

# Representational analysis with Fullprof and SARAh to refine $\text{MnPSe}_3$ data collected on HB2A

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MagStr, ORNL, 2022

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# MnPSe<sub>3</sub>

- *R*-3 space group (148)  
Setting 1, hexagonal
- $a=b=6.387 \text{ \AA}$ ,  $c=19.996 \text{ \AA}$ .
- $\alpha=90^\circ$ ,  $\beta=90^\circ$ ,  $\gamma=120^\circ$
- Mn<sup>2+</sup>,  $S=5/2$

Solid State Communications, Vol. 40, pp. 1067–1072.  
Pergamon Press Ltd. 1981. Printed in Great Britain.

0038–1098/81/481067–06\$02.00/0

## NEUTRON DIFFRACTION STUDY OF THE LAYERED COMPOUNDS MnPSe<sub>3</sub> AND FePSe<sub>3</sub>\*

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(Received 11 August 1981 by E.F. Bertaut)

In the insulating compounds MnPSe<sub>3</sub> (1) and FePSe<sub>3</sub> (2) transition metal ions form planar honeycomb lattices. A neutron study revealed a collinear antiferromagnetic order below  $T_N$  (1) and  $T_N = 119 \pm 1 \text{ K}$  (2) with the corresponding wave vector  $[000]$  (1) and  $k = [1/2 \ 0 \ 1/2]$  (2). In MnPSe<sub>3</sub> the magnetic ions ( $m_0 = 4.74 \mu_B$ ) lie within the basal plane and in FePSe<sub>3</sub> (they are pointing along the *c*-axis. The collinear structures are determined by the dominating intralayer interactions between first ( $J_1$ ) and third neighbours ( $J_3$ ) which in MnPSe<sub>3</sub> are all antiferromagnetic whereas in FePSe<sub>3</sub>  $J_1$  is ferromagnetic and  $J_2$  and  $J_3$  are antiferromagnetic.

**Originally investigated in 1981. Renewed interest due to quasi-2D van der Waal layered structure.**

PHYSICAL REVIEW B **103**, 024414 (2021)

## Magnetic exchange interactions in the van der Waals layered antiferromagnet MnPSe<sub>3</sub>

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<sup>1</sup>Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

<sup>2</sup>Department of Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee 37996, USA

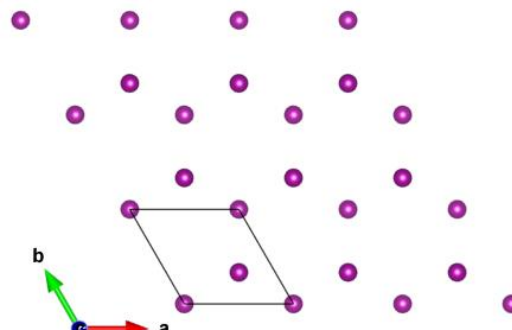
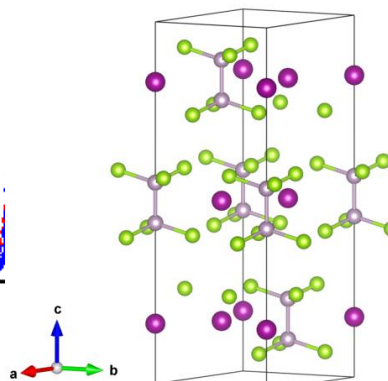
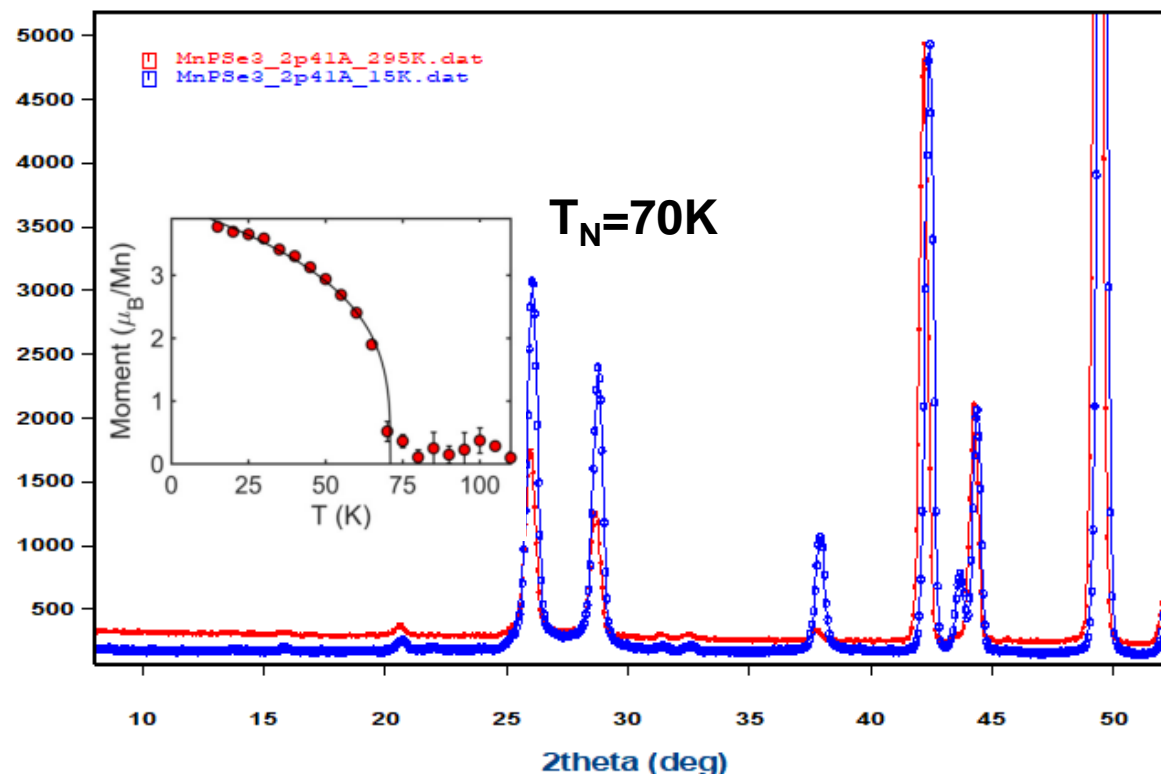
<sup>3</sup>Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

(Received 16 October 2020; accepted 21 December 2020; published 11 January 2021)

Two-dimensional van der Waals compounds with magnetic ions on a honeycomb lattice are hosts to a variety of exotic behavior. The magnetic interactions in one such compound, MnPSe<sub>3</sub>, are investigated with elastic and inelastic neutron scattering. Magnetic excitations are observed in the magnetically ordered regime and persist to temperatures well above the ordering temperature,  $T_N = 74 \text{ K}$ , consistent with low dimensional magnetic interactions. The inelastic neutron scattering results allow a model spin Hamiltonian to be presented that includes dominant intralayer interactions of  $J_{1ab} = 0.45 \text{ meV}$ ,  $J_{2ab} = 0.03 \text{ meV}$ ,  $J_{3ab} = 0.19 \text{ meV}$ , consistent with theoretical predictions. Despite the quasi-2D behavior, appreciable interlayer interactions of  $J_c = 0.031(5) \text{ meV}$  are required to model the data. No evidence for anisotropy in the form of a spin gap is observed in the data collected. The measurements on MnPSe<sub>3</sub> are contrasted with those on MnPS<sub>3</sub> and reveal a large increase in the interlayer exchange interaction in MnPSe<sub>3</sub> that may stabilize the similar ordering temperatures in the bulk compounds.

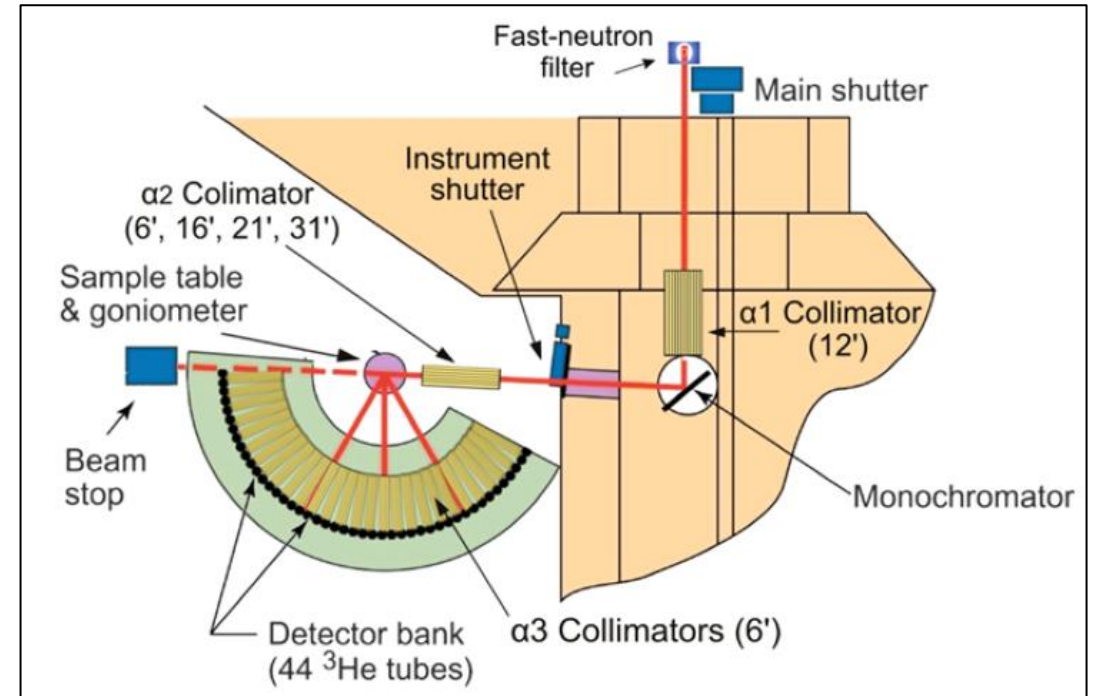
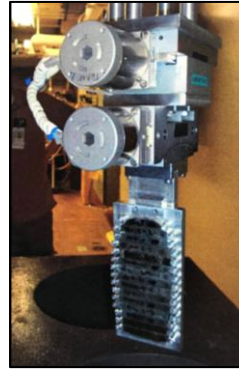
DOI: 10.1103/PhysRevB.103.024414

Intensity (arb. units)



# HB-2A: Powder diffractometer at HFIR

- Constant wavelength
- Germanium monochromator
  - $\sim 90^\circ$  take off angle for medium-high resolution
  - Variety of complex sample environments: 50mK, 8 Tesla, pressure...
- Detector is an array of 44 individual  $^3\text{He}$  tubes
  - Low background and robust to magnetic field
  - Covers  $\sim 2$ - $150^\circ$  in  $2\theta$  through scanning detector



<https://neutrons.ornl.gov/powder>


Ge(hkl)	$\lambda$ (Å)	$d_{\text{max}}$ (Å)	$4\pi\sin\theta/\lambda$	Flux (n/cm <sup>2</sup> s)
<b>(113)</b>	<b>2.41</b>	<b>27.6</b>	<b>0.2-5.1</b>	<b><math>5 \times 10^6</math></b>
<b>(115)</b>	<b>1.54</b>	<b>17.6</b>	<b>0.35-7.9</b>	<b><math>1 \times 10^7</math></b>
(117)	1.12	12.8	0.5-10.9	$4 \times 10^6$

# Details of this $\text{MnPSe}_3$ example

- Neutron powder diffraction data collected at HB2A, HFIR
- $\lambda = 2.41 \text{ \AA}$ . Collimation: open-open-21'
- Data at 15K (**MnPSe3\_HB2A\_15K.dat**) and 295K (**MnPSe3\_HB2A\_295K.dat**)
- Sample in a vanadium can
- Instrument resolution file: **hb2a\_resolution.irf**
- Crystal structure: **MnPSe3.cif**

Name

 hb2a\_resolution.irf

 MnPSe3.cif

 MnPSe3\_HB2A\_15K.dat

 MnPSe3\_HB2A\_295K.dat



# MnPSe<sub>3</sub>

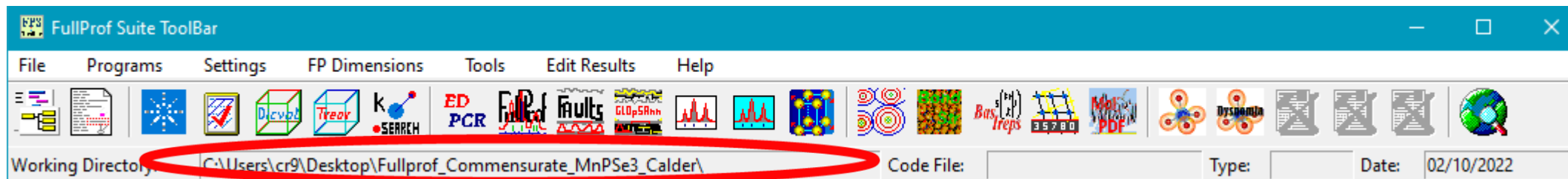
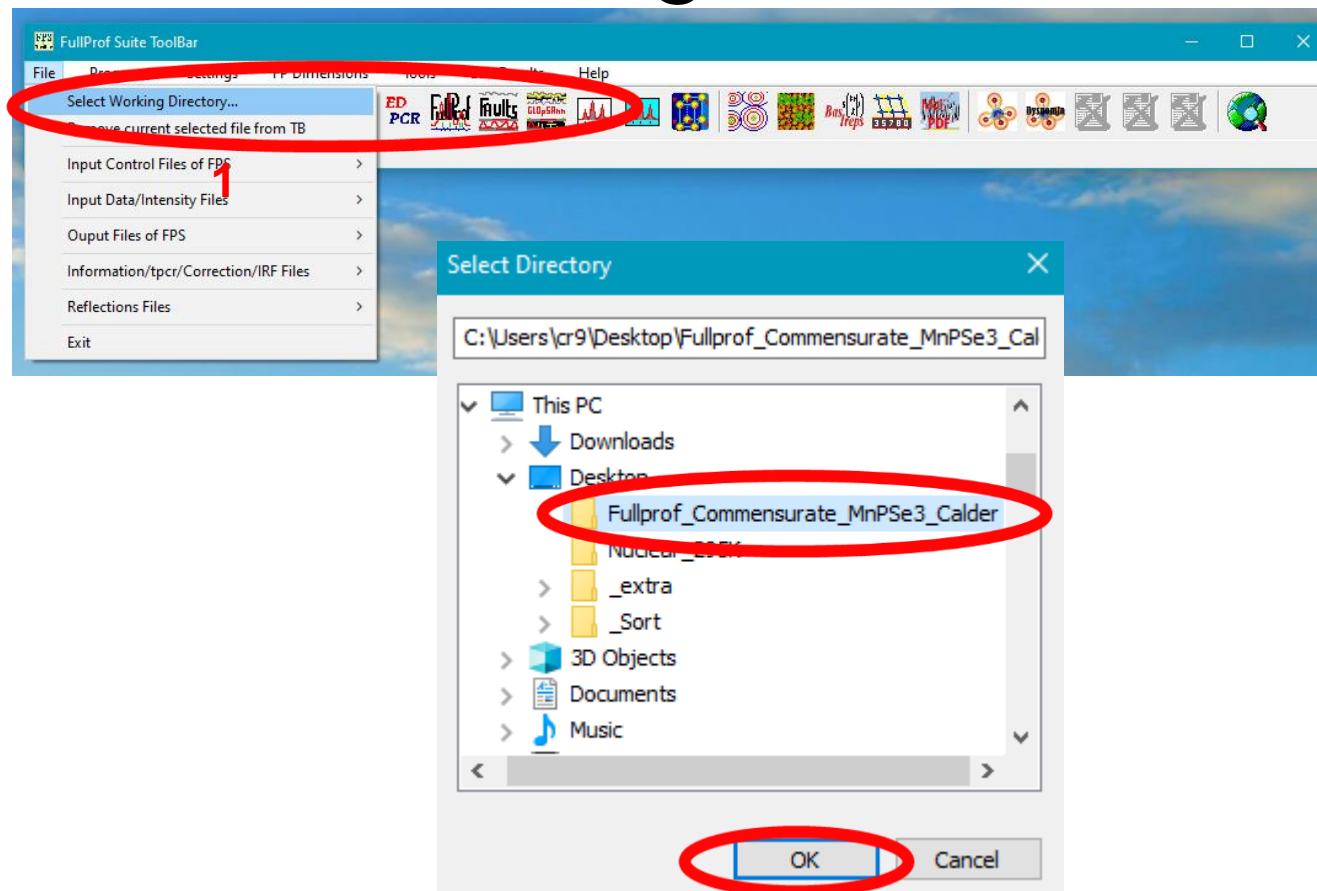
- This example will use Fullprof and SARAh  
<http://fermat.chem.ucl.ac.uk/spaces/willsgroup/web-software/sarah-refine-fullprof/>
  - Step 1: Refine the crystal structure using FullProf
  - Step 2: Determine the k-vector by indexing the magnetic reflections using k-search
  - Step 3: Create candidate magnetic models using SARAh
  - Step 4: Refine the magnetic model and nuclear phase in Fullprof.
  - Step 5: Visualize the magnetic model

