

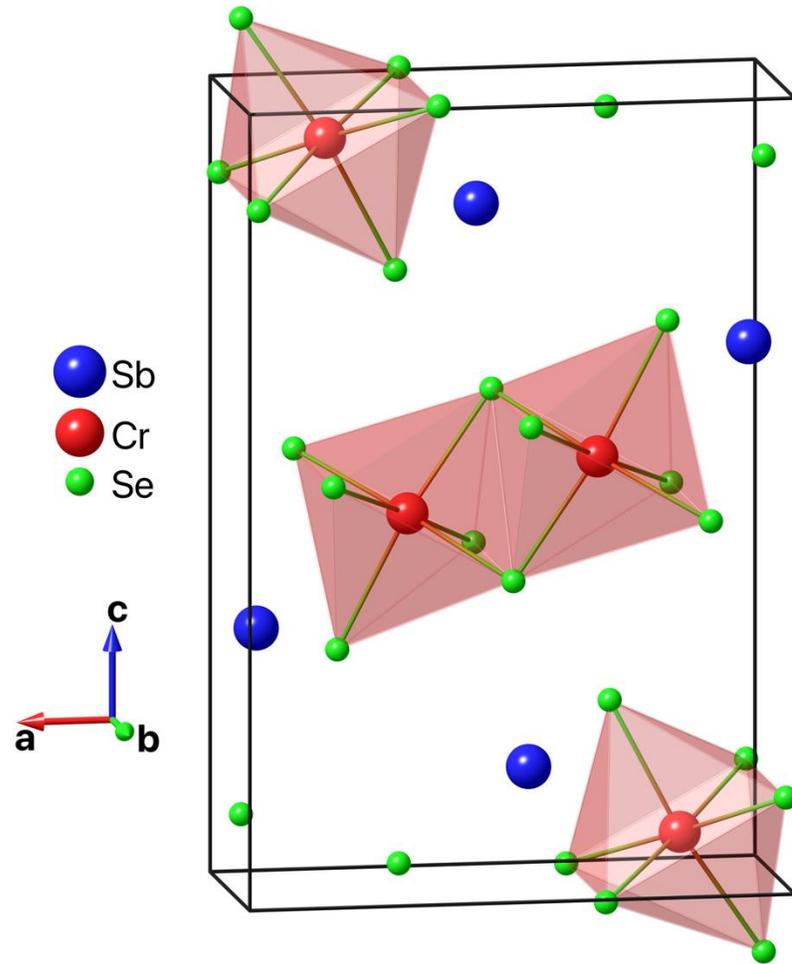
A visual guide for crystal and commensurate magnetic structure refinement using Mag2Pol

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Details of the compound, data and software



Orthorhombic structure: *Pnma* (No. 62)

$a = 9.143086 \text{ \AA}$, $b = 3.784552 \text{ \AA}$, $c = 13.416915 \text{ \AA}$

Time-of-flight diffraction data at POWGEN:

[PG3_42702-2_300K.dat](#) (Paramagnetic phase @ 300 K)

[PG3_42704-2_10K.dat](#) (Magnetically ordered phase @ 10 K)

Instrumental resolution file:

[PG2018B_HighRes_60Hz_b2_Ddep.irf](#)

Crystal Information File for crystal structure:

[CrSbSe3.cif](#)

Mag2Pol version used: [7.0.4](#)

The main interface of Mag2Pol

The main window of Mag2Pol - GUI

Running the Mag2Pol application, the main window 'Mag2Pol' will open. By default, the interface may look slightly different. You can modify this under the menu 'View'

This window should remain open as long as any other Mag2Pol utility or window is running. The current version of Mag2Pol will not save the project automatically, so make sure to save any project before closing this window.

The screenshot displays the Mag2Pol GUI interface. The main window is titled 'Mag2Pol' and features a menu bar (File, Generate, Structure, Fit, Geometry, Form factors, Tools, View, Help) and a toolbar with various icons. The interface is divided into several panels:

- Symmetry Panel:** Contains fields for 'Space group', 'Cell' parameters (a, b, c, α , β , γ), and 'Number of symmetry operators' and 'Number of irreps'. A table lists symmetry operators with columns for x, y, z, u, v, w, and ϕ .
- Atoms Panel:** Shows 'Number of sites' and a table with columns for Atom, x, y, z, B, occ, plot, color, R, and S.
- Spins Panel:** Includes 'Propagation vector: q' and a table with columns for Spin, Rx, Ry, Rz, Ix, Iy, Iz, and ϕ .

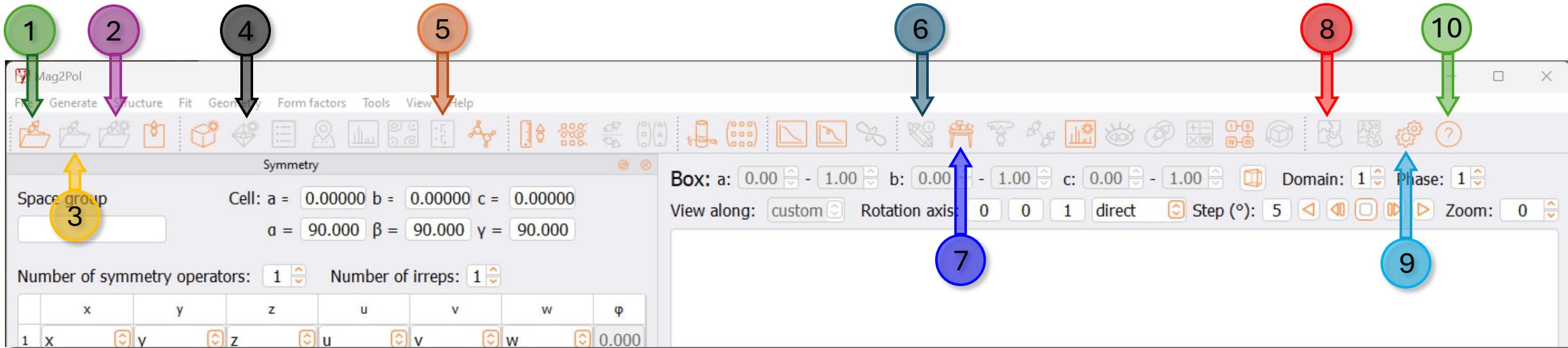
On the right side, there are controls for 'Box' (a, b, c), 'Domain', 'Phase', 'View along', 'Rotation axis', 'Step', and 'Zoom'. A large empty area is reserved for the main visualization.

	x	y	z	u	v	w	ϕ
1	x	y	z	u	v	w	0.000

Atom	x	y	z	B	occ	plot	color	R	S
1	0.00000	0.00000	0.00000	0.000	1.000	<input checked="" type="checkbox"/>	■	10	1.0

Spin	Rx	Ry	Rz	Ix	Iy	Iz	ϕ
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Menu items (icons) on the main window relevant for this tutorial



- 1 Open:** Load a structure file (cif) or an existing Mag2Pol project (xml).
- 2 Save as:** Save a new Mag2Pol project (as *.xml).
- 3 Save:** Append the currently working project with the same name.
- 4 Bonds:** Opens a new window that is used to modify the visuals of the structural model [active after loading the structure file, if it is not active even after loading the cif file, press *Ctrl+U* (on Windows) or *Cmd+U* (on Mac)].
- 5 Irreducible representations:** Opens a new window that provides details of irreps and lets you select one or more irreps for the refinement of magnetic structure (active when at least one magnetic ion is defined)
- 6 Sample info:** Opens a new window that provides details of, lattice and magnetic structures and the results of the last refinements.
- 7 Spacegroup tables:** Opens a window on which you can select magnetic space group (Shubnikov group) instead of irreps, to refine the magnetic structure.
- 8 Fit:** Opens the window where you can choose the data file, and instrument resolution file, and perform the refinements.
- 9 Settings:** Opens a new window that lets you modify a few important settings about GUI, a graphical rendering of plots and figures, and also the refinement procedure.
- 10 Manual:** Opens Mag2Pol manual in pdf format.

Refining high temperature NPD data, collected in paramagnetic phase

Step 1: Loading the structure or an existing project

The structure file (*.cif, *.mcif) or existing Mag2Pol project file (*.xml) can be loaded by clicking this icon or through the menu tree: File→Open

In this case: CrSbSe3.cif

1

2

If the structure file is loaded properly, several sections in the main window are populated automatically.

Legend:

- Sb (blue sphere)
- Cr (red sphere)
- Se (green sphere)

Unit cell diagram showing axes a, b, and c.

Symmetry Panel:

Space group: **Pnma**

Cell: a = 9.14600 b = 3.78510 c = 13.4240

$\alpha = 90.000$ $\beta = 90.000$ $\gamma = 90.000$

Number of symmetry operators: 1 Number of irreps: 1

	x	y	z	u	v	w	ϕ
1	x	y	z	u	v	w	0.000

Atoms Panel:

Number of sites: 5

Atom	x	y	z	B	occ	plot	color	R	S
1 Sb	0.02950	0.25000	0.65786	1.000	1.000	<input checked="" type="checkbox"/>	blue	10	1.0
2 Cr	0.15490	0.25000	0.04460	1.000	1.000	<input checked="" type="checkbox"/>	red	10	1.0
3 Se	0.17180	0.25000	0.48450	1.000	1.000	<input checked="" type="checkbox"/>	green	10	1.0
4 Se	0.28480	0.25000	0.21280	1.000	1.000	<input checked="" type="checkbox"/>	green	10	1.0
5 Se	0.50190	0.25000	0.60870	1.000	1.000	<input checked="" type="checkbox"/>	green	10	1.0

Spins Panel:

Propagation vector: q = 0.000 0.000 0.000 +q ≠ -q

Spin	Rx	Ry	Rz	Ix	Iy	Iz	ϕ
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Optional: Editing structure plot to produce publication-quality figure

Click on **Bonds** icon, a **new window** 'Bonds and polyhedra' will pop out. You can define and edit the bonds and polyhedral of the graphic here. If the Bonds icon is inactive even after loading the structure file it can be activated by pressing key board short-cut, Ctrl+U (on Windows) or Cmd+U (on Mac).

The screenshot shows the Mag2Pol software interface. The 'Atoms' table is highlighted with a red box, and a red arrow points to it. The table contains the following data:

Atom	x	y	z	B	occ	plot	color	R	S
1 Sb	0.02950	0.25000	0.65786	1.000	1.000	<input checked="" type="checkbox"/>	blue	15	1.0
2 Cr	0.15490	0.25000	0.04460	1.000	1.000	<input checked="" type="checkbox"/>	red	14	1.0
3 Se	0.17180	0.25000	0.48450	1.000	1.000	<input checked="" type="checkbox"/>	green	8	1.0
4 Se	0.28480	0.25000	0.21280	1.000	1.000	<input checked="" type="checkbox"/>	green	8	1.0
5 Se	0.50190	0.25000	0.60870	1.000	1.000	<input checked="" type="checkbox"/>	green	8	1.0

The 3D structure plot shows a unit cell with atoms represented by spheres: Sb (blue), Cr (red), and Se (green). Polyhedra are shown as semi-transparent pink planes. A legend on the left identifies the atoms: Sb (blue sphere), Cr (red sphere), and Se (green sphere). A coordinate system with axes a, b, and c is shown at the bottom left.

The 'Bonds and polyhedra' dialog box is shown. It has two sections: 'Bonds' and 'Polyhedra'. The 'Bonds' section has a table with the following data:

Atom 1	Atom 2	dmin Å	dmax Å	add	style	Color 1	Color 2	alpha	radius	show
1 CR	SE	0.10	3.00	<input checked="" type="checkbox"/>	Gradient	red	green	0.06		<input checked="" type="checkbox"/>

The 'Polyhedra' section has a table with the following data:

Atom 1	Atom 2	polyhedra	face color	alpha	min. d Å	edge color	alpha	radius
1 CR	SE	face Color 1, edge Color2	red	0.30	green		0.01	

Buttons for 'Apply', 'OK', and 'Cancel' are at the bottom.

Once you are satisfied with the structure plot, you can export it as *.png following the menu:

File→Export→Graphic

It is also possible to export the graphic as *.cif and *.mcif (in the case of magnetic structure).

Step 2: Enter the refinement (Fit) window

To load the experimental data we need to open the 'Fit' window, by clicking on the icon as shown in the screenshot below (or the keyboard shortcut 'Ctrl+F').

Within the 'Fit' window, you can load the data, load the instrument resolution file, and perform Le Bail Profile fit or Rietveld refinement.

