector (*k*).
Spin density wave vs canonical (spin spiral)
Alternative of two propagation vectors considered as extension to model.

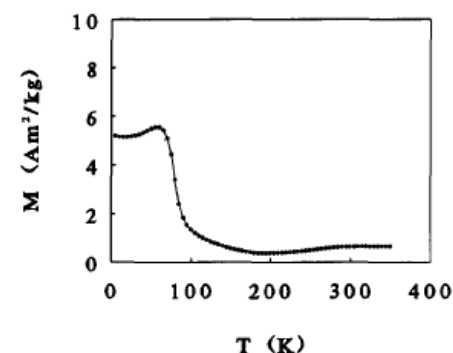


Fig. 1. Temperature dependence of the magnetization of DyMn₆Ge₆ measured in a field of 0.1 T.

Experimental details of measurements on DyMn₆Ge₆

- Neutron powder diffraction collected on DMC at PSI, Switzerland.
- $\lambda=1.7037\text{\AA}$
- Background file: dy_nuc_background.BGR
This can be created from winplotr, but file is already generated for this example.
- Manually input instrument parameter files U, V, W, asym1 (irf file not needed)
- CIF file obtained for crystal structure from ICSD:
dymn6ge6_nuc.cif

Steps for magnetic structure determination:

1. Import known crystal structure and input instrument parameters to create PCR file for Nuclear phase
2. Refine crystal structure at 11 K (***EdPcr / Winplotr***)
3. Identify magnetic reflections and determine propagation vector (**k-search**)
4. Use crystal structure and propagation vector to perform symmetry analysis to find the allowed irreducible representations (IRs) and Basis vectors (BVs) for magnetic phase. (***SARAh / Basireps***)
5. Select a magnetic model and add it as additional phase(s) to the crystal structure refinement (***EdPcr / SARAh***)
6. Refine both nuclear phase and magnetic phase(s) (**Fullprof**)
7. Visualize the magnetic structure model (**FpStudio**)

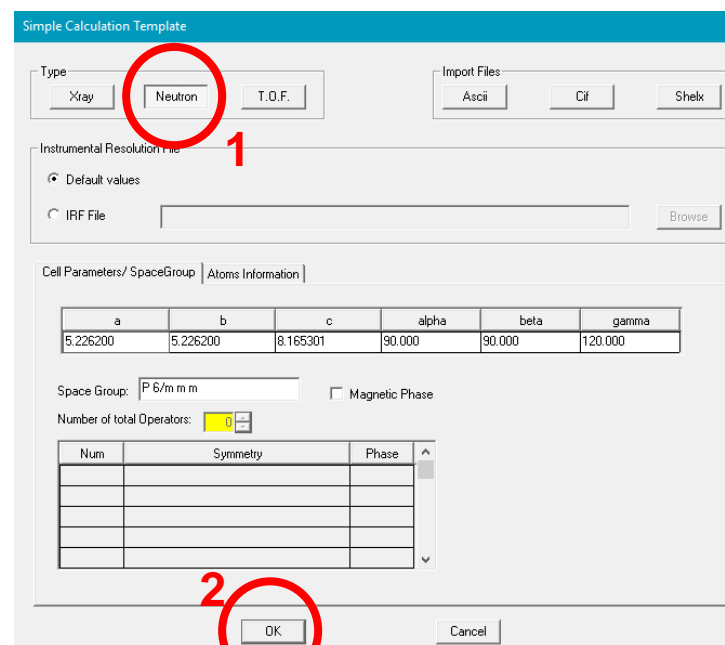
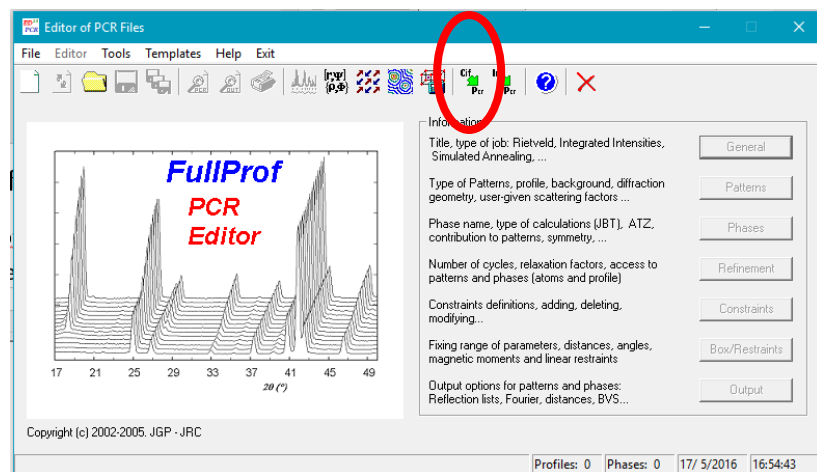
Step 1: Refine the crystal structure of DyMn₆Ge₆

Use EdPCR to create the input file for FullProf (.pcr):

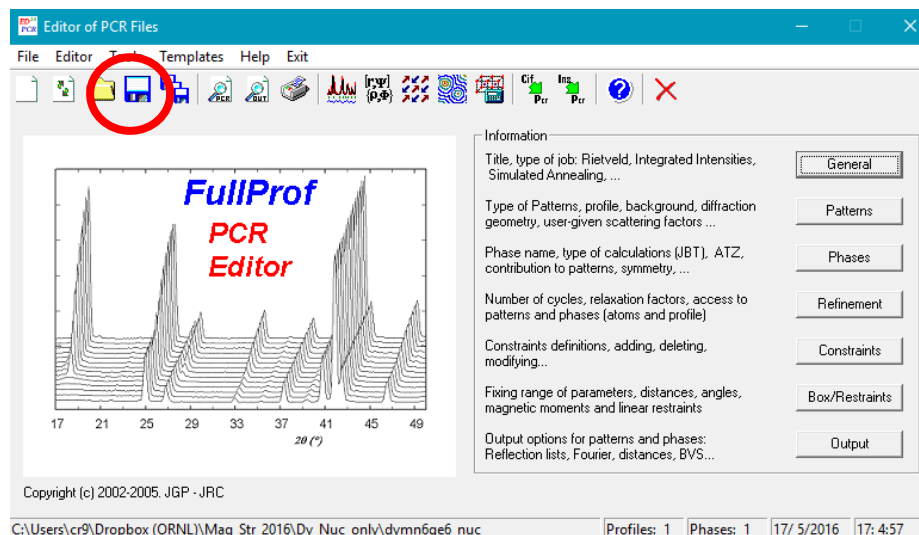
- Import the crystallographic information file (CIF)
dymn6ge6_nuc.cif



In the new “simple calculation template” window select “Neutron”

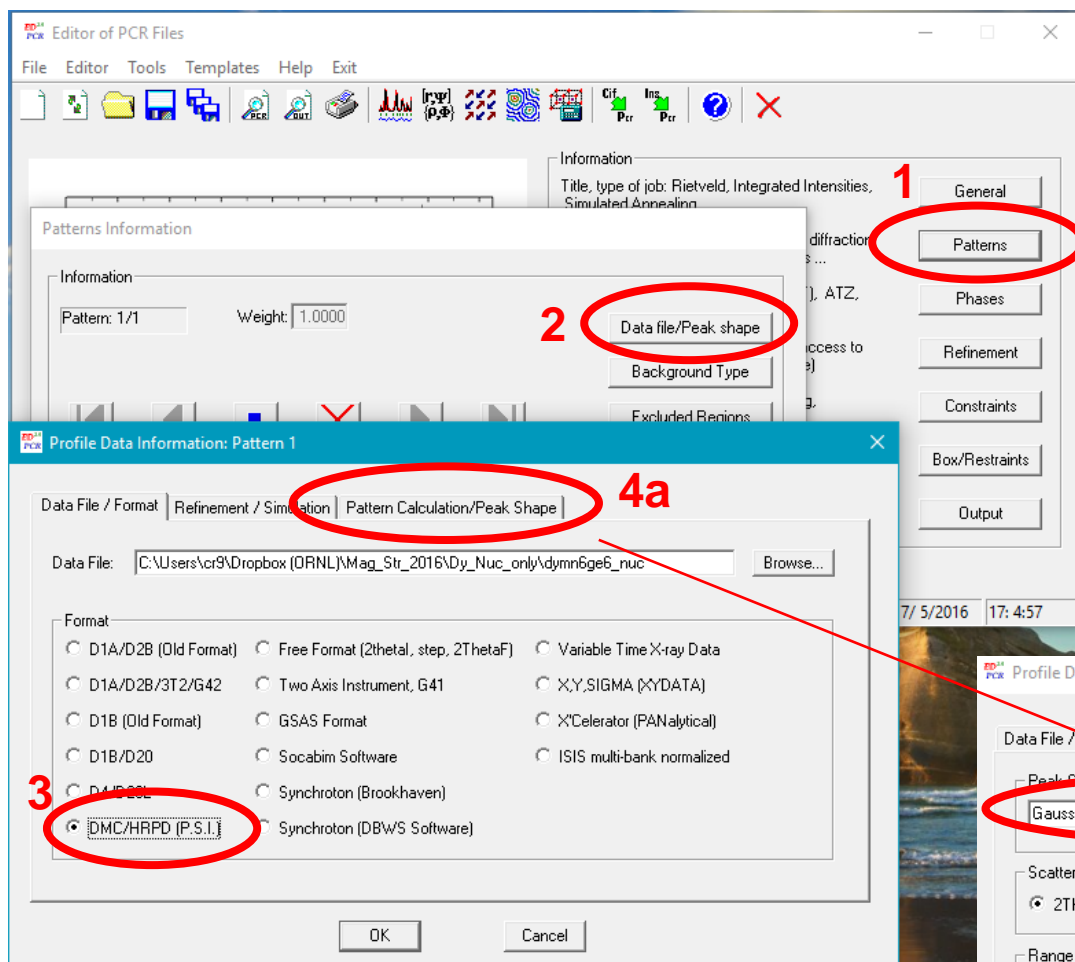


Step 1: Refine the crystal structure of DyMn₆Ge₆

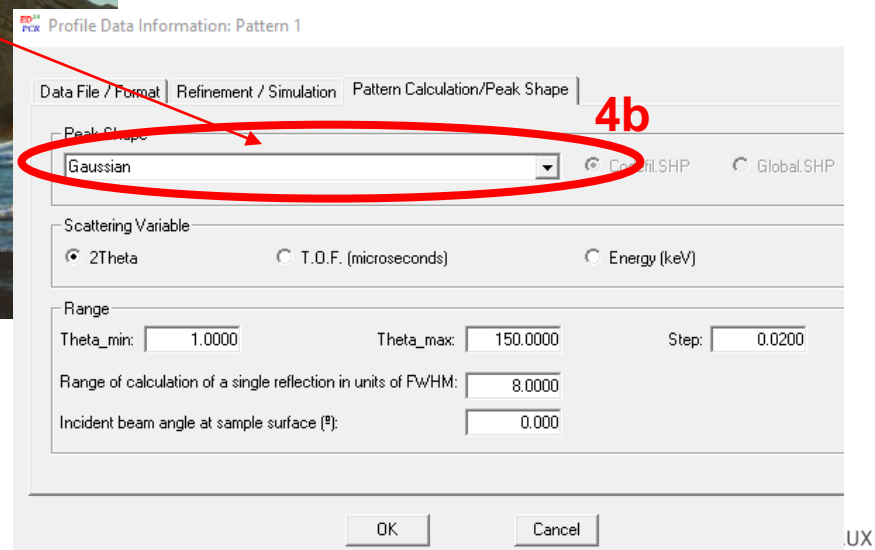


After each step click “OK” to get back to main EdPCR window and save to ensure the changes are accepted

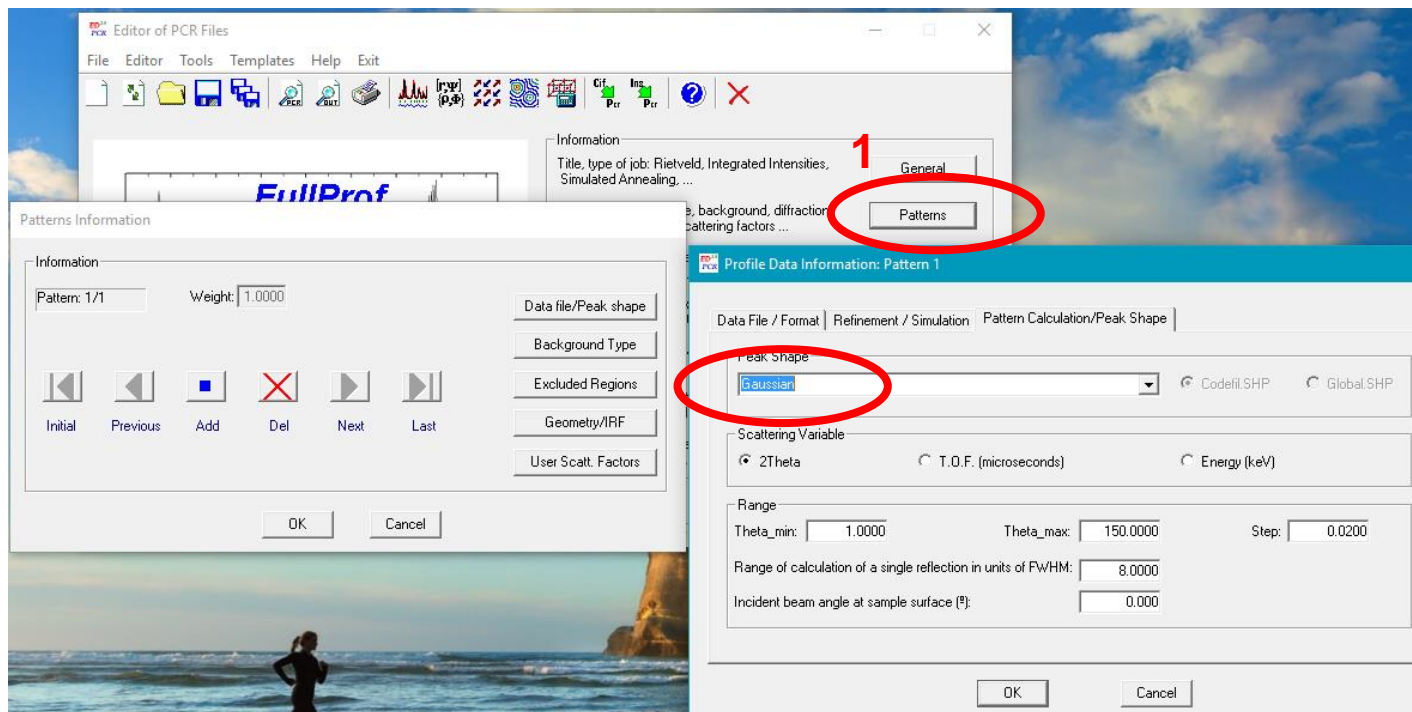
Step 1: Refine the crystal structure of DyMn₆Ge₆



Open tabs “Patterns”,
then “DataFile/Peak shape”
and select “DMC/HRPD (P.S.I)”
Steps 1,2,3
Next select “Pattern
Calculations/Peak Shape” tab and
change peak shape to Gaussian
Steps 4a-4b



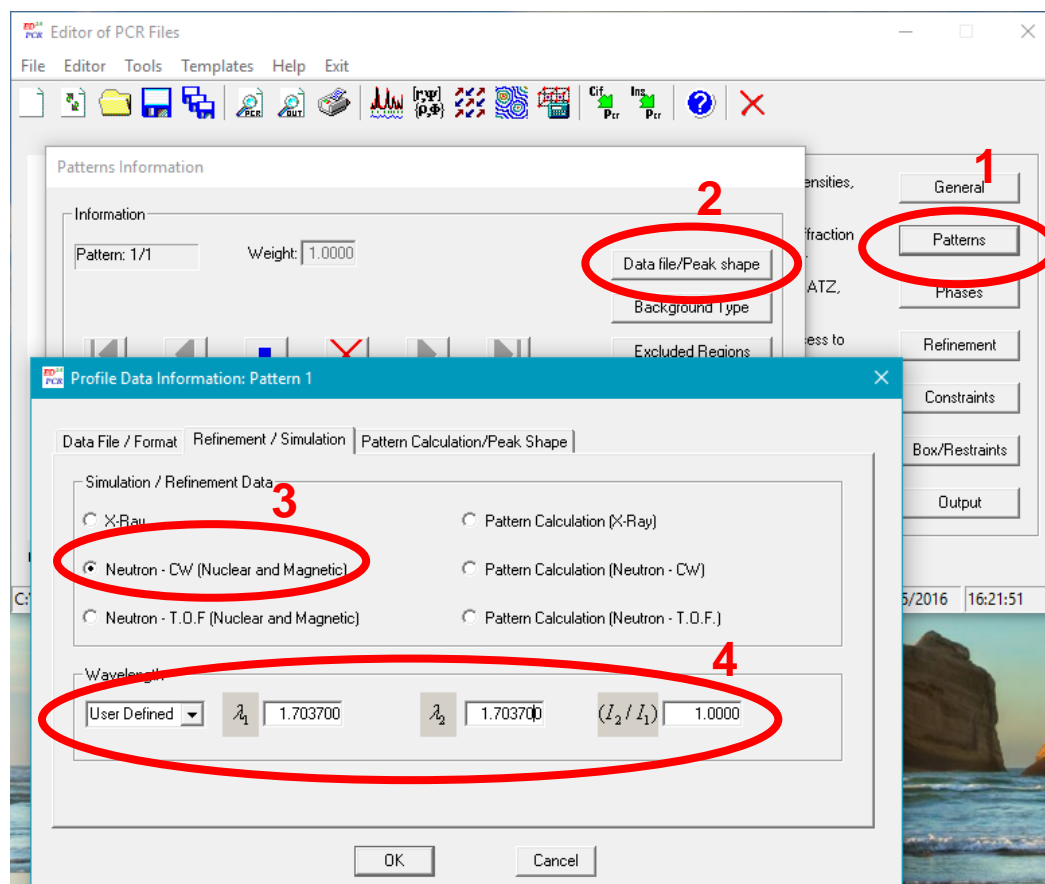
Step 1: Refine the crystal structure of DyMn_6Ge_6