# MnPSe<sub>3</sub>

- This example will use Fullprof and SARAh  
<http://fermat.chem.ucl.ac.uk/spaces/willsgroup/web-software/sarah-refine-fullprof/>
  - **Step 1: Refine the crystal structure using FullProf**
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  - Step 4: Refine the magnetic model and nuclear phase in Fullprof.
  - Step 5: Visualize the magnetic model

# Step 1: Refine the crystal structure using FullProf

- Open Fullprof Suite toolbar.
  - **1.** Select working directory with data  
“File>Select Working directory...”
  - **2.** Browse to wherever your folder  
“Ho2Ba2NiO5\_MagSpaceGroup” is located on your computer and select “ok”
  - **3.** Path on FP studio toolbar should now be updated. This helps with interacting with other features of Fullprof



# Step 1: Refine the crystal structure using FullProf

- 1. From FullProf Suite Toolbar open EdPCR.
- 2. Import crystallographic information file by clicking on "CIF→PCR"
- 3. Select the file "MnPSe3.cif"

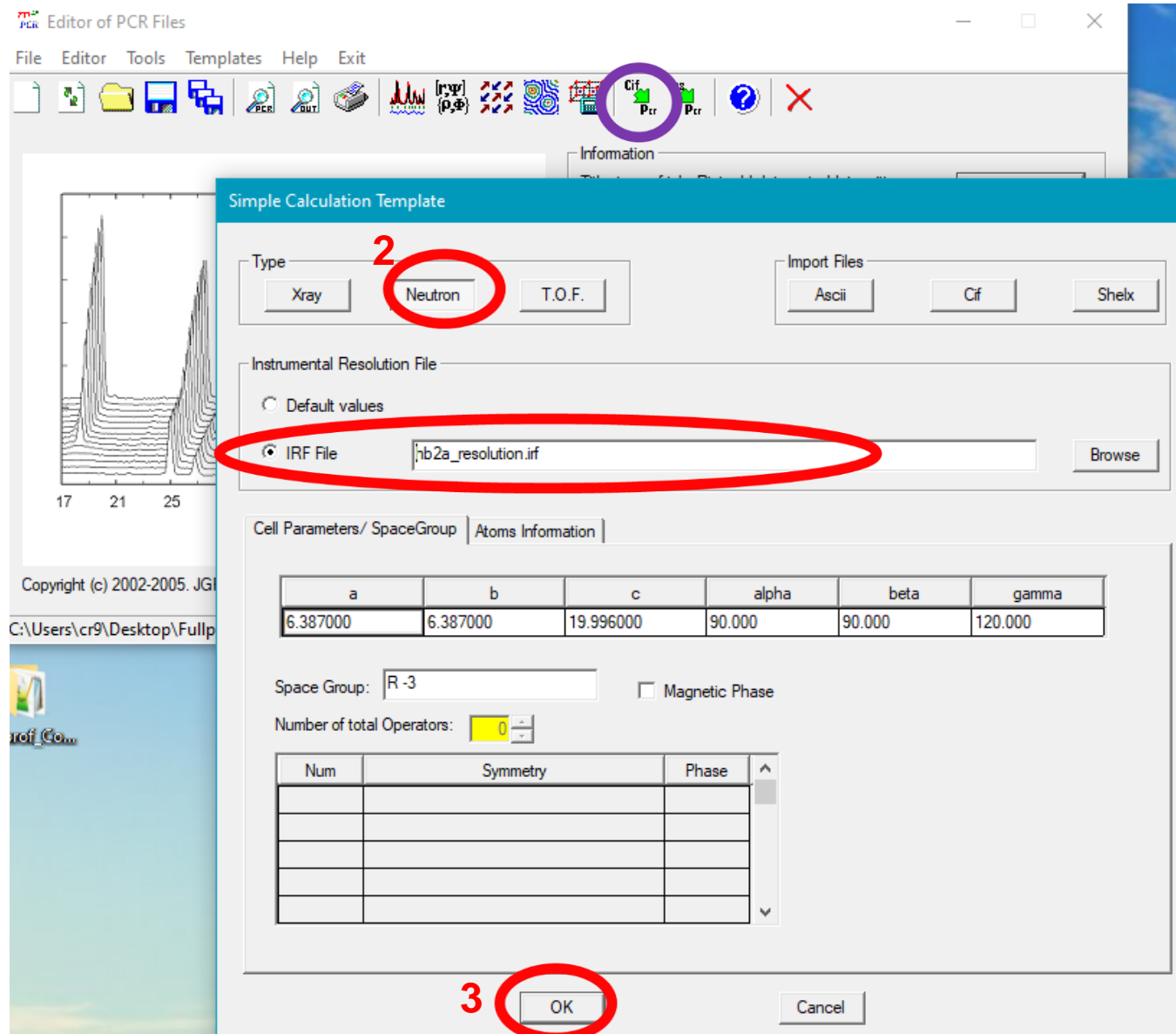
The image shows two screenshots of the FullProf Suite software interface. The top screenshot is the 'FullProf Suite Toolbar' with a red circle around the 'ED PCR' button, labeled with a red '1'. A large red arrow points from this button to the bottom screenshot. The bottom screenshot is the 'Editor of PCR Files' window. In its toolbar, the 'Cif → Pcr' button is circled in red and labeled with a red '2'. The main window of the editor shows a plot of intensity versus  $2\theta$  (°) with the text 'FullProf PCR Editor' overlaid. On the right, there is an 'Information' panel with tabs for General, Patterns, Phases, Refinement, Constraints, Box/Restrains, and Output. The 'General' tab is selected, showing fields for Title, Type of Patterns, Phase name, Number of cycles, Constraints definitions, Fixing range of parameters, and Output options. To the right of the editor, a file explorer shows a list of files: 'hb2a\_resolution.irf', 'MnPSe3.cif' (circled in red and labeled with a red '3'), 'MnPSe3\_HB2A\_15K.dat', and 'MnPSe3\_HB2A\_295K.dat'.



# Step 1: Refine the crystal structure using FullProf

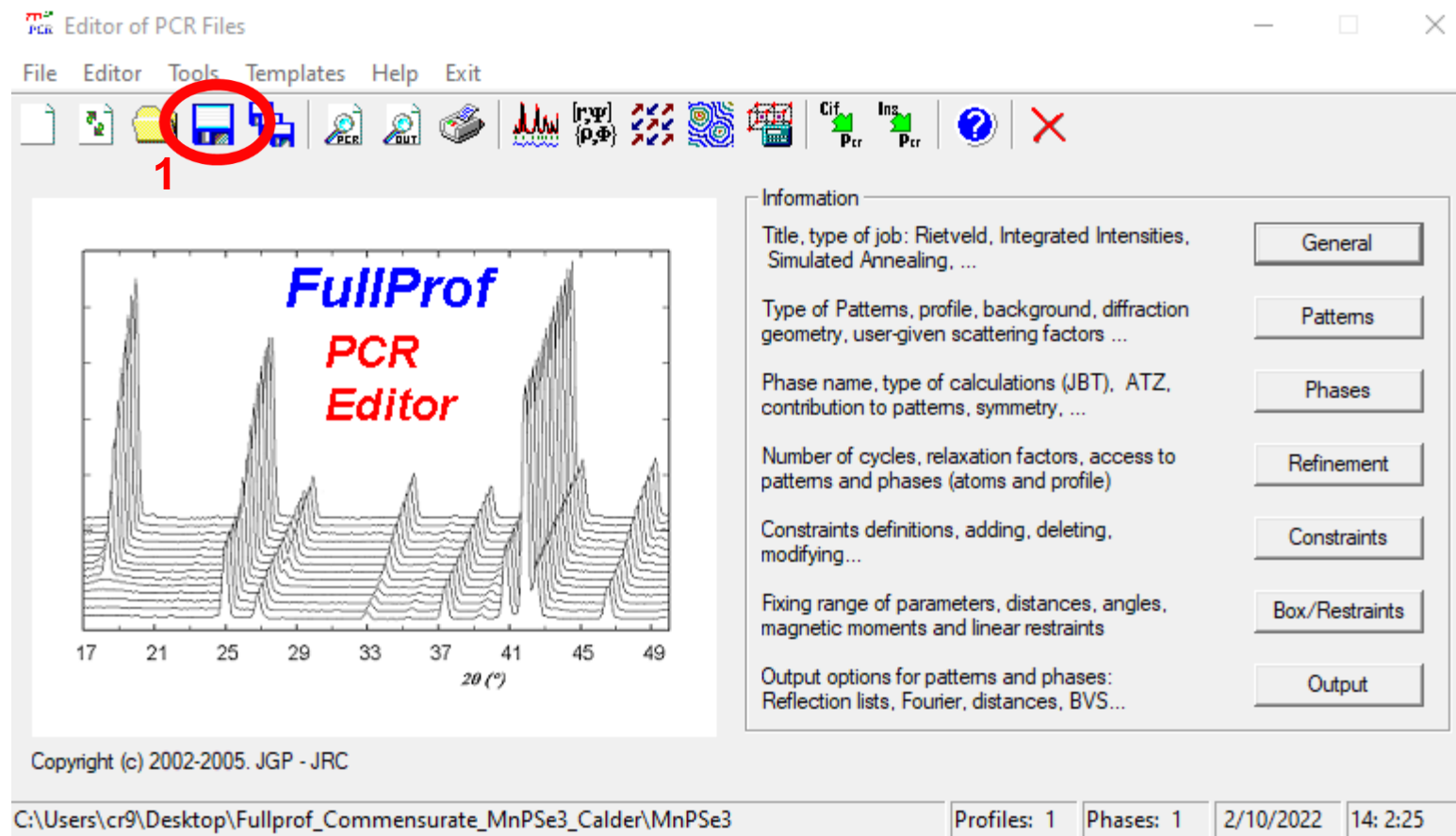
Cif→PCR opens a window to input instrument and show structural info.

- 1. Load the instrument resolution file "hb2a\_resolution.irf". *NOTE: remove the full path to just keep "dib\_ill.irf". If you don't and move the pcr file to a different directory (or share the pcr with someone else) it will create problems*
- 2. Change "Type" to "Neutron" for constant wavelength
- Starting **Cell Parameters**, **Space Group** and **Atoms Information** are now loaded.
- Note: occ = site multip./general multip. Always check this has been correctly calculated after importing the .cif file.
- 3. Hit "OK"



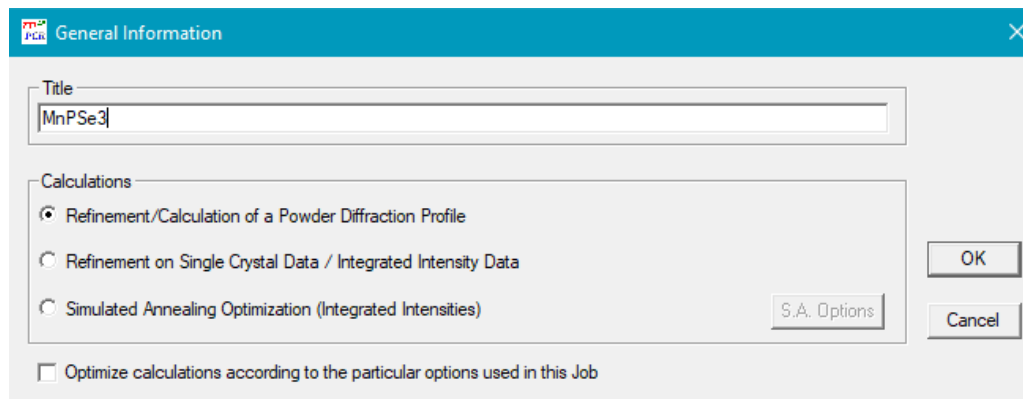
# Step 1: Refine the crystal structure using FullProf

- **1.** Save the changes.
- This should be done whenever changes are made in the GUI.



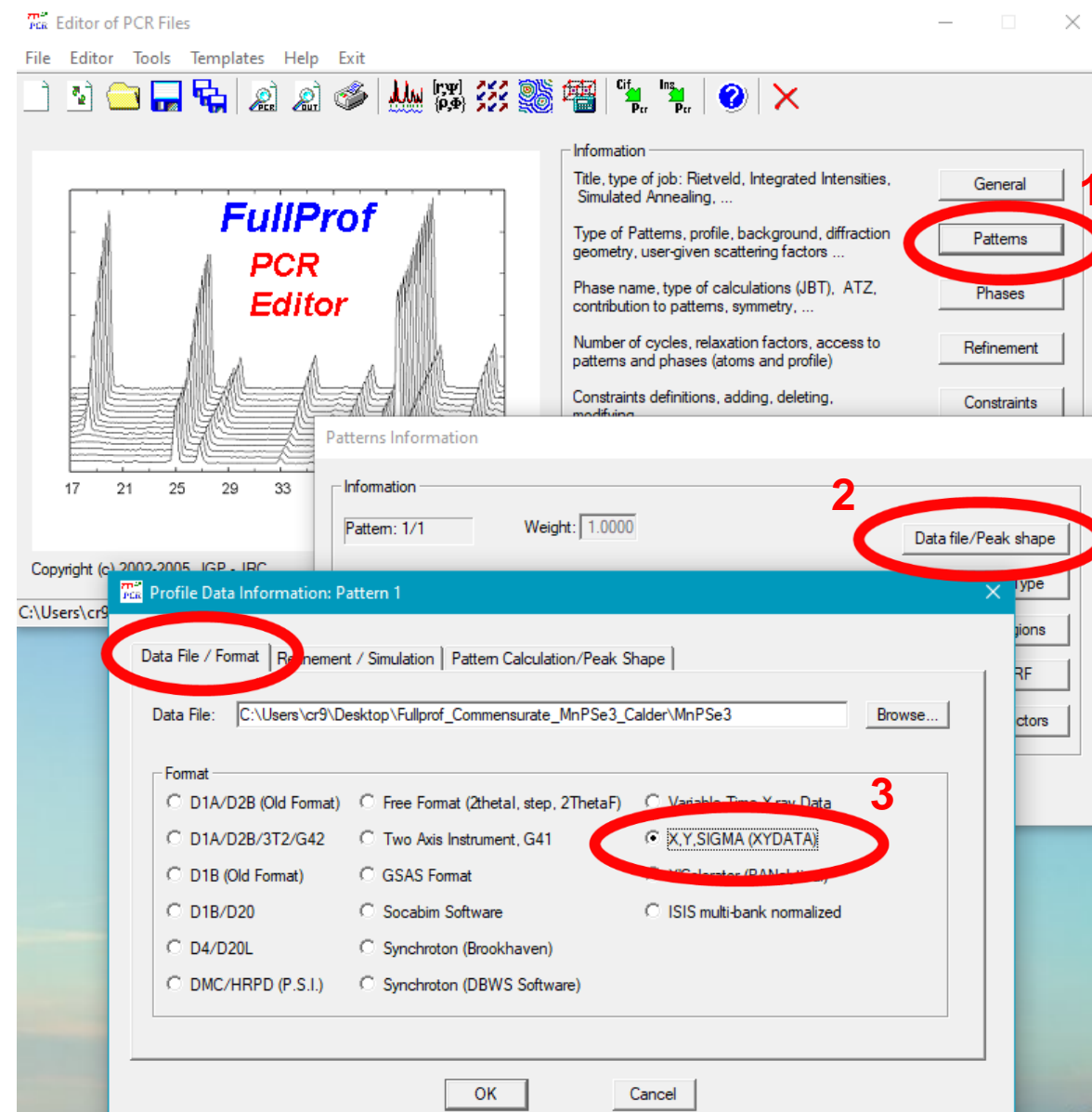
# Step 1: Refine the crystal structure using FullProf

“General” tab has refinement of powder data as default. Can edit title as wanted.