Symmetry

Space group: **Pnma**
Cell: a = 9.14600 b = 3.78510 c = 13.4240
α = 90.000 β = 90.000 γ = 90.000

Number of symmetry operators: 1 Number of irreps: 1

	x	y	z	u	v	w	φ
1	x	y	z	u	v	w	0.000

Atoms

Number of sites: 5

Atom	x	y	z	B	occ	plot	color	R	S
1 Sb	0.02950	0.25000	0.65786	1.000	1.000	<input checked="" type="checkbox"/>	blue	15	1.0
2 Cr	0.15490	0.25000	0.04460	1.000	1.000	<input checked="" type="checkbox"/>	red	14	1.0
3 Se	0.17180	0.25000	0.48450	1.000	1.000	<input checked="" type="checkbox"/>	green	8	1.0
4 Se	0.28480	0.25000	0.21280	1.000	1.000	<input checked="" type="checkbox"/>	green	8	1.0
5 Se	0.50190	0.25000	0.60870	1.000	1.000	<input checked="" type="checkbox"/>	green	8	1.0

Spins

Propagation vector: q = 0.000 0.000 0.000 +q ≠ -q

Spin	Rx	Ry	Rz	Ix	Iy	Iz	φ
------	----	----	----	----	----	----	---

Fit

Polarization data

Load *.fli Load *.int Load Numors

View data Save data

Integrated intensities

Load *.int Load *.col/*.fsq/*.sf/*.bra

View data Save data

Powder patterns

Load pattern Mag2Pol format

View data Save data

Step 2a: Load the experimental data

The data can be loaded under the 'Data' tab of the 'Fit' window. Mag2Pol can accept three kinds of data sets. In this example, we will start with 'Powder diffraction data' of CrSbSe₃ collected at 300 K (Paramagnetic phase). **Follow the order indicated below.**

The screenshot shows the 'Fit' window with the 'Data' tab selected. The window is divided into two main sections: 'Polarization data' and 'Powder patterns'. The 'Data' tab is highlighted with a red circle and the number '1'. The text 'We are under the 'Data' tab' is written in red. In the 'Polarization data' section, there are buttons for 'Load *.fli', 'Load *.int', and 'Load Numors'. In the 'Powder patterns' section, there is a 'Load pattern' button, a dropdown menu showing 'x y sigma (Ins 10)', and a green circle with the number '2'. A text box next to it says 'Select the data format 'x y Sigma (Ins 10)'. Below the dropdown, a file 'PG3_42702-2_300K.dat (weight = 1)' is listed. A purple circle with the number '3' is next to the 'Load pattern' button, with a text box that says 'Click on 'Load pattern' and select the data file when prompted. In this case: PG3_42702-2_300K.dat'. At the bottom, there is a checkbox for 'Refine nuclear structure' which is checked, and a radio button for 'Purely magnetic scattering' which is unselected. A black circle with the number '4' is next to the 'Refine nuclear structure' checkbox, with the text 'Activate 'Refine nuclear structure''. There are also 'View data' and 'Save data' buttons in both sections.

Step 2b: Confirm all the atoms are loaded properly

Under the 'Atoms' tab, check if all the atoms are loaded properly and the occupancies nominally follow the chemical formula. Do not select any of these parameters for refinement, at this stage.

Fit We are under the 'Atoms' tab ? x

Data **Atoms** Moments Domains Constraints Patterns Fit

	Atom	x	y	z	B	occ
A1	SB	0.02950	0.25000	0.65786	1.000	1.000
A2	CR	0.15490	0.25000	0.04460	1.000	1.000
A3	SE	0.17180	0.25000	0.48450	1.000	1.000
A4	SE	0.28480	0.25000	0.21280	1.000	1.000
A5	SE	0.50190	0.25000	0.60870	1.000	1.000

Scale factor and $\lambda/2$: 1.00000 0.00000

Extinction parameters:
 anisotropic ShelX-like model

χ_{11} χ_{12} χ_{13}
0.00000 0.00000 0.00000

χ_{22} χ_{23}
0.00000 0.00000

χ_{33}
0.00000

Becker-Coppens model

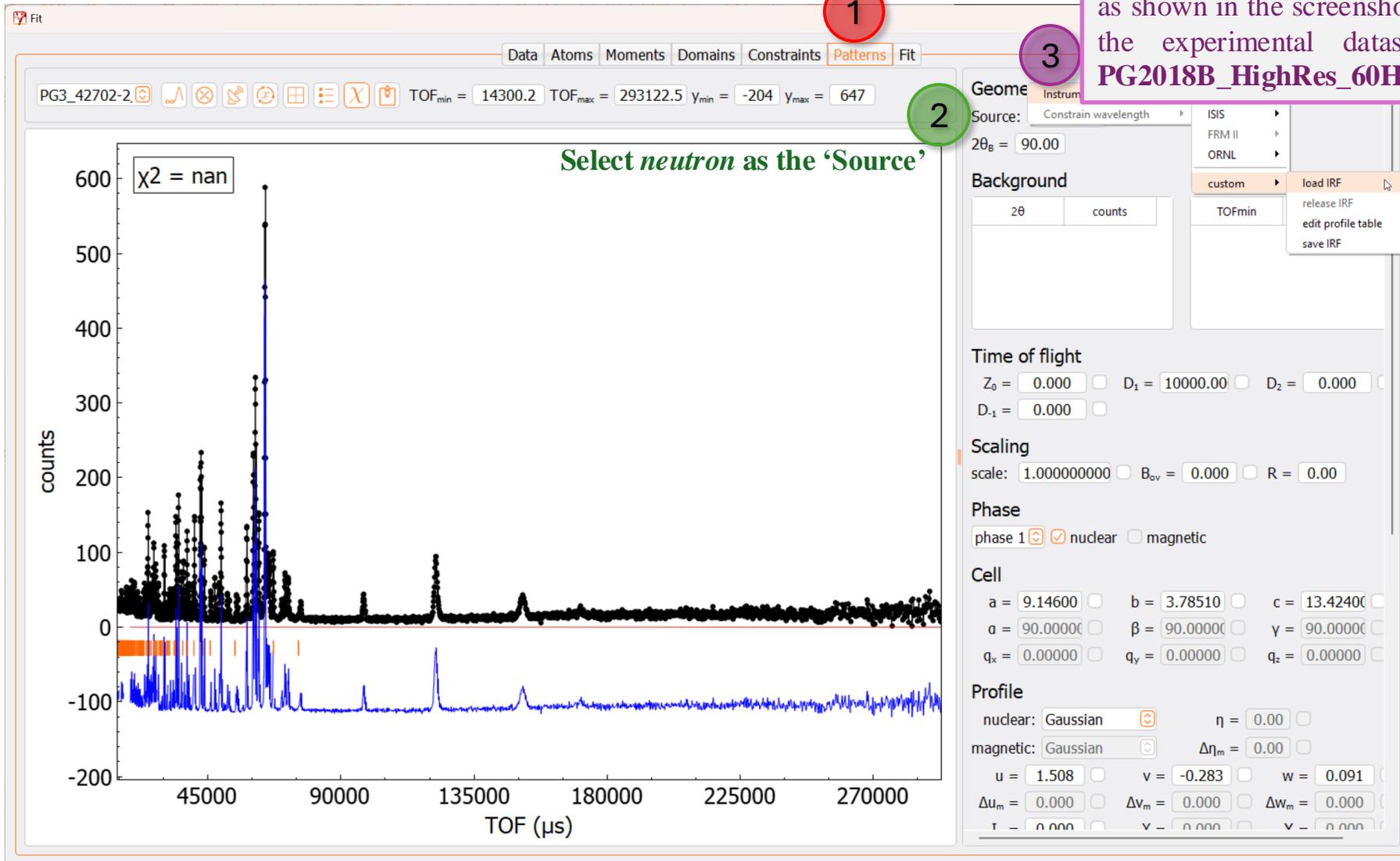
r_D : 0.000

θ_D : 0.000 Lorentzian

Step 2c: Load the instrument resolution (irf) file

Under the 'Patterns' tab

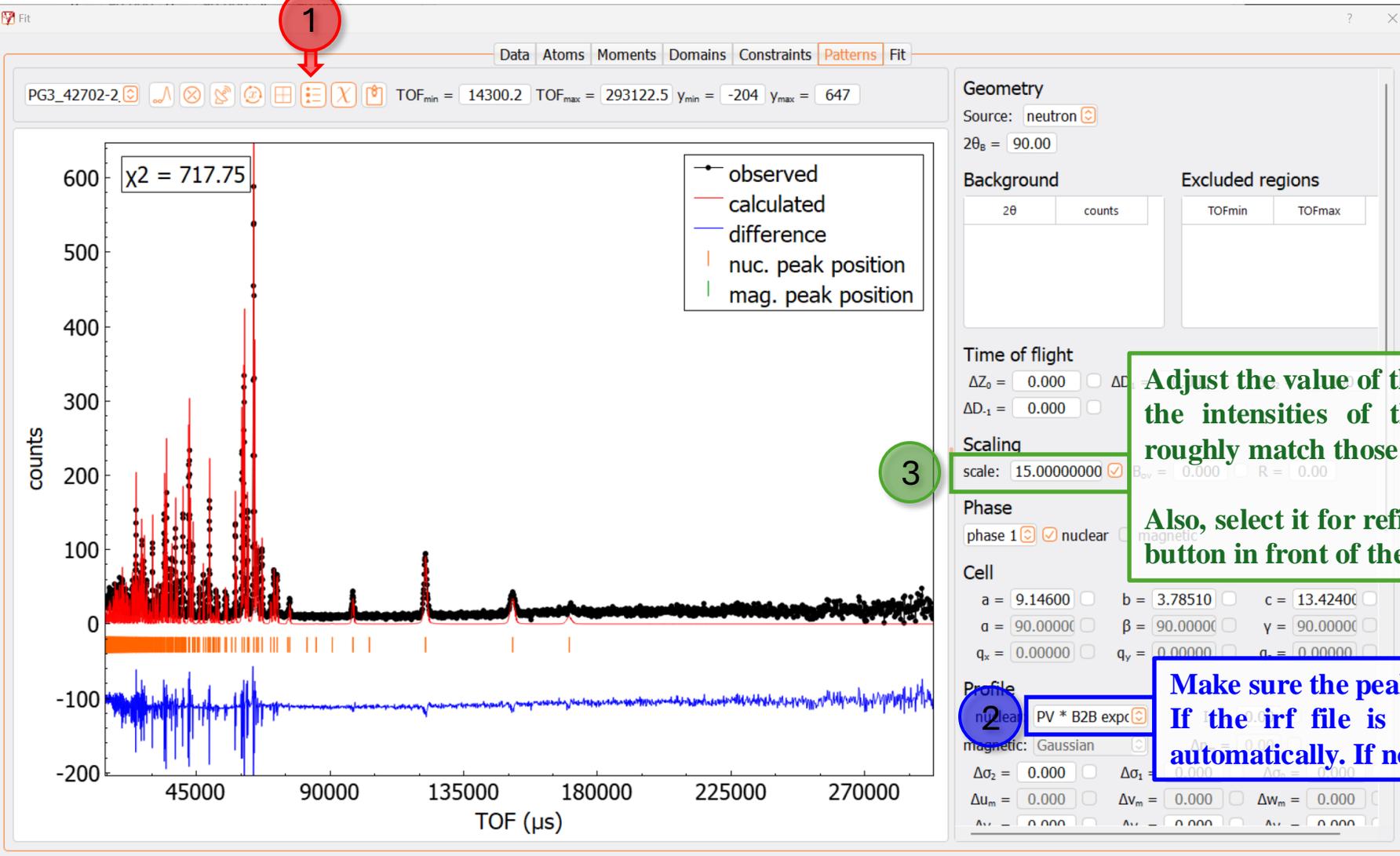
Right-click on the text 'Geometry' and follow the menu items as shown in the screenshot, to load the appropriate irf file for the experimental dataset (data bank). In this case: **PG2018B_HighRes_60Hz_b2_Ddep.irf**



Step 2d: Check the peak function and set an appropriate scale factor

Toggle the legend ON/OFF

1



3

Adjust the value of the 'scale' factor so that the intensities of the calculated pattern roughly match those of observed data.

Also, select it for refinement, by ticking the button in front of the scale factor value.