Open tabs “Patterns”,
then “DataFile/Peak shape”
and select “DMC/HFPR (P.S.I)”
Steps 1,2,3
Close tabs by selecting OK

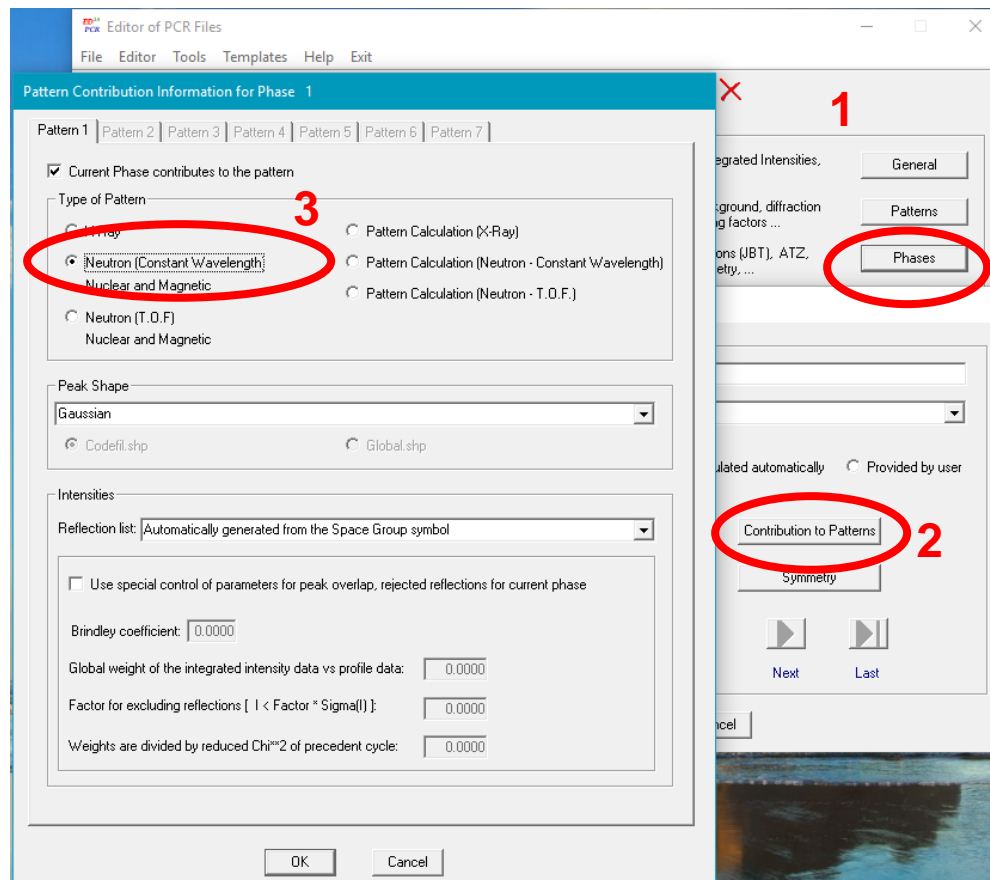
Step 1: Refine the crystal structure of DyMn₆Ge₆

- From main window of EdPCR select “Patterns” tab, click on “Data file/Peak shape” and then select “Neutron – CW (Nuclear and Magnetic)” Under “Wavelength” from drop-down select “User defined” input 1.7037 for λ_1 and λ_2 and 1 for (I_2/I_1) Steps 1,2,3,4
- Close tabs (select “OK”) and save.



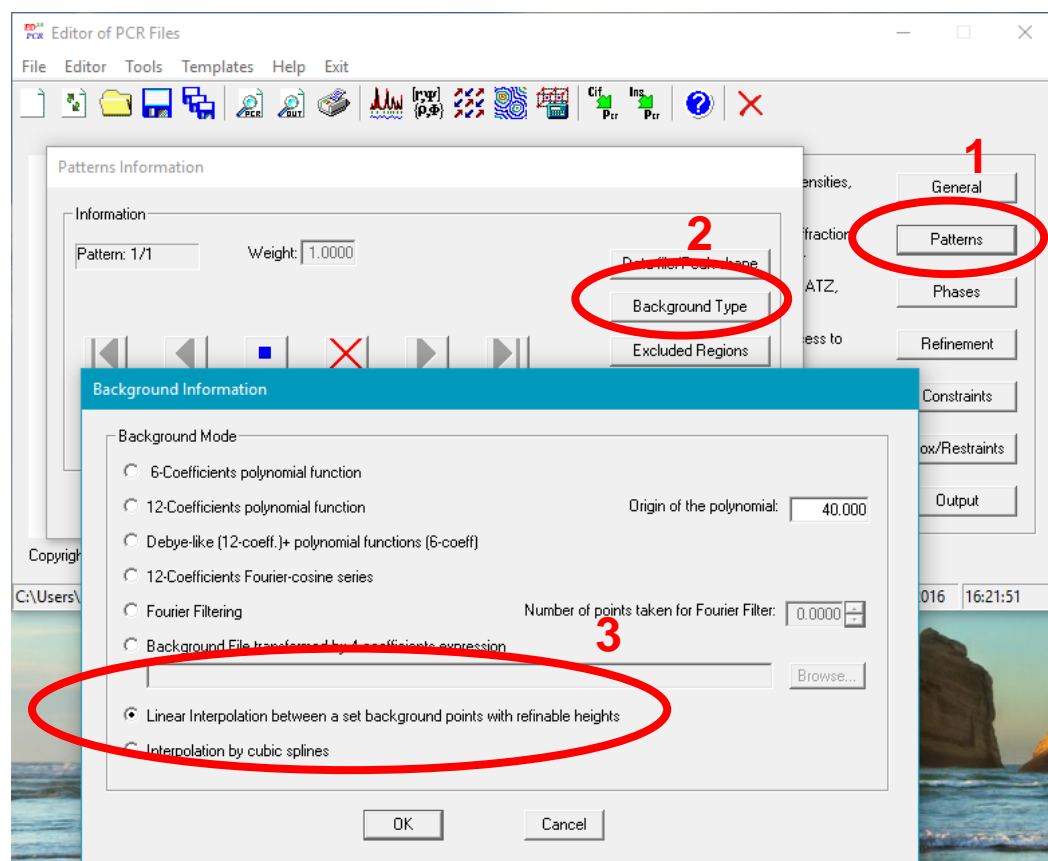
Step 1: Refine the crystal structure of DyMn₆Ge₆

- From main window of EdPCR select “Phases” tab, click on “Contribution to patterns” and then select “current phase contributes to the pattern”
- Steps 1,2,3



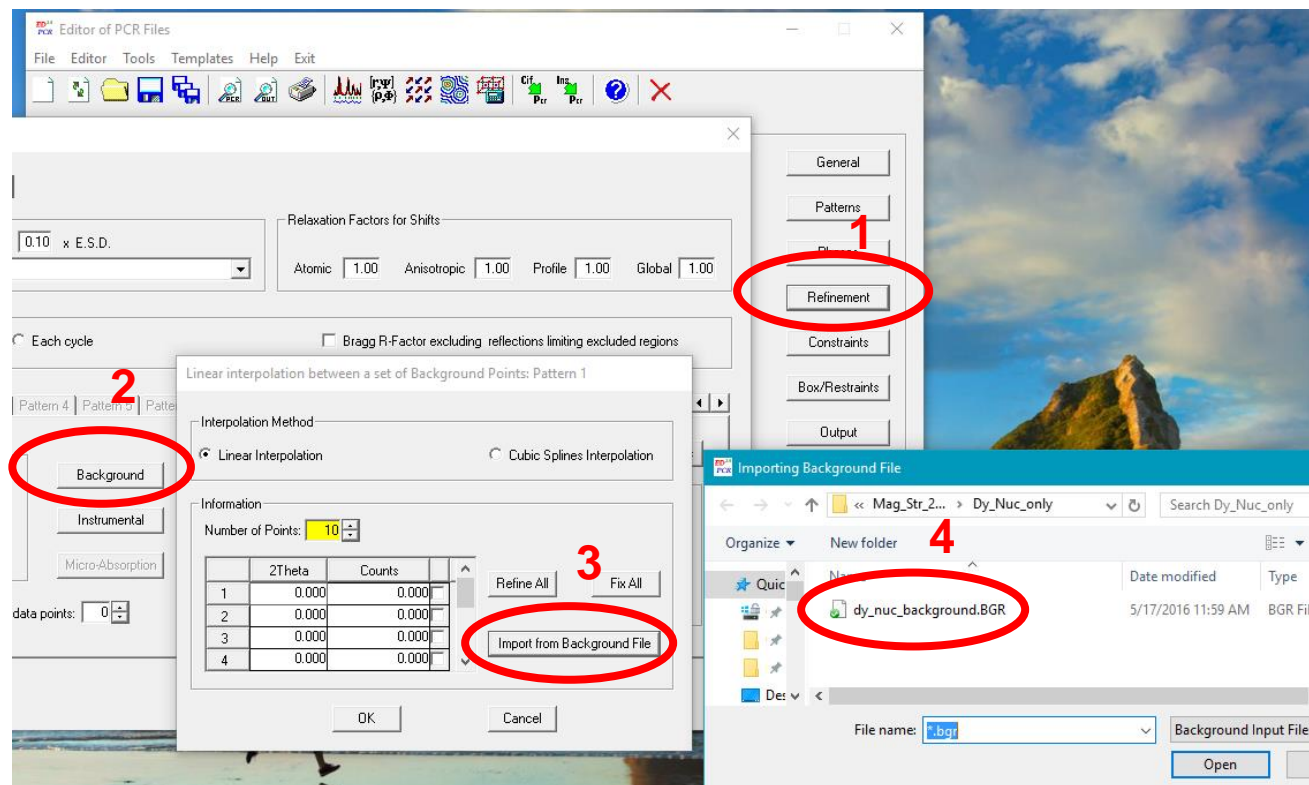
Step 1: Refine the crystal structure of DyMn₆Ge₆

- From main window of EdPCR select “Patterns” tab, click on “Background type” and then select “Linear Interpolation between a set background points with refinable heights” Steps 1,2,3
- Close tabs (select “OK”) and save.
- A background file can now be loaded.



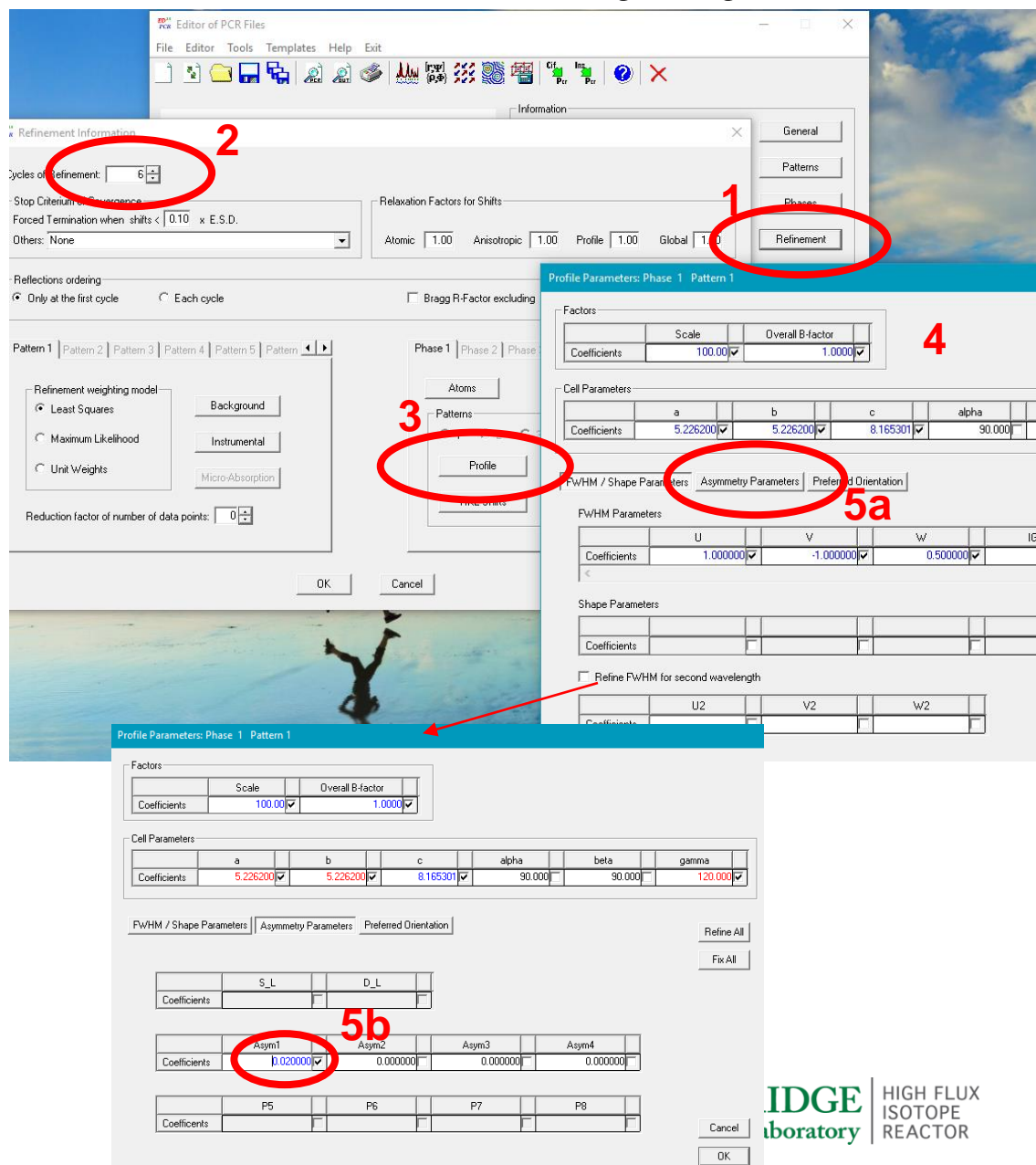
Step 1: Refine the crystal structure of DyMn₆Ge₆

- Select “Refinement” tab on main EdPCR window. Then “background” and “Import from Background File”. Import “dy_nuc_backg round.BGR”
- Select OK and save.



Step 1: Refine the crystal structure of DyMn₆Ge₆

- Select “Refinement” tab again on main EdPCR window [1]. Increase number “Cycles of refinement” to 6 [2]. Then select “Profile” [3] and alter Scale, Overall B-factor, U, V, W and along with a,b,c cell paramaters set them all to refine by checking the boxes (4).
- [5ab]: Select “Asymmetry Paramaters” tab and “Asymm1” to refine
- Select OK and save.