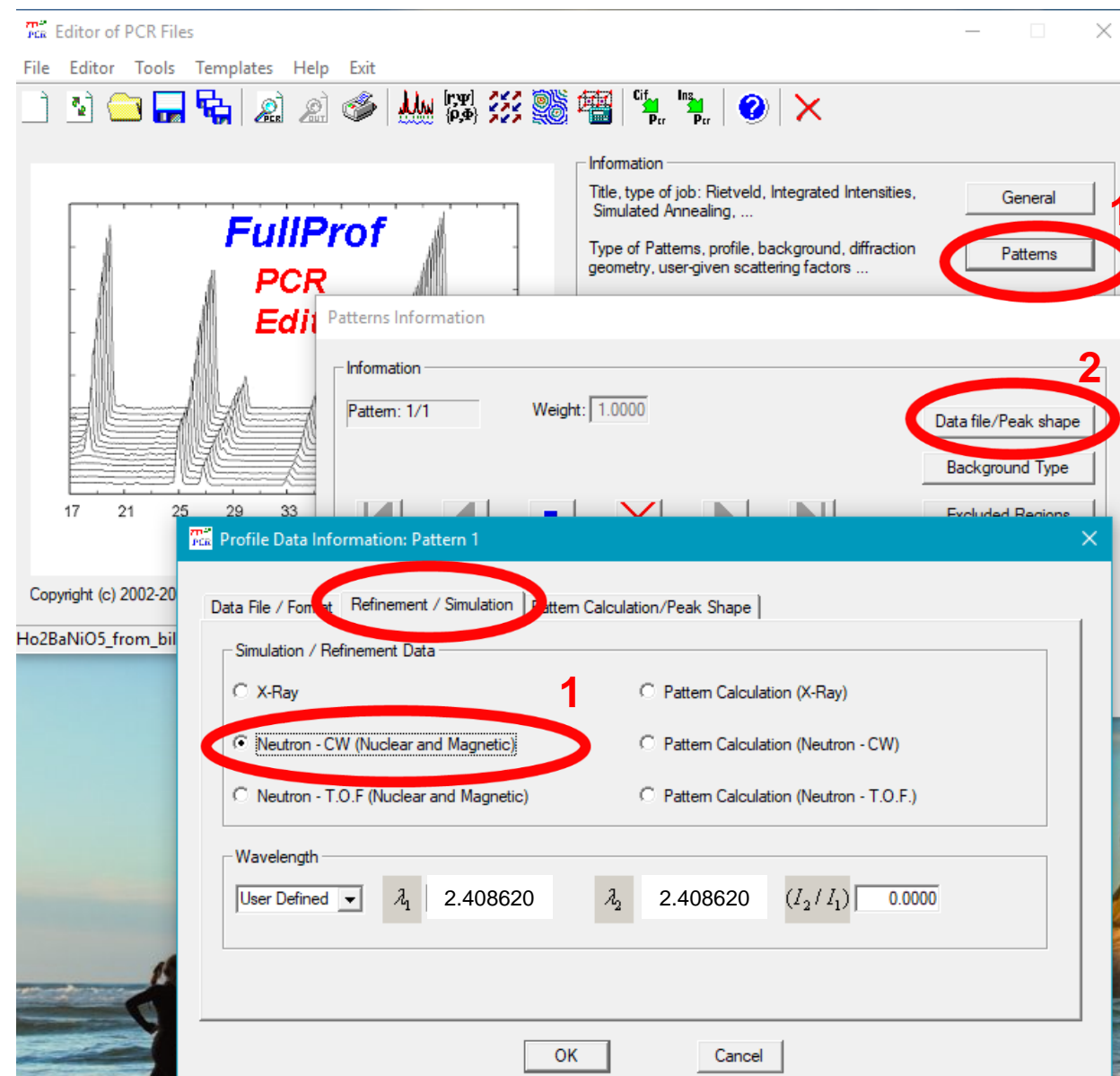
## 1. “Patterns” tab

- 2. Select the format of the data file Fullprof should refine.
- 3. X,YSIGMA (XYDATA).



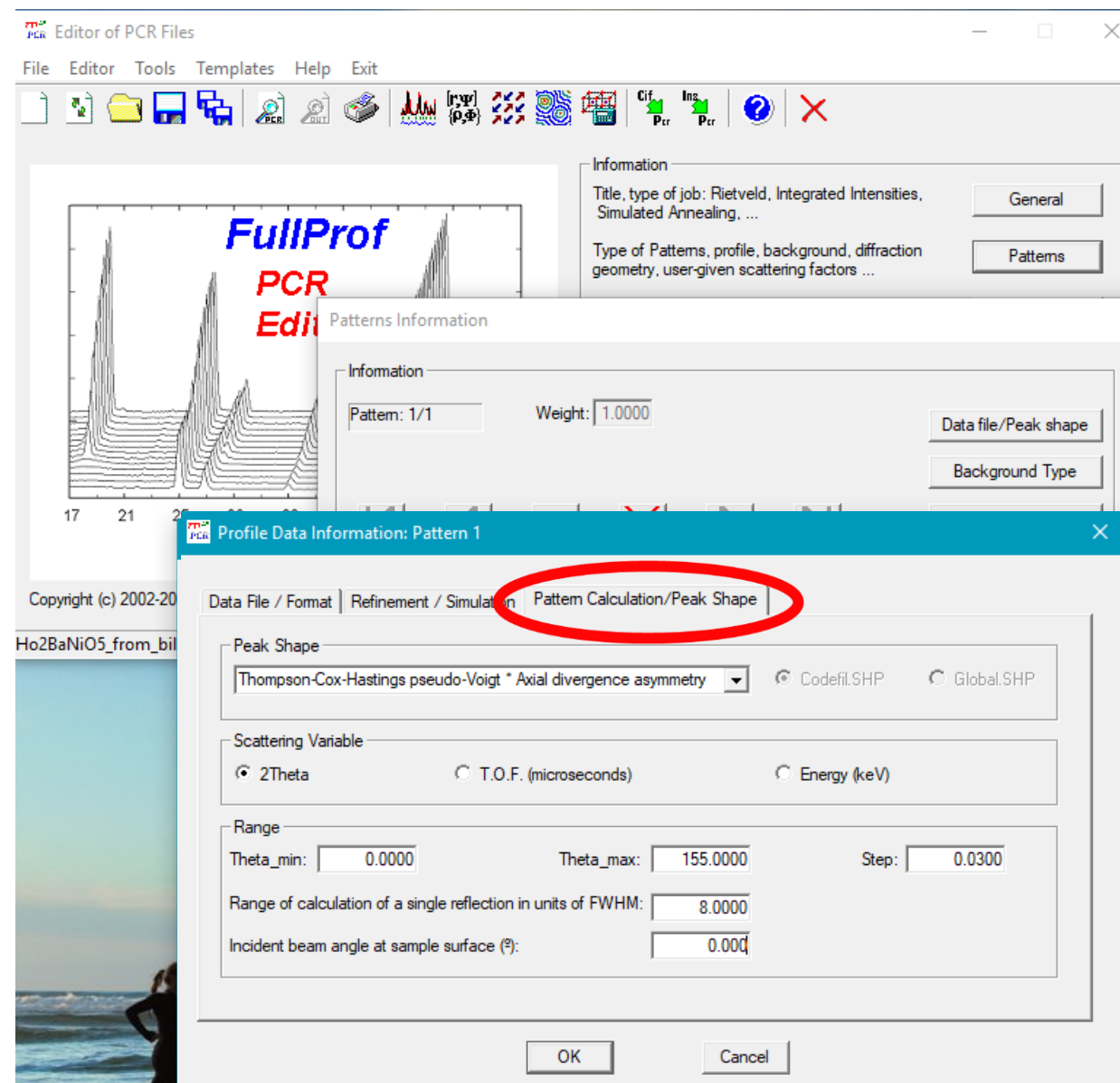
# Step 1: Refine the crystal structure using FullProf

- Patterns → Data file/Peak Shape → Refinement/Simulation
- **[1]** Select “**Neutron – CW (nuclear and Magnetic)**”
- Wavelength is already set by irf file, 2.40862 in this example.



# Step 1: Refine the crystal structure using FullProf

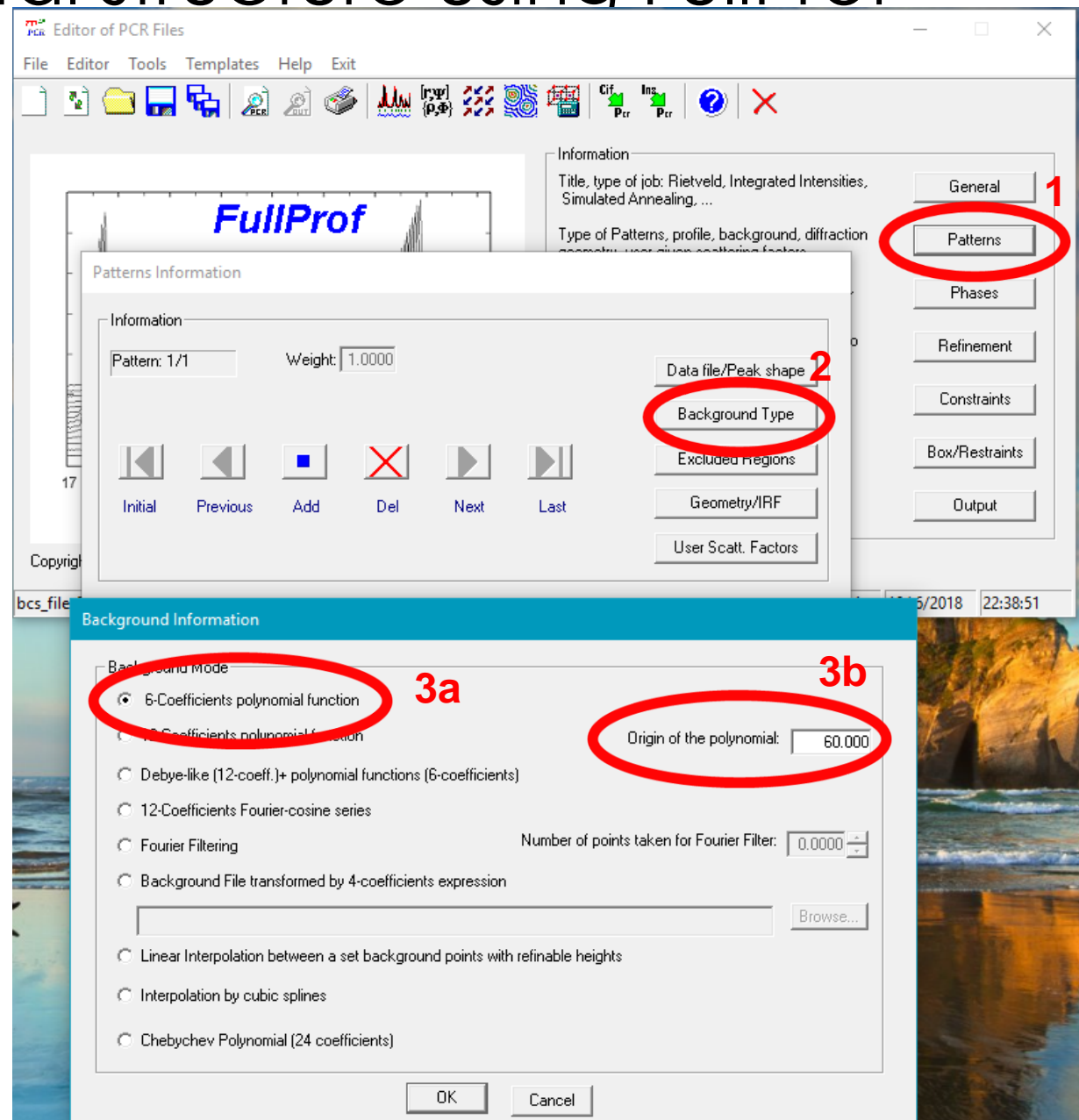
- Check final tab:
- Patterns → Data file/Peak Shape  
→ Pattern Calculation/Peak Shape
- Peak shape is already loaded from irf file.





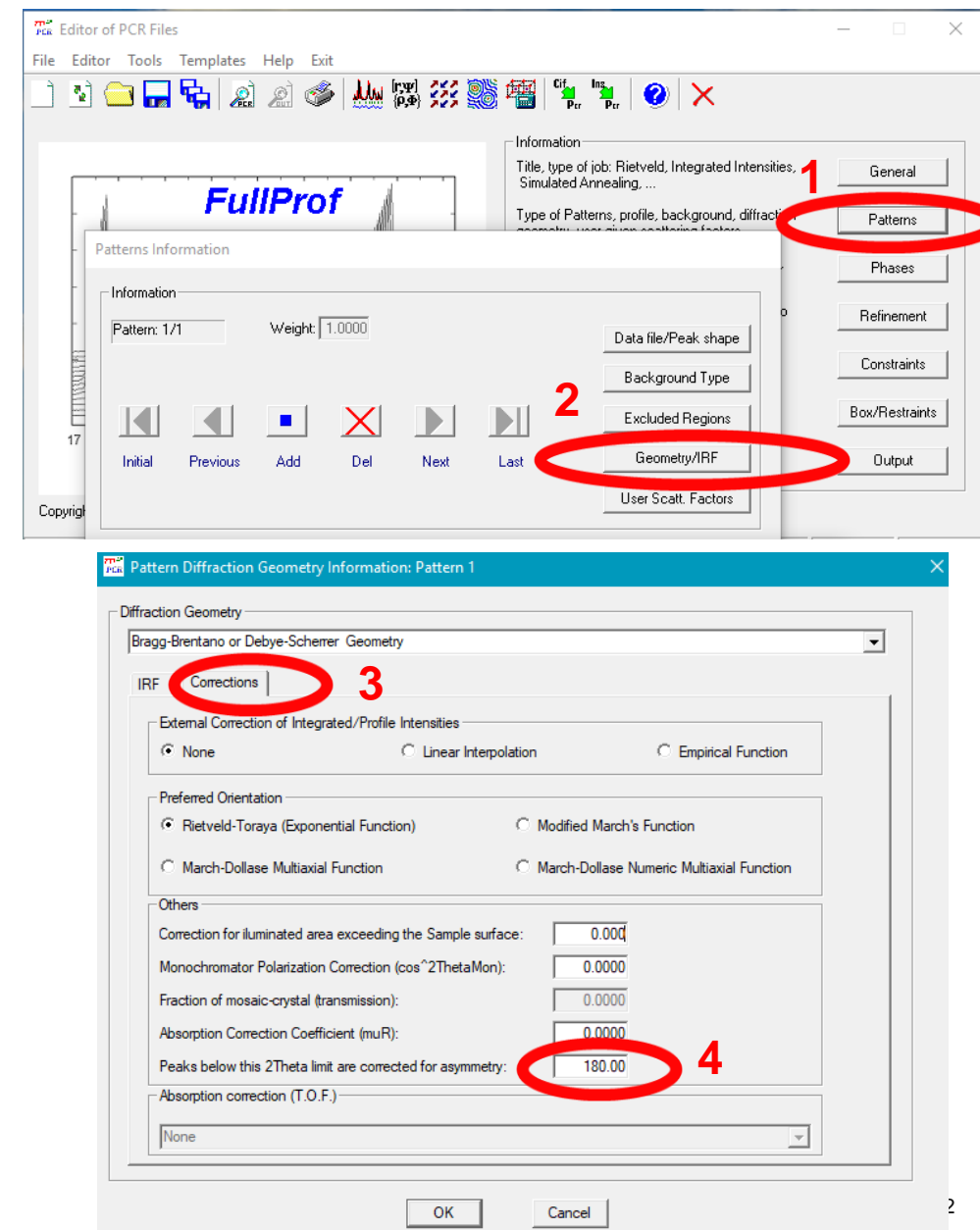
# Step 1: Refine the crystal structure using FullProf

- Move to next tab down to select background type
- Patterns → Background Type  
Check “6-coefficient”
- Put origin of polynomial at 60 for this example.