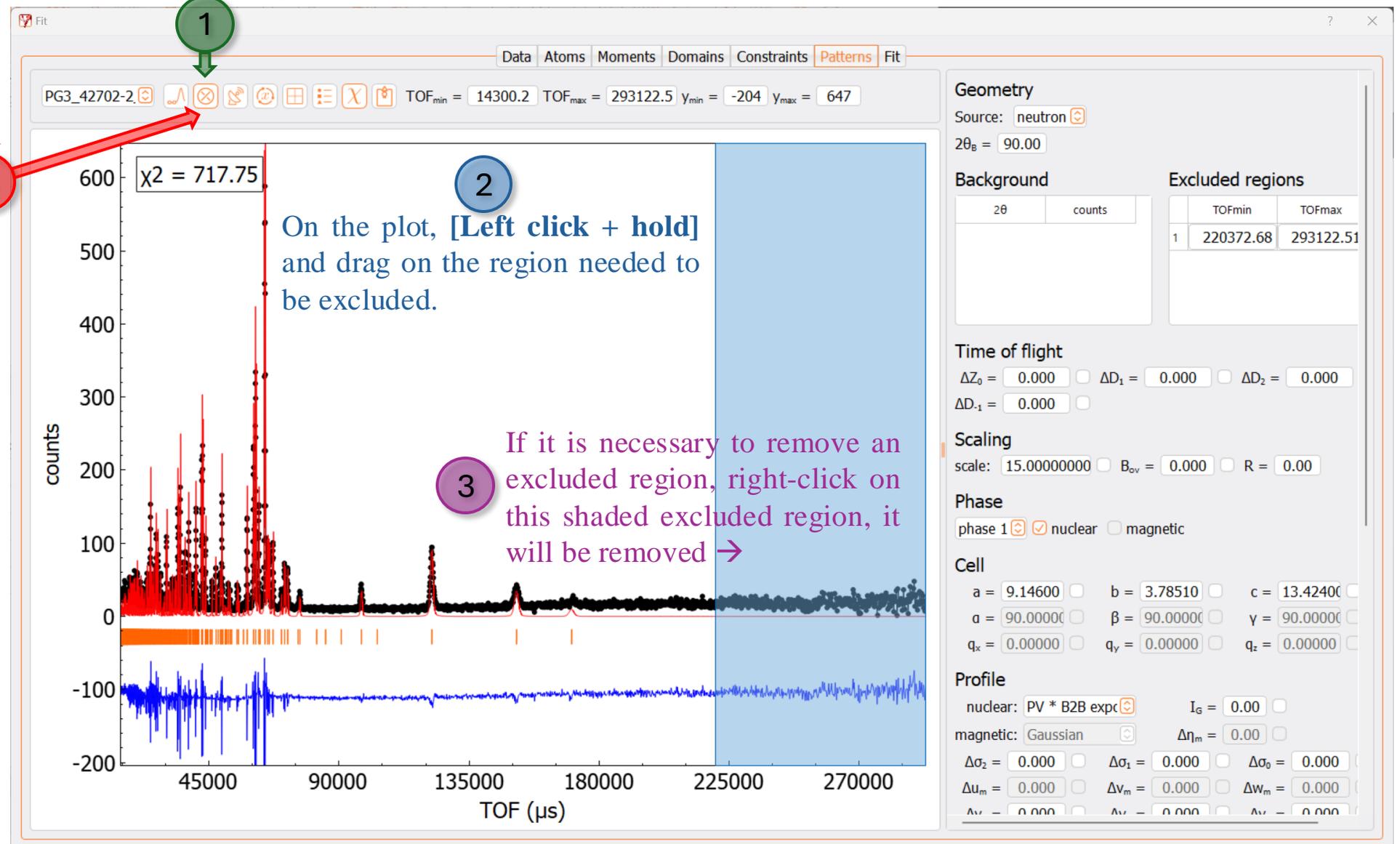
2

Make sure the peak function is: $PV * B2B \text{ exp}(Tof1)$
If the irf file is loaded properly this should be updated automatically. If not choose it manually.

Step 2e: Select the region to exclude from the fit 'Excluded region'

Toggle the 'excluded regions' ON

Toggle the 'excluded regions' OFF



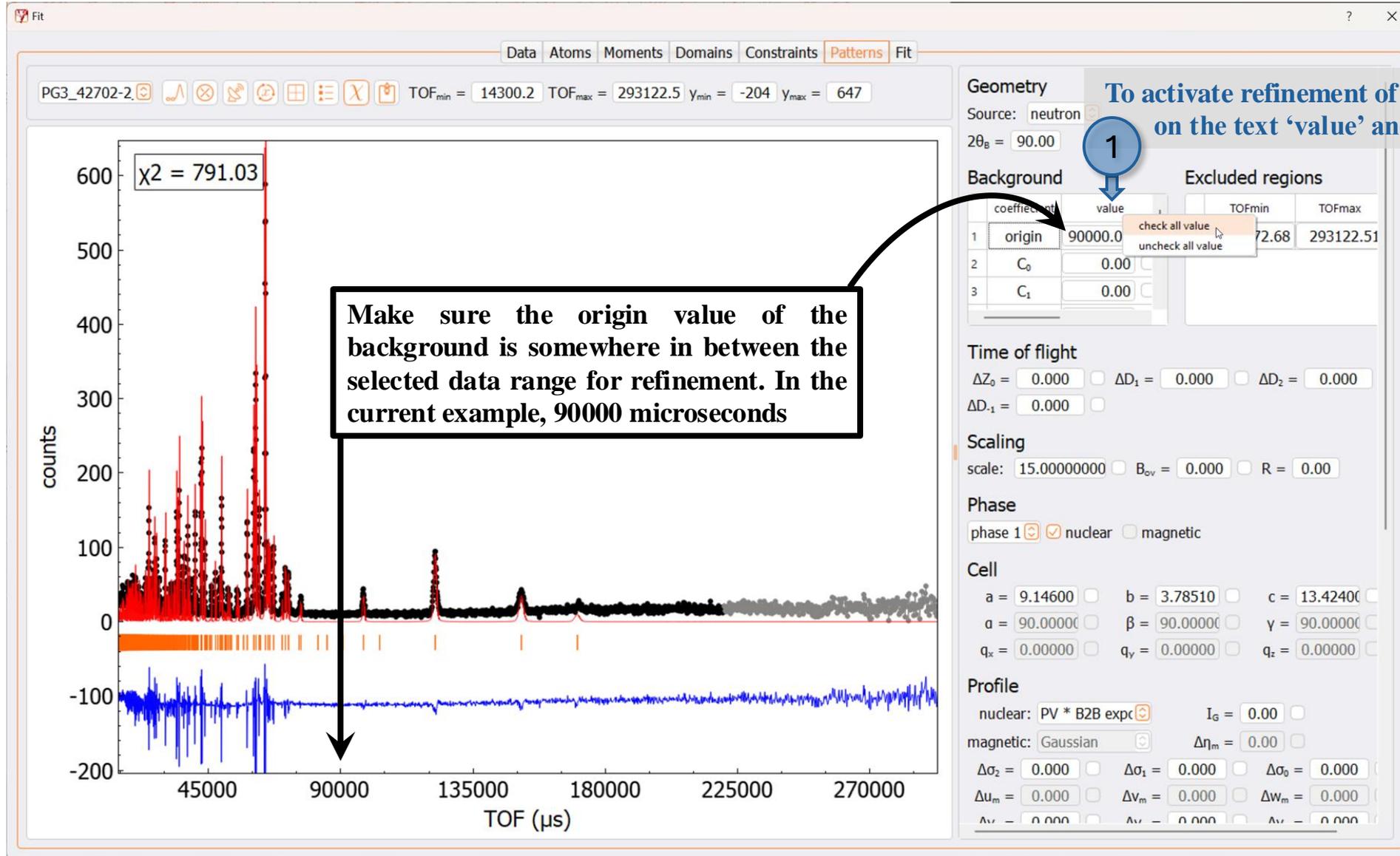
Step 2f: Select the background

(Only for BG type 'linear interpolation')

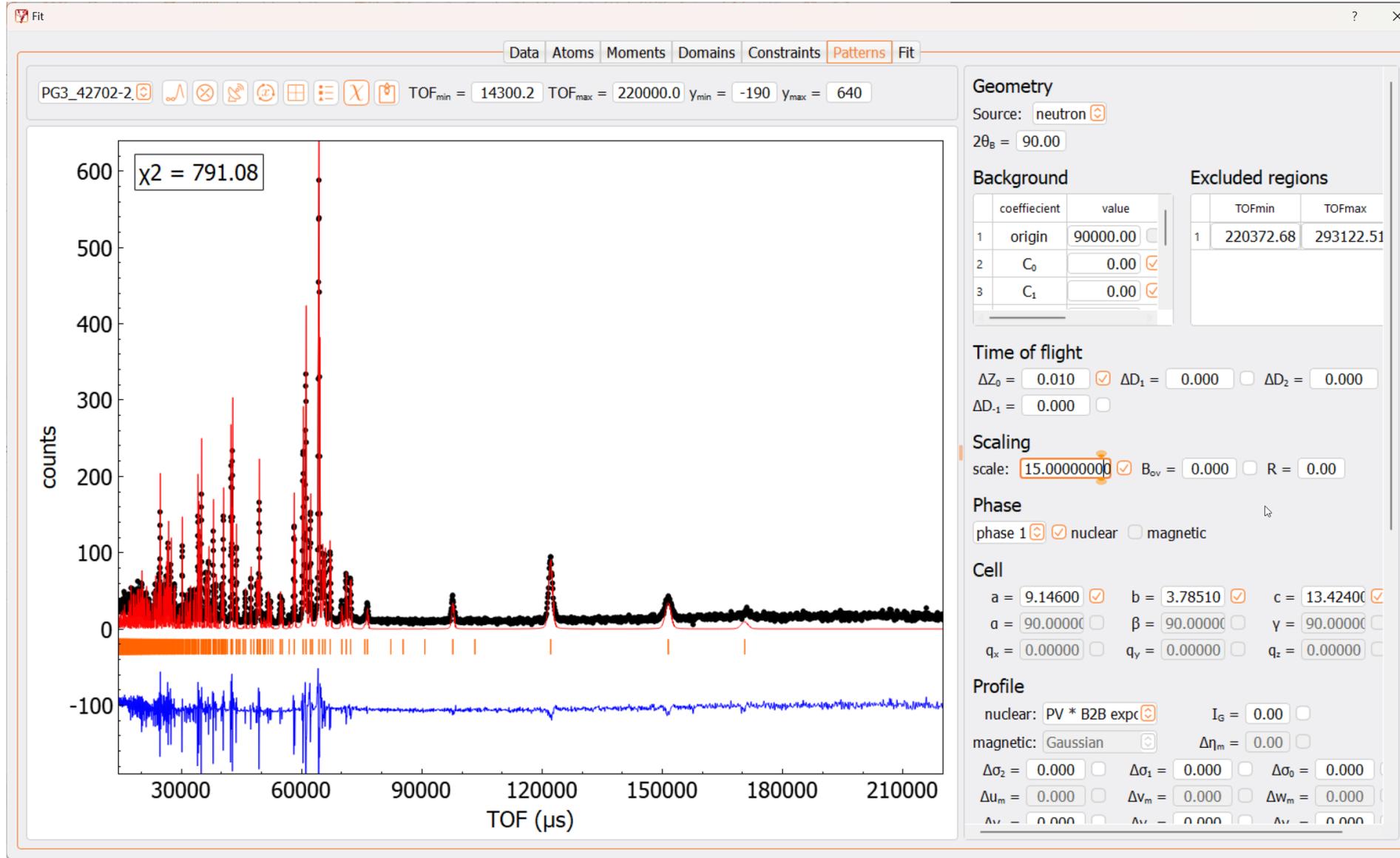
For manual background selection toggle this ON
(toggle it OFF after selection is complete)

The screenshot shows the 'Fit' software interface. The main plot displays a diffraction pattern with counts on the y-axis (ranging from -200 to 600) and TOF (μs) on the x-axis (ranging from 45000 to 270000). A red line represents the fit, and a blue line represents the residual. A box in the top left of the plot indicates $\chi^2 = 791.03$. A blue arrow points to the baseline of the diffraction pattern, with a text box stating: "If the 'Background' type is 'linear interpolation', then one can select an appropriate number of background points by right-clicking on the baseline of the diffraction pattern." A second blue arrow points to the 'Background' dropdown menu in the right-hand panel, which is open and showing options: 'linear interpolation', 'polynomial (6 coeffs)', 'polynomial (12 coeffs)', and 'polynomial (6 coeffs) + Debye-like'. A green circle with the number '1' is placed over the 'polynomial (6 coeffs)' option. A green text box on the right side of the interface states: "Right-click on the text 'Background' and pick a background type. In this case background is fairly flat so a polynomial with 6 coefficients should be sufficient." The right-hand panel also shows various other settings like Geometry, Time of flight, Scaling, Phase, Cell, and Profile.