Step 1: Refine the crystal structure of DyMn₆Ge₆

```

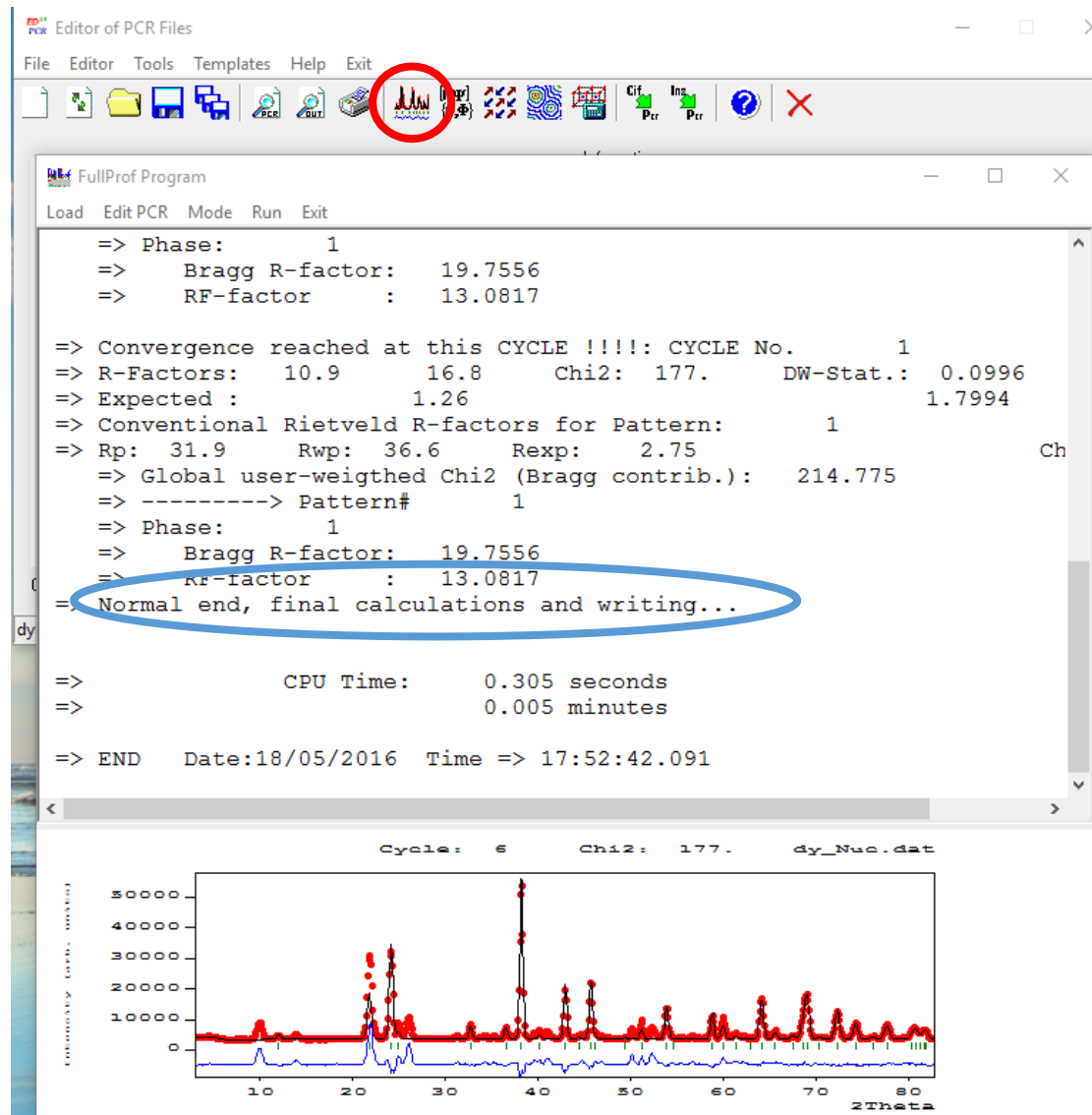
PC External PCR Text Editor - [C:\Users\cr9\Dropbox (ORNL)\Mag_Str_2016\Di_Nuc_only\dymn6ge6_nuc.pcr]
File Edit Search
[Icons]
COMM ;
! Files => DAT-file: , PCR-file: dymn6ge6_nuc
!Job Npr Nph Nba Nex Nsc Nor Dum Iwg Ilo Ias Res Ste Nre Cry Uni Cor Opt Aut
1 0 1 38 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
!
!Ipr 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 0 0 0 0 0 0
!
! Lambda1 Lambda2 Ratio Bkpos Wdt Cthm muR AsyLin Rplarz 2nd-muR -> Patt# 1
1.703700 1.703700 1.00000 40.000 0.0000 0.0000 1.2800 180.00 0.0000 0.0000
!
! NCY Eps R_at R_an R_pr R_gl Thmin Step Thmax PSD Sent0
6 0.10 1.00 1.00 1.00 1.00 1.0000 0.020000 150.0000 0.000 0.000
!
!2Theta/T0F/E(Kev) Background for Pattern# 1
3.1300 4310.0000 0.00
3.9800 4111.0000 0.00
5.1100 4111.0000 0.00
6.4900 3316.0000 0.00
7.4100 3361.0000 0.00
8.9300 3427.0000 0.00
11.1000 3471.0000 0.00
12.7000 3471.0000 0.00
13.2000 3471.0000 0.00
14.7000 3515.0000 0.00
17.1000 3515.0000 0.00
19.3000 3581.0000 0.00
20.1000 3626.0000 0.00
20.9000 3846.0000 0.00
23.2000 3891.0000 0.00
26.9000 3692.0000 0.00
29.6000 3670.0000 0.00
31.0000 3692.0000 0.00
33.4000 3692.0000 0.00
36.0000 3758.0000 0.00
39.1000 3846.0000 0.00
41.9000 3824.0000 0.00
42.3000 3802.0000 0.00
43.7000 3846.0000 0.00
47.3000 3846.0000 0.00
48.2000 3648.0000 0.00
48.9000 3581.0000 0.00
55.0000 3581.0000 0.00
55.9000 3626.0000 0.00
63.4000 3626.0000 0.00
66.8000 3648.0000 0.00
71.5000 3802.0000 0.00
75.1000 3603.0000 0.00
76.9000 3603.0000 0.00
78.7000 3515.0000 0.00
79.1000 3515.0000 0.00
82.5000 3581.0000 0.00
82.8000 3581.0000 0.00
!
!
9 !Number of refined parameters
! Zero Code SyCos Code SySin Code Lambda Code MORE -> Patt# 1
0.04000 0.0 0.00000 0.0 0.00000 0.0 0.000000 0.00 0
!
!
Line:10 Col:40 NUM INS

```

- Select the PCR button:  
- This opens the text for the .pcr file
- Edit the values circled

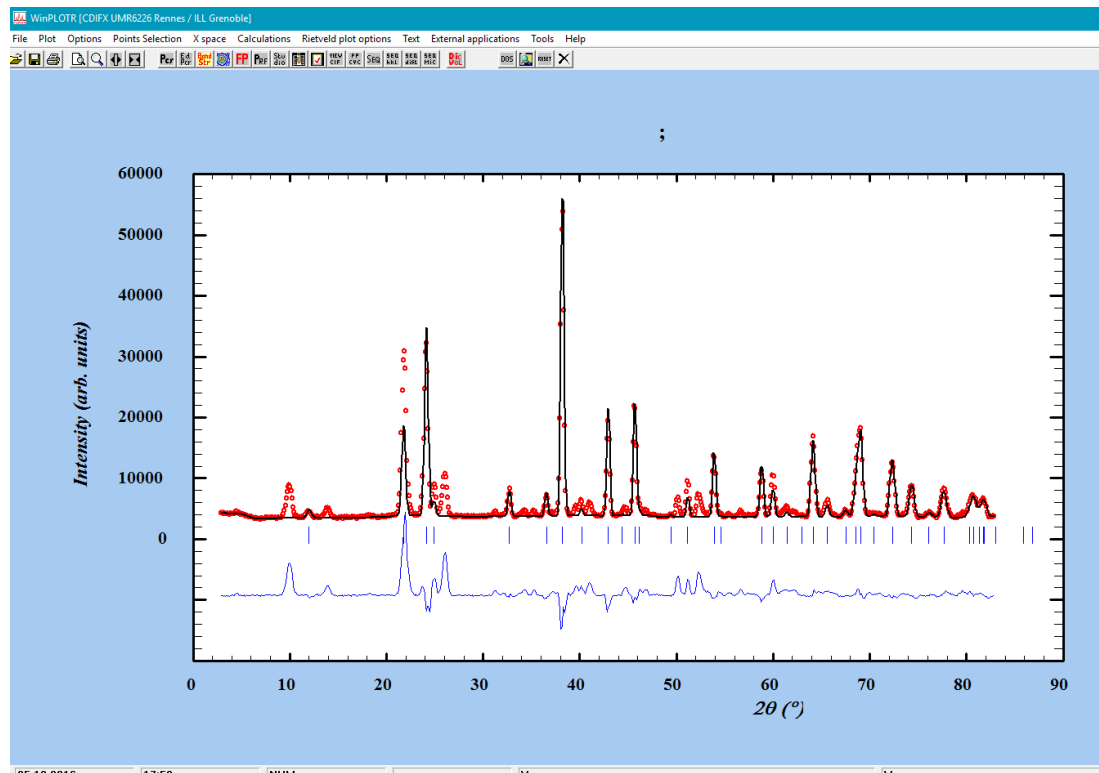
Step 1: Refine the crystal structure of DyMn₆Ge₆

- PCR file is set-up for refinement.
- Press circled tab and refinement runs.
- Number of cycles set to 6 in earlier step, more cycles can be performed by pressing “Run” until it reads: “Normal end, final calculations and writing....”



Step 1: Refine the crystal structure of DyMn₆Ge₆

- Open PRF file created after each refinement.
- Several “extra” peaks or intensity is present. Comparing with high temperature data show these are magnetic.
- The next step is to determine how these magnetic peaks are related to the nuclear peaks.

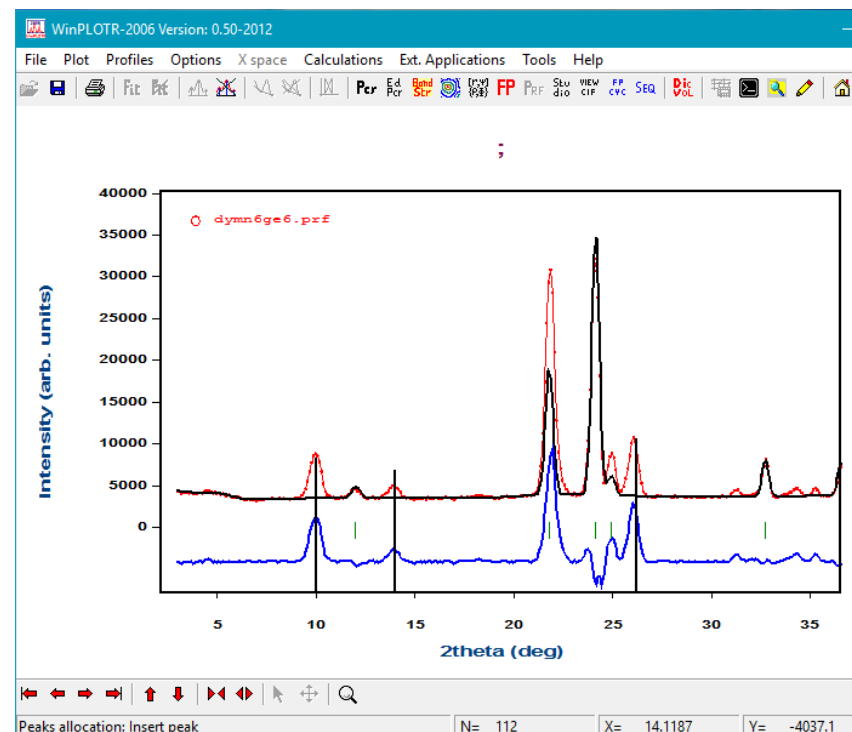


Step 2: Determine the propagation vector (k-wave vector)



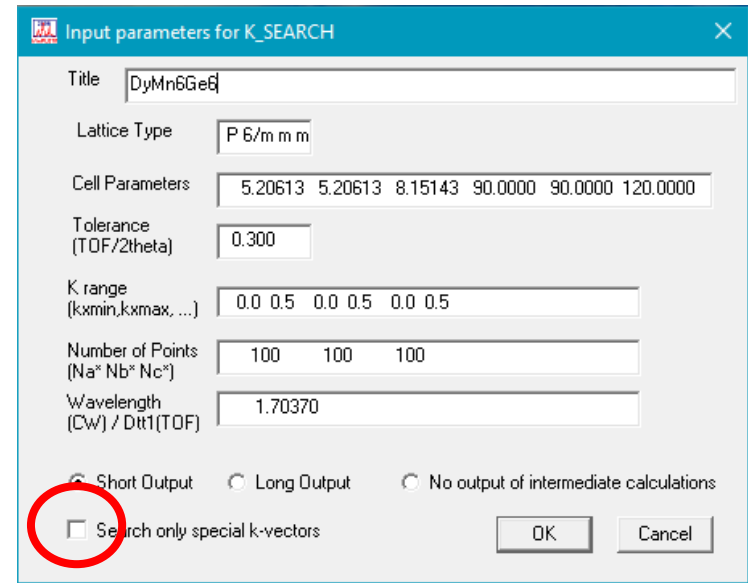
- Open prf with WinPLOTR-2006 from FPtoolbar.
(Otherwise open WinPLOTR then load the .prf file using
File → Open Rietveld/Profile file (.prf))

- Zoom into low 2theta range to observe magnetic scattering.
- To select peaks for k-search click:
Calculations → peak detection → enable
Then:
Calculations → peak detection → insert peak
User cursor to select peaks at 2theta
9.9, 13.9 and 26.1 deg.
- Run k-search by selecting
Calculations → peak detection → save peaks → K_Search Format



Step 2: Determine the propagation vector (k-wave vector)

- Along with the peak positions the Input parameters for K_SEARCH are loaded from the refinements.
- Run k-search by selecting OK, save .sat file and then “Yes” to run k-search.
- No solution are found with the “Search only special k-vectors” box ticked indicating the solution is not commensurate.
- Uncheck the “Search only special k-vectors” box and rerun k-search
- $k=(0\ 0\ 0.165)$** appears a good candidate.
- Note – an alternative solution exists for this particular sample with two propagation vectors that goes beyond initial publication in literature.



```
C:\windows\SYSTEM32\cmd.exe
99.47% S: 20200 k =( 0.5000 0.2300 0.2100) R-F: 5.3791 R-best: 0.1770
99.59% S: 20300 k =( 0.5000 0.2950 0.2950) R-F: 1.6963 R-best: 0.1770
99.68% S: 20400 k =( 0.5000 0.3400 0.1450) R-F: 3.8553 R-best: 0.1770

=> List of the best 10 solutions for 3 satellites

  kx      Ky      kz      R-factor
0.010000  0.005000  0.165000  0.177039
0.005000  0.010000  0.165000  0.177039
0.005000  0.015000  0.165000  0.188981
0.015000  0.005000  0.165000  0.188981
0.000000  0.025000  0.165000  0.227686
0.025000  0.000000  0.165000  0.227686
0.140000  0.495000  0.170000  0.291242
0.495000  0.140000  0.170000  0.291242
0.140000  0.365000  0.170000  0.291264
0.365000  0.140000  0.170000  0.291264

=> A probable solution is the special kvector ks =( 0.0000 0.0000 0.0000)
=> The corresponding R-factor is: 0.0000

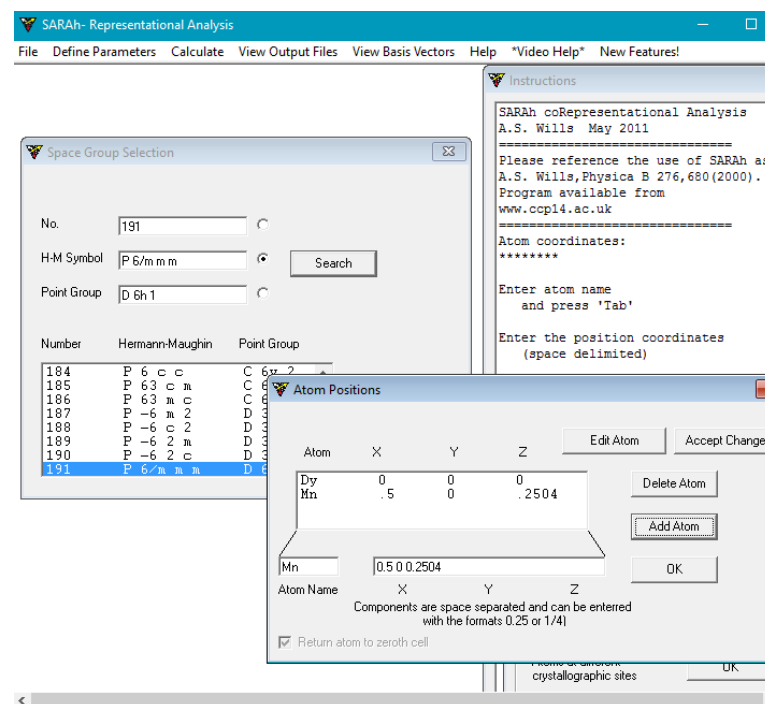
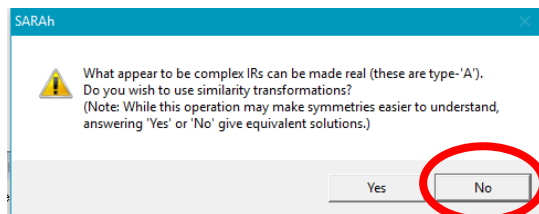
Total CPU-Time
CPU-seconds: 0.28
CPU-minutes: 0.00
CPU-hours : 0.00

=> Press <enter> to finish
```

- Following was using complex output for SARAh.
- This makes interpreting the BVs potentially more complicated than keeping everything real. But the solutions are equivalent.

Step 3: Symmetry analysis

- Use SARAh (or Baslreps) to generate the Irreducible Representations (IRs) and basis vectors (BVs) associated with the propagation vectors, crystal structure and magnetic atom positions.
- Open SARAh- Representational analysis
- Under “Define Parameters” input:
 “Space group” No. 191 or H_M Symbol P 6/m m m
 “K-vector” 0 0 0.165
 “Atoms” Dy 0 0 0
 Mn 0.5 0 0.2504
- Run program using “Calculate”
 Select directory where the created output files will go (i.e. current directory).
 Some pop windows will appear during calculation. For source of IR select Kovalev and “**No**” so the solution will be easier to interpret, although not imaginary.



Step 3: Symmetry analysis

- SARAh outputs several files to explain the allowed symmetries.
- From pdf created from .tex file:

IR	BV	Atom	BV components					
			$m_{\parallel a}$	$m_{\parallel b}$	$m_{\parallel c}$	$im_{\parallel a}$	$im_{\parallel b}$	$im_{\parallel c}$
Γ_2	ψ_1	1	0	0	12	0	0	0
Γ_5	ψ_2	1	6	6	0	0	0	0
	ψ_3	1	3.464	-3.464	0	0	0	0

Table 1: Basis vectors for the space group P 6/m m m with $\mathbf{k}_{11} = (0, 0, .165)$. The decomposition of the magnetic representation for the *Dy* site $(0, 0, 0)$ is $\Gamma_{Mag} = 0\Gamma_1^1 + 1\Gamma_2^1 + 0\Gamma_3^1 + 0\Gamma_4^1 + 1\Gamma_5^2 + 0\Gamma_6^2$. The atom of the primitive basis is defined according to 1: $(0, 0, 0)$.