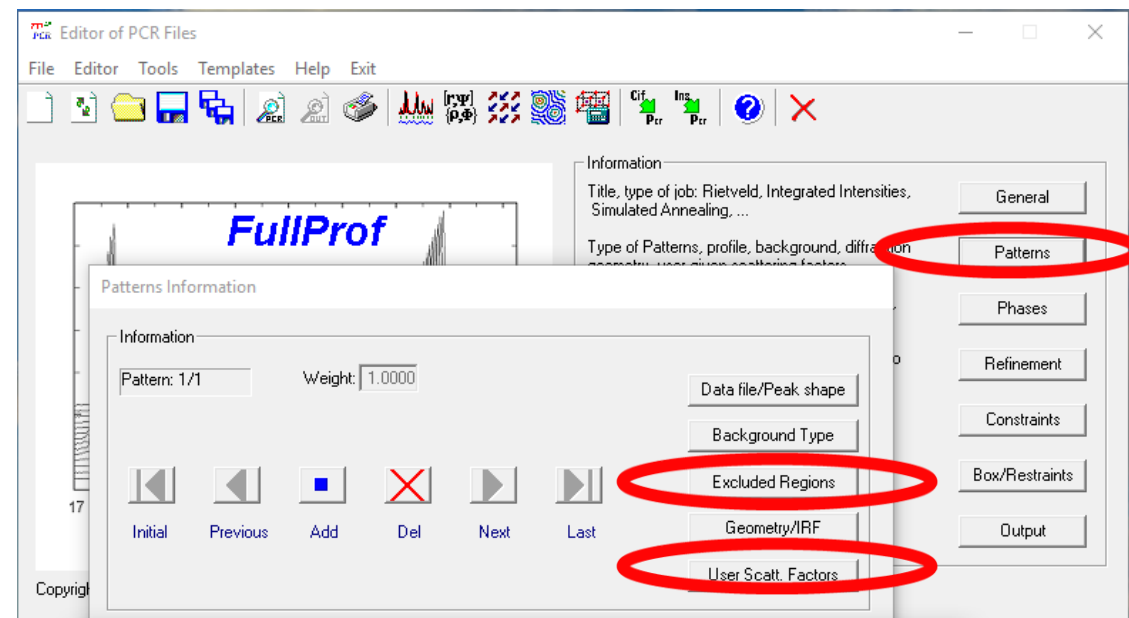
# Step 1: Refine the crystal structure using FullProf

- No further editing should be needed of the remaining “Patterns” → “Geometry/irf”:
  - The irf tab is populated since we loaded the file
  - Corrections tab [3]
  - 4. Change asymmetry to 180. If this is kept 0 then you will get errors if you refine asymmetry.
  - Can add absorption if needed. Check <https://www.ncnr.nist.gov/resources/activation/>



# Step 1: Refine the crystal structure using FullProf

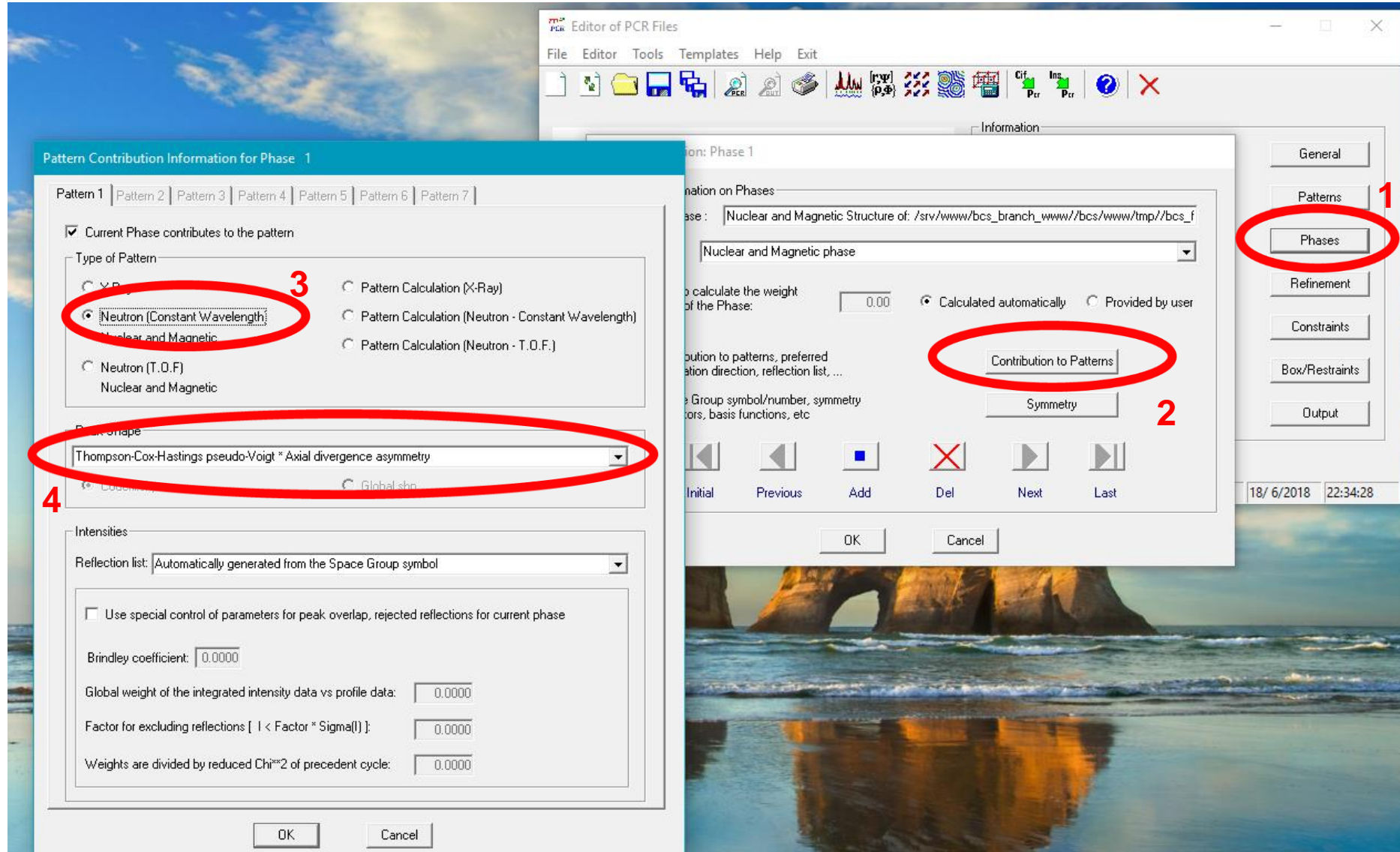
- No further editing should be needed of the remaining “Patterns” tabs:
  - Excluded Region  
Use with care, but can cut out background.
  - User Scatt. Factors  
This can be used to add e.g. a form factor that isn't tabulated



# Step 1: Refine the crystal structure using FullProf

## PHASES tab

- Make phase contribute to refinement.
- **[1]** Phases → **[2]** Contribution to Patterns → **[3]** Neutron (constant wavelength)
- Set peak shape to “**Thompson-Cox-Hastings pseudo-Voigt**”





# Step 1: Refine the crystal structure using FullProf

## REFINEMENT tab:

- Setting starting values for refinements
- Starting background value of 200 (check data)

The screenshot shows the FullProf software interface. The 'Refinement' tab is selected in the right-hand menu (1). The 'Refinement Information' dialog box is open, showing various settings for refinement. The 'Background' button is circled in red (2). The '6 Coefficients Polynomial Background: Pattern 1' dialog box is open, showing a table of coefficients. The 'd\_0' coefficient is set to 200 (3).

	d_0	d_1	d_2	d_3	d_4	d_5
Coefficients	200	0.0000	0.0000	0.0000	0.0000	0.0000
	d_6	d_7	d_8	d_9	d_10	d_11
Coefficients						
	d_12	d_13	d_14	d_15	d_16	d_17
Coefficients						
	d_18	d_19	d_20	d_21	d_22	d_23
Coefficients						

Intensity (arb. units)

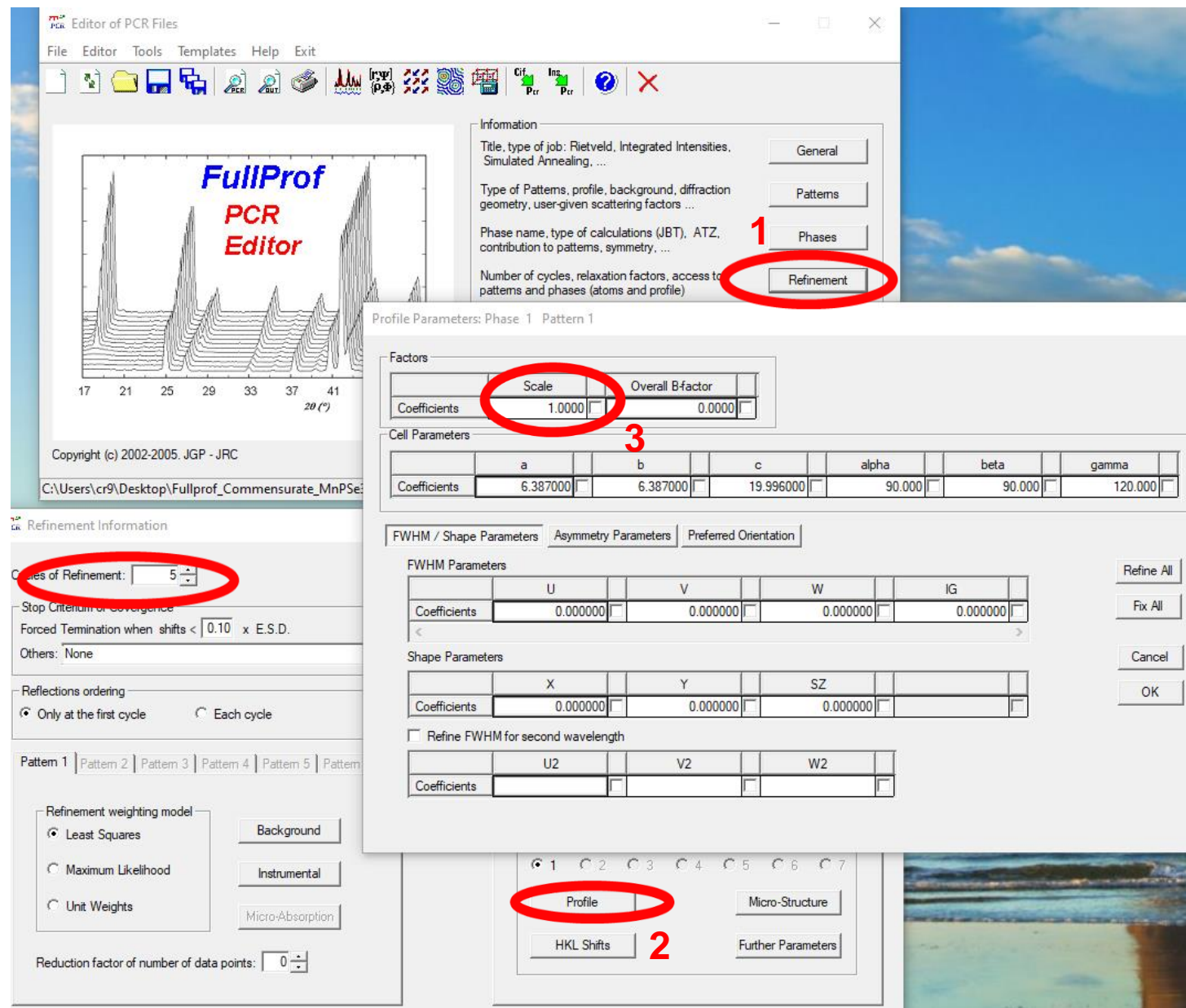
2theta (deg)

of data points: 0



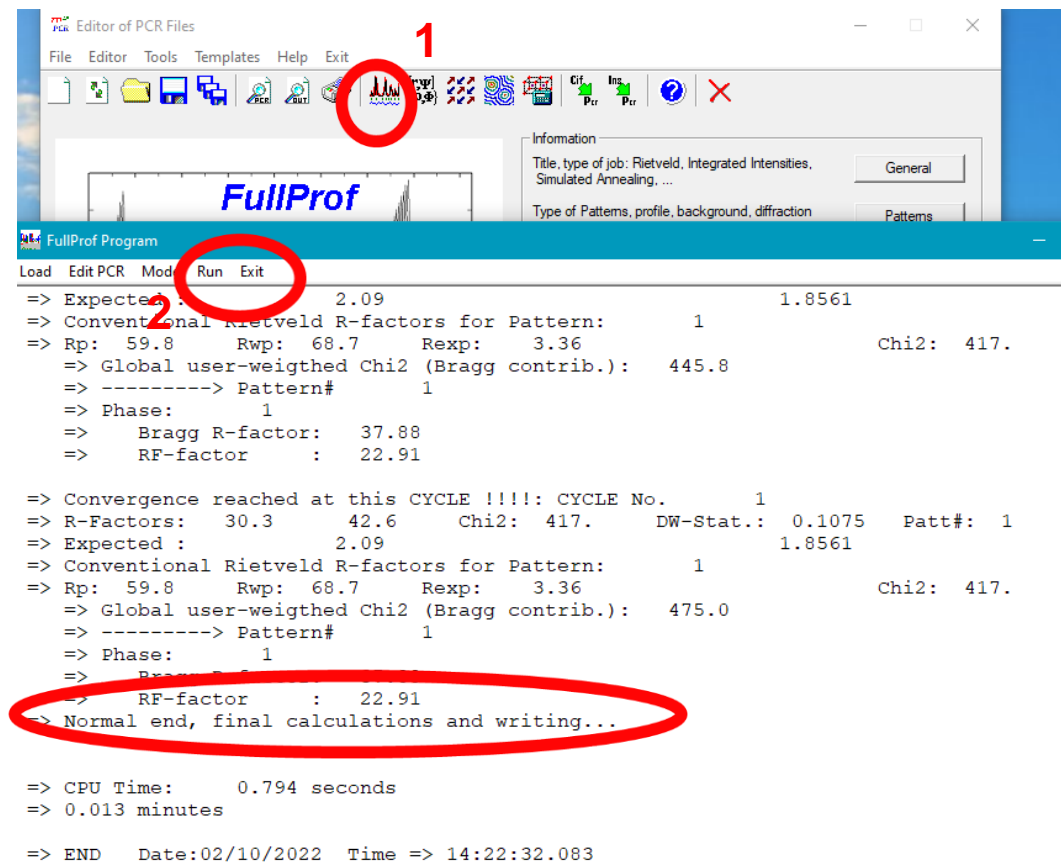
# Step 1: Refine the crystal structure using FullProf

- **1.** Select “Refinement” tab again. Update “Cycle of Refinement” to 5
- From “Refinement” tab select: Refinement>Profile
- Change scale to 1.0
- Note U, V, W, X are set to zero. BUT, the values are being read from the .irf file. So if we refine these then they add on to the irf values.