Step 2g: Activate refinement of background



Step 2h: Select Cell parameters and ΔZ_0 for refinement



Step 3a: Run the first refinement run

Fit

Data Atoms Moments Domains Constraints Patterns **Fit**

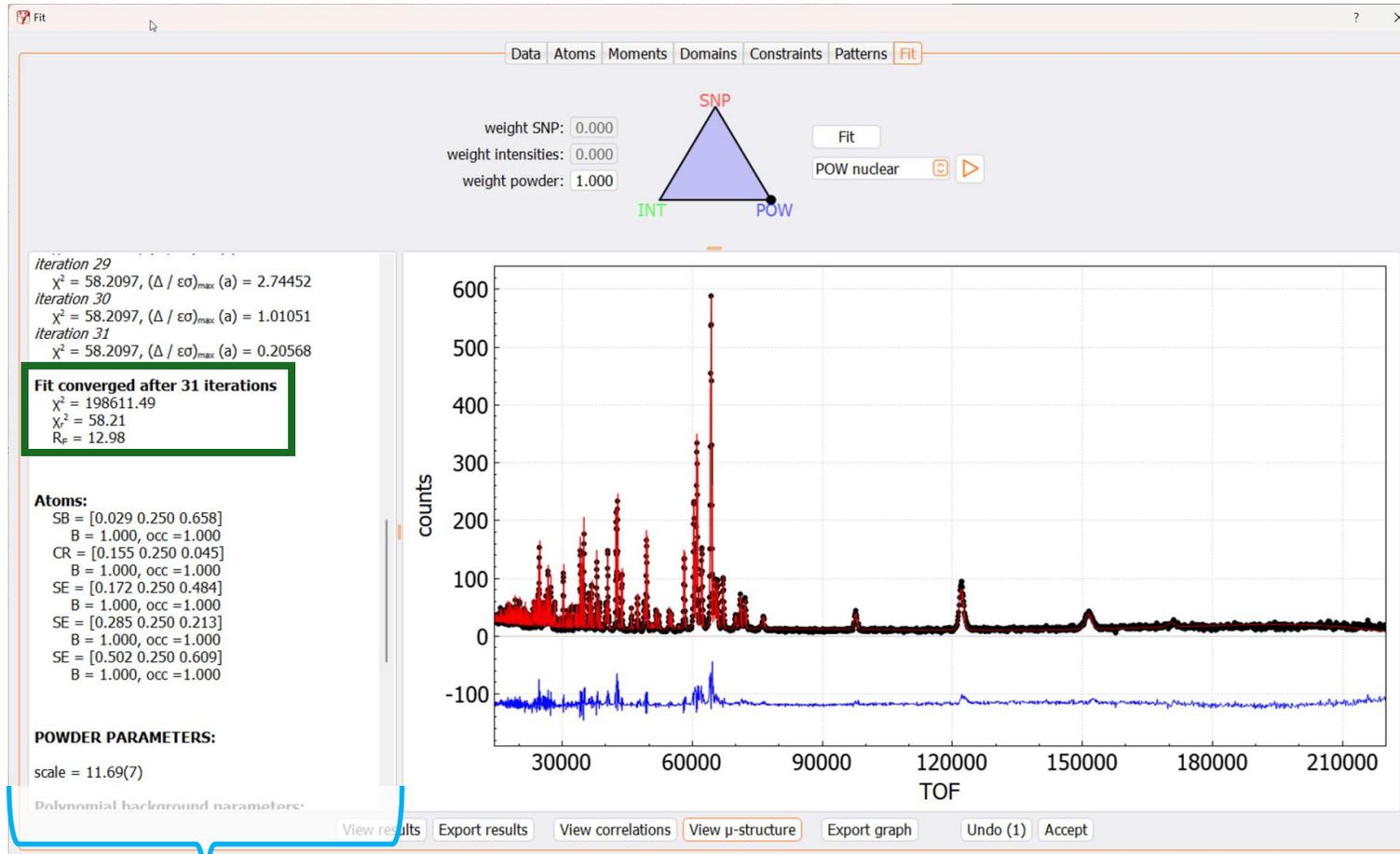
weight SNP: 0.000
weight intensities: 0.000
weight powder: 1.000

SNP
INT POW

Fit POW nuclear

View results Export results View correlations View μ -structure Export graph Undo Accept

Step 3b: Results after the first run of the refinement



Time of flight:
 $Z_0 = 3.3(6)$ $D_1 = 0.000$ $D_2 = 0.000$ $D_3 = 0.000$

Profile:
 $\sigma_2 = 0.000$ $\sigma_1 = 0.000$ $\sigma_0 = 0.000$ $\sigma_Q = 0.000$ $I_G = 0.000$
 $\gamma_2 = 0.000$ $\gamma_1 = 0.000$ $\gamma_0 = 0.000$
 $a_0 = 0.000$ $a_1 = 0.000$ $a_Q = 0.000$
 $\beta_0 = 0.000$ $\beta_1 = 0.000$ $\beta_Q = 0.000$
 $P_1 = 0.000$ $P_2 = 0.000$

Lattice:
 $a = 9.1429(3)$ $b = 3.7839(1)$ $c = 13.4147(4)$
 $\alpha = 90.000$ $\beta = 90.000$ $\gamma = 90.000$
Volume = 464.09(2)

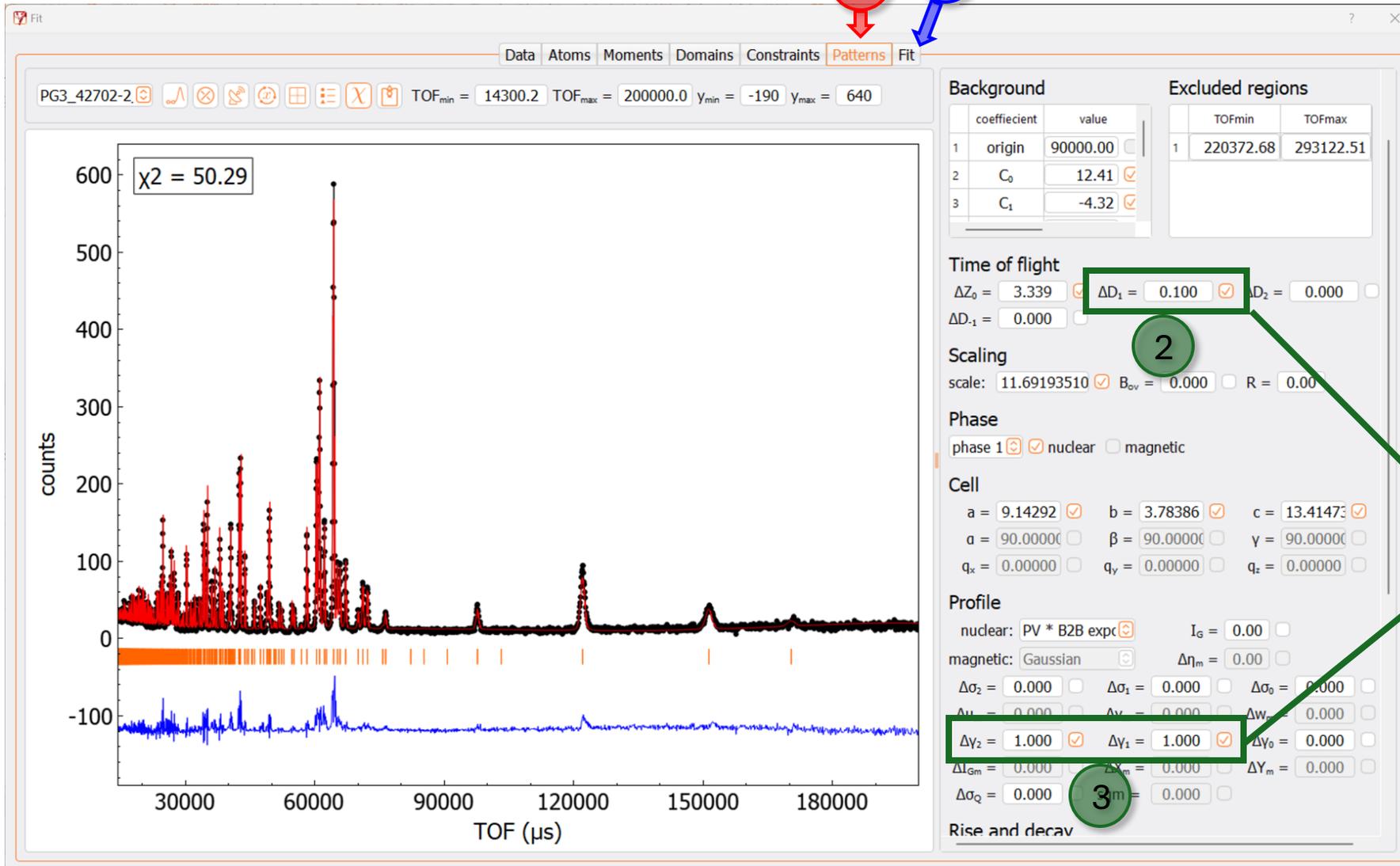
Convergence reached after 31 cycles! Discrepancy parameters and all the refined parameters can be found in the left window.

Step 3c: Refine instrument parameters

1

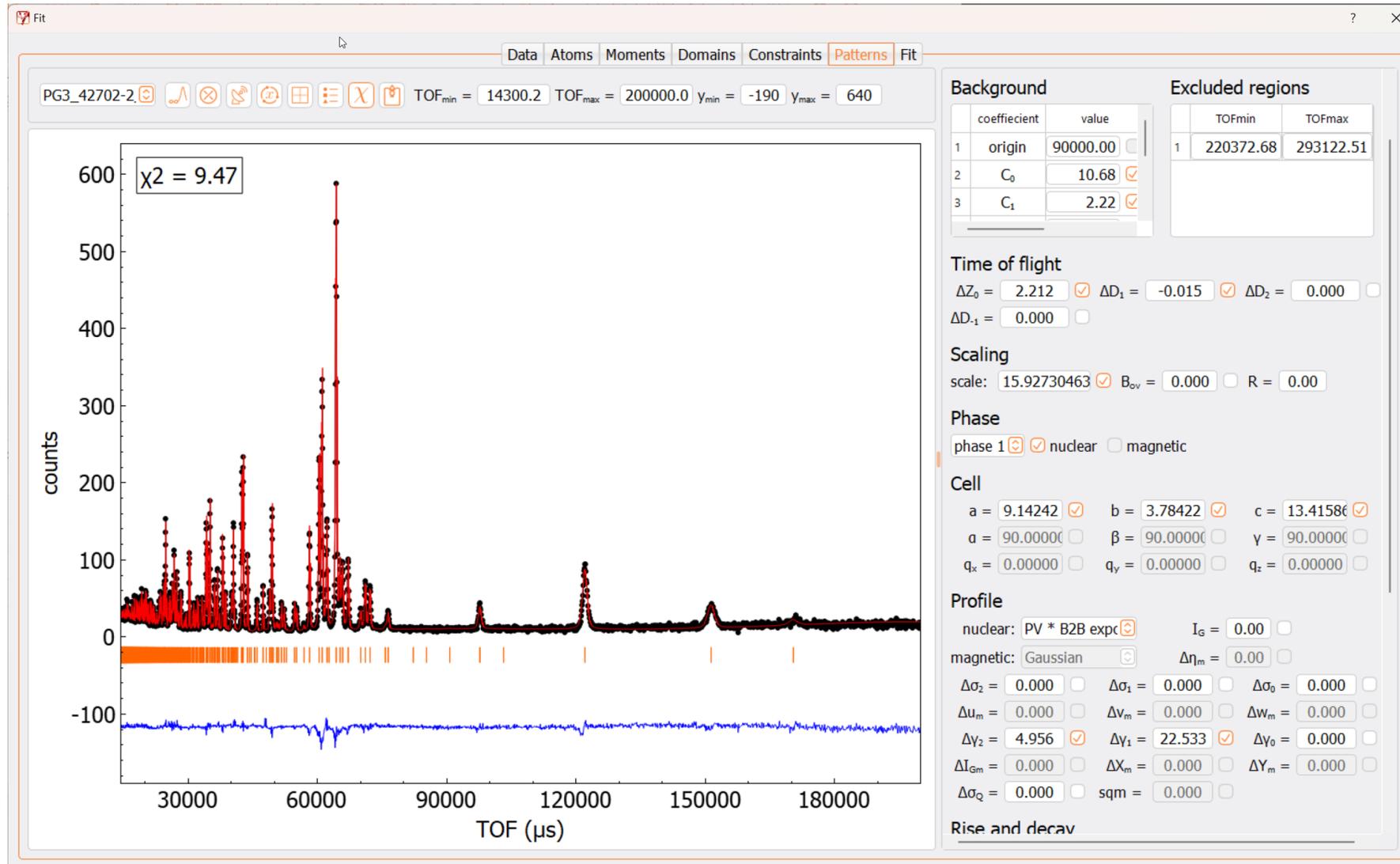
4

Back to the fitting tab and run fitting again till the fit converges.



In the current version, it is necessary to choose a small value when starting the refinement of a new parameter. Leaving them to be zero won't work.

Step 3d: Significant improvement in the fit



Step 3e: Refine atomic parameters

1

2

Back to the fitting tab and run fitting again till the fit converges.