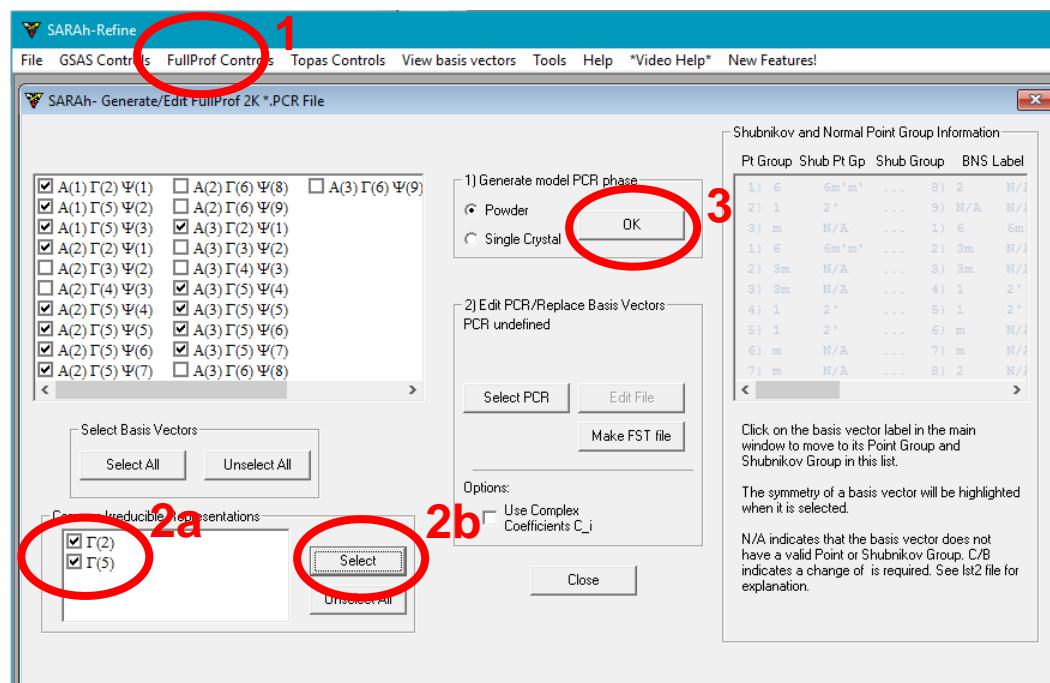
- Γ_2 and Γ_5 form the common IRs. Both Γ_2 (c-axis) and Γ_5 (ab-plane) will be needed. Note complex BVs.
- The Mn is split into 2 orbits (3 atoms at $z=0.2504$ and 3 at $z=0.7496$). For this exercise we will fix both orbits to be the same (in or out of phase). This reduces the free parameters to make the problem more tractable. Moreover for in this kind of compound generally the Mn-Mn interactions are ferromagnetic suggesting constrained orbits.

IR	BV	Atom	BV components					
			$m_{\parallel a}$	$m_{\parallel b}$	$m_{\parallel c}$	$im_{\parallel a}$	$im_{\parallel b}$	$im_{\parallel c}$
Γ_2	ψ_1	1	0	0	4	0	0	0
		2	0	0	4	0	0	0
		3	0	0	4	0	0	0
Γ_3	ψ_2	1	2	0	0	0	0	0
		2	-2	-2	0	0	0	0
		3	0	2	0	0	0	0
Γ_4	ψ_3	1	2	4	0	0	0	0
		2	2	-2	0	0	0	0
		3	4	2	0	0	0	0
Γ_5	ψ_4	1	2	2	0	0	0	0
		2	0	1	0	0	-1.732	0
		3	1	0	0	1.732	0	0
	ψ_5	1	2	-2	0	0	0	0
		2	2	1	0	-3.464	-1.732	0
		3	-1	-2	0	-1.732	-3.464	0
	ψ_6	1	0	1	0	0	1.732	0
		2	-2	0	0	0	0	0
		3	-1	-1	0	1.732	1.732	0
Γ_6	ψ_7	1	-2	-1	0	-3.464	-1.732	0
		2	-2	-4	0	0	0	0
		3	1	-1	0	-1.732	1.732	0
	ψ_8	1	0	0	4	0	0	0
		2	0	0	-2	0	0	0
		3	0	0	-2	0	0	0
	ψ_9	1	0	0	0	0	0	0
		2	0	0	3.464	0	0	0
		3	0	0	-3.464	0	0	0

Table 2: Basis vectors for the space group P 6/m m m with $\mathbf{k}_{11} = (0, 0, .165)$. The decomposition of the magnetic representation for the *Mn* site $(.5, 0, .2504)$ is $\Gamma_{Mag} = 0\Gamma_1^1 + 1\Gamma_2^1 + 1\Gamma_3^1 + 1\Gamma_4^1 + 2\Gamma_5^2 + 1\Gamma_6^2$. The atoms of the nonprimitive basis are defined according to 1: $(.5, 0, .2504)$, 2: $(.5, .5, .2504)$, 3: $(0, .5, .2504)$.

Step 4: Adding the magnetic phase

- Open SARAh-Refine.
- Under “Fullprof Controls” [1] select “Load SARAh MAT file” and open file created by SARAh (sarah191.mat)
- Under “Common Irreducible Representations” check boxes next to both $\Gamma(2)$ and $\Gamma(5)$ and press select to associate all BVs. [2]



- Create the magnetic phase part of the PCR file by selecting “OK” next to “Generate model PCR phase” [3]. This creates a file “sarah191.pcr” that can be copied and pasted into the crystal structure pcr file from Step 1.
Note: only open the created “sarah191.pcr” with a text editor and not EdPCR.

Step 4: Adding the magnetic phase

- Open “sarah191.pcr” with a text editor (notepad, notepad++) and open the text of the structural refinement “dymn6ge6.pcr”.
- Change the number of phases to 2 since we will now have a nuclear and magnetic phase. [1]
- Copy and paste the created magnetic phase just before line
! 2Th1/TOF1 [2]
- Make sure there are no blank lines before or after the pasted section.

```

External EdPCR Text Editor - [C:\Users\cr9\Dropbox (ORNL)\Mag_Str_2016\Di...
File Edit Search

COMM ;
! Current global Chi2 (Bragg contrib.) = 214.8
! Files => DAT-file: dymn6ge6.dat, PCR-file: dymn6ge6
! Job Np Nph Nba Nex Nsc Nor Dum Iwg Ilo Ias Res Ste N
1 0 2 8 0 0 0 0 0 0 0 0 0 0
!
! Ipr Pp1 Ioc Mat Pcr Ls1 Ls2 Ls3 NLI Prf Ins Rpa Sym H
0 0 1 0 1 0 4 0 0 3 8 0 0
!
! Lambda1 Lambda2 Ratio Bkpos Wdt Cthm
1.703700 1.703700 1.00000 40.000 5.0000 0.0000
!
! NCY Eps R_at R_an R_pr R_gl Thmin Step
6 0.10 1.00 1.00 1.00 1.00 3.0000 0.1000
!
! 2Theta/TOF/E(Kev) Background for Pattern# 1
3.1300 4310.0000 0.00
0.0000 0.0000 0.00

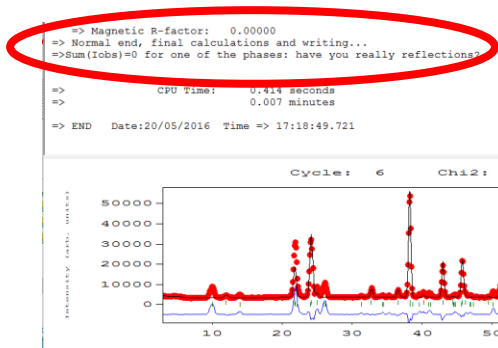
! Zero Code SyCos Code SySin Code Lambda Code MORE -> Patt# 1
0.04000 0.0 0.00000 0.0 0.00000 0.0 0.00000 0.00 0
!
! Data for PHASE number: 1 ==> Current R_Bragg for Pattern# 1: 19.75
!
! Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nuk Npr More
5 0 0 0.0 0.0 1.0 0 0 0 0 0 927.738 0 0 0
!
! 6/m m n <--Space group symbol
! Atom Typ X Y Z Biso Occ In Fin N_t Spc /Codes
Dy1 Dy 0.00000 0.00000 0.00000 0.00000 0.04167 0 0 0 0
0.00 0.00 0.00 0.00 0.00
Mn1 Mn 0.50000 0.00000 0.25040 0.00000 0.25000 0 0 0 0
0.00 0.00 0.00 0.00 0.00
Ge1 Ge 0.33330 0.66670 0.00000 0.00000 0.08333 0 0 0 0
0.00 0.00 0.00 0.00 0.00
Ge2 Ge 0.33330 0.66670 0.50000 0.00000 0.08333 0 0 0 0
0.00 0.00 0.00 0.00 0.00
Ge3 Ge 0.00000 0.00000 0.34530 0.00000 0.08333 0 0 0 0
0.00 0.00 0.00 0.00 0.00
!-----> Profile Parameters for Pattern # 1
! Scale Shape1 Bvo Str1 Str2 Str3 Strain-Model
117.38 0.00000 1.72597 0.00000 0.00000 0.00000 0
21.00000 0.000 81.000 0.000 0.000 0.000
! U U W X Y GauSiz LorSiz Size-Modi
1.702200 -1.352255 0.422342 0.000000 0.000000 0.000000 0
31.000 41.000 51.000 0.000 0.000 0.000
! a b c alpha beta gamma #Cell Info
5.206125 5.206125 8.151433 90.000000 90.000000 120.000000
11.00000 11.00000 61.00000 0.00000 0.00000 11.00000
! Pref1 Pref2 Asu1 Asu2 Asu3 Asu4
0.00000 0.00000 -0.01184 0.00000 0.00000 0.00000
0.00 0.00 71.00 0.00 0.00 0.00
! 2Th1/TOF1 2Th2/TOF2 Pattern to plot
0.00 82.900 1

```

2→insert
magnetic
phase

Step 4: Adding the magnetic phase

- The correct profile parameters were refined for the nuclear phase and should be copied into the magnetic phase. Paste in the line before
! Propagation vectors:
- Close and save the Text of the pcr with both the magnetic and nuclear phases.
- To check the phases were added correctly run a refinement. Since no intensity has been added to the coefficients for the magnetic phase this should give the same refinement as for just the nuclear phase, but with a comment to indicate zero intensity is coming from one of the phases.



Copy

```

76.9000 3603.0000 0.00
78.7000 3515.0000 0.00
79.1000 3515.0000 0.00
82.5000 3581.0000 0.00
82.8000 3581.0000 0.00

8 #Number of refined parameters
Zero Code SyCos Code SySin Code Lambda Code MORE -> Patt# 1
0.04000 0.0 0.00000 0.0 0.00000 0.0 0.000000 0.00 0

Data for PHASE number: 1 ==> Current R_Bragg for Pattern# 1: 19.75

Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nuk Npr More
5 0 0 0.0 0.0 1.0 0 0 0 0 0 0 0 0 0 0 0 0

P 6/m m m <--Space group symbol
taton Typ X Y Z Biso Occ In Fin H t Spc /Codes
Dy1 Dy 0.00000 0.00000 0.00000 0.00000 0.04167 0 0 0 0 0
Hn1 Hn 0.50000 0.00000 0.25040 0.00000 0.25000 0 0 0 0 0
Ge1 Ge 0.33330 0.66670 0.00000 0.00000 0.08333 0 0 0 0 0
Ge2 Ge 0.33330 0.66670 0.50000 0.00000 0.08333 0 0 0 0 0
Ge3 Ge 0.00000 0.00000 0.34530 0.00000 0.08333 0 0 0 0 0

Profile Parameters for Pattern # 1
Scale Shape1 Bov STR1 STR2 STR3 Strain-Model
117.38 0.00000 1.72597 0.00000 0.00000 0.00000 0
21.00000 0.000 81.000 0.000 0.000 0.000
U U V X Y GausSiz LorSiz Size-Model
1.702209 -1.352255 0.422342 0.00000 0.00000 0.00000 0
31.000 41.000 51.000 0.000 0.000 0.000 0
a b c alpha beta gamma NCell Info
5.206125 5.206125 8.151433 90.000000 90.000000 120.000000
11.00000 11.00000 61.00000 0.00000 0.00000 11.00000
Pref1 Pref2 Asy1 Asy2 Asy3 Asy4
0.00000 0.00000 -0.01184 0.00000 0.00000 0.00000
0.00 0.00 71.00 0.00 0.00 0.00

Data for PHASE number: 1 ==> Current R_Bragg for Pattern# 1: 1.00

Magnetic Phase
Nat Dis Mon Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nuk Npr More
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

C4 C5 C6 C7 C8 C9 MagPh
DY1 MDY3 1 0 0.00000 0.00000 0.00000 0.00000 0.00000 0.000 0.000 0.000
0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
NM2 NMN3 2 0 0.50000 0.00000 0.25040 0.00000 1.00000 0.000 0.000 0.000
0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
NM3 NMN3 3 0 0.00000 0.50000 0.74960 0.00000 1.00000 0.000 0.000 0.000
0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

Profile Parameters for Pattern # 1
Scale Shape1 Bov STR1 STR2 STR3 Strain-Model
117.38 0.00000 1.72597 0.00000 0.00000 0.00000 0
21.00000 0.000 81.000 0.000 0.000 0.000
U U V X Y GausSiz LorSiz Size-Model
1.702209 -1.352255 0.422342 0.00000 0.00000 0.00000 0
31.000 41.000 51.000 0.000 0.000 0.000 0
a b c alpha beta gamma NCell Info
5.206125 5.206125 8.151433 90.000000 90.000000 120.000000
11.00000 11.00000 61.00000 0.00000 0.00000 11.00000
Pref1 Pref2 Asy1 Asy2 Asy3 Asy4
0.00000 0.00000 -0.01184 0.00000 0.00000 0.00000
0.00 0.00 71.00 0.00 0.00 0.00

Propagation vectors:
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
2Th1/TOF1 2Th2/TOF2 Pattern to plot
3.000 82.900 1

```

Paste

Step 5: Fitting a magnetic model: SDW

- Consider first a real only solution $\Gamma(2)$ that will yield a spin-density-wave for the incommensurate k-vector.
- As discussed fix MN2 to be proportional to MN3 [1]
- Model with $\Gamma(2)$ corresponds to C1. Put anti-parallel moments on Dy and Mn as shown in [2].
- Close and save.
- Run the refinement until it has converged.