# Step 1: Refine the crystal structure using FullProf

- 1. Can now run the refinement  
Select the “MnPS<sub>3</sub>\_HB2A\_295K.dat” data
  - Note: we have not set anything to refine yet. It is good to check your model is close to the data and makes sense before refining.
- 2. Refinement runs for the number of cycles (in this case 5). You can repeat this by pushing run until “Normal end, final calculation and writing...” shows rather than “Convergence not reached”
- Select **yes** to save.  
If you're doing a refinement and the fit gets worse then you can select “no” and the starting values will remain.

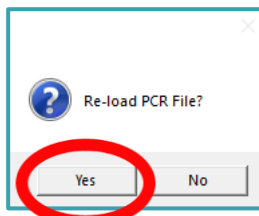
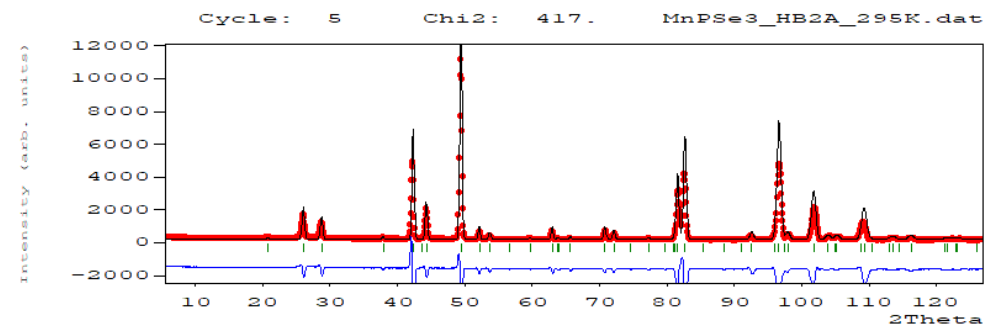


```
FullProf Program
Load Edit PCR Mod Run Exit
=> Expected: 2.09 1.8561
=> Conventional Rietveld R-factors for Pattern: 1
=> Rp: 59.8 Rwp: 68.7 Rexp: 3.36 Chi2: 417.
=> Global user-weighted Chi2 (Bragg contrib.): 445.8
=> -----> Pattern# 1
=> Phase: 1
=> Bragg R-factor: 37.88
=> RF-factor : 22.91

=> Convergence reached at this CYCLE !!!!: CYCLE No. 1
=> R-Factors: 30.3 42.6 Chi2: 417. DW-Stat.: 0.1075 Patt#: 1
=> Expected: 2.09 1.8561
=> Conventional Rietveld R-factors for Pattern: 1
=> Rp: 59.8 Rwp: 68.7 Rexp: 3.36 Chi2: 417.
=> Global user-weighted Chi2 (Bragg contrib.): 475.0
=> -----> Pattern# 1
=> Phase: 1
=> Bragg R-factor: 37.88
=> RF-factor : 22.91
=> Normal end, final calculation and writing...

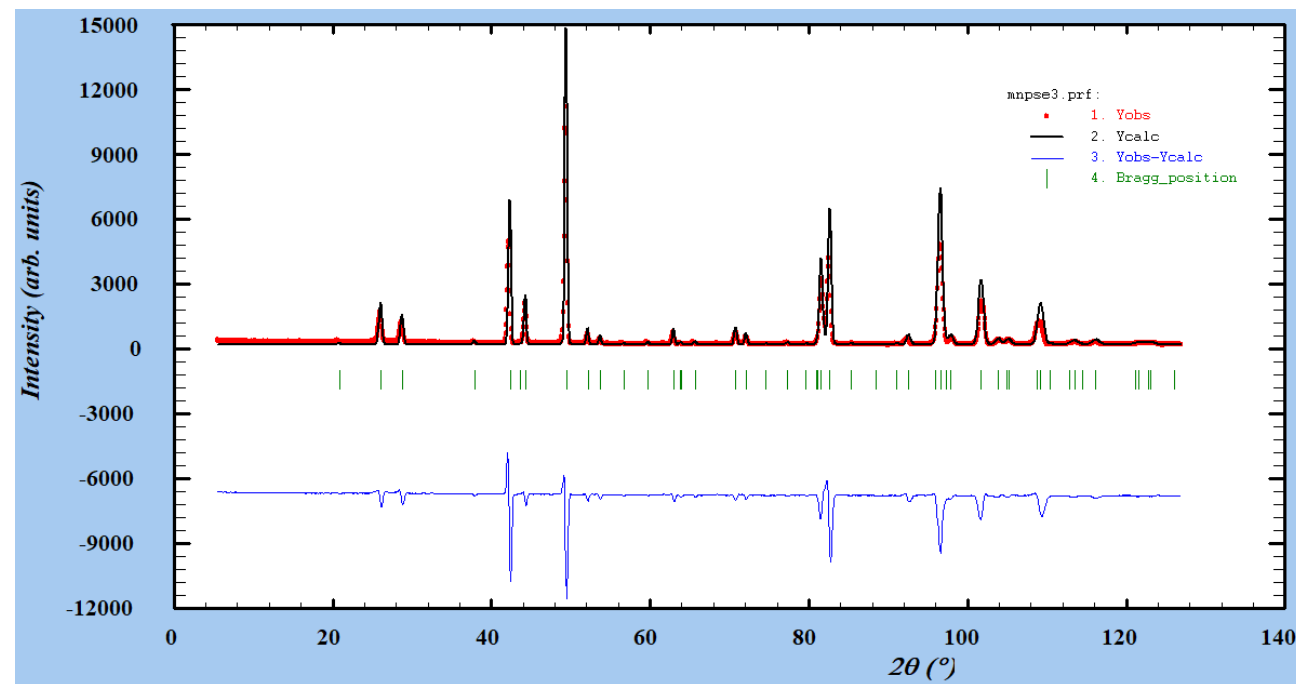
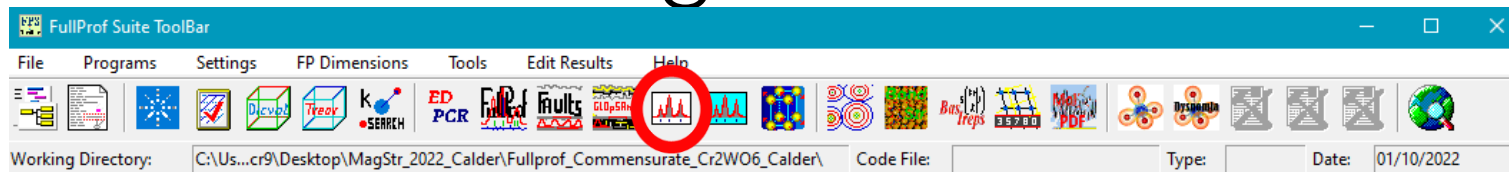
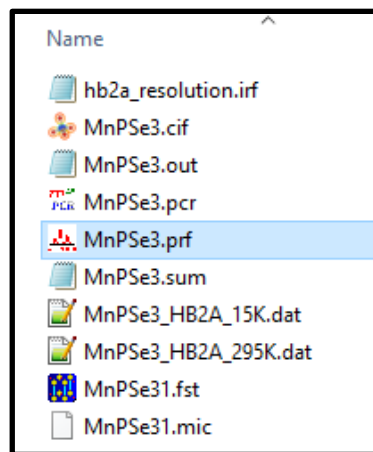
=> CPU Time: 0.794 seconds
=> 0.013 minutes

=> END Date:02/10/2022 Time => 14:22:32.083
```



# Step 1: Refine the crystal structure using FullProf

- Open the .prf file to check the fit.
- You might have to open the file after clicking on the toolbar. Or open it from the file directly.
- The peaks are fit at slightly different 2theta. So need to refine the lattice constants first. Also scale is a bit off. *NOTE: refine lattice constants before peak shape parameters.*



# Step 1: Refine the crystal structure using FullProf

- Now allow the following to refine to fit the nuclear crystal:
  - Scale factor (*Refinement>Profile*)
  - Lattice parameters (*Refinement>Profile*)
  - Background (*Refinement>Background*)
  - 2theta zero. (*Refinement>Instrumental*)
- Can also try to refine atomic parameters  
Refinement→Phase tab→Atoms
- If B is 0 in atom information, put in 0.3

Checking the box turns the number **blue** to show they are set to refine. If they are **red** then they are constrained to refine with another parameter. Looking in the text of the pcr file shows refined parameters by codes ending in 1.

Those constrained have the same code e.g. 11 and 11 or 511 and 511.

Profile Parameters: Phase 1 Pattern 1

Factors	
Scale	Overall B-factor
Coefficients	1.0000

Cell Parameters						
	a	b	c	alpha	beta	gamma
Coefficients	6.387001	6.387001	19.996000	90.000	90.000	120.000

FWHM / Shape Parameters    Asymmetry Parameters    Preferred Orientation

FWHM Parameters				
	U	V	W	IG
Coefficients	0.000000	0.000000	0.000000	0.000000

Shape Parameters			
	X	Y	SZ
Coefficients	0.000000	0.000000	0.000000

☐ Refine FWHM for second wavelength

	U2	V2	W2
Coefficients			

Buttons: Refine All, Fix All, Cancel, OK

6 Coefficients Polynomial Background: Pattern 1

	d_0	d_1	d_2	d_3	d_4	d_5
Coefficients	200.00	0.0000	0.0000	0.0000	0.0000	0.0000

	d_6	d_7	d_8	d_9	d_10	d_11
Coefficients						

Buttons: Refine All, Fix All

Instrumental Parameters Refinement: Pattern 1

2\_Theta

	Zero	Displacement	Transparency	Wavelength
Coefficients	0.000000	0.000000	0.000000	0.000000

Buttons: Refine All, Fix All, Cancel, OK

Atoms Information: Phase 1

List of Atoms  
Number of Atoms: 3

	Label	Ntyp	X	Y	Z	B	Occ	Therm. Fact.
Atom # 1	Mn1	Mn	0.00000	0.00000	0.16610	0.00000	0.33333	Isotropic
Atom # 2	P1	P	0.00000	0.00000	0.44430	0.00000	0.33333	Isotropic
Atom # 3	Se1	Se	0.33050	-0.00160	0.08180	0.00000	1.00000	Isotropic

Buttons: Refine Positions, Refine B\_iso, Refine B\_aniso, Fix All

Anisotropic Thermal Factors / Form Factors

# Step 1: Refine the crystal structure using FullProf

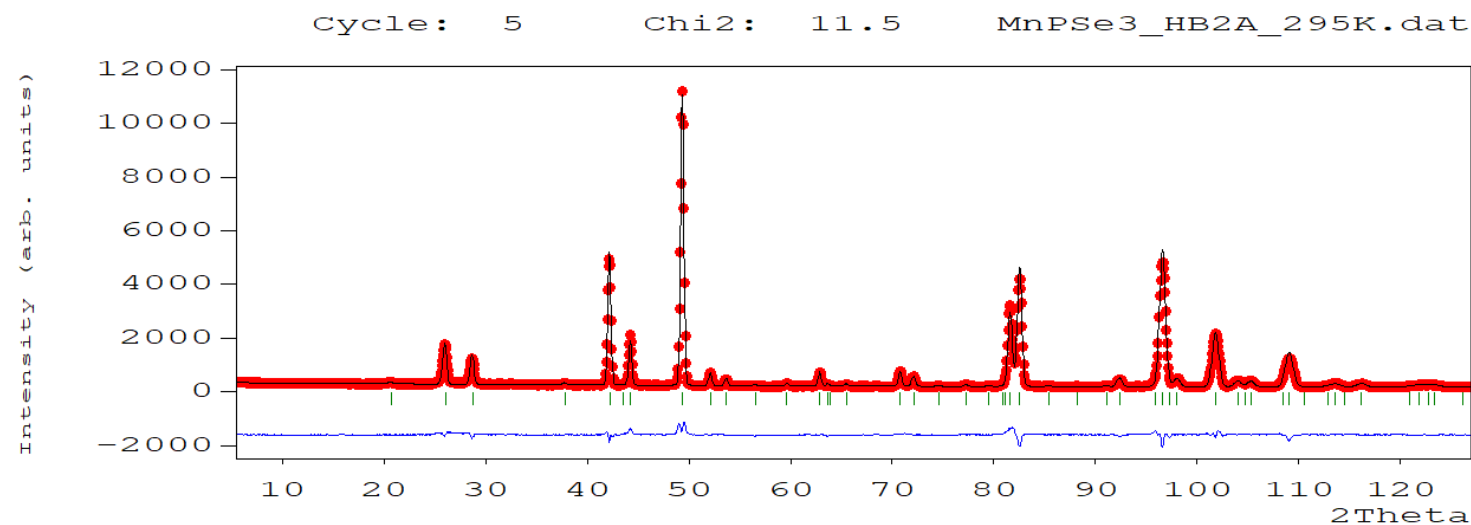
- The refinement to the 295K data is now close.
- You can add in refinements to the peak shape, since the sample may add some broadening beyond the parameters loaded in with the irf file.

```
FullProf Program
Load Edit PCR Mode Run Exit
=> Expected : 2.08 1.8701
=> Conventional Rietveld R-factors for Pattern: 1
=> Rp: 12.3 Rwp: 11.8 Rexp: 3.49 Chi2: 11.5
=> Global user-weighted Chi2 (Bragg contrib.): 12.73
=> -----> Pattern# 1
=> Phase: 1
=> Bragg R-factor: 7.624
=> RF-factor : 6.833

=> Convergence reached at this CYCLE !!!!: CYCLE No. 2
=> R-Factors: 5.21 7.04 Chi2: 11.5 DW-Stat.: 0.1937 Patt#: 1
=> Expected : 2.08 1.8701
=> Conventional Rietveld R-factors for Pattern: 1
=> Rp: 12.3 Rwp: 11.8 Rexp: 3.49 Chi2: 11.5
=> Global user-weighted Chi2 (Bragg contrib.): 13.06
=> -----> Pattern# 1
=> Phase: 1
=> Bragg R-factor: 7.624
=> RF-factor : 6.833
=> Normal end, final calculations and writing...

=> CPU Time: 1.136 seconds
=> 0.019 minutes

=> END Date:02/10/2022 Time => 14:37:37.528
```





# Step 1: Refine the crystal structure using FullProf

- Refinement → Profile → Refine U,V,W,X. Also refine asymmetry parameters.