Atom	x	y	z	B	occ	
A1	SB	0.02950 <input checked="" type="checkbox"/>	0.25000 <input type="checkbox"/>	0.65786 <input checked="" type="checkbox"/>	1.00 <input checked="" type="checkbox"/>	<input type="checkbox"/>
A2	CR	0.15490 <input checked="" type="checkbox"/>	0.25000 <input type="checkbox"/>	0.04460 <input checked="" type="checkbox"/>	1.000 <input type="checkbox"/>	1.000 <input type="checkbox"/>
A3	SE	0.17180 <input checked="" type="checkbox"/>	0.25000 <input type="checkbox"/>	0.48450 <input checked="" type="checkbox"/>	1.000 <input type="checkbox"/>	1.000 <input type="checkbox"/>
A4	SE	0.28480 <input checked="" type="checkbox"/>	0.25000 <input type="checkbox"/>	0.21280 <input checked="" type="checkbox"/>	1.000 <input type="checkbox"/>	1.000 <input type="checkbox"/>
A5	SE	0.50190 <input checked="" type="checkbox"/>	0.25000 <input type="checkbox"/>	0.60870 <input checked="" type="checkbox"/>	1.000 <input type="checkbox"/>	1.000 <input type="checkbox"/>

Scale factor and $\lambda/2$: 1.00000 0.00000

Extinction parameters:

anisotropic ShelX-like model

X_{11} X_{12} X_{13}
 0.00000 0.00000 0.00000

X_{22} X_{23}
 0.00000 0.00000

X_{33}
 0.00000

Becker-Coppens model

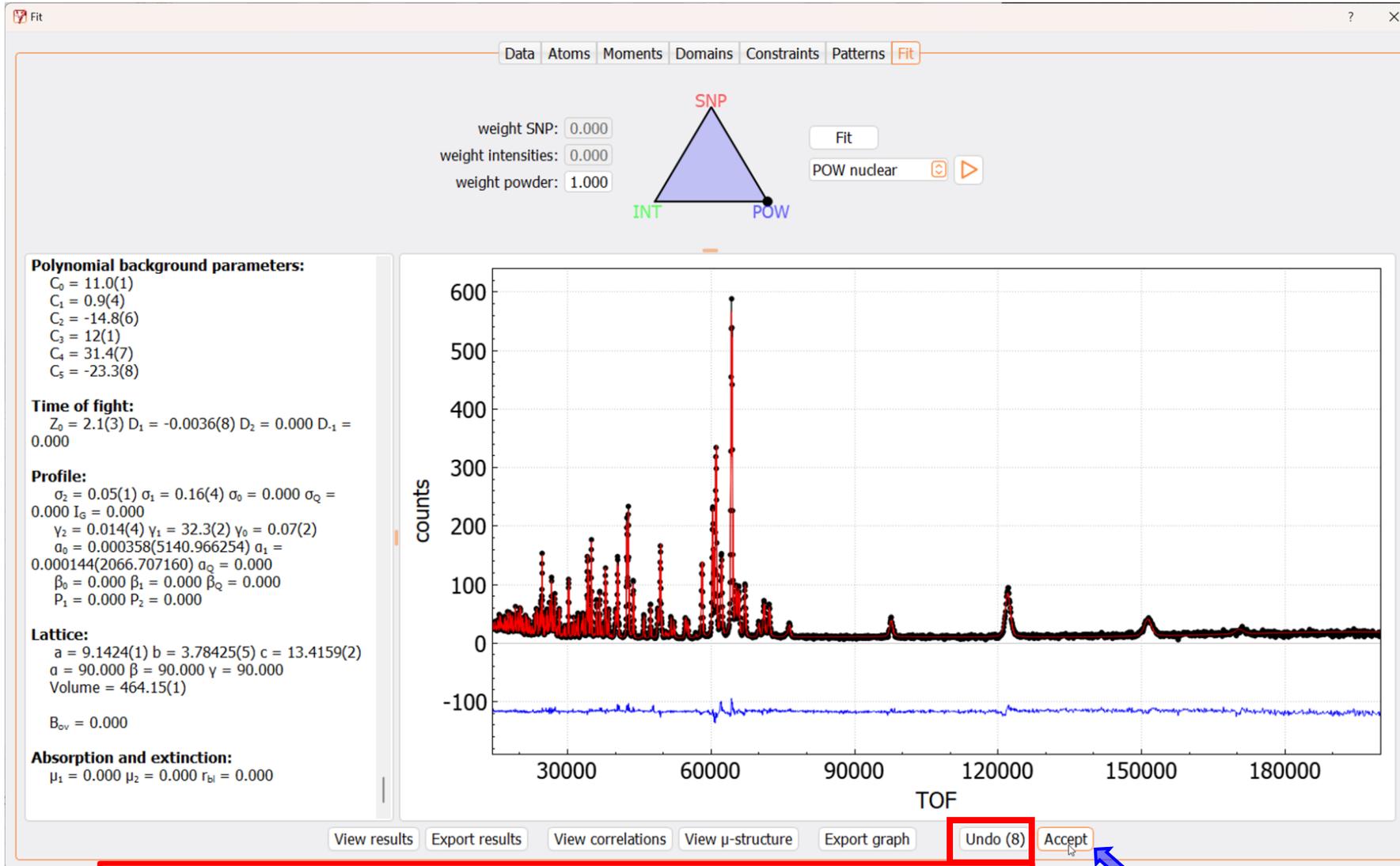
r_D : 0.000

θ_D : 0.000 Lorentzian

Refinement of atomic parameters can be activated by right-clicking on the text, 'x', 'z', and 'B' and selecting 'check all x/y/B'. They can also be selected one by one.

In some cases, starting the refinement of both positions and thermal parameters might lead to divergence or local minima, so refine positions (x , y , z) first and then activate and refine thermal parameters (B).

Step 3f: The fit looks good; accept this as final refinement result.

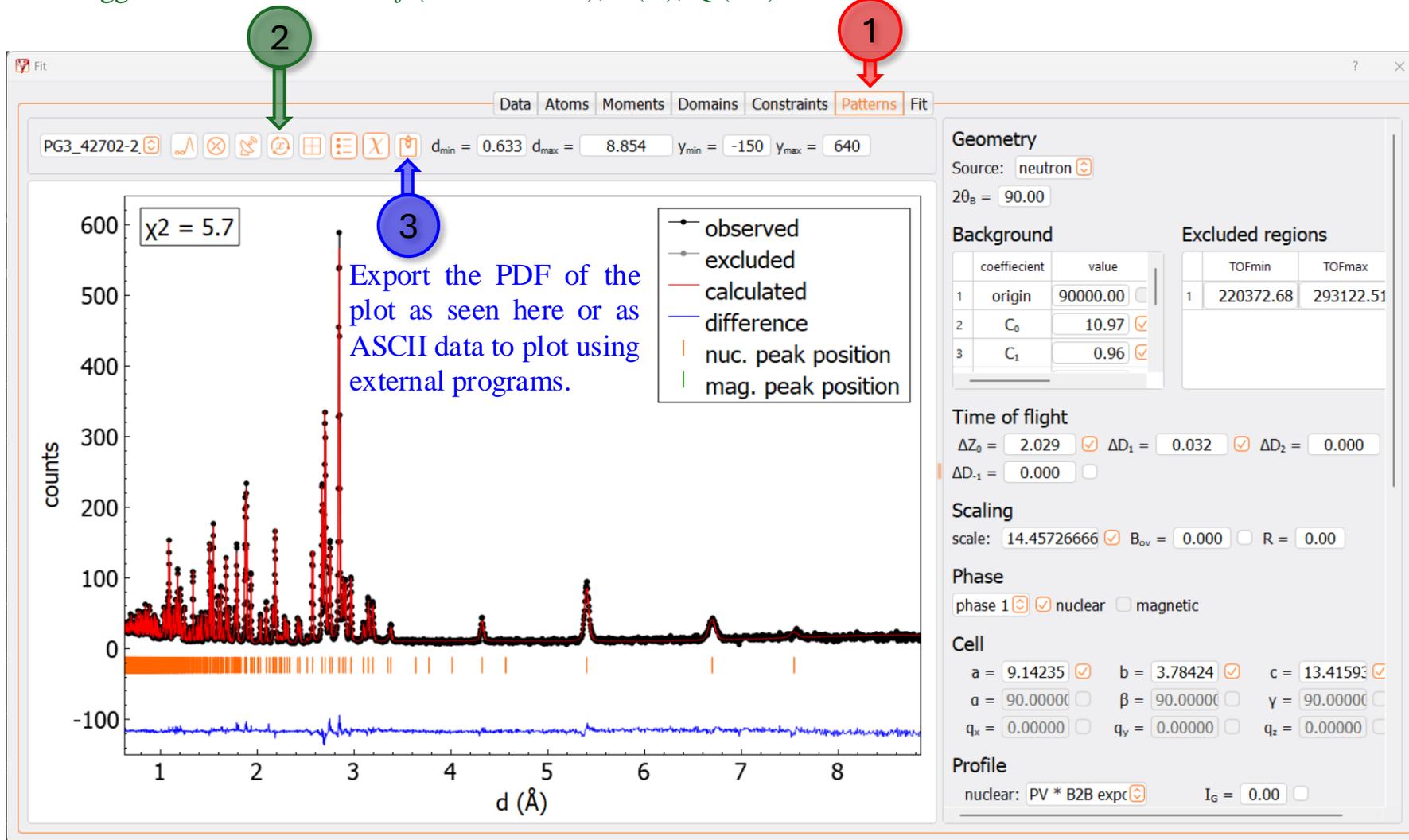


At any stage, if the fit diverges, you can recover previous states by pressing 'Undo' button. It can go back as many steps as you want, all the way back to the initial state of the refinements of the current session.

1 Accept the fit results by clicking on this button.

Step 3g: Export the refinement profile as a PDF or ASCII file.

Can toggle x-axis between - *t.o.f* (microseconds); *d* (Å); *Q* (Å⁻¹)



4 Close the 'Fit' window, and go back to the main Mag2Pol window.

Step 3h: Save the Mag2Pol project (*.xml). It's a very crucial step!

1 Save the project with an appropriate name. In this case, **CrSbSe3_300K.xml**

2 Export the new Graphic as *.png or structure as *.cif file

The screenshot shows the Mag2Pol software interface. The main window displays a 3D crystal structure model of CrSbSe3. The structure is shown within a unit cell, with atoms represented by colored spheres: Sb (blue), Cr (red), and Se (green). The structure is viewed along the 'a' axis, with the 'b' and 'c' axes also indicated. The model shows the arrangement of atoms and the resulting magnetic structure, with red and blue spheres representing the magnetic ions and green spheres representing the Se ions. The structure is shown within a unit cell, with the axes labeled 'a', 'b', and 'c'. The 'a' axis is horizontal, 'b' is vertical, and 'c' is diagonal. The structure is shown within a unit cell, with the axes labeled 'a', 'b', and 'c'. The 'a' axis is horizontal, 'b' is vertical, and 'c' is diagonal. The structure is shown within a unit cell, with the axes labeled 'a', 'b', and 'c'. The 'a' axis is horizontal, 'b' is vertical, and 'c' is diagonal.

Number of sites: 5

Atom	x	y	z	B	occ	plot	color	R	S
1 Sb	0.02984	0.25000	0.65781	0.938	1.000	<input checked="" type="checkbox"/>	blue	15	1.0
2 Cr	0.15608	0.25000	0.04475	0.331	1.000	<input checked="" type="checkbox"/>	red	14	1.0
3 Se	0.17196	0.25000	0.48416	0.595	1.000	<input checked="" type="checkbox"/>	green	8	1.0
4 Se	0.28484	0.25000	0.21309	0.568	1.000	<input checked="" type="checkbox"/>	green	8	1.0
5 Se	0.50201	0.25000	0.60882	0.509	1.000	<input checked="" type="checkbox"/>	green	8	1.0

Propagation vector: q = 0.000 0.000 0.000 +q ≠ -q

Spin	Rx	Ry	Rz	Ix	Iy	Iz	φ
------	----	----	----	----	----	----	---

In the current version of Mag2Pol, the project (*.xml) file will have all the refined parameters and absolute paths for data and irf files. The project file can be reloaded without any issue later. But if it is opened in a different computer with a different folder structure, it will complain about missing data and irf files file and prompts to choose the file path. Choose the right file format and indicate the file path; it will reload the project in its original.

Refining low temperature NPD data, collected in the magnetically ordered phase

Step 4a: Start with the project created for the high-temperature phase in Step 7f.

Save as a new project, with appropriate name for the low-temperature phase. To begin with, we will only consider lattice contribution.

1

The screenshot shows the Mag2Pol software interface. The 'Fit' window icon in the top toolbar is highlighted with a blue circle containing the number 2. The interface includes a menu bar (File, Generate, Structure, Fit, Geometry, Form factors, Tools, View, Help), a toolbar, and several panels: Symmetry, Atoms, and Spins. The Symmetry panel shows the space group Pnma and unit cell parameters. The Atoms panel shows a table of 5 sites. The Spins panel shows the propagation vector q = 0.000, 0.000, 0.000. The main 3D view shows a crystal structure with atoms represented by colored spheres (Sb, Cr, Se) and a legend below it.

Atom	x	y	z	B	occ	plot	color	R	S
1 Sb	0.02984	0.25000	0.65781	0.938	1.000	<input checked="" type="checkbox"/>	blue	15	1.0
2 Cr	0.15608	0.25000	0.04475	0.331	1.000	<input checked="" type="checkbox"/>	red	14	1.0
3 Se	0.17196	0.25000	0.48416	0.595	1.000	<input checked="" type="checkbox"/>	green	8	1.0
4 Se	0.28484	0.25000	0.21309	0.568	1.000	<input checked="" type="checkbox"/>	green	8	1.0
5 Se	0.50201	0.25000	0.60882	0.509	1.000	<input checked="" type="checkbox"/>	green	8	1.0

We will be using the refinement results of high-temperature data as a starting point for the refinement of low-temperature data.