P -1 <--Space group symbol for hkl generation

† Nsym Cen Laue Irep N_Bas

5 1 10 -3 5

† Real(0)-Imaginary(1) indicator for Ci

0 0 0 0 0

†

SYMM X Y Z $\Gamma(2)$ $\Gamma(5)$

BASR	0	0	12	6	6	0	3.46	-3.5	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	2	2	0	2	-2	0	0	1	0	-2	-1	0	0
BASI	0	0	0	0	0	0	0	0	0	0	1.73	0	-3.5	-1.7	0	0
BASR	0	0	4	2	2	0	2	-2	0	-2	0	0	-2	-4	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SYMM	-	X-Y, Z														
BASR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	1	0	0	-1	-2	0	-1	-1	0	1	-1	0	0
BASI	0	0	0	3	0	0	-1.7	-3.5	0	1.73	1.73	0	-1.7	1.73	0	0
BASR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SYMM	-	+Y+1, -X+1, Z														
BASR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	0	1	0	2	1	0	-2	0	0	-2	-4	0	0
BASI	0	0	0	0	-1.7	0	-3.5	-1.7	0	0	0	0	0	0	0	0
BASR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SYMM	-	+1, X-Y+1, Z														
BASR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	1	0	0	-1	-2	0	0	1	0	-2	-1	0	0
BASI	0	0	0	3	0	0	-1.7	-3.5	0	0	1.73	0	-3.5	-1.7	0	0
SYMM	-	+Y, -X, Z														
BASR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	0	1	0	2	1	0	-1	-1	0	1	-1	0	0
BASI	0	0	0	0	-1.7	0	-3.5	-1.7	0	1.73	1.73	0	-1.7	1.73	0	0

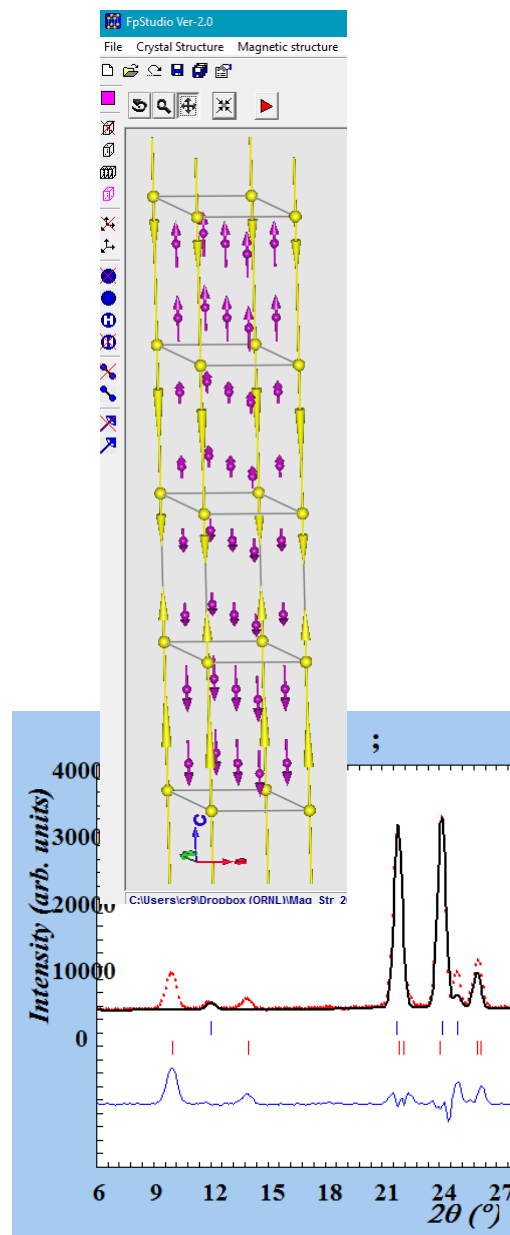
† Atom

Atom	Typ	Mag	Ueq	X	Y	Z	Biso	Occ	C1	C2	C3
DY1	MDY3	1	0	0.00000	0.00000	0.00000	0.30000	1.00000	1.000	0.000	0.000
				0.00	0.00	0.00	0.00	0.00	711.00	0.00	0.00
				0.000	0.000	0.000	0.000	0.00000			
				0.00	0.00	0.00	0.00	0.00			
MN2	MMN3	2	0	0.50000	0.00000	0.25040	0.30000	1.00000	-1.000	0.000	0.000
				0.00	0.00	0.00	0.00	0.00	811.00	0.00	0.00
				0.000	0.000	0.000	0.000	0.00000			
				0.00	0.00	0.00	0.00	0.00			
MN3	MMN3	2	0	0.00000	0.50000	0.74960	0.30000	1.00000	-1.000	0.000	0.000
				0.00	0.00	0.00	0.00	0.00	811.00	0.00	0.00
				0.000	0.000	0.000	0.000	0.00000			
				0.00	0.00	0.00	0.00	0.00			

1 2

Step 5: Fitting a magnetic model: SDW

- Spin structure can be visualized by opening .fst file for magnetic phase (created name ends in 2) with FPStudio.
- Visualized unit cells can be increased to follow the SDW as the magnitude of the moment varies along c-axis.
- Check prf file and fst to see $\Gamma(2)$ model
- Recall neutrons measure the moment perpendicular to Q. So intensity at these reflections correspond to c-axis spins.
- Zero intensity at 10 and 14 degs corresponding to (001) reflections. Only ab-plane will give intensity.
- The spins form a SDW. To define a helical structure the Real and Imaginary components have to be orthogonal. As an example edit the BVs in the pcr file for the Dy atom to create a helical structure.



Step 5: Fitting a magnetic model: Helical

- Consider ab-plane spins only $\Gamma(5)$. Note complex nature.
- Reasonable starting model given knowledge of compound is to have Dy-Dy and Mn-Mn ferromagnetic and Dy-Mn antiferromagnetic.
- This is achieved using BV(1) and BV(2) for Dy (c2,c3 in Fullprof) and BV(3) and BV(5) for Mn (c3,c5 in Fullprof). Combining these BVs will give spins for Mn along the b-axis.
- Save and refine.

P -1 <--Space group symbol for hkl generation

! Nsym Cen Laue Irep N_Bas

5 1 10 -3 5

! Real(0)-Imaginary(1) indicator for Ci

0 0 0 0 0

!

SYMM X, Y, Z

BASR	0	0	12	6	6	0	3.46	-3.5	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	2	2	0	2	-2	0	0	1	0	-2	-1	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	1.73	0	-3.5	-1.7	0	0	0	0
BASR	0	0	4	2	2	0	2	-2	0	-2	0	0	2	-1	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

SYMM -Y, X-Y, Z

BASR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	1	0	0	-1	-2	0	-1	-1	0	1	-1	0	0	0	0
BASI	0	0	0	1.73	0	0	-1.7	-3.5	0	1.73	1.73	0	-1.7	1.73	0	0	0	0
BASR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

SYMM -X+Y+1, -X+1, Z

BASR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	0	1	0	2	1	0	-2	0	0	-2	-4	0	0	0	0
BASI	0	0	0	0	-1.7	0	-3.5	-1.7	0	0	0	0	0	0	0	0	0	0
BASR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

SYMM -Y+1, X-Y+1, Z

BASR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	1	0	0	-1	-2	0	0	1	0	-2	-1	0	0	0	0
BASI	0	0	0	1.73	0	0	-1.7	-3.5	0	0	1.73	0	-3.5	-1.7	0	0	0	0

SYMM -X+Y, -X, Z

BASR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	0	1	0	2	1	0	-1	-1	0	1	-1	0	0	0	0
BASI	0	0	0	0	-1.7	0	-3.5	-1.7	0	1.73	1.73	0	-1.7	1.73	0	0	0	0

!

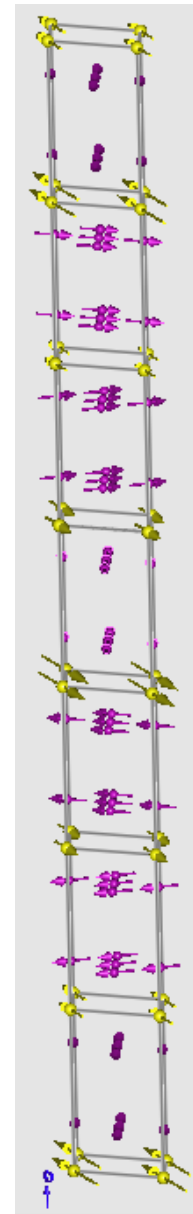
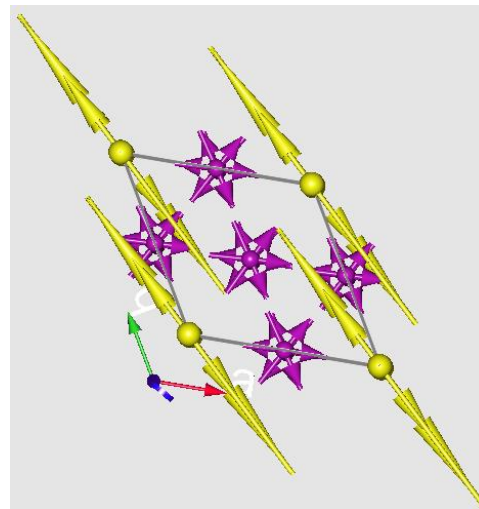
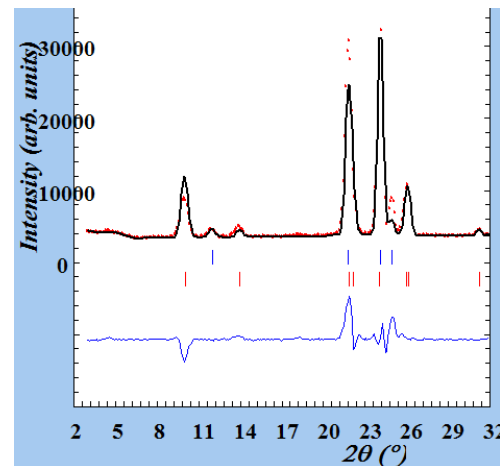
!Atom Typ Mag Vek X Y Z Biso Occ C1 C2 C3

! C4 C5 C6 C7 C8 C9 MagPh

DY1	MDY3	1	0	0.00000	0.00000	0.00000	0.30000	1.00000	0.000	0.500	-1.000
				0.00	0.00	0.00	0.00	0.00	0.00	21.00	11.00
				0.00	0.00	0.00	0.00	0.00	0.00		
				0.00	0.00	0.00	0.00	0.00	0.00		
				0.00	0.00	0.00	0.00	0.00	0.00		
MN2	MMN3	2	0	0.50000	0.00000	0.25040	0.30000	1.00000	0.000	0.000	1.000
				0.00	0.00	0.00	0.00	0.00	0.00	0.00	701.00
				1.000	0.000	0.000	0.000	0.000	0.000		
				701.00	0.00	0.00	0.00	0.00	0.00		
MN3	MMN3	2	0	0.00000	0.50000	0.74960	0.30000	1.00000	0.000	0.000	1.000
				0.00	0.00	0.00	0.00	0.00	0.00	0.00	701.00
				1.000	0.000	0.000	0.000	0.000	0.000		
				701.00	0.00	0.00	0.00	0.00	0.00		

Step 5a: Fitting a magnetic model ***edit***

- Check prf file and fst to see fit for the $\Gamma(5)$ model with chosen BVs.
- Intensity at 10 and 14 degs corresponding to (001) reflections.
- Spin structure can be visualized by opening .fst file for magnetic phase (created name ends in 2) with FPStudio.
- Visualized unit cells can be increased to follow the Helical Mn and SDW Dy.
- To define a helical structure the Real and Imaginary components have to be orthogonal. This occurs for the chosen of BVs of Mn.

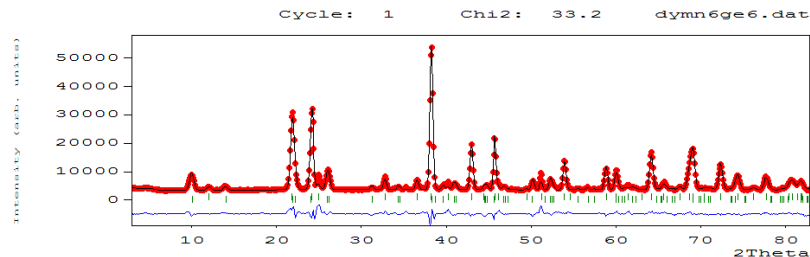


Step 5a: Fitting a magnetic model

- Neither $\Gamma(2)$ or $\Gamma(5)$ alone is a suitable model, so combine both by allowing c1 [$\Gamma(2)$, BV(1)] to refine, along with $\Gamma(5)$.
- The model now gives intensity to all measured peaks.

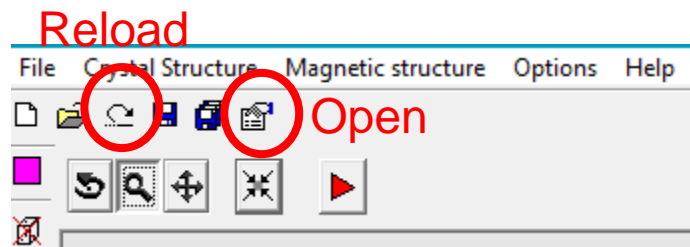
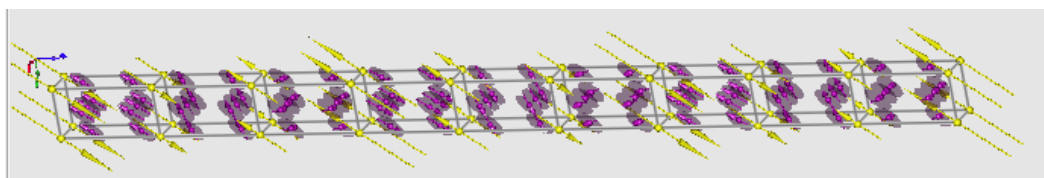
```
FullProf Program
Load Edit PCR Mode Run Exit
=> Conventional Rietveld R-factors for Pattern: 1
=> Rp: 14.6 Rwp: 15.8 Rexp: 2.75 Chi2: 33.2
=> Global user-weighted Chi2 (Bragg contrib.): 35.3369
=> -----> Pattern# 1
=> Phase: 1
=> Bragg R-factor: 8.89069
=> RF-factor: 6.02289
=> Phase: 2
=> Magnetic R-factor: 12.3464
=> Normal end, final calculations and writing...

=> CPU Time: 0.328 seconds
=> 0.005 minutes
=> END Date:23/05/2016 Time => 13:52:06.774
```

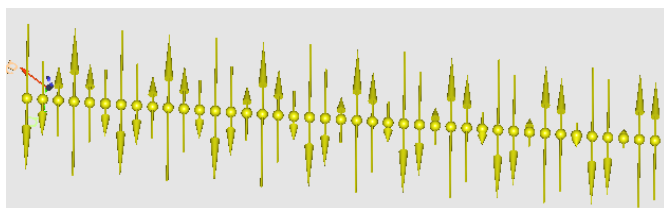


```
P -1 <--Space group symbol for hkl generation
! Nsym Cen Laue Irep N_Bas
! 5 1 10 -3 5
! Real(0)-Imaginary(1) indicator for Ci
0 0 0 0 0
!
SYMM X, Y, Z
BASF 0 0 12 6 6 0 3.46 -3.5 0 0 0 0 0 0 0
BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASF 0 0 4 2 2 0 2 -2 0 0 1 0 -2 -1 0
BASI 0 0 0 0 0 0 0 0 0 0 1.73 0 -3.5 -1.7 0
BASF 0 0 4 2 2 0 2 -2 0 -2 0 0 -2 -4 0
BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
SYMM -Y, X-Y, Z
BASF 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASF 0 0 4 1 0 0 -1 -2 0 -1 -1 0 1 -1 0
BASI 0 0 0 1.73 0 0 -1.7 -3.5 0 1.73 1.73 0 -1.7 1.73 0
BASF 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
SYMM -X+Y+1, -X+1, Z
BASF 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASF 0 0 4 0 1 0 2 1 0 -2 0 0 -2 -4 0
BASI 0 0 0 0 -1.7 0 -3.5 -1.7 0 0 0 0 0 0 0
BASF 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
SYMM -Y+1, X-Y+1, Z
BASF 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASF 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASF 0 0 4 1 0 0 -1 -2 0 0 1 0 -2 -1 0
BASI 0 0 0 1.73 0 0 -1.7 -3.5 0 0 1.73 0 -3.5 -1.7 0
SYMM -X+Y, -X, Z
BASF 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASF 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASF 0 0 4 0 1 0 2 1 0 -1 -1 0 1 -1 0
BASI 0 0 0 0 -1.7 0 -3.5 -1.7 0 1.73 1.73 0 -1.7 1.73 0
!
!Atom Typ Mag Vek X Y Z Biso Occ C1 C2 C3
! C4 C5 C6 C7 C8 C9 MagPh
DY1 MDY3 1 0 0.00000 0.00000 0.00000 0.30000 1.00000 1.000 0.363 -1.490
0.000 0.000 0.000 0.000 0.000 0.000 0.000000
0.000 0.000 0.000 0.000 0.000 0.000 0.000000
MN2 MDY3 2 0 0.50000 0.00000 0.25040 0.30000 1.00000 -1.000 0.000 0.736
0.000 0.736 0.000 0.000 0.000 0.000 0.000000
0.000 11.00 0.00 0.00 0.00 0.00 0.000000
MN3 MDY3 2 0 0.00000 0.50000 0.74960 0.30000 1.00000 -1.000 0.000 0.736
0.000 0.736 0.000 0.000 0.000 0.000 0.000000
0.000 11.00 0.00 0.00 0.00 0.00 0.000000
```

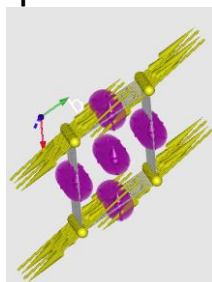
Step 5b: Fitting a magnetic model ***edit***



- Fst file can be edited to show envelope.



SDW for Dy



Helical for Mn

- Pitch of the rotation can be altered and unfixed from the real components to create a cycloidal structure, but this doesn't improve the fit.
- The magnitude of the magnetic moment size at any specific position can be seen with Fpstudio under:
"Magnetic structure" → "list moments"

```
File Edit Search
! FILE for FullProf Studio: generated automatically by FullProf
!Title: Magnetic Phase
SPACEG P 1
CELL 5.206289 5.206289 8.148093 90.0000 90.0000 120.0000 DISPLAY MULTIPLE
BOX -0.15 1.15 -0.15 1.15 -0.15 9.15

{
LATTICE P
K 0.00000 0.00000 0.16500
SYMM x,y,z
MSYM u,v,w,0.0
MATOM DY1_1
SKP Dy 0.00000 0.00000 0.00000 SCALE 1.0 GROUP
1 1 -1.43962 7.79939 7.43255 0.00000 0.00000 0.00000 0.00000
MATOM DY1_2
SKP Dy 0.00000 0.00000 0.00000 SCALE 1.0 GROUP
1 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
MATOM DY1_3
SKP Dy 1.00000 1.00000 0.00000 SCALE 1.0 GROUP
1 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
MATOM DY1_4
SKP Dy 1.00000 1.00000 0.00000 SCALE 1.0 GROUP
1 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
MATOM DY1_5
SKP Dy 0.00000 0.00000 0.00000 SCALE 1.0 GROUP
1 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
MATOM MN2_1
SKP Mn 0.50000 0.00000 0.25040 SCALE 1.0 GROUP ENVELOP
1 1 0.00000 -1.67971 -1.92814 -1.95966 -0.95184 0.00000 0.00000
MATOM MN2_2
SKP Mn 0.00000 0.50000 0.25040 SCALE 1.0 GROUP ENVELOP
1 1 0.00000 -1.67971 -1.92814 -1.90367 -0.99103 0.00000 0.00000
MATOM MN2_3
SKP Mn 0.50000 0.50000 0.25040 SCALE 1.0 GROUP ENVELOP
1 1 0.00000 -1.67971 -1.92814 -1.95966 -0.95184 0.00000 0.00000
MATOM MN2_4
SKP Mn 1.00000 1.50000 0.25040 SCALE 1.0 GROUP ENVELOP
1 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
MATOM MN2_5
SKP Mn -0.50000 -0.50000 0.25040 SCALE 1.0 GROUP ENVELOP
1 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
MATOM MN3_1
SKP Mn 0.00000 0.50000 0.74960 SCALE 1.0 GROUP ENVELOP
1 1 0.00000 -1.67971 -1.92814 -1.95966 -0.95184 0.00000 0.00000
MATOM MN3_2
SKP Mn -0.50000 -0.50000 0.74960 SCALE 1.0 GROUP ENVELOP
1 1 0.00000 -1.67971 -1.92814 -1.90367 -0.99103 0.00000 0.00000
MATOM MN3_3
SKP Mn 1.50000 1.00000 0.74960 SCALE 1.0 GROUP ENVELOP
1 1 0.00000 -1.67971 -1.92814 -1.95966 -0.95184 0.00000 0.00000
MATOM MN3_4
SKP Mn 0.50000 0.50000 0.74960 SCALE 1.0 GROUP ENVELOP
1 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
MATOM MN3_5
SKP Mn 0.50000 0.00000 0.74960 SCALE 1.0 GROUP ENVELOP
1 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
}
```

Alternative solution with two k-vectors

- While the magnetic fit to SDW or Helical is good, it is not the final solution.
- An alternative solution is to use two propagation vectors, $k_1=(0,0,0)$ and $k_2=(0,0,0.165)$.