Profile Parameters: Phase 1 Pattern 1

Factors

	Scale	Overall B-factor
Coefficients	0.73943 ✓	0.0000

Cell Parameters

	a	b	c	alpha	beta	gamma
Coefficients	6.378181 ✓	6.378181 ✓	20.016632 ✓	90.000	90.000	120.000 ✓

FWHM / Shape Parameters / Asymmetry Parameters / Preferred Orientation

FWHM Parameters

	U	V	W	IG
Coefficients	0.000 ✓	0.000 ✓	0.000 ✓	0.000000

Shape Parameters

	X	Y	SZ
Coefficients	0.000 ✓	0.000000	0.000000

☐ Refine FWHM for second wavelength

	U2	V2	W2
Coefficients			

Refine All  
Fix All  
Cancel  
OK

Profile Parameters: Phase 1 Pattern 1

Factors

	Scale	Overall B-factor
Coefficients	0.73943 ✓	0.0000

Cell Parameters

	a	b	c	alpha	beta	gamma
Coefficients	6.378181 ✓	6.378181 ✓	20.016632 ✓	90.000	90.000	120.000 ✓

FWHM / Shape Parameters / Asymmetry Parameters / Preferred Orientation

S\_L D\_L

	S_L	D_L
Coefficients	0.000000	0.000000

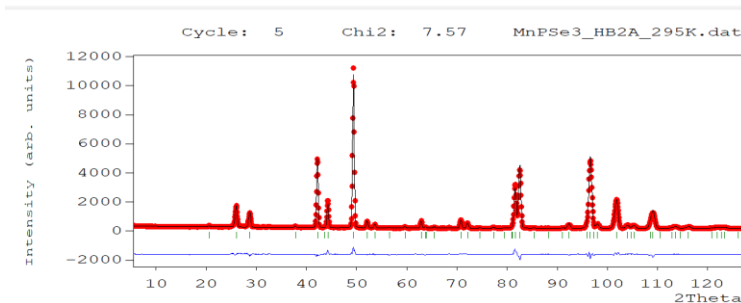
Asym1 Asym2 Asym3 Asym4

	Asym1	Asym2	Asym3	Asym4
Coefficients	0.000000 ✓	0.000000 ✓	0.000000 ✓	0.000000 ✓

Refine All  
Fix All  
Cancel  
OK

=> Phase: 1  
=> Bragg R-factor: 6.354  
=> RF-factor: 5.194  
=> Normal end, final calculations and writing...  
=> CPU Time: 1.521 seconds  
=> 0.025 minutes  
=> END Date:02/10/2022 Time => 14:42:13.490

- The refinement to the 295K data is now very close.
- At this point you should copy the pcr file or rename it so you can go back to this point if the refinement crashes or you have issues.



# Step 1: Refine the crystal structure using FullProf

- The previous steps were refining the crystal structure at 295K, where there was no long range magnetic order.
- We now want to refine the crystal structure in the magnetically ordered region (15K).
- Then we will add on the magnetic phase based on that refinement in steps 2 and 3.

# Step 1: Refine the crystal structure using FullProf

- Before refining the 4K data **FIRST TURN OFF PEAK SHAPE REFINEMENTS.** Since the peaks shift with temperature, refining both the lattice constants and peak shape may become unstable if all done at the same time.
  - The peak shapes should not change with temperature (we're measuring the same sample on the same instrument!)
  - The lattice constants and structural parameters would be expected to vary with temperature.

Profile Parameters: Phase 1 Pattern 1

Factors

	Scale	Overall B-factor
Coefficients	0.76115	0.0000

Cell Parameters

	a	b	c	alpha	beta	gamma
Coefficients	6.377378	6.377378	20.015066	90.000	90.000	120.000

FWHM / Shape Parameters | Asymmetry Parameters | Preferred Orientation

FWHM Parameters

	U	V	W	IG
Coefficients	0.016	-0.057	0.020	0.000000

Shape Parameters

	X	Y	SZ
Coefficients	0.052	0.000000	0.000000

☐ Refine FWHM for second wavelength

	U2	V2	W2
Coefficients			

Refine All  
Fix All  
Cancel  
OK

Profile Parameters: Phase 1 Pattern 1

Factors

	Scale	Overall B-factor
Coefficients	0.76115	0.0000

Cell Parameters

	a	b	c	alpha	beta	gamma
Coefficients	6.377378	6.377378	20.015066	90.000	90.000	120.000

FWHM / Shape Parameters | Asymmetry Parameters | Preferred Orientation

S\_L

	S_L	D_L
Coefficients	0.000000	0.000000

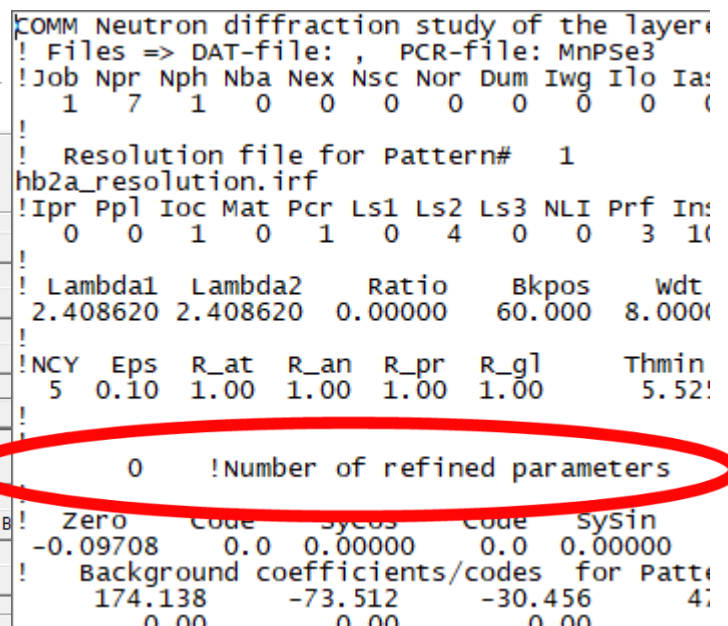
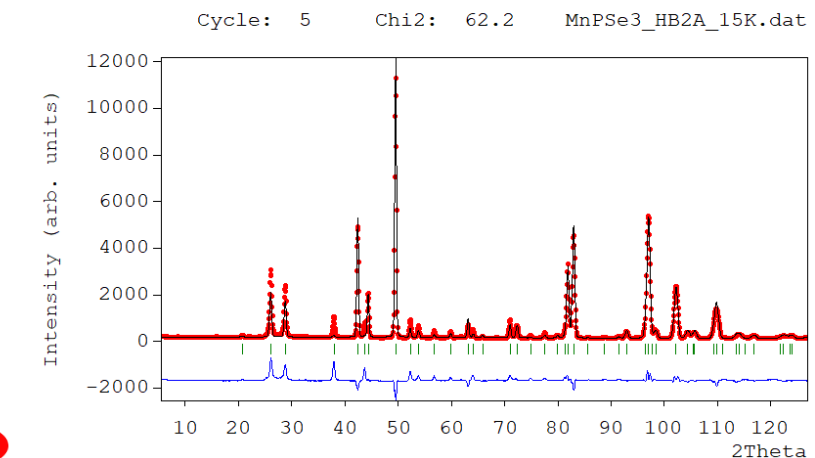
Asym1

	Asym1	Asym2	Asym3	Asym4
Coefficients	0.252470	0.097520	-0.446240	-0.169800

Refine All  
Fix All  
Cancel  
OK

- Now refine the 4K data (**MnPSe3\_HB2A\_295K.dat**).

- **TURN OFF ALL THE REFINEMENT PARAMETERS.**  
**\*\*\*Check in pcr text\*\*\***



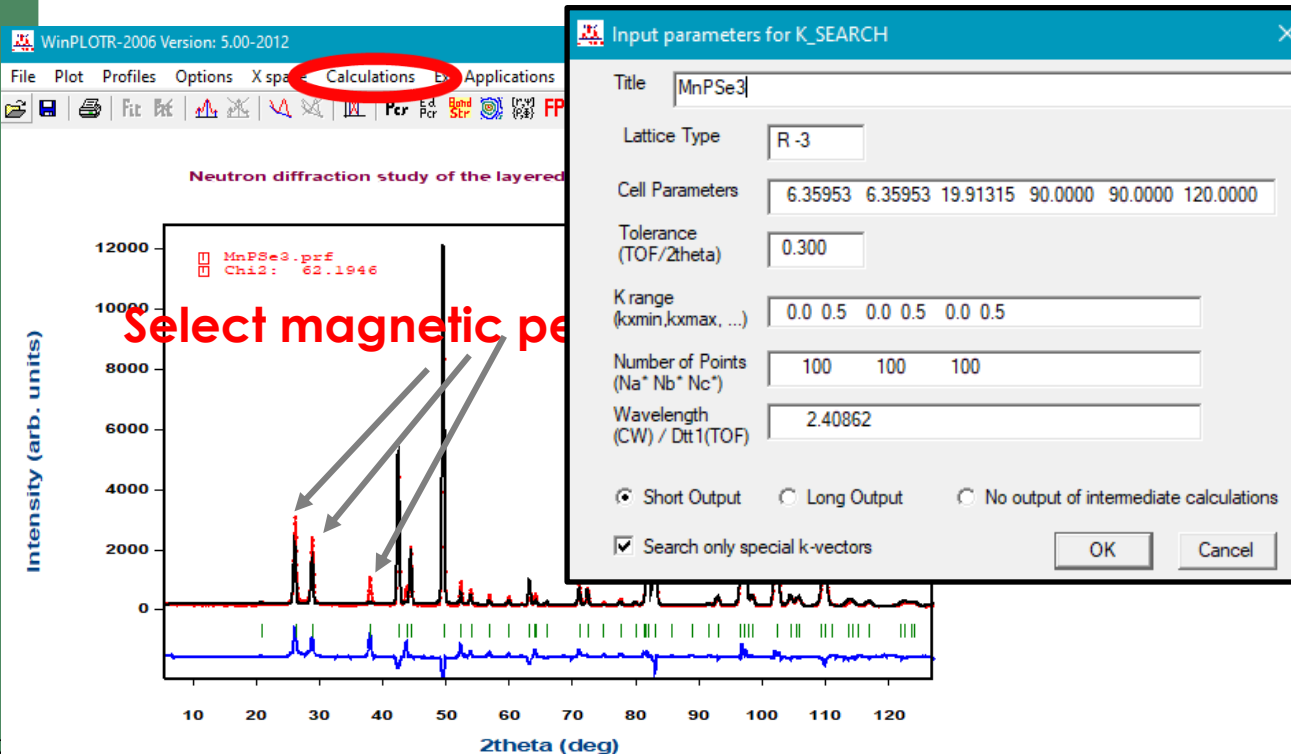
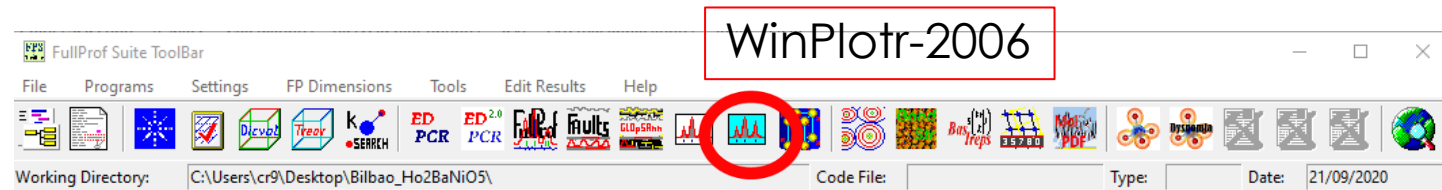
# MnPSe<sub>3</sub>

- This example will use Fullprof and SARAh  
<http://fermat.chem.ucl.ac.uk/spaces/willsgroup/web-software/sarah-refine-fullprof/>
  - Step 1: Refine the crystal structure using FullProf
  - **Step 2: Determine the k-vector by indexing the magnetic reflections using k-search**
  - Step 3: Create candidate magnetic models using SARAh
  - Step 4: Refine the magnetic model and nuclear phase in Fullprof.
  - Step 5: Check the magnetic model



# Determine the k-vector

- Now the magnetic peaks need to be indexed to find the propagation vector that defines the magnetic unit cell.
- Open the refinement .prf file using **WinPlotr-2006 > File > Open Rietveld/Profile (\*.prf)**
- Select “Calculations”> “peak detection”>”enable” . After enabling, go again to “Calculations”> “peak detection” > “insert peak”. After clicking on magnetic peaks, go to “save peaks” to save them as “K-search format”. Run k-search.



```
C:\WINDOWS\SYSTEM32\cmd.exe

Solution:      4 k = ( 0.1250 0.2500 0.0000) R-F:   2.0948
Solution:      5 k = ( 0.2500 0.1250 0.0000) R-F:   2.0948
Solution:      6 k = ( 0.1250 0.5000 0.1250) R-F:   1.7787
=> Special k-vector solutions found!

=> List of the best incommensurate 10 solutions for 8 satellites

      Kx      Ky      Kz      R-factor
0.000000  0.000000  0.000000  0.553222
1.000000  0.000000  0.000000  0.553230
0.000000  1.000000  0.000000  0.553230
0.125000  0.500000  0.125000  1.778686
0.125000  0.250000  0.000000  2.094841
0.250000  0.125000  0.000000  2.094841

=> The best commensurate solution is the special kvector ks = ( 0.0000 0.0000 0.0000)
=> The corresponding R-factor is:      0.5532 to be compared with incommensurate R-factor

=> Powder diffraction may give wrong results even if the R-factors for the solutions are "good"
    The best way to verify the solutions is to perform a full profile fitting and look for mismatches
```

**k=(0,0,0)**

# MnPSe<sub>3</sub>

- This example will use Fullprof and SARAh  
<http://fermat.chem.ucl.ac.uk/spaces/willsgroup/web-software/sarah-refine-fullprof/>
  - Step 1: Refine the crystal structure using FullProf
  - Step 2: Determine the k-vector by indexing the magnetic reflections using k-search
  - **Step 3: Create candidate magnetic models using SARAh**
  - Step 4: Refine the magnetic model and nuclear phase in Fullprof.
  - Step 5: Visualize the magnetic model

# Step 3: Create candidate magnetic models using SARAh

- We will use the SARAh software that is web based.
- There is an example of refining  $\text{Cr}_2\text{WO}_6$  using the stand alone software.
- Use the SARAh webrefine – Fullprof
- <http://fermat.chem.ucl.ac.uk/spaces/willsgroup/web-software/sarah-refine-fullprof/>

## Wills Group

Magnetism and magnetic materials

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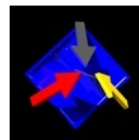
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## SARAh – Simulated Annealing and Representation Analysis



**News – Feb 2022. The web version of SARAh Refine for FullProf has been released. It reproduces the core features of SARAh Refine for Windows in a browser and has introduced new refinement ideas :**

<http://fermat.chem.ucl.ac.uk/spaces/willsgroup/web-software/sarah-refine-fullprof/>

(Click icon to download combined install file from Dropbox)

- k search – finding the propagation vector with SARAh
- SARAh – Simulated Annealing and Representation Analysis
  - SARAh Installation Instructions
  - SARAh – Introduction video
  - SARAh with FullProf
  - SARAh with GSAS
- Valist – Bond Valence Calculations and Listing
- Downloads

*The SARAh suite is made up of 2 separate programs that perform symmetry calculations and magnetic structure analysis :*

### SARAh Representational Analysis –

Performs the calculations of Representational Analysis. These allow the determination of atomic displacements or magnetic structures that can accompany a second-order phase transition. Output files includes a tailored summary with cut-and-paste tables written in LaTeX. (Win9x, 2000, Vista and Windows 7) [1]

### SARAh Refine –

Is an example of a 'metaprogram'. SARAh refine was developed to add new functionality to the standard Rietveld programs GSAS, FullProf and TOPAS, i.e. to allow them to refine magnetic structures in terms of the basis vectors (symmetry modes) generated by SARAh Representational Analysis and the calculations of group theory. [1]

# Step 3: Create candidate magnetic models using SARAh

Help with technical settings and refinement strategies

<http://fermat.chem.ucl.ac.uk/spaces/willsgroup/web-software/sarah-refine-fullprof/>

*Technical information: (ASW version Oct 2022 :-)*

## Open information about browser settings (this is really important!)

Most browsers have a default directory where they save files. webSARAh-Refine works best if you can select the location for each download. This will enable you to save the template magnetic phase .pcr file to your current refinement directory or to edit a file by replacing it. If you use more than one browser, perhaps for compatibility or as part of your internet security, it may be easiest to have one set to using a default folder and another that asks each time for the download location.