Click this icon to open the 'Fit' window.

Step 4b: Replace the old data with the new data.

The screenshot shows the 'Fit' software interface with the 'Data' tab selected. The 'Powder patterns' section is active, displaying a list of patterns. The first pattern is 'PG3_42702-2_300K.dat (weight)'. A context menu is open over this pattern, with the 'Replace' option highlighted. A blue circle with the number '1' points to the dropdown menu in the 'Load pattern' field, which is currently set to 'x y sigma (Ins 10)'. A green circle with the number '2' points to the 'Replace' option in the context menu.

Right-click on the old data, select the 'Replace' option and pick the new data set when prompted. In this case loading: **PG3_42704-2_10K.dat**

Select the data format 'x y sigma (Ins 10)'

Step 4c: Fix all the atomic parameters

1

2

At this stage do not refine any of the atomic parameters. Fix them by unchecking one by one or by right-clicking on the column name and selecting 'uncheck all'

Atom	x	y	z	B	occ	
A1	SB	0.02984	0.25000	0.65781	0.938	
A2	CR	0.15608	0.25000	0.04475	0.331	1.000
A3	SE	0.17196	0.25000	0.48416	0.595	1.000
A4	SE	0.28484	0.25000	0.21309	0.568	1.000
A5	SE	0.50201	0.25000	0.60882	0.509	1.000

Scale factor and $\lambda/2$: 1.00000 0.00000

Extinction parameters:
 anisotropic ShelX-like model

χ_{11} χ_{12} χ_{13}
0.00000 0.00000 0.00000

χ_{22} χ_{23}
0.00000 0.00000

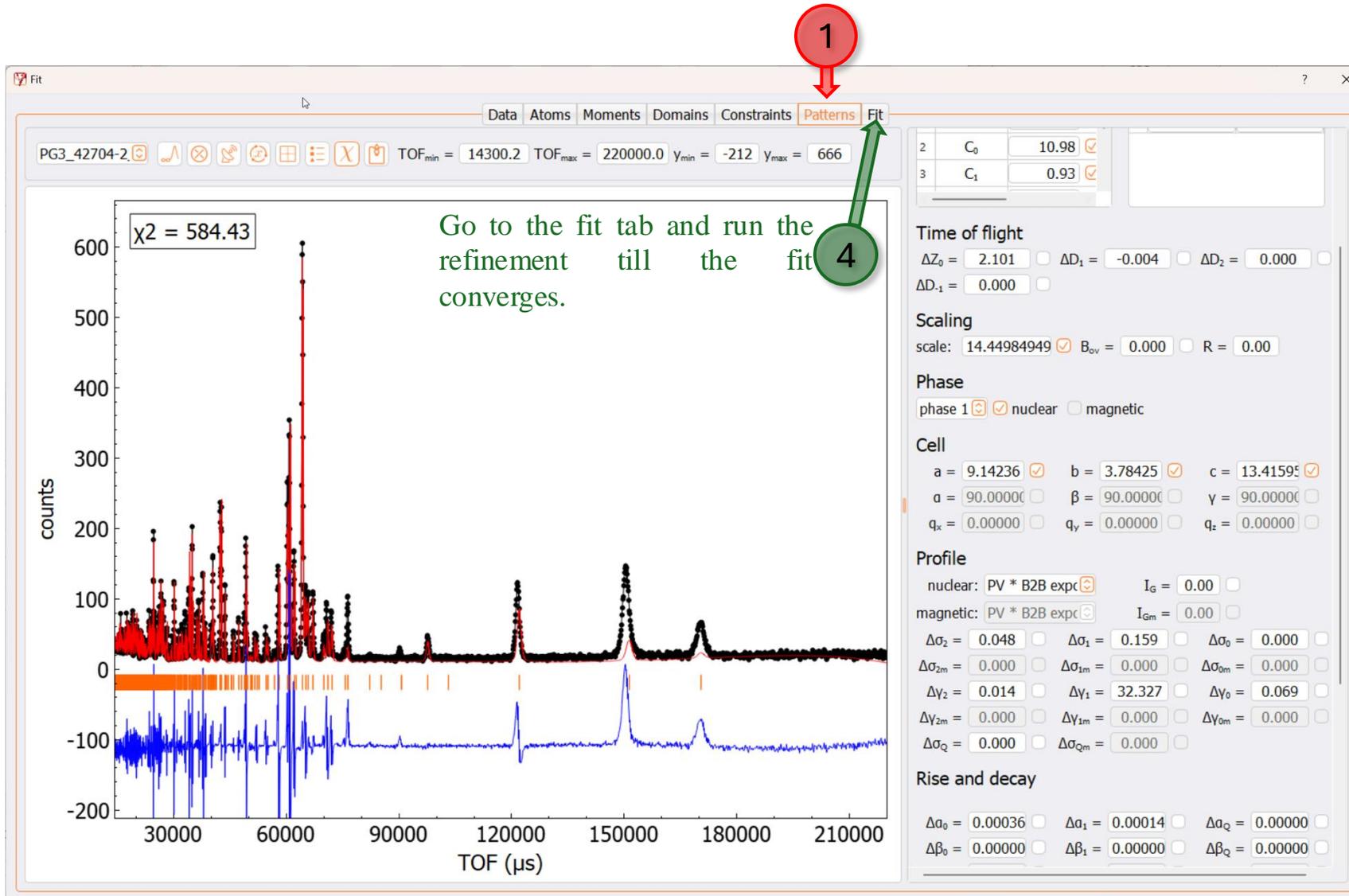
χ_{33}
0.00000

Becker-Coppens model

r_D : 0.000

θ_D : 0.000 Lorentzian

Step 4d: Refine the scale and Cell parameters



2

NOTE: If the new data set that was loaded in this section is measured with a different center wavelength (data bank) than the previous data set, then make sure to load the corresponding irf file. And need to refine the profile, Time of flight, and Rise and decay parameters as necessary, before proceeding to the next point (3).

In the current case, both 300 K and 10K data sets were collected with the same center wavelength neutrons, so no need to change the irf file.

3

Fix all parameters except the 'scale' and 'Cell' parameters.

Step 4e: Refine profile parameters as necessary

1

2 The fit profile looks good except for the data set at the higher d -range, where the contribution from magnetic scattering is significant.

3 Select profile parameters for the refinement

4 Go to the fit tab and run the refinement till the fit converges.

5 After convergence is reached click on the 'Accept' button (under Fit tab) and close this 'Fit' window.

The screenshot displays the 'Fit' software interface. The main window shows a plot of counts versus TOF (μs) with a fit line and a residual plot. The plot is annotated with a green box around the high-d region and a green circle with the number '2' and a text box explaining the fit quality. The parameter panel on the right is annotated with a blue box around the Profile section and a blue circle with the number '3'. A yellow circle with the number '1' points to the 'Patterns' tab, a purple circle with the number '4' points to the 'Fit' tab, and a red circle with the number '5' points to the 'Accept' button. The parameter panel includes sections for Time of flight, Scaling, Phase, Cell, Profile, and Rise and decay.

Parameter	Value	Status
C_0	16.20	Checked
C_1	2.57	Checked
$\Delta\sigma_2$	0.058	Checked
$\Delta\sigma_{2m}$	0.000	Unchecked
$\Delta\gamma_2$	0.013	Checked
$\Delta\gamma_{2m}$	0.000	Unchecked
$\Delta\sigma_Q$	0.000	Unchecked
$\Delta\sigma_1$	0.111	Checked
$\Delta\sigma_{1m}$	0.000	Unchecked
$\Delta\gamma_1$	33.224	Checked
$\Delta\gamma_{1m}$	0.000	Unchecked
$\Delta\sigma_{Qm}$	0.000	Unchecked
$\Delta\sigma_0$	0.000	Unchecked
$\Delta\sigma_{0m}$	0.000	Unchecked
$\Delta\gamma_0$	0.080	Checked
$\Delta\gamma_{0m}$	0.000	Unchecked
$\Delta\alpha_0$	0.00036	Unchecked
$\Delta\alpha_1$	0.00014	Unchecked
$\Delta\alpha_Q$	0.00000	Unchecked
$\Delta\beta_0$	0.00000	Unchecked
$\Delta\beta_1$	0.00000	Unchecked
$\Delta\beta_Q$	0.00000	Unchecked

Step 4f: Back to the main window of Mag2Pol

Save as a new project, with an appropriate name for the low-temperature phase. In this example, CrSbSe₃_10K_Lattice.xml

1

Mag2Pol

File Generate Structure Fit Geometry Form factors Tools View Help

Symmetry

Space group: **Pnma** Cell: a = 9.14953 b = 3.78322 c = 13.3306
a = 90.000 β = 90.000 γ = 90.000

Number of symmetry operators: 1 Number of irreps: 1

	x	y	z	u	v	w	φ
1	x	y	z	u	v	w	0.000

Atoms

Number of sites: 5

Atom	x	y	z	B	occ	plot	color	R	S
1 SB	0.02915	0.25000	0.65833	0.153	1.000	<input checked="" type="checkbox"/>	blue	15	1.0
2 MCR3	0.15654	0.25000	0.04386	0.118	1.000	<input checked="" type="checkbox"/>	red	14	1.0
3 SE	0.17118	0.25000	0.48383	0.120	1.000	<input checked="" type="checkbox"/>	green	8	1.0
4 SE	0.28581	0.25000	0.21378	0.129	1.000	<input checked="" type="checkbox"/>	green	8	1.0
5 SE	0.50057	0.25000	0.60810	0.136	1.000	<input checked="" type="checkbox"/>	green	8	1.0

Spins

Propagation vector: q = 0.000 0.000 0.000 +q ≠ -q

Spin	Rx	Ry	Rz	lx	ly	lz	φ
1 MCR3	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Box: a: 0.00 - 1.00 b: 0.00 - 1.00 c: 0.00 - 1.00 Domain: 1 Phase: 1
View along: custom Rotation axis: 0 0 1 direct Step (°): 5 Zoom: 0

Legend:
Sb (blue sphere)
Cr (red sphere)
Se (green sphere)

We have refined only the lattice contribution so far, and now we can define the magnetic ion and proceed with the refinement of the magnetic structure.

Refinement of magnetic structure

Step 9: Define the magnetic ion

Under the 'Atoms' section:

Depending on the type of magnetic contribution, simply add the prefix M or J to the magnetic ion followed by the ionic state. In this case only Cr^{3+} is magnetic.

After this, update the structure by the keyboard shortcut [Ctrl+U] (on Windows) or [Cmd+U] (on Mac)

As soon as a Magnetic atom is defined under the 'Atoms' section, the 'Spins' section will be populated automatically with the Magnetic ions. By default, the Propagation vector is set to (0, 0, 0). Leave everything default.

1

Atom	x	y	z	B	occ	plot	color	R	S
1 SB	0.02915	0.25000	0.65833	0.153	1.000	<input checked="" type="checkbox"/>	■	15	1.0
2 MCR3	0.15654	0.25000	0.04386	0.118	1.000	<input checked="" type="checkbox"/>	■	14	1.0
3 SE	0.17118	0.25000	0.48383	0.120	1.000	<input checked="" type="checkbox"/>	■	8	1.0
4 SE	0.28581	0.25000	0.21378	0.129	1.000	<input checked="" type="checkbox"/>	■	8	1.0
5 SE	0.50057	0.25000	0.60810	0.136	1.000	<input checked="" type="checkbox"/>	■	8	1.0