Rodriguez-Carvajal & Bouree EPJ 22, 00010 (2012)

- Check with SARAh the solutions for $k=(0,0,0)$.
→ The same IRs are solutions as previously used.
- The physics tells us $k=(000)$ is the FM c-axis.
- $\Gamma(2)$ corresponds to k_1 and $\Gamma(5)$ corresponds to k_2 .
- This solution is included in the folders, but can be readily produced by following the previous steps in this example.

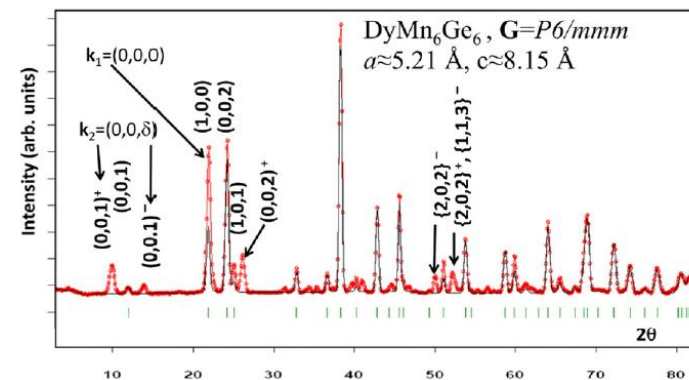
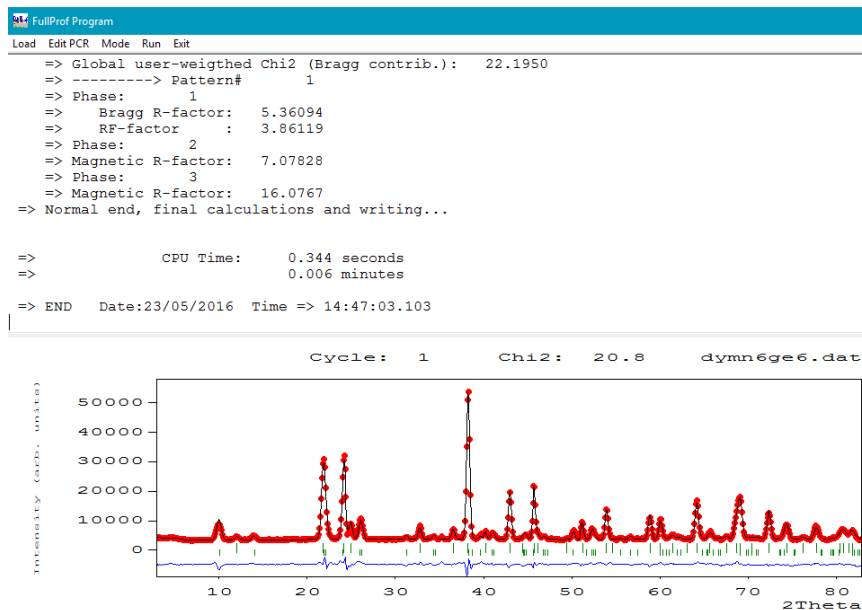


Figure 19. Powder diffraction pattern of DyMn_6Ge_6 at 11 K taken at DMC (PSI) with $\lambda = 2.425 \text{ \AA}$. The first propagation vector is $k_1 = (0, 0, 0)$ and the second one is $k_2 = (0, 0, \delta)$ with $\delta \approx 0.1651(4)$, quite close to $\delta = 1/6$. The calculated nuclear diffraction pattern is shown as a continuous line.

Alternative solution with two k-vectors

- Change number of phases to 3.
- Create the 3rd magnetic phase by copying and pasting the current magnetic phase.
- Alter the propagation vector of phase 2 to $k=(0,0,0)$ and make all coefficients apart from C1 zero. i.e. $k=(0,0,0)$ corresponds only to $\Gamma(2)$.
- For phase 3 make C1 values zero i.e $k=(0,0,0.165)$ corresponds only to $\Gamma(2)$.
- Refinement now is improved further.



```

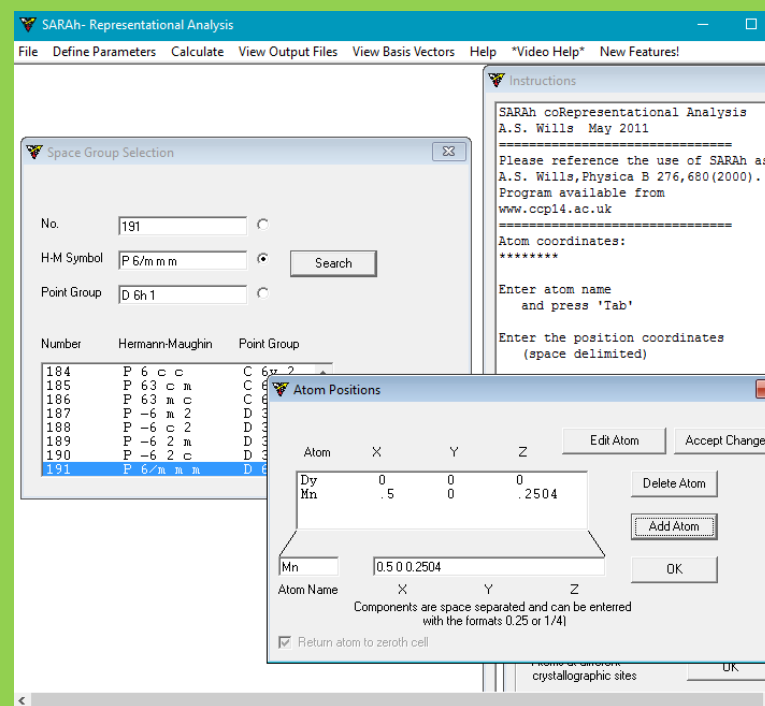
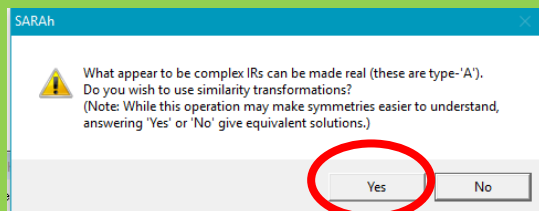
COMM ;
! Files -> DLT-file: XXXXXXXXXXXXXXXXXXXX, PCR-file: dymn6ge6
! Job Np Nph Npa Npc Npc Nor Dum Iwg Ilo Ias Res Ste Nre Cry Uni
! 1 3 38 0 0 0 0 0 0 0 0 0 0 0 0
!
! Ipr Ppl Ioc Mat Pcr Ls1 Ls2 Ls3 NLI Prf Ins Rpa Sym Hkl Fou Sho
! 0 0 1 0 1 0 4 0 0 3 8 0 0 0 0 0
!
! Lambda1 Lambda2 Ratio Bkpos Wdt Cthm muR As
! 1.703700 1.703700 1.00000 40.000 5.0000 0.0000 1.2800 18
!
! NNCY Eps R_at R_an R_pr R_gl Thmin Step Thm
! 6 0.50 1.00 1.00 1.00 1.00 3.0000 0.100000 82.9
!
! 2Theta/TOF/E (Kev) Background for Pattern# 1
! -----
!
! Atom Type Mag Vet X Y Z Biso Occ C1 C2 C3
! C4 C5 C6 C7 C8 C9 MagPh
! DT1 MDY3 1 0 0.00000 0.00000 0.00000 0.30000 1.00000 0.411 0.000 0.000
! 0.000 0.000 0.000 0.000 0.000 0.000 0.000
! 0.00 0.00 0.00 0.00 0.00 0.00 0.00
! MN2 MDY3 2 0 0.50000 0.00000 0.25000 0.30000 1.00000 -0.288 0.000 0.000
! 0.000 0.000 0.000 0.000 0.000 0.000 0.000
! 0.00 0.00 0.00 0.00 0.00 0.00 0.00
! MN3 MDY3 2 0 0.00000 0.50000 0.74960 0.30000 1.00000 -0.288 0.000 0.000
! 0.000 0.000 0.000 0.000 0.000 0.000 0.000
! 0.00 0.00 0.00 0.00 0.00 0.00 0.00
!
! -----> Profile Parameters for Pattern# 1
! Scale Shap1 Bwv Str1 Str2 Str3 Strain-Model
! 95.044 0.00000 0.96612 0.00000 0.00000 0.00000 0
! 51.00000 0.000 0.000 0.000 0.000 0.000
! U V W X Y GauSis LorSis Size-Model
! 1.932143 -1.589736 0.469940 0.000000 0.000000 0.000000 0.000000 0
! 61.000 71.000 81.000 0.000 0.000 0.000 0.000
! a b c alpha beta gamma #Cell Info
! 5.206095 5.206095 8.149457 90.000000 90.000000 120.000000
! 41.00000 41.00000 51.00000 0.00000 0.00000 41.00000
! Pref1 Pref2 Asy1 Asy2 Asy3 Asy4
! 0.00000 0.00000 0.01425 0.00000 0.00000 0.00000
! 0.00 0.00 51.00 0.00 0.00 0.00
! Propagation vectors:
! 0.000000 0.000000 0.000000 Propagation Vector 1
! 0.000000 0.000000 0.000000
!
! -----> Data for PHASE number: 3 ==> Current R_Bragg for Pattern# 1: 0.00
!
! Magnetic Phase
!
! Nat Dis Mom Pr1 Pr2 Pr3 Ubt Irf Isy Str Furth ATZ Nvk Npr More
! 2 0 0 0.0 0.0 1.0 1 0 -1 -2 0 0 0.000 -1 0 0
!
! P -1
!
! -----> Space group symbol for hkl generation
! Nsym Cen Laue Irep N_Bas
! 5 1 10 -2 5
  
```

Supplemental Material:

- Fit solution using only real BVs outputted from SARAh Representational Analysis
- More intuitive, but requires knowledge of system.
- Makes BVs for commensurate and SDW easier to interpret.
- Imaginary component can be added to create e.g. Helical, BUT care should be taken to make sure it is appropriate (loose symmetry constraints).

Step 3(Real IRs): Symmetry analysis

- Use SARAh (or Baslreps) to generate the Irreducible Representations (IRs) and basis vectors (BVs) associated with the propagation vectors, crystal structure and magnetic atom positions.
- Open SARAh- Representational analysis
- Under “Define Parameters” input:
 “Space group” No. 191 or H_M Symbol P 6/m m m
 “K-vector” 0 0 0.165
 “Atoms” Dy 0 0 0
 Mn 0.5 0 0.2504
- Run program using “Calculate”
 Select directory where the created output files will go (i.e. current directory).
 Some pop windows will appear during calculation. For source of IR select Kovalev and “Yes” so the solution will be easier to interpret, although not imaginary.



Step 3(Real IRs): Symmetry analysis

- SARAh outputs several files to explain the allowed symmetries.
- From pdf created from .tex file:

IR	BV	Atom	BV components					
			$m_{\parallel a}$	$m_{\parallel b}$	$m_{\parallel c}$	$im_{\parallel a}$	$im_{\parallel b}$	$im_{\parallel c}$
Γ_2	ψ_1	1	0	0	12	0	0	0
Γ_5	ψ_2	1	0	3	0	0	0	0
	ψ_3	1	3.464	1.732	0	0	0	0

Table 1: Basis vectors for the space group P 6/m m m with $\mathbf{k}_{11} = (0, 0, .165)$. The decomposition of the magnetic representation for the Dy site $(0, 0, 0)$ is $\Gamma_{Mag} = 0\Gamma_1^1 + 1\Gamma_2^1 + 0\Gamma_3^1 + 0\Gamma_4^1 + 1\Gamma_5^2 + 0\Gamma_6^2$. The atom of the primitive basis is defined according to 1: $(0, 0, 0)$.

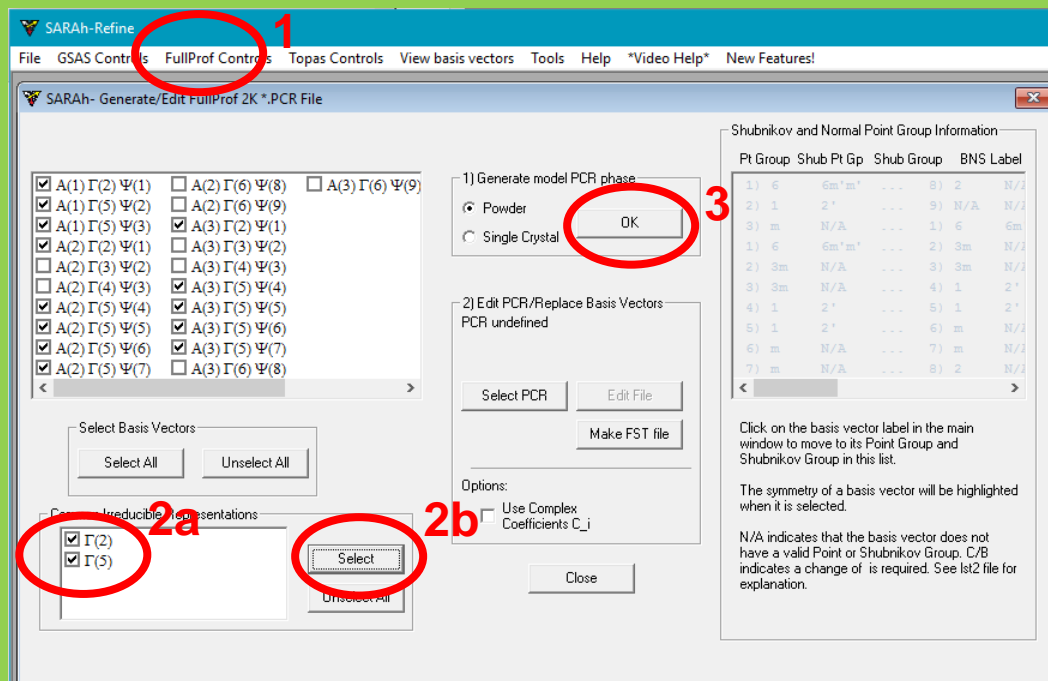
- Γ_2 and Γ_5 form the common IRs. Both Γ_2 (c-axis) and Γ_5 (ab-plane) will be needed.
- The Mn is split into 2 orbits (3 atoms at $z=0.2504$ and 3 at $z=0.7496$). For this exercise we will fix both orbits to be the same (in or out of phase). This reduces the free parameters to make the problem more tractable. Moreover for in this kind of compound generally the Mn-Mn interactions are ferromagnetic suggesting constrained orbits.

IR	BV	Atom	BV components					
			$m_{\parallel a}$	$m_{\parallel b}$	$m_{\parallel c}$	$im_{\parallel a}$	$im_{\parallel b}$	$im_{\parallel c}$
Γ_2	ψ_1	1	0	0	4	0	0	0
		2	0	0	4	0	0	0
		3	0	0	4	0	0	0
Γ_3	ψ_2	1	2	0	0	0	0	0
		2	-2	-2	0	0	0	0
		3	0	2	0	0	0	0
Γ_4	ψ_3	1	2	4	0	0	0	0
		2	2	-2	0	0	0	0
		3	-4	-2	0	0	0	0
Γ_5	ψ_4	1	2	3	0	0	0	0
		2	-2	1	0	0	0	0
		3	0	-1	0	0	0	0
	ψ_5	1	0	-3	0	0	0	0
		2	0	-3	0	0	0	0
		3	0	-3	0	0	0	0
	ψ_6	1	0	1.732	0	0	0	0
		2	0	-1.732	0	0	0	0
		3	3.464	1.732	0	0	0	0
Γ_6	ψ_7	1	-3.464	-1.732	0	0	0	0
		2	-3.464	-1.732	0	0	0	0
		3	-3.464	-1.732	0	0	0	0
	ψ_8	1	0	0	3	0	0	0
		2	0	0	-3	0	0	0
		3	0	0	0	0	0	0
	ψ_9	1	0	0	1.732	0	0	0
		2	0	0	1.732	0	0	0
		3	0	0	-3.464	0	0	0

Table 2: Basis vectors for the space group P 6/m m m with $\mathbf{k}_{11} = (0, 0, .165)$. The decomposition of the magnetic representation for the Mn site $(.5, 0, .2504)$ is $\Gamma_{Mag} = 0\Gamma_1^1 + 1\Gamma_2^1 + 1\Gamma_3^1 + 1\Gamma_4^1 + 2\Gamma_5^2 + 1\Gamma_6^2$. The atoms of the nonprimitive basis are defined according to 1: $(.5, 0, .2504)$, 2: $(.5, .5, .2504)$, 3: $(0, .5, .2504)$.