Below are some settings for common browsers that turn on 'Ask where to save each file before downloading':

**Google Chrome** : 1) Click the menu icon (aka 3 dots) in the upper right corner of the Chrome window. 2) Select 'Settings'. 3) Scroll down and click 'Show Advanced Settings'. 4) Scroll down to the 'Downloads' section and click 'Ask where to save each file before downloading'

**Firefox - Mac**: 1) Select 'Firefox' → 'Preferences' from the menu bar. 2) In the General panel scroll down to 'Files and Applications'. 3) In Downloads select 'Always ask where to save files'

**Firefox - Windows 11**: 1) Click the menu button (the 3 line burger button) and select 'Settings'. 2) In the General panel scroll down to 'Files and Applications'. 3) In Downloads select 'Always ask where to save files'

**Safari - Mac**: 1) Select 'Safari' → 'Preferences' from the menu bar. 2) In the General tab, click the dropdown menu next to 'File download location'. 3) Select 'Ask for Each Download'

# Step 3: Create candidate magnetic models using SARAh

- Input the crystal structure information. All we need is the
  - Space group
  - Propagation vector
  - Magnetic ion position

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## SARAh webRefine – FullProf (beta version)

Two pieces of advice for using SARAh webRefine : 1. change your browser settings to allow you to select where you save downloads (and overwrite files), 2. when you click <evaluate>, it will look like nothing is happening for a few seconds. Look in the tab '4. Help and Strategies' for more information.

-Andrew (February 2022)



Space group : {148:H, R -3:H, C 3i 2} ▼

Propagation vector :

0 0 0

Crystallographic coordinates in the form :  
or Cu2 1/2 1/2 -1/2

Mn1 0 0 0.17521

Submit



# Step 3: Create candidate magnetic models using SARAh

- SARAh produces the basis vectors.
- These can be viewed on the webpage
- See next slide for details

## SARAh webRefine – FullProf (beta version)

Two pieces of advice for using SARAh webRefine : 1. change your browser settings to allow you to select where you save downloads (and overwrite files), 2. when you click <evaluate>, it will look like nothing is happening for a few seconds. Look in the tab '4. Help and Strategies' for more information.

-Andrew (February 2022)



1. Conventional basis vectors (as projected)	2. Stationary vector combinations	3. Exchange multiplets	4. Help and strategies
---	-----------------------------------	------------------------	------------------------

### Method 1. Conventional analysis - as projected basis vectors

Select command (generate template for magnetic phase for pcr; edit pcr with magnetic phase present):

1. powder format ▼

2. make template pcr ▼

☐ Mn1  $\Gamma_1 \psi_1$

☐ Mn1  $\Gamma_2 \psi_1$

☐ Mn1  $\Gamma_3 \psi_1$

☐ Mn1  $\Gamma_4 \psi_1$

☐ Mn1  $\Gamma_5 \psi_1$

☐ Mn1  $\Gamma_6 \psi_1$

(Your browser should be set to ask for the download location so the pcr file can be overwritten. Please look in '4. Help and strategies' for an explanation/help.)

Submit

# Step 3: Create candidate magnetic models using SARAh

$$\left\{ \begin{array}{cc} \Gamma_1 & \psi_1 \\ \text{Mn1} & \begin{array}{l} 1) \ 0. \ 0. \ 3. \\ 2) \ 0. \ 0. \ 3. \end{array} \end{array} \right\}$$



$\Gamma_1$ : c-axis moment (FM)

$$\left\{ \begin{array}{cc} \Gamma_2 & \psi_1 \\ \text{Mn1} & \begin{array}{l} 1) \ 0. \ 0. \ 3. \\ 2) \ 0. \ 0. \ -3. \end{array} \end{array} \right\}$$



$\Gamma_2$ : c-axis moment (AFM)

$$\left\{ \begin{array}{cc} \Gamma_3 & \psi_1 \\ \text{Mn1} & \begin{array}{l} 1) \ 1.5 - 0.866025 i \ 0. \ -1.73205 i \ 0. \\ 2) \ 1.5 - 0.866025 i \ 0. \ -1.73205 i \ 0. \end{array} \end{array} \right\}$$



$\Gamma_3$ : ab-plane moment (FM)

$$\left\{ \begin{array}{cc} \Gamma_4 & \psi_1 \\ \text{Mn1} & \begin{array}{l} 1) \ 1.5 - 0.866025 i \ 0. \ -1.73205 i \ 0. \\ 2) \ -1.5 + 0.866025 i \ 0. \ +1.73205 i \ 0. \end{array} \end{array} \right\}$$



$\Gamma_4$ : ab-plane moment (AFM)

$$\left\{ \begin{array}{cc} \Gamma_5 & \psi_1 \\ \text{Mn1} & \begin{array}{l} 1) \ 1.5 + 0.866025 i \ 0. \ +1.73205 i \ 0. \\ 2) \ 1.5 + 0.866025 i \ 0. \ +1.73205 i \ 0. \end{array} \end{array} \right\}$$



$\Gamma_5$ : ab-plane moment (FM)

$$\left\{ \begin{array}{cc} \Gamma_6 & \psi_1 \\ \text{Mn1} & \begin{array}{l} 1) \ 1.5 + 0.866025 i \ 0. \ +1.73205 i \ 0. \\ 2) \ -1.5 - 0.866025 i \ 0. \ -1.73205 i \ 0. \end{array} \end{array} \right\}$$



$\Gamma_6$ : ab-plane moment (AFM)

**Most reflections have zero h or k. No change at (110). This suggests spins in ab-plane. Bulk measurements indicated AFM and no FM.**

**So try  $\Gamma_4$  and  $\Gamma_6$  first, but all should be checked.**

# Step 3: Create candidate magnetic models using SARAh

- There are different options for the magnetic phase output
  - 1. add new phase to pcr
  - 2. make template pcr  
*This is similar to the older stand alone SARAh that creates the magnetic phase in a text file that needs to be pasted into the pcr. See other examples for this.*
  - 3. edit pcr
- We'll use 1. to add the new magnetic phase directly to the pcr file.
- Choose the "MnPSe3.pcr" file from STEP 1
- Click submit and again choose the "MnPSe3.pcr" file to overwrite it
- "MnPSe3.pcr" should now contain the additional magnetic phase

## SARAh webRefine – FullProf (beta version)

Two pieces of advice for using SARAh webRefine : 1. change your browser settings to allow you to select where you save downloads (and overwrite files), 2. when you click <evaluate>, it will look like nothing is happening for a few seconds. Look in the tab '4. Help and Strategies' for more information.

-Andrew (February 2022)



1. Conventional basis vectors (as projected)	2. Stationary vector combinations	3. Exchange multiplets	4. Help and strategies
--	-----------------------------------	------------------------	------------------------

### Method 1. Conventional analysis - as projected basis vectors

Select command (generate template for magnetic phase for pcr; edit pcr with magnetic phase present):

1. powder format ▾ 1. add new phase to pcr ▾ Choose File MnPSe3.pcr

☐ Mn1  $\Gamma_1 \psi_1$   
☐ Mn1  $\Gamma_2 \psi_1$   
☐ Mn1  $\Gamma_3 \psi_1$   
☐ Mn1  $\Gamma_4 \psi_1$   
☐ Mn1  $\Gamma_5 \psi_1$

1. add new phase to pcr  
2. make template pcr  
3. edit pcr

(Your browser should be set to ask for the download location so the pcr file can be overwritten. Please look in '4. Help and strategies' for an explanation/help.)

Submit

### Method 1. Conventional analysis - as projected basis vectors

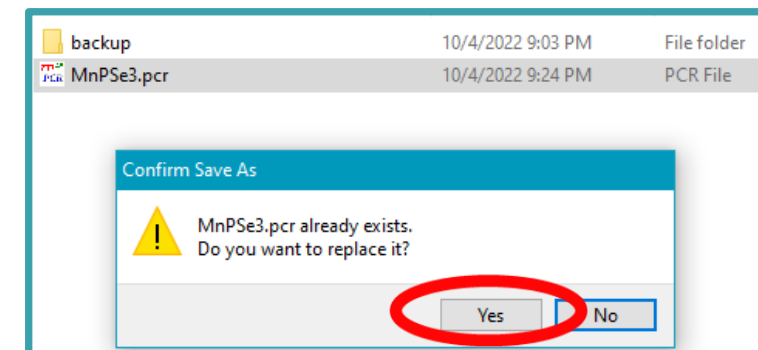
Select command (generate template for magnetic phase for pcr; edit pcr with magnetic phase present):

1. powder format ▾ 1. add new phase to pcr ▾ Choose File MnPSe3.pcr

☐ Mn1  $\Gamma_1 \psi_1$   
☐ Mn1  $\Gamma_2 \psi_1$   
☐ Mn1  $\Gamma_3 \psi_1$   
☒ Mn1  $\Gamma_4 \psi_1$   
☐ Mn1  $\Gamma_5 \psi_1$   
☒ Mn1  $\Gamma_6 \psi_1$

(Your browser should be set to ask for the download location so the pcr file

Submit



# MnPSe<sub>3</sub>

- This example will use Fullprof and SARAh  
<http://fermat.chem.ucl.ac.uk/spaces/willsgroup/web-software/sarah-refine-fullprof/>
  - Step 1: Refine the crystal structure using FullProf
  - Step 2: Determine the k-vector by indexing the magnetic reflections using k-search
  - Step 3: Create candidate magnetic models using SARAh
  - **Step 4: Refine the magnetic model and nuclear phase in Fullprof.**
  - Step 5: Check the magnetic model

## Step 4: Refine the magnetic model and nuclear phase in Fullprof

- The SARA web interface directly adds the magnetic phase.
  - For representational analysis there are two phases
    - Nuclear
    - Magnetic
- *NOTE: The scale for nuclear and magnetic phase should always be kept the SAME.*

```

COMM Neutron diffraction study of the layered compounds Mn P Se3 and Fe P Se3
Files ==> DAT-file: , PCR-file: MNPSe3
Job Npr Nph Nba Nex Nsc Nor Dum Iwg Ilo Ias Res Ste Nre Cry uni Cor Opt Aut
1 7 2 0 0 1 0 4 0 0 3 10 0 0 0 0 0 0 0 0 1

! Resolution file for Pattern# 1
hb2a_resolution.irf
! Ipr Ppl Ioc Mat Pcr Ls1 Ls2 Ls3 NLI Prf Ins Rpa Sym Hk1 Fou Sho Ana
0 0 1 0 1 0 4 0 0 3 10 0 0 0 0 0 0 0 0 0 0

! Lambda1 Lambda2 Ratio Bkpos wdt cthm muR AsyLim Rpolarz 2nd-muR -> Patt# 1
2.408620 2.408620 0.00000 60.000 8.0000 0.0000 0.0000 180.00 0.0000 0.0000

! NCY Eps R_at R_an R_pr R_g| Thmin Step Thmax PSD Sent0
5 0.10 1.00 1.00 1.00 1.00 5.5250 0.064983 155.0000 0.000 0.000

0 !Number of refined parameters

! Zero code SysCos Code Sysin Code Lambda Code MORE ->Patt# 1
-0.09708 0.0 0.00000 0.0 0.00000 0.0 0.000000 0.00 0
! Background coefficients/codes for Pattern# 1 (Polynomial of 6th degree)
174.138 -73.512 -30.454 47.759 0.000 0.000
0.00 0.00 0.00 0.00 0.00 0.00

-----
! Data for PHASE number: 1 ==> Current_R_Bragg for Pattern# 1: 0.0000
-----
Neutron diffraction study of the layered compounds Mn P Se3 and Fe P Se3

! Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nvk Npr More
3 0 0 0 0.0 0.0 1.0 0 0 0 0 0 1936.726 0 7 0

R -3 <--Space group symbol
! Atom Typ X Y Z B1so Occ In Fin N_Lt Spc /Codes
Mn1 Mn 0.00000 0.00000 0.1751 0.30000 0.33333 0 0 0 0
0.00 0.00 0.00 0.00 0.00 0.00
P1 P 0.00000 0.00000 0.44848 0.30000 0.33333 0 0 0 0
0.00 0.00 0.00 0.00 0.00 0.00
Se1 Se 0.32983 -0.01193 0.08193 0.30000 1.00000 0 0 0 0
0.00 0.00 0.00 0.00 0.00 0.00

!-----> Profile Parameters for Pattern # 1 -----> Phase # 1
! Scale Shape1 Bov Str1 Str2 Str3 Strain-Model
0.8798522 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0
0.00000 0.000 0.000 0.000 0.000 0.000 0.000

! U V W X Y Gaussiz Lorsiz Size-Model
0.015521 -0.057189 0.020187 0.052448 0.000000 0.000000 0.000000 0
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

! a b c alpha beta gamma #Cell Info
6.359528 6.359528 19.913155 90.00000 90.00000 120.000000
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
! Pref1 Pref2 Asy1 Asy2 Asy3 Asy4 S_L D_L
0.00000 0.00000 0.25247 0.09752 -0.44624 -0.16980 0.0000 0.00000
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

-----
! Data for PHASE number: 2 ==> Current_R_Bragg for Pattern# 1: 46.66
-----
Template magnetic phase by SARAH - web Representational Analysis

! Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nvk Npr More
1 0 0 0 0.0 0.0 1.0 1 0 -2 0 0 1936.726 1 7 0

R -1 <--Space group symbol
! Nsym Cen Laue Ireps N_Bas
2 1 1 -1 2
! Real(0)-Imaginary(1) indicator for ci
0 0

! SYMM X, Y, Z
BASR 1.5 0 0 1.5 0 0
BASi 0.866 1.732 0 -0.866 -1.732 0
SYMM 4/3 - X, 2/3 - Y, 2/3 - Z
BASR -1.5 0 0 -1.5 0 0
BASi -0.866 -1.732 0 0.866 1.732 0
! Atom Typ Mag Vek C6 X C7 Y C8 Z B1so Occ C1 C2 C3
Mn1 MN5 1 0 0 0 0 0 0 0.17521 30000 1.00000 0.000 0.000 0.000
0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.00000
0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

!-----> Profile Parameters for Pattern # 1 -----> Phase # 1
! Scale Shape1 Bov Str1 Str2 Str3 Strain-Model
0.8798522 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0
0.00000 0.000 0.000 0.000 0.000 0.000 0.000

! U V W X Y Gaussiz Lorsiz Size-Model
0.015521 -0.057189 0.020187 0.052448 0.000000 0.000000 0.000000 0
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

! a b c alpha beta gamma #Cell Info
6.359528 6.359528 19.913155 90.00000 90.00000 120.000000
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
! Pref1 Pref2 Asy1 Asy2 Asy3 Asy4 S_L D_L
0.00000 0.00000 0.25247 0.09752 -0.44624 -0.16980 0.0000 0.00000
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

! Propagation vectors:
0.0 0.0 Propagation vector 1
0.000000 0.000000 0.000000

```

## Nuclear phase

## Magnetic phase



# Step 4: Refine the magnetic model and nuclear phase in Fullprof

- The basis vectors can be seen in the magnetic phase.
- In this case we loaded two:  
☒ Mn1  $\Gamma_4 \psi_1$   
☒ Mn1  $\Gamma_6 \psi_1$
- To give these basis vectors magnitude put values in the coefficients C1 and C2