2

Spin	Rx	Ry	Rz	lx	ly	lz	φ
1 MCR3	0.000	0.000	0.000	0.000	0.000	0.000	0.000

3

Open the fit window by clicking this icon

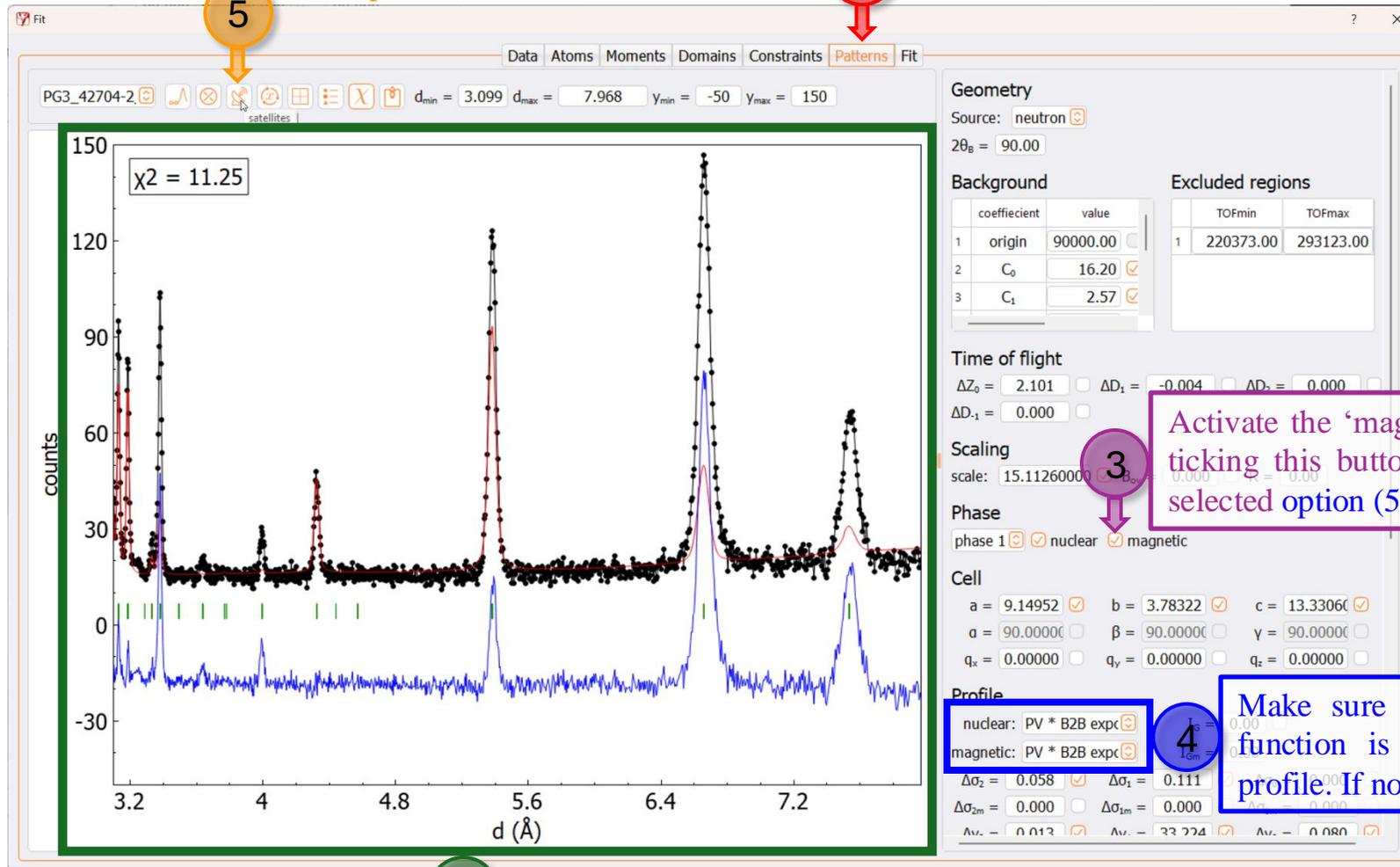
Legend:
Sb (blue sphere)
Cr (red sphere)
Se (green sphere)

Coordinate system: a, b, c

Searching for propagation vector (q -vector) from the satellite peaks

Step 5a: Zoom into the diffraction pattern and activate 'Satellites' window

Click on the 'satellites' tab which will open a new window

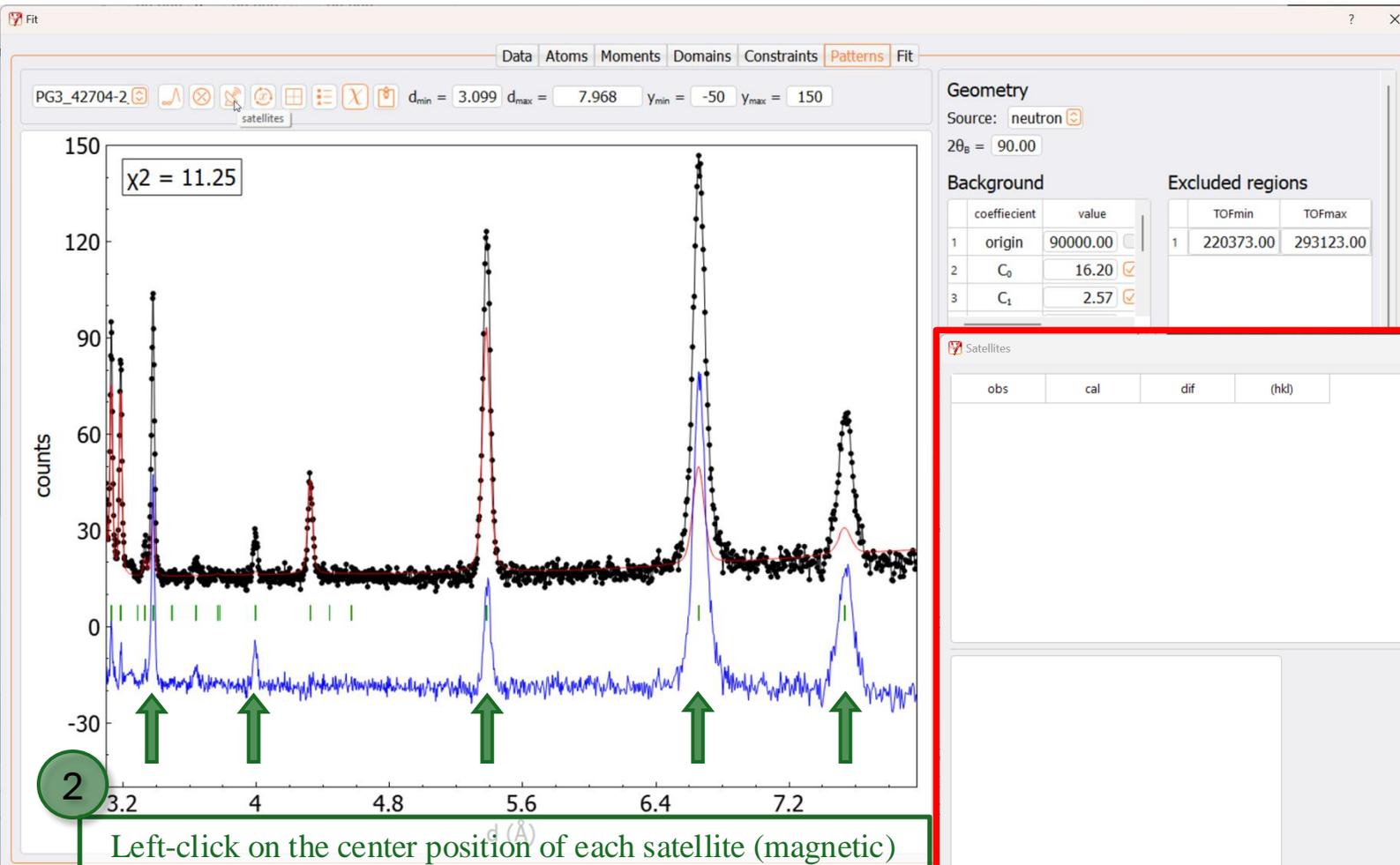


Activate the 'magnetic' option by ticking this button. If this is not selected option (5) will not work.

Make sure the magnetic peak profile function is the same as the nuclear profile. If not select it manually.

Zoom into the section of the diffraction pattern where you see magnetic peaks (at higher d -range)

Step 5b: Select satellite (magnetic) peaks



1 Move this 'Satellites' window away so that the diffraction profile on the 'Fit' window is accessible.

obs cal dif (hkl)

q-vector symmetries:

- (a 0 0)
- (0 b 0)
- (0 0 c)
- (a a 0)
- (a a a)
- (a b 0)
- (a 0 c)
- (0 b c)
- (a a c)
- (a b c)

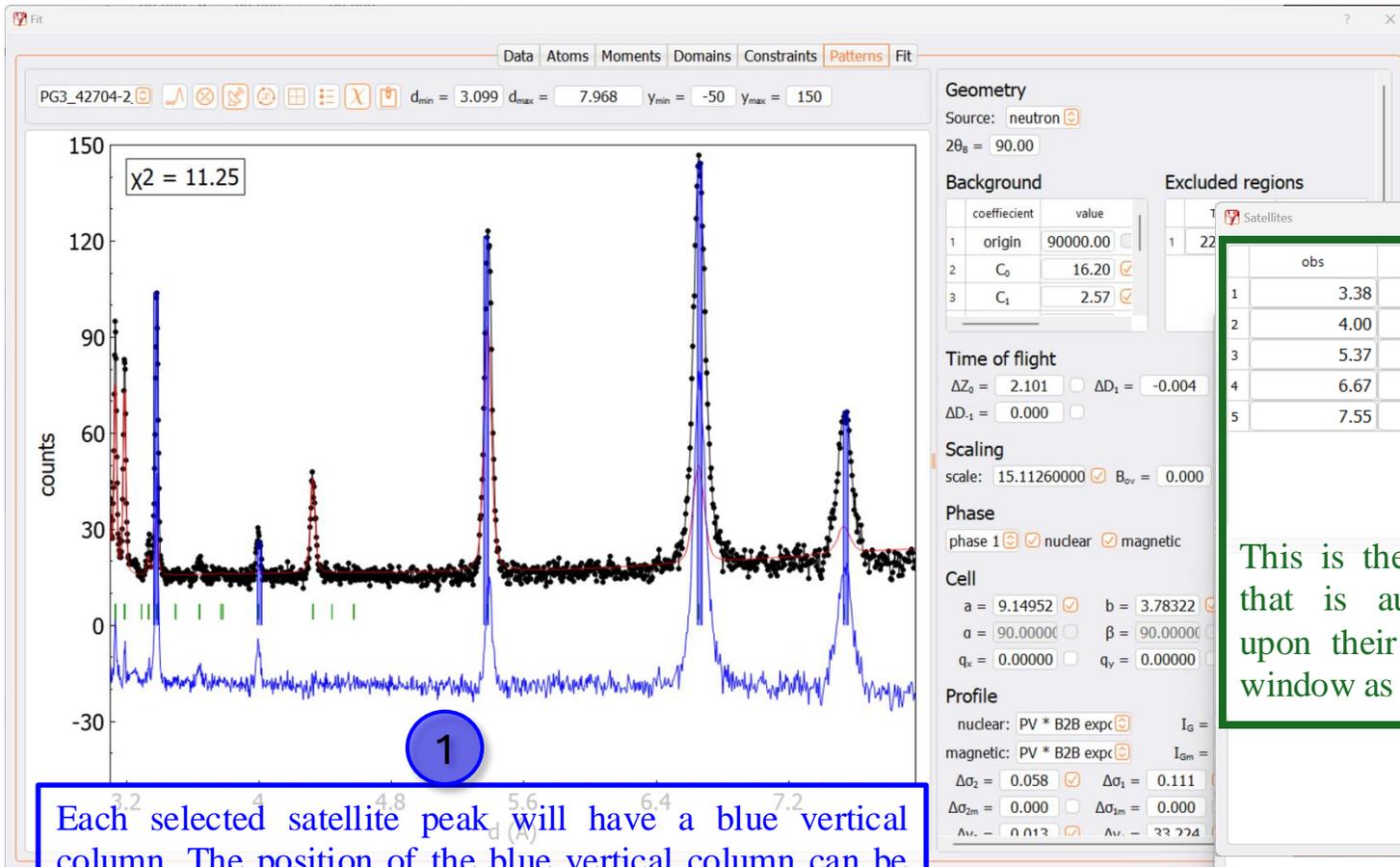
Step sizes: 0.05 0.05 0.05 Fit best 20

Find q-vector

q = 0.000 0.000 0.000

OK Cancel

Step 5b: Select satellite (magnetic) peaks



Each selected satellite peak will have a blue vertical column. The position of the blue vertical column can be altered using a mouse (left-click + hold + move) and can be removed by right-clicking on it

Select an appropriate q-vector type expected based on the lattice symmetry and 'Step size', to limit the search time. I will go with defaults in this example.