Step 4(Real IRs): Adding the magnetic phase

- Open SARAh-Refine.
- Under “Fullprof Controls” [1] select “Load SARAh MAT file” and open file created by SARAh (sarah191.mat)
- Under “Common Irreducible Representations” check boxes next to both $\Gamma(2)$ and $\Gamma(5)$ and press select to associate all BVs. [2]



- Create the magnetic phase part of the PCR file by selecting “OK” next to “Generate model PCR phase” [3]. This creates a file “sarah191.pcr” that can be copied and pasted into the crystal structure pcr file from Step 1.
Note: only open the created “sarah191.pcr” with a text editor and not EdPCR.

Step 4(Real IRs): Adding the magnetic phase

- Open “sarah191.pcr” with a text editor (e.g. notepad++) and open the text of the structural refinement “dymn6ge6.pcr” (either from EdPCR or text editor).
- Change the number of phases to 2 since we will now have a nuclear and magnetic phase. [1]
- Copy and paste the created magnetic phase just before line
! 2Th1/TOF1 [2]
- Make sure there are no blank lines before or after the pasted section.

```
External EdPCR Text Editor - [C:\Users\cr9\Dropbox (ORNL)\Mag_Str_2016\Dy...
File Edit Search
! COMM ;
! Current global Chi2 (Bragg contrib.) = 214.8
! Files => DAT-file: dymn6ge6.dat, PCR-file: dymn6ge6
! Job Np Nph Nba Nex Nsc Nor Dum Iwg Ilo Ias Res Ste N
! 1 0 2 8 0 0 0 0 0 0 0 0 0 0
!
! Ipr Pp1 Ioc Mat Pcr Ls1 Ls2 Ls3 NLI Prf Ins Rpa Sym H
! 0 0 1 0 1 0 4 0 0 3 8 0 0
!
! Lambda1 Lambda2 Ratio Bkpos Wdt Cthm
! 1.703700 1.703700 1.00000 40.000 5.0000 0.0000
!
! NCY Eps R_at R_an R_pr R_gl Thmin Step
! 6 0.10 1.00 1.00 1.00 1.00 3.0000 0.1000
!
! 2Theta/TOF/E(Kev) Background for Pattern# 1
! 3.1300 4310.0000 0.00
! 2.0000 1111.0000 0.00
```

```
! Zero Code SyCos Code SySin Code Lambda Code MORE -> Patt# 1
! 0.04000 0.0 0.00000 0.0 0.00000 0.0 0.00000 0
!
! Data for PHASE number: 1 ==> Current R_Bragg For Pattern# 1: 19.75
!
! Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nuk Npr More
! 5 0 0 0.0 0.0 1.0 0 0 0 0 0 927.738 0 0 0
!
! P 6/m m m <--Space group symbol
! Atom Typ X Y Z Biso Occ In Fin N_t Spc /Codes
! Dy1 Dy 0.00000 0.00000 0.00000 0.00000 0.04167 0 0 0 0
! 0.00 0.00 0.00 0.00 0.00
! Mn1 Mn 0.50000 0.00000 0.25040 0.00000 0.25000 0 0 0 0
! 0.00 0.00 0.00 0.00 0.00
! Ge1 Ge 0.33330 0.66670 0.00000 0.00000 0.08333 0 0 0 0
! 0.00 0.00 0.00 0.00 0.00
! Ge2 Ge 0.33330 0.66670 0.50000 0.00000 0.08333 0 0 0 0
! 0.00 0.00 0.00 0.00 0.00
! Ge3 Ge 0.00000 0.00000 0.34530 0.00000 0.08333 0 0 0 0
! 0.00 0.00 0.00 0.00 0.00
!
! -----> Profile Parameters for Pattern # 1
! Scale Shape1 Bvo Str1 Str2 Str3 Strain-Model
! 117.38 0.00000 1.72597 0.00000 0.00000 0.00000 0
! 21.00000 0.000 81.000 0.000 0.000
!
! U U W X Y GauSiz LorSiz Size-Mod
! 1.702200 -1.352255 0.422342 0.000000 0.000000 0.000000 0
! 31.000 41.000 51.000 0.000 0.000 0.000
!
! a b c alpha beta gamma #Cell Info
! 5.206125 5.206125 8.151433 90.000000 90.000000 120.000000
! 11.00000 11.00000 61.00000 0.00000 0.00000 11.00000
!
! Pref1 Pref2 Asu1 Asu2 Asu3 Asu4
! 0.00000 0.00000 -0.01184 0.00000 0.00000 0.00000
! 0.00 0.00 71.00 0.00 0.00 0.00
!
! 2Th1/TOF1 2Th2/TOF2 Pattern to plot
! 3.1300 82.900 1
```

2→insert
magnetic
phase

Step 4(Real IRs): Adding the magnetic phase

- The correct profile parameters were refined for the nuclear phase and should be copied into the magnetic phase. Paste in the line before
! Propagation vectors:
- Close and save the Text of the pcr with both the magnetic and nuclear phases.
- To check the phases were added correctly run a refinement. Since no intensity has been added to the coefficients for the magnetic phase this should give the same refinement as for just the nuclear phase, but with a comment to indicate zero intensity is coming from one of the phases.

Copy

Paste

```

Zero Code SyCos Code SySin Code Lambda Code MORE ->Pat
0.04000 0.0 0.00000 0.0 0.00000 0.0 0.00000 0.00 0

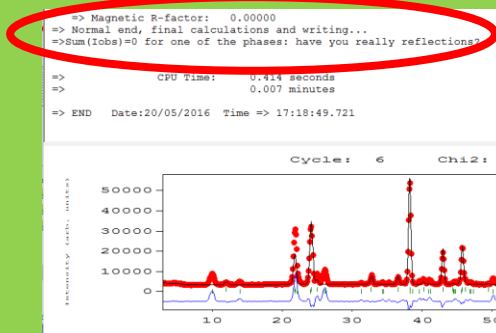
Data for PHASE number: 1 ==> Current R_Bragg for Pattern# 1: 0.00

!Mat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nuk Npr More
5 0 0 0.0 0.0 1.0 0 0 0 0 0 0 927.738 0 0 0

P 6/n m n <--Space group symbol
!Atom Typ X Y Z Biso Occ In Fin N t Spc
Dy1 Dy 0.00000 0.00000 0.00000 0.00000 0.04167 0 0 0 0 0
0.00 0.00 0.00 0.00 0.00 0.00
Mn1 Mn 0.50000 0.00000 0.25003 0.00000 0.25000 0 0 0 0 0
0.00 0.00 0.00 0.00 0.00 0.00
Ge1 Ge 0.33330 0.66670 0.00000 0.00000 0.08333 0 0 0 0 0
0.00 0.00 0.00 0.00 0.00 0.00
Ge2 Ge 0.33330 0.66670 0.50000 0.00000 0.08333 0 0 0 0 0
0.00 0.00 0.00 0.00 0.00 0.00
Ge3 Ge 0.00000 0.00000 0.34354 0.00000 0.08333 0 0 0 0 0
0.00 0.00 0.00 0.00 0.00 0.00

Profile Parameters for Pattern # 1
Scale Shape1 Bov Str1 Str2 Str3 Strain-Model
117.75 0.00000 1.73631 0.00000 0.00000 0.00000 0
21.00000 0.000 31.000 0.000 0.000 0.000
U V X Y GauSiz LorSiz
1.690659 -1.328530 0.421520 0.000000 0.000000 0.000000 0.000000
41.000 51.000 61.000 0.000 0.000 0.000 0.000
a b c alpha beta gamma #Cell I
5.206196 5.206196 8.151175 90.000000 90.000000 120.000000
11.00000 11.00000 71.00000 0.00000 0.00000 11.00000
Pref1 Pref2 Asy1 Asy2 Asy3 Asy4
0.00000 0.00000 -0.00944 0.00000 0.00000 0.00000
0.00 0.00 81.00 0.00 0.00 0.00

Data for PHASE number: 1 ==> Current R_Bragg for Pattern# 1: 1.00
Magnetic Phase
  
```



```

!Atom Typ Mag Ueq X Y Z Biso Occ C1 C2
DY1 DY1 1 0 0.00000 0.00000 0.00000 0.30000 1.00000 0.000 0.000
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
MN2 MN2 2 0 0.00000 0.00000 0.25000 0.30000 1.00000 0.000 0.000
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
MN3 MN3 3 0 0.00000 0.50000 0.74960 0.30000 1.00000 0.000 0.000
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

Profile Parameters for Pattern # 1
Scale Shape1 Bov Str1 Str2 Str3 Strain-Model
117.75 0.00000 1.73631 0.00000 0.00000 0.00000 0
21.00000 0.000 31.000 0.000 0.000 0.000
U V X Y GauSiz LorSiz
1.690659 -1.328530 0.421520 0.000000 0.000000 0.000000 0.000000
41.000 51.000 61.000 0.000 0.000 0.000 0.000
a b c alpha beta gamma #Cell I
5.206196 5.206196 8.151175 90.000000 90.000000 120.000000
11.00000 11.00000 71.00000 0.00000 0.00000 11.00000
Pref1 Pref2 Asy1 Asy2 Asy3 Asy4
0.00000 0.00000 -0.00944 0.00000 0.00000 0.00000
0.00 0.00 81.00 0.00 0.00 0.00

Propagation vectors:
0.000000 0.000000 0.165000 0.000000
0.000000 0.000000 0.000000 0.000000

Propagation Vector 1
  
```

Step 5a(Real IRs): Fitting a magnetic model: SDW

- Consider first a solution that will yield a spin-density-wave for the incommensurate k-vector. (BVs real)
- As discussed fix MN2 to be proportional to MN3 [1]
- Start model with $\Gamma(2)$. There is only one BV, corresponding to coefficients C1 in Fullprof. There is evidence for a ferrimagnetic component along the c-axis so put anti-parallel moments on Dy and Mn as shown in [2].
- Close and save.
- Run the refinement until it has converged.

P -1 <--Space group symbol for hkl generation

! Nsym Cen Laue Irep N_Bas

5 1 10 -3 5

! Real(0)-Imaginary(1) indicator for Ci

0 0 0 0 0

!

SYMM X, Y, Z $\Gamma(2)$ $\Gamma(5)$

BASR	0	0	12	0	3	0	3.46	1.73	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	2	3	0	0	-3	0	0	1.73	0	-3.5	-1.7	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	0	2	0	0	0	0	0	0	0	0	4	2	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SYMM	-Z, X-Y, Z															
BASR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	0	-1	0	0	-3	0	3.46	1.73	0	-3.5	-1.7	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SYMM	-Z+Y+1, -X+1, Z															
BASR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	-2	1	0	0	-3	0	0	-1.7	0	-3.5	-1.7	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SYMM	-Z+1, X-Y+1, Z															
BASR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	1	1	0	-1.7	1.73	0	1.73	1.73	0	1	-1	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SYMM	-Z+Y, -X, Z															
BASR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	-1	0	0	1.73	3.46	0	1.73	0	0	1	2	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

! Atom Typ Mag Vek X Y Z Biso Occ C1 C2 C3

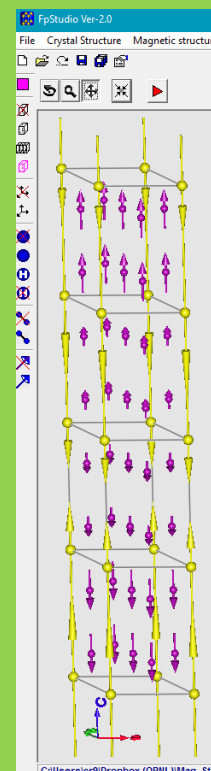
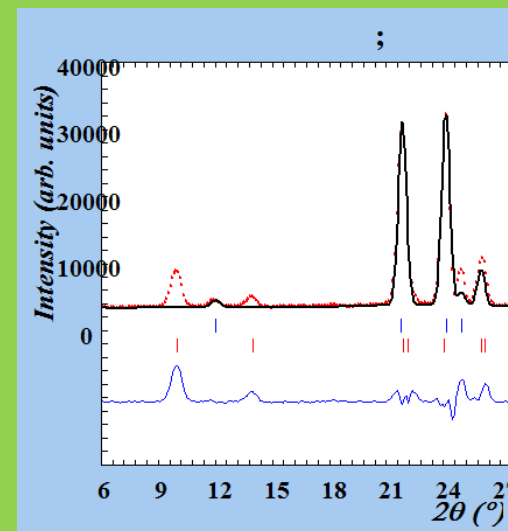
! C4 C5 C6 C7 C8 C9 MagPh

DY1	MDY3	1	0	0.00000	0.00000	0.00000	0.30000	1.00000	1.000	0.000	0.000
				0.00	0.00	0.00	0.00	0.00	711.00	0.00	0.00
				0.00	0.00	0.00	0.00	0.00000			
				0.00	0.00	0.00	0.00	0.00			
MN2	MN3	2	0	0.50000	0.00000	0.25040	0.30000	1.00000	-1.000	0.000	0.000
				0.00	0.00	0.00	0.00	0.00	811.00	0.00	0.00
				0.00	0.00	0.00	0.00	0.00000			
				0.00	0.00	0.00	0.00	0.00			
MN3	MN3	2	0	0.00000	0.50000	0.74960	0.30000	1.00000	-1.000	0.000	0.000
				0.00	0.00	0.00	0.00	0.00	811.00	0.00	0.00
				0.00	0.00	0.00	0.00	0.00000			
				0.00	0.00	0.00	0.00	0.00			

1 2

Step 5a(Real IRs): Fitting a magnetic model: SDW

- Check prf file and fst to see fit for the $\Gamma(2)$ model.
- Recall neutrons measure the moment perpendicular to Q. So intensity from $\Gamma(2)$ at reflections with H or L equal to zero, e.g around $2\theta=22^\circ$.
- Zero intensity at 10 and 14 degs corresponding to (001) reflections. Only ab-plane spins will give intensity for these reflections.
- Spin structure can be visualized by opening .fst file for magnetic phase (created name ends in 2) with FPStudio.
- Visualized unit cells can be increased to follow the SDW.



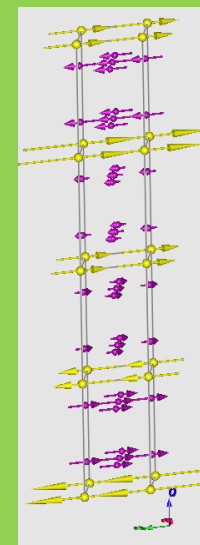
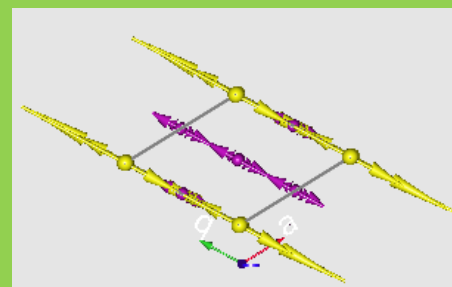
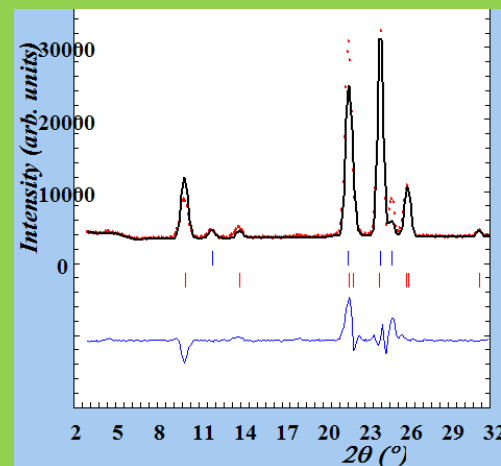
Step 5a(Real IRs): Fitting a magnetic model: SDW

- Consider ab-plane spins only $\Gamma(5)$.
- Reasonable starting model given knowledge of compound is to have Dy-Dy and Mn-Mn ferromagnetic and Dy-Mn antiferromagnetic.
- This is achieved using BV(1) for Dy (c2 in Fullprof) and BV(3) for Mn (c3 in Fullprof).
- Save and refine.