## Magnetic phase

```
-----
Data for PHASE number: 2 ==> Current R_Bragg for Pattern# 1: 46.66
-----
Template magnetic phase by SARAh - web Representational Analysis
Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nvk Npr More
1 0 0 0.0 0.0 1.0 1 0 -2 0 0 1936.726 1 7 0
!
! R -1 <--Space group symbol
! Nsym Cen Laue Ireps N_Bas
! 2 1 1 -1 2
! Real(0)-Imaginary(1) indicator for Ci
! 0 0
!
! MM X, Y, Z
! 1.5 0 0
! 0.866 1.732 0
! 4/3 - X, 2/3 - Y, 2/3 - Z
! -1.5 0 0
! -0.866 -1.732 0
! Atom Typ Mag Vek X Y Z Biso Occ
! C4 C5 C6 C7 C8 C9
Mn1 MMN5 1 0 0 0 0 0.17521 30000 1.00000
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
!-----> Profile Parameters for Pattern # 1 -----> Phase # 1
! Scale Shape1 Bov Str1 Str2 Str3 Strain-Model
! 0.8798522 0.00000 0.00000 0.00000 0.00000 0.00000 0
! U V W X Y GauSiz Lorziz Size-Model
! 0.015521 -0.057189 0.020187 0.052448 0.000000 0.000000 0.000000 0
! a b c alpha beta gamma #Cell Info
! 6.359528 6.359528 19.913155 90.000000 90.000000 120.000000
! 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
! Pref1 Pref2 Asy1 Asy2 Asy3 Asy4 S_L D_L
! 0.00000 0.00000 0.25247 0.09752 -0.44624 -0.16980 0.00000 0.00000
! 0.00 0.00 0.00 0.00 0.00 0.00 0.00
! Propagation vectors:
! 0. 0. 0. Propagation Vector 1
! 0.000000 0.000000 0.000000
```

Mn1  $\Gamma_4 \psi_1$

Mn1  $\Gamma_6 \psi_1$

C1 C2 C3

# Step 4: Refine the magnetic model and nuclear phase in Fullprof

- Turn on C1 to refine in the pcr text file.
- Also update the Mn ion to MMN2 (this is magnetic  $\text{Mn}^{2+}$ ). The form factor is selected by the valence state, so might vary slightly if the valence label is wrong.

```
!----- Data for PHASE number: 2 ==> Current R_Bragg for Pattern# 1: 46.66 -----!
!----- Template magnetic phase by SARAh - web Representational Analysis -----!
! Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nvk Npr More
! 1 0 0 0.0 0.0 1.0 1 0 -2 0 0 1936.726 1 7 0
!
! R -1 <--Space group symbol
! Nsym Cen Laue Ireps N_Bas
! 2 1 1 -1 2
! Real(0)-Imaginary(1) indicator for ci
! 0 0
!
! SYMM X , Y , Z
! BASR 1.5 0 0 1.5 0 0
! BASI 0.866 1.732 0 -0.866 -1.732 0
! SYMM 4/3 - X , 2/3 - Y , 2/3 - Z
! BASR -1.5 0 0 -1.5 0 0
! BASI -0.866 -1.732 0 0.866 1.732 0
! Atom Typ Mag Vek X Y Z Biso Occ C1 C2 C3
! c4 c5 c6 c7 c8 c9 MagPh 1.0000 2 0.000 0.000
Mn MMN2 0 0.00 0.00 0.00 0.00 0.00 0.00 0.00 1 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
!-----> Profile Parameters for Pattern # 1 -----> Phase # 1
! Scale Shape1 Bov Str1 Str2 Str3 Strain-Model
! 0.8798522 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0
! 0.00000 0.000 0.000 0.000 0.000 0.000 0.000
! U V W X Y GauSiz LorsiZ Size-Model
! 0.015521 -0.057189 0.020187 0.052448 0.000000 0.000000 0.000000 0.000000 0
! 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
! a b c alpha beta gamma #Cell Info
! 6.359528 6.359528 19.913155 90.000000 90.000000 120.000000
! 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
! Pref1 Pref2 Asy1 Asy2 Asy3 Asy4 S_L D_L
! 0.00000 0.00000 0.25247 0.09752 -0.44624 -0.16980 0.00000 0.00000
! 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
! Propagation vectors:
! 0. 0. 0. Propagation vector 1
! 0.000000 0.000000 0.000000
```

# Step 4: Refine the magnetic model and nuclear phase in Fullprof

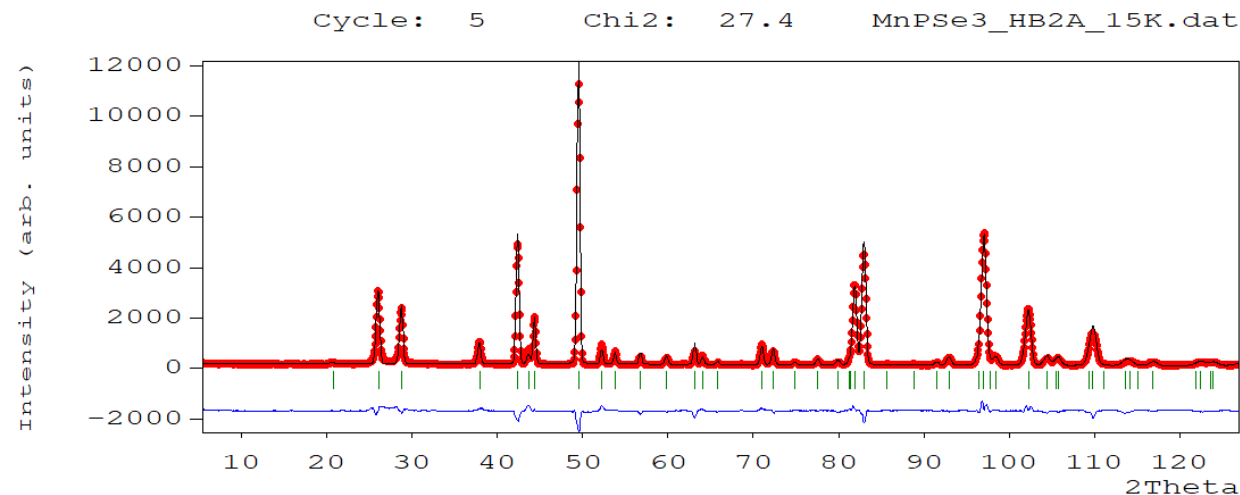
- Refine the 15K data.
- This captures the magnetic peaks well.
- Put the C1 back to zero and refine C2. The fit is identical.
- These are related solutions.
- Try refining C1 and C2 (with the constraint that they are equal).
- *To improve the fit, try refining the peak shapes, background, atom positions, thermal parameters, etc*

```
FullProf Program
Load Edit PCR Mode Run Exit
=> -----> Pattern#      1
=> Phase:      1
=> Bragg R-factor:  9.407
=> RF-factor      :  6.532
=> Phase:      2
=> Magnetic R-factor: 18.65

=> Convergence reached at this CYCLE !!!!: CYCLE No.      4
=> R-Factors:  8.59      11.2      Chi2: 27.4      DW-Stat.: 0.1143      Patt#: 1
=> Expected :      2.13
=> Conventional Rietveld R-factors for Pattern:      1
=> Rp: 14.9      Rwp: 15.7      Rexp: 3.00
=> Global user-weighted Chi2 (Bragg contrib.): 31.12      Chi2: 27.4
=> -----> Pattern#      1
=> Phase:      1
=> Bragg R-factor:  9.407
=> RF-factor      :  6.532
=> Phase:      2
=> Magnetic R-factor: 18.65
=> Normal end, final calculations and writing...

=> CPU Time:      2.662 seconds
=> 0.044 minutes

=> END      Date:02/10/2022      Time => 16:25:16.376
```

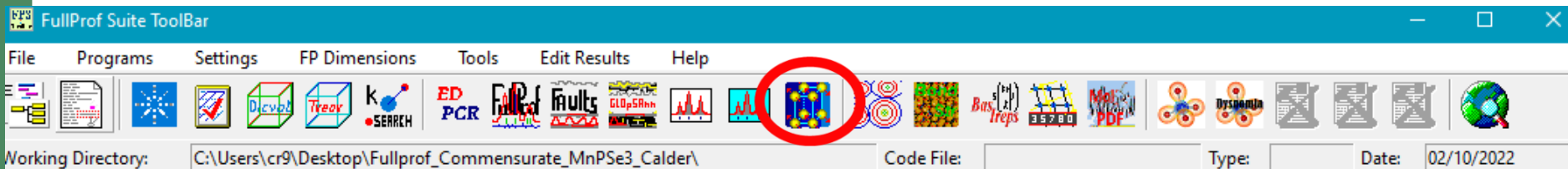
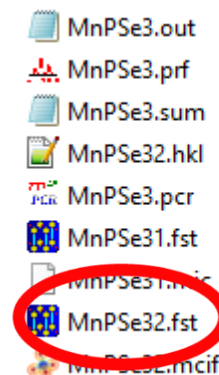


# MnPSe<sub>3</sub>

- This example will use Fullprof and SARAh  
<http://fermat.chem.ucl.ac.uk/spaces/willsgroup/web-software/sarah-refine-fullprof/>
  - Step 1: Refine the crystal structure using FullProf
  - Step 2: Determine the k-vector by indexing the magnetic reflections using k-search
  - Step 3: Create candidate magnetic models using SARAh
  - Step 4: Refine the magnetic model and nuclear phase in Fullprof.
  - **Step 5: Check the magnetic model**

# Step 5: Check the magnetic model

- The model can be checked in FPStudio

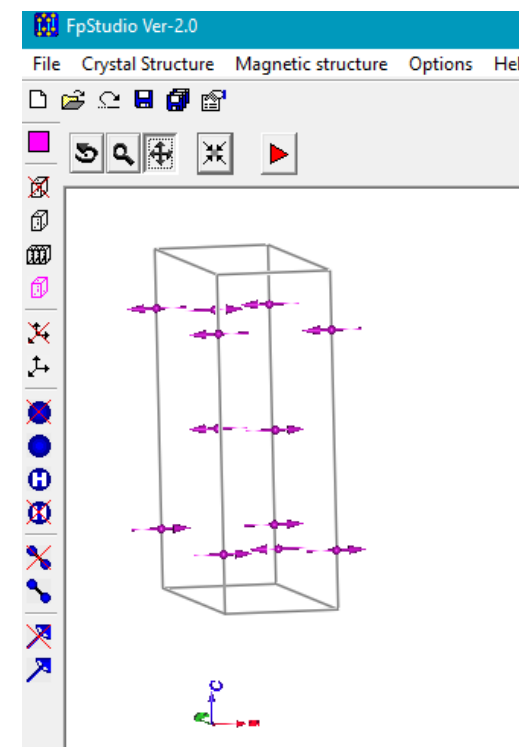


- There are two .fst files, these are for the 2 phases. Open the magnetic phase (file ending in 2.fst)
- In Fpstudio click on the drop-down menu "Magnetic Structure" and select "List magnetic moments"

```

Magnetic lattice type : R
Unit cell:      6.3595      6.3595      19.9132      90.0000      90.0000      120.0000
Current Box:    0  1  0  1  0  1
Magnetic k-vectors :
0.00000 0.00000 0.00000
Symmetry operations :
SYMM x,y,z
u,v,w,0.0
Atom : Mn1_1  Mn
-----
      x      y      z      Translation      k MSYM      m(a)      m(b)      m(c)      Mtot
0.00000 0.00000 0.17521
      ( 0,  0,  0)      1  1  3.34510  0.00000  0.00000
                                     3.34510  0.00000  0.00000  3.34510
      ( 0,  1,  0)      1  1  3.34510  0.00000  0.00000
                                     3.34510  0.00000  0.00000  3.34510
      ( 1,  0,  0)      1  1  3.34510  0.00000  0.00000

```

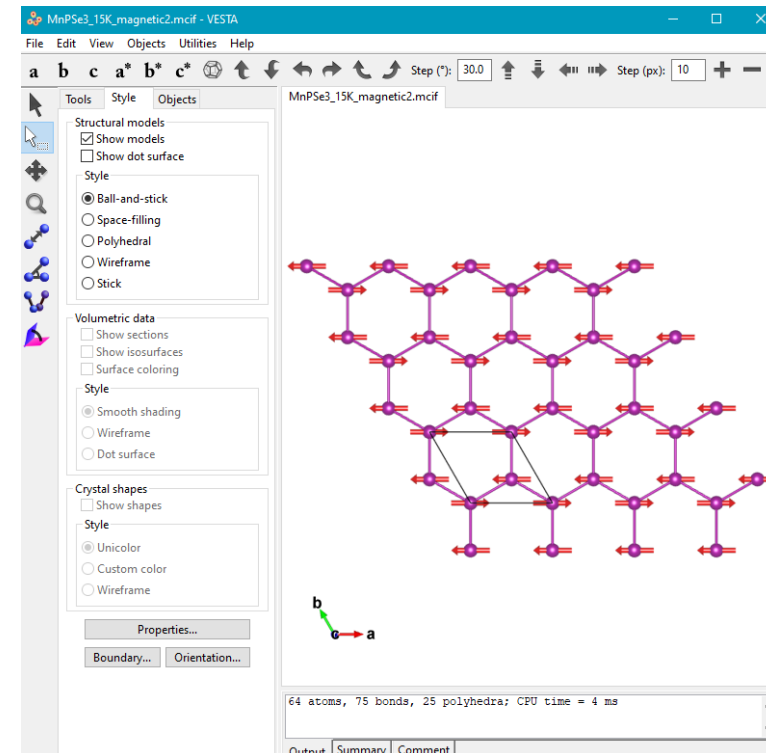
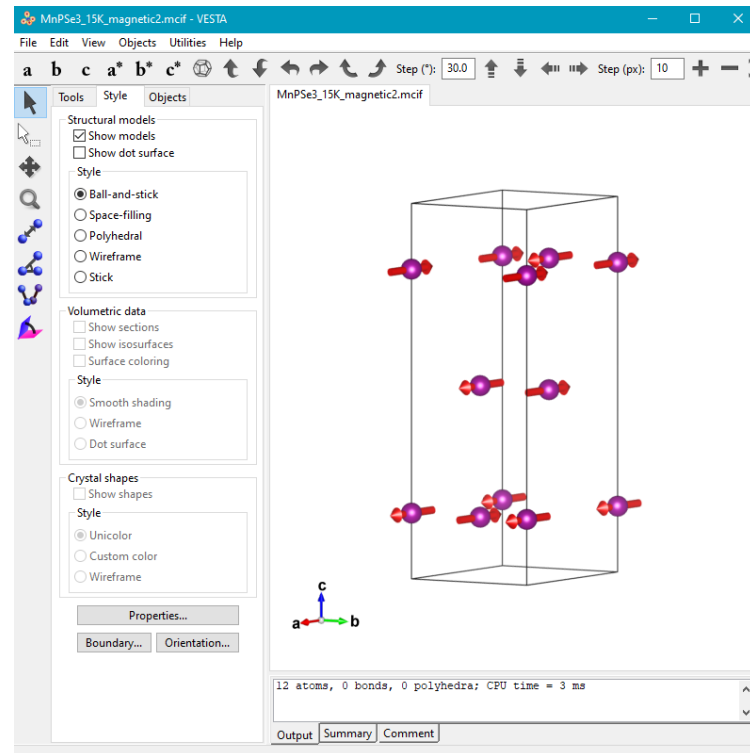


Note the assignment of moments along the a-axis is arbitrary. Symmetry allows for any direction in the *ab*-plane. c-axis moment should also be checked.



# Step 5: Check the magnetic model

- The .mcif file output by Fullprof can be used to visualize the magnetic structure in vesta



- This is the published magnetic structure.