SYMM X, Y, Z												
BASR	0	0	12	0	3	0	3.46	1.73	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	2	3	0	0	-3	0	1.73	0	-3.5
BASI	0	0	0	0	0	0	0	0	0	0	0	-1.7
BASR	0	0	4	0	2	0	0	0	0	0	4	2
BASI	0	0	0	0	0	0	0	0	0	0	0	0
SYMM -Y, X-Y, Z												
BASR	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	0	-1	0	0	-3	0	3.46	1.73	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0
SYMM -X+Y+1, -X+1, Z												
BASR	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	-2	1	0	0	-3	0	0	-1.7	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0
SYMM -Y+1, X-Y+1, Z												
BASR	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	1	1	0	-1.7	1.73	0	1.73	1.73	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0
SYMM -X+Y, -X, Z												
BASR	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	-1	0	0	1.73	3.46	0	1.73	0	1
BASI	0	0	0	0	0	0	0	0	0	0	0	2
?												
!Atom	Typ	Mag	Ueq	X	Y	Z	Biso	Occ	C1	C2	C3	
!C4		C5	C6	C7	C8	C9	MagPh					
DY1	MDY3	1	0	0.00000	0.00000	0.00000	0.30000	1.00000	0.000	1.0	0.000	
				0.00	0.00	0.00	0.00	0.00	0.00	811.0	0.00	
		0.000	0.000	0.000	0.000	0.000	0.000	0.00000				
		0.00	0.00	0.00	0.00	0.00	0.00	0.00				
MN2	MMN3	2	0	0.50000	0.00000	0.25040	0.30000	1.00000	0.000	0.00	1.000	
				0.00	0.00	0.00	0.00	0.00	0.00	0.0	711.00	
		0.000	0.000	0.000	0.000	0.000	0.000	0.00000				
		0.00	0.00	0.00	0.00	0.00	0.00	0.00				
MN3	MMN3	2	0	0.00000	0.50000	0.74960	0.30000	1.00000	0.000	0.0	1.000	
				0.00	0.00	0.00	0.00	0.00	0.00	0.00	711.00	
		0.000	0.000	0.000	0.000	0.000	0.000	0.00000				
		0.00	0.00	0.00	0.00	0.00	0.00	0.00				

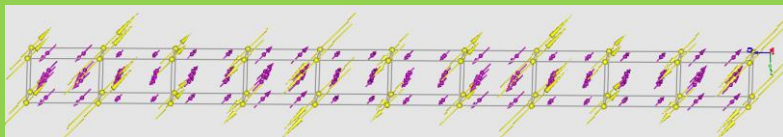
Step 5a(Real IRs): Fitting a magnetic model: SDW

- Check prf file and fst to see fit for the $\Gamma(5)$ model with chosen BVs.
- Intensity at 10 and 14 degs corresponding to (001) reflections.
- Spin structure can be visualized by opening .fst file for magnetic phase (created name ends in 2) with FPStudio.
- Visualized unit cells can be increased to follow the SDW.

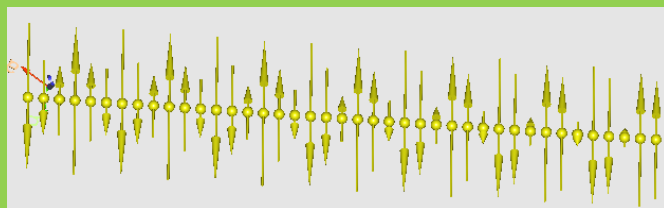


Step 5a(Real IRs): Fitting a magnetic model: SDW

- Neither $\Gamma(2)$ or $\Gamma(5)$ alone is a suitable model, so combine both by allowing c1 [$\Gamma(2)$, BV(1)] to refine.
- The model now gives intensity to all measured peaks.



SDW



- The magnitude of the magnetic moment size at any specific position can be seen with Fpstudio under: “Magnetic structure” → “list moments”

SYMM X, Y, Z												
BASR	0	0	12	0	3	0	3.46	1.73	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	2	3	0	0	-3	0	0	1.73	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	0	2	0	0	0	0	0	0	4
BASI	0	0	0	0	0	0	0	0	0	0	0	0
SYMM -Y, X-Y, Z												
BASR	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	0	-1	0	0	-3	0	3.46	1.73	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0
SYMM -X+Y+1, -X+1, Z												
BASR	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	-2	1	0	0	-3	0	0	-1.7	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0
SYMM -Y+1, X-Y+1, Z												
BASR	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	1	1	0	-1.7	1.73	0	1.73	1.73	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0
SYMM -X+Y, -X, Z												
BASR	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	0	0	0	0	0	0	0	0	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0
BASR	0	0	4	-1	0	0	1.73	3.46	0	1.73	0	0
BASI	0	0	0	0	0	0	0	0	0	0	0	0
!												
!Atom	Typ	Mag	Ueq	X	Y	Z	Biso	Occ	C1	C2	C3	
?	C4	C5	C6	C7	C8	C9		MagPh				
DY1	MDY3	1	0	0.00000	0.00000	0.00000	0.30000	1.00000	1.000	3.061	0.000	
				0.00	0.00	0.00	0.00	0.00	911.00	91.00	0.00	
		0.000	0.000	0.000	0.000	0.000	0.000	0.000000				
		0.00	0.00	0.00	0.00	0.00	0.00	0.00				
MN2	MMN3	2	0	0.50000	0.00000	0.25000	0.30000	1.00000	-1.000	0.000	0.826	
				0.00	0.00	0.00	0.00	0.00	811.00	0.00	101.00	
		0.000	0.000	0.000	0.000	0.000	0.000	0.000000				
		0.00	0.00	0.00	0.00	0.00	0.00	0.00				
MN3	MMN	2	0	0.00000	0.50000	0.74960	0.30000	1.00000	-1.000	0.000	0.826	
				0.00	0.00	0.00	0.00	0.00	811.00	0.00	101.00	
		0.000	0.000	0.000	0.000	0.000	0.000	0.000000				
		0.00	0.00	0.00	0.00	0.00	0.00	0.00				

Model can be slightly improved by adding equal and opposite components to C5

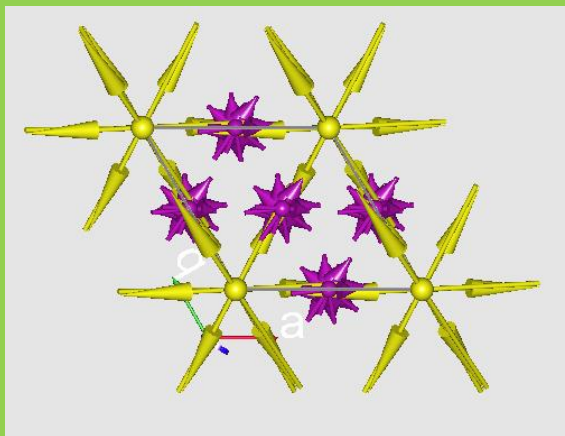
Step 5b(Real IRs): Fitting a magnetic model: Helical

- An alternative to a SDW (varying spin magnitude) is rotating spins forming a helical or cycloidal structure.
- To define a helical structure the Real and Imaginary components have to be orthogonal. This dictates the choice of BVs.
- Copy and paste C2-C5 and make these new coefficients (C6-C9) imaginary by adding 1s to the circled indicator.
- Alter N bas to 9

P -1
 ! Nsym Cen Laua Irepas Bas
 ! 5 1 10 -3 9
 ! Real(0)-Imaginary(1) and Cartesian for Ci
 0 0 0 0 0 1 1 1 1
 !
 SYMM X, Y, Z
 BASR 0 0 0 12
 BASI 0 0 0 0
 BASR 0 0 0 4
 BASI 0 0 0 0
 BASR 0 0 0 4
 BASI 0 0 0 0
 SYMM -Y, X-Y, Z
 BASR 0 0 0 0
 BASI 0 0 0 0
 BASR 0 0 0 4
 BASI 0 0 0 0
 BASR 0 0 0 0
 BASI 0 0 0 0
 SYMM -X+Y+1, -X+1, Z
 BASR 0 0 0 0
 BASI 0 0 0 0
 BASR 0 0 0 4
 BASI 0 0 0 0
 BASR 0 0 0 0
 BASI 0 0 0 0
 SYMM -Y+1, X-Y+1, Z
 BASR 0 0 0 0
 BASI 0 0 0 0
 BASR 0 0 0 0
 BASI 0 0 0 0
 BASR 0 0 0 4
 BASI 0 0 0 0
 SYMM -X+Y, -X, Z
 BASR 0 0 0 0
 BASI 0 0 0 0
 BASR 0 0 0 0
 BASI 0 0 0 0
 BASR 0 0 0 4
 BASI 0 0 0 0
 !
 Atom Typ Mag Vek X Y Z Biso Occ C1 C2 C3
 ! C4 C5 C6 C7 C8 C9 MagPh
 DY1 MDY3 1 0 0.000000 0.000000 0.000000 0.300000 1.000000 0.647 2.863 0.000
 0.00 0.00 0.00 0.00 0.00 0.00 0.00 111.00 91.00 0.00
 0.00 0.00 0.00 0.00 0.00 0.00 0.00
 MN2 MN3 2 0 0.500000 0.000000 0.25040 0.300000 1.000000 -0.476 0.000 0.690
 0.00 0.00 0.00 0.00 0.00 0.00 0.00 121.00 0.00 101.00
 0.00 0.00 0.00 0.00 0.00 0.00 0.00
 MN3 MN3 2 0 0.000000 0.500000 0.74960 0.300000 1.000000 -0.476 0.000 0.690
 0.00 0.00 0.00 0.00 0.00 0.00 0.00 121.00 0.00 101.00
 0.00 0.00 0.00 0.00 0.00 0.00 0.00
 0.00 0.00 0.00 0.00 0.00 0.00 0.00

Step 5b(Real IRs): Fitting a magnetic model: Helical

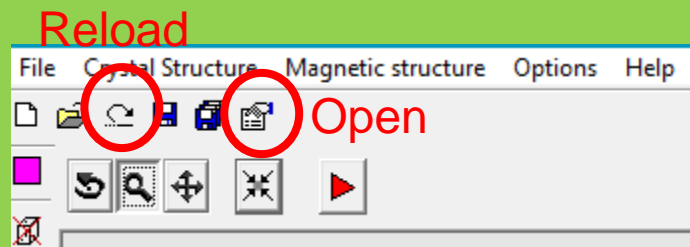
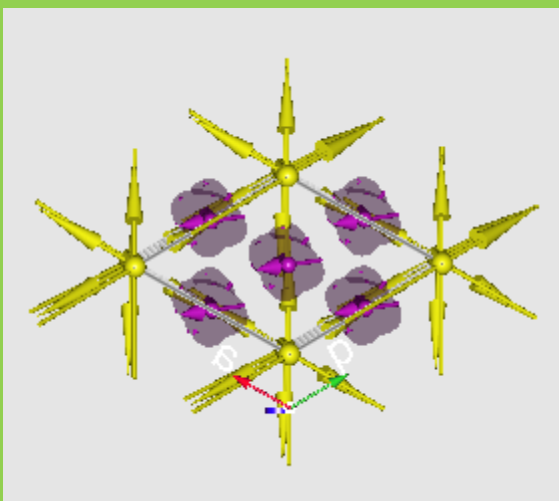
- Refining the imaginary BVs of C5 yields the same solution as purely real.
- Instead need to refine orthogonal BVs. Try C9 with equal value to C3.
For Dy refine C7 equal to C2



```
P -1 <--Space group symbol for hkl generation
! Nsym Cen Lauz Irep N_Bas
   5      1    10    -3     9
! Real(0)-Imaginary(1) indicator for Ci
  0 0 0 0 0 1 1 1 1
!
SYMM X, Y, Z
BASR 0 0 12 0 3 0 3.46 1.73 0 0 0 0 0 0 0 0 0 3 0 3.46 1.73 0 0 0 0 0 0 0 0
BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASR 0 0 4 2 3 0 0 -3 0 0 1.73 0 -3.5 -1.7 0 2 3 0 0 -3 0 0 1.73 0 -3.5 -1.7 0 0
BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASR 0 0 4 0 2 0 0 0 0 0 0 0 0 0 4 2 0 0 2 0 0 0 0 0 0 0 4 2 0 0
BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
SYMM -Y, X-Y, Z
BASR 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASR 0 0 4 0 -1 0 0 -3 0 3.46 1.73 0 -3.5 -1.7 0 0 -1 0 0 -3 0 3.46 1.73 0 -3.5 -1.7 0 0
BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASR 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
SYMM -X+Y+1, -X+1, Z
BASR 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASR 0 0 4 -2 1 0 0 -3 0 0 -1.7 0 -3.5 -1.7 0 -2 1 0 0 -3 0 0 -1.7 0 -3.5 -1.7 0 0
BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASR 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
SYMM -Y+1, X-Y+1, Z
BASR 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASR 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASR 0 0 4 1 1 0 -1.7 1.73 0 1.73 1.73 0 1 -1 0 1 1 0 -1.7 1.73 0 1.73 1.73 0 1 -1 0 0
BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
SYMM -X+Y, -X, Z
BASR 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASR 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
BASR 0 0 4 -1 0 0 1.73 3.46 0 1.73 0 0 1 2 0 -1 0 0 1.73 3.46 0 1.73 0 0 1 2 0 0
BASI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
!
!Atom Typ Mag Wek X Y Z Biso Occ C1 C2 C3
! C4 C5 C6 C7 C8 C9 MagPh
DY1 MDY3 1 0 0.00000 0.00000 0.00000 0.30000 1.00000 0.609 2.879 0.000
        0.00 0.00 0.00 0.00 0.00 0.00 111.00 91.00 0.00
        0.000 0.000 0.000 0.000 0.000 0.000 0.00000
        0.00 0.00 0.00 0.00 0.00 0.00 0.00
MN2 MNZ3 2 0 0.50000 0.00000 0.25040 0.30000 1.00000 -0.484 0.000 0.552
        0.00 0.00 0.00 0.00 0.00 0.00 101.00 0.00 121.00
        0.000 -0.239 0.000 0.000 0.000 0.552 0.00000
        0.00 0.00 0.00 0.00 0.00 121.00 0.00
MN3 MNZ3 2 0 0.00000 0.50000 0.74960 0.30000 1.00000 -0.484 0.000 0.552
        0.00 0.00 0.00 0.00 0.00 0.00 101.00 0.00 121.00
        0.000 0.239 0.000 0.000 0.000 0.552 0.00000
        0.00 0.00 0.00 0.00 0.00 121.00 0.00
```

Step 5b(Real IRs): Fitting a magnetic model: Helical

- Fst file can be edited to show envelope.



```
File Edit Search
[Icons]
! FILE for FullProf Studio: generated automatically by FullProf
!Title: Magnetic Phase
SPACEG P 1
CELL 5.206226 5.206226 8.147879 90.0000 90.0000 120.0000 DISPLAY MULTIPLE
BOX -0.15 1.15 -0.15 1.15 -0.15 6.15

{
LATTICE P
K 0.00000 0.00000 0.16500
SYMM x,y,z
MSYM u,v,w,0.0
MATOM DY1_1 Dy 0.00000 0.00000 0.00000 SCALE 1.0 GROUP ENVELOP
SKP 1 1 0.00000 6.55141 6.38451 7.55596 3.77798 0.00000 0.00000
MATOM DY1_2 Dy 0.00000 0.00000 0.00000 SCALE 1.0 GROUP ENVELOP
SKP 1 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
MATOM DY1_3 Dy 1.00000 1.00000 0.00000 SCALE 1.0 GROUP ENVELOP
SKP 1 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
MATOM DY1_4 Dy 1.00000 1.00000 0.00000 SCALE 1.0 GROUP ENVELOP
SKP 1 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
MATOM DY1_5 Dy 0.00000 0.00000 0.00000 SCALE 1.0 GROUP ENVELOP
SKP 1 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
MATOM MN2_1 Mn 0.50000 0.00000 0.25040 SCALE 1.0 GROUP ENVELOP
SKP 1 1 0.83650 -1.36435 -1.45472 -2.06576 -1.00337 0.00000 0.00000
MATOM MN2_2 Mn 0.00000 0.50000 0.25040 SCALE 1.0 GROUP ENVELOP
SKP 1 1 0.83650 -1.36435 -1.45472 -2.06576 -1.00337 0.00000 0.00000
MATOM MN2_3 Mn 0.50000 0.50000 0.25040 SCALE 1.0 GROUP ENVELOP
SKP 1 1 0.83650 -1.36435 -1.45472 -2.06576 -1.00337 0.00000 0.00000
MATOM MN2_4 Mn 1.00000 1.50000 0.25040 SCALE 1.0 GROUP ENVELOP
SKP 1 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
MATOM MN2_5 Mn -0.50000 -0.50000 0.25040 SCALE 1.0 GROUP ENVELOP
SKP 1 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
MATOM MN3_1 Mn 0.00000 0.50000 0.74960 SCALE 1.0 GROUP ENVELOP
SKP 1 1 -0.83650 -2.17695 -1.45472 -2.06576 -1.00337 0.00000 0.00000
MATOM MN3_2 Mn -0.50000 -0.50000 0.74960 SCALE 1.0 GROUP ENVELOP
SKP 1 1 -0.83650 -2.17695 -1.45472 -2.06576 -1.00337 0.00000 0.00000
MATOM MN3_3 Mn 1.50000 1.00000 0.74960 SCALE 1.0 GROUP ENVELOP
SKP 1 1 -0.83650 -2.17695 -1.45472 -2.06576 -1.00337 0.00000 0.00000
MATOM MN3_4 Mn 0.50000 0.50000 0.74960 SCALE 1.0 GROUP ENVELOP
SKP 1 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
MATOM MN3_5 Mn 0.50000 0.00000 0.74960 SCALE 1.0 GROUP ENVELOP
SKP 1 1 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
}
```