3

q-vector symmetries:
 (a 0 0) (0 b 0) (0 0 c) (a a 0) (a a a)
 (a b 0) (a 0 c) (0 b c) (a a c)
 (a b c)

Step sizes: 0.05 0.05 0.05 Fit best 20

Find q-vector

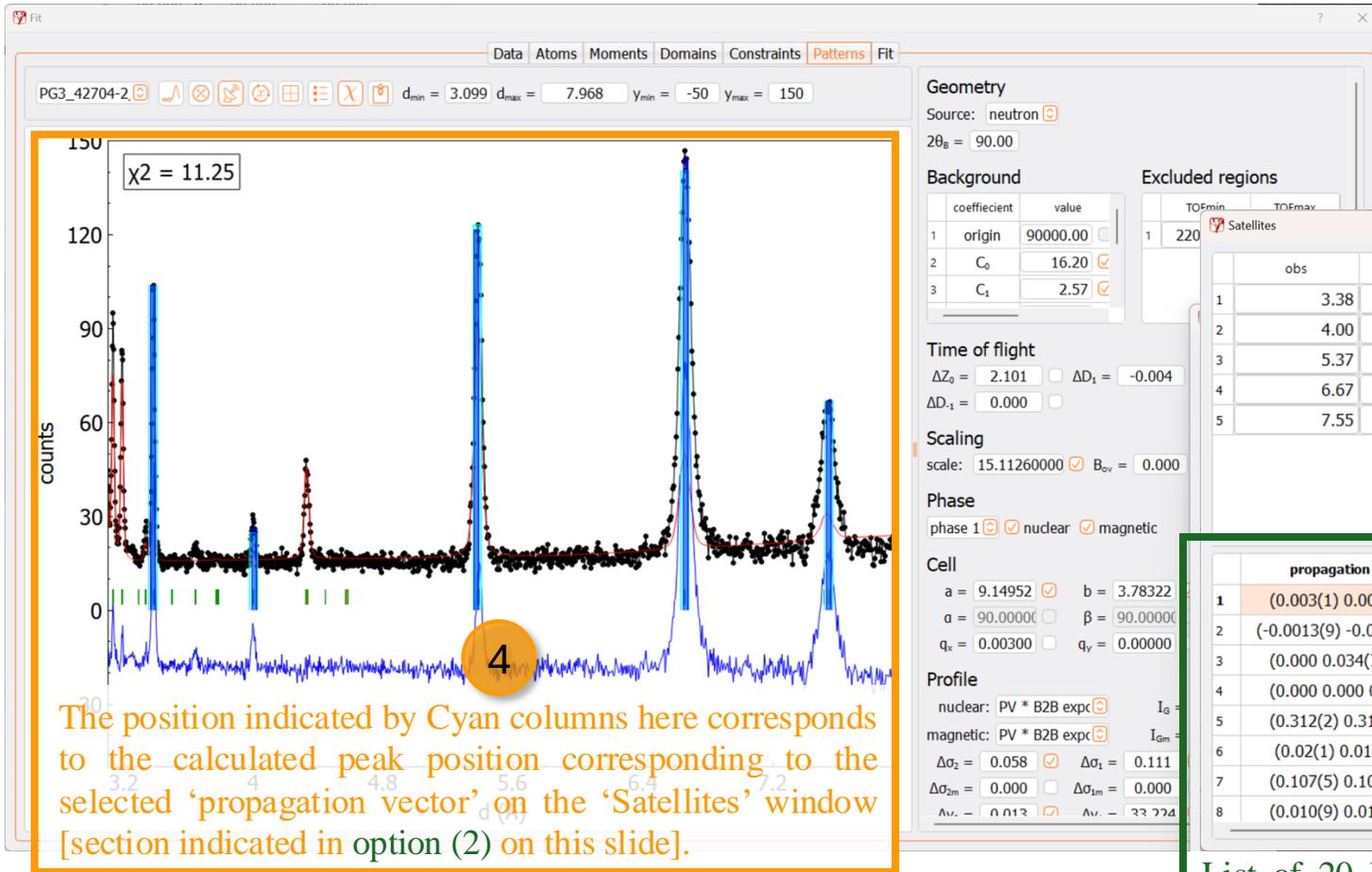
q = 0.000 0.000 0.000

OK Cancel

2

This is the list of satellite peaks that is automatically populated upon their selection on the 'Fit' window as indicated by option (1)

Step 5c: Run the q-vector search, and note down the best q-vectors



The position indicated by Cyan columns here corresponds to the calculated peak position corresponding to the selected 'propagation vector' on the 'Satellites' window [section indicated in option (2) on this slide].

obs cal dif (hkl)

1	3.38	3.38	0.00	(1 1 1)+
2	4.00	4.00	0.00	(1 0 3)-
3	5.37	5.38	0.00	(1 0 2)+
4	6.67	6.66	0.01	(0 0 2)+
5	7.55	7.55	0.00	(1 0 1)-

q-vector symmetries:
 (a 0 0) (0 b 0) (0 0 c) (a a 0) (a a a)
 (a b 0) (a 0 c) (0 b c) (a a c)
 (a b c)

Step sizes: 0.05 0.05 0.05 Fit best 20

1 Find q-vector

Clicking on 'Find q-vector' will run the search routine.

	propagation vector	chisq
1	(0.003(1) 0.000 0.000)	67518.078
2	(-0.0013(9) -0.001 -0.001)	151149.46
3	(0.000 0.034(7) 0.000)	949423.55
4	(0.000 0.000 0.006(5))	1027480.4
5	(0.312(2) 0.312 0.312)	2825092.2
6	(0.02(1) 0.017 0.017)	4220851.4
7	(0.107(5) 0.107 0.107)	4673941.1
8	(0.010(9) 0.010 0.000)	5226642.5

2

List of 20 best q-vectors that fit the selected satellites best, Populated automatically after running 'Find q-vector'.

3 q = 0.003 0.000 0.000

The best q-vector is listed here by default, after running 'Find q-vector'. In this case it is (0, 0, 0)

- 5** Note down all the propagation vectors that you wish to try out. Close both the 'Satellites' and 'Fit' windows. And go back to the main window of Mag2Pol.

Refinement of Magnetic structure

Step 6a: Update propagation vector and open the 'Irreducible representations' window

2 Clicking on this icon will open a new window, 'Irreducible representations'. This may not be active if the structure is not updated using the keyboard shortcut after updating the q -vector.

Mag2Pol

File Generate Structure Fit Geometry Form factors Tools View Help

Symmetry Irreducible representations

Space group: **Pnma** Cell: a = 9.14952 b = 3.78322 c = 13.3306
 $\alpha = 90.000^\circ \beta = 90.000^\circ \gamma = 90.000^\circ$

Box: a: 0.00 - 1.00 b: 0.00 - 1.00 c: 0.00 - 1.00 Domain: 1 Phase: 1
 View along: custom Rotation axis: 0 0 1 direct Step (°): 5 Zoom: 0

Number of symmetry operators: 1 Number of irreps: 1

	x	y	z	u	v	w	ϕ
1	x	y	z	u	v	w	0.000

Atoms

Number of sites: 5

Atom	x	y	z	B	occ	plot	color	R	S
1 SB	0.02915	0.25000	0.65833	0.153	1.000	<input checked="" type="checkbox"/>	blue	15	1.0
2 MCR3	0.15654	0.25000	0.04386	0.118	1.000	<input checked="" type="checkbox"/>	red	14	1.0
3 SE	0.17118	0.25000	0.48383	0.120	1.000	<input checked="" type="checkbox"/>	green	8	1.0
4 SE	0.28581	0.25000	0.21378	0.129	1.000	<input checked="" type="checkbox"/>	green	8	1.0
5 SE	0.50057	0.25000	0.60810	0.136	1.000	<input checked="" type="checkbox"/>	green	8	1.0

Spins

Propagation vector: $q = 0.000 \ 0.000 \ 0.000$ $+q \neq -q$

Spin: $R_x \ R_y \ R_z \ t_x \ t_y \ t_z$

1 If the propagation vector is other than (0,0,0), change it here. And update it by pressing the keyboard shortcut 'Ctrl + U' (Windows) or 'cmd + U' (on Mac). In the current case, it is the default value.

3 The newly opened 'Irreducible representations' window contains details of magnetic representations for the given wave vector.

Irreducible representations

Symmetry Multiplication table Irreps Basis vectors

8 operators in space group Pnma:

(1)	$x \ y \ z$	1
(2)	$-x+1/2 \ -y \ z+1/2$	$2(0,0,1/2) \ 1/4,0,z$
(3)	$-x \ y+1/2 \ -z$	$2(0,1/2,0) \ 0,y,0$
(4)	$x+1/2 \ -y+1/2 \ -z+1/2$	$2(1/2,0,0) \ x,1/4,1/4$
(5)	$-x \ -y \ -z$	$-1 \ 0,0,0$
(6)	$x+1/2 \ -y \ -z+1/2$	$a \ x,y,1/4$
(7)	$x \ -y+1/2 \ z$	$m \ x,1/4,z$
(8)	$-x+1/2 \ y+1/2 \ z+1/2$	$n(0,1/2,1/2) \ 1/4,y,z$

8 operators in little group with $q = (0 \ 0 \ 0)$:

(1)	$x \ y \ z$	1
(2)	$-x+1/2 \ -y \ z+1/2$	$2(0,0,1/2) \ 1/4,0,z$
(3)	$-x \ y+1/2 \ -z$	$2(0,1/2,0) \ 0,y,0$
(4)	$x+1/2 \ -y+1/2 \ -z+1/2$	$2(1/2,0,0) \ x,1/4,1/4$
(5)	$-x \ -y \ -z$	$-1 \ 0,0,0$
(6)	$x+1/2 \ -y \ -z+1/2$	$a \ x,y,1/4$
(7)	$x \ -y+1/2 \ z$	$m \ x,1/4,z$
(8)	$-x+1/2 \ y+1/2 \ z+1/2$	$n(0,1/2,1/2) \ 1/4,y,z$

Atomic positions:

Site 1

(1.1)	MCR3	(0.15728 0.25 0.04407)
(1.2)	MCR3	(0.34272 0.75 0.54407)
(1.3)	MCR3	(0.84272 0.75 0.95593)
(1.4)	MCR3	(0.65728 0.25 0.45593)

Atoms within primitive unit cell:

Site 1

(1.1)	MCR3	(0.15728 0.25 0.04407)
(1.2)	MCR3	(0.34272 0.75 0.54407)
(1.3)	MCR3	(0.84272 0.75 0.95593)
(1.4)	MCR3	(0.65728 0.25 0.45593)

Decomposition of the magnetic representation:

$$\Gamma = 1\Gamma_1 + 2\Gamma_2 + 2\Gamma_3 + 1\Gamma_4 + 1\Gamma_5 + 2\Gamma_6 + 2\Gamma_7 + 1\Gamma_8$$

41

Step 6b: On the 'Irreducible representation' window select an irrep (Γ_n) for the refinement

The 'Symmetry' tab provides some details of symmetry analysis and magnetic representation

1

8 operators in space group Pnma:

(1) x y z	1
(2) -x+1/2 -y z+1/2	2(0,0,1/2) 1/4,0,z
(3) -x y+1/2 -z	2(0,1/2,0) 0,y,0
(4) x+1/2 -y+1/2 -z+1/2	2(1/2,0,0) x,1/4,1/4
(5) -x -y -z	-1 0,0,0
(6) x+1/2 y -z+1/2	a x,y,1/4
(7) x -y+1/2 z	m x,1/4,z
(8) -x+1/2 y+1/2 z+1/2	n(0,1/2,1/2) 1/4,y,z

8 operators in little group with q = (0 0 0):

(1) x y z	1
(2) -x+1/2 -y z+1/2	2(0,0,1/2) 1/4,0,z
(3) -x y+1/2 -z	2(0,1/2,0) 0,y,0
(4) x+1/2 -y+1/2 -z+1/2	2(1/2,0,0) x,1/4,1/4
(5) -x -y -z	-1 0,0,0
(6) x+1/2 y -z+1/2	a x,y,1/4
(7) x -y+1/2 z	m x,1/4,z
(8) -x+1/2 y+1/2 z+1/2	n(0,1/2,1/2) 1/4,y,z

Atomic positions:

Site 1

(1.1) MCR3 (0.15728 0.25 0.04407)
(1.2) MCR3 (0.34272 0.75 0.54407)
(1.3) MCR3 (0.84272 0.75 0.95593)
(1.4) MCR3 (0.65728 0.25 0.45593)

Atoms within primitive unit cell:

Site 1

(1.1) MCR3 (0.15728 0.25 0.04407)
(1.2) MCR3 (0.34272 0.75 0.54407)
(1.3) MCR3 (0.84272 0.75 0.95593)
(1.4) MCR3 (0.65728 0.25 0.45593)

Decomposition of the magnetic representation:

$$\Gamma = 1\Gamma_1 + 2\Gamma_2 + 2\Gamma_3 + 1\Gamma_4 + 1\Gamma_5 + 2\Gamma_6 + 2\Gamma_7 + 1\Gamma_8$$

The 'Basis vectors' tab provides some details of Basis vectors of all magnetic sites for an irrep.

2

Choose an irrep to see the Basis vector details

Basis vectors of Γ_1

Display of basis vectors: normalized

		Site 1			
		(0.15728 1/4 0.04407)	(0.34272 3/4 0.54407)	(0.84272 3/4 0.95593)	(0.65728 1/4 0.45593)
ψ_1	0 0 0	0 -1 0	0 1 0	0 -1 0	0 -1 0

Basis vector ψ_1 of irrep Γ_1 for the Site 1 of the magnetic ion.

If the magnetic moment is not allowed at a site this space will be empty for that site.

If there is more than one magnetic site they appear as different tabs: Site 1, Site 2, etc.

The 'Irreps' tab lists all irreps. Right-click on one of the irreps symbols (Γ_1 in this example), consequently click on 'Use Γ_1 ' Go back to the main window of Mag2Pol

1

	1	21z	21y	21x	-1	az	my	nx
Γ_1	1	1	1	1	1	1	1	1
Γ_2	1	1	1	1	-1	-1	-1	-1
Γ_3	1	1	-1	-1	1	1	-1	-1
Γ_4	1	1	-1	-1	-1	-1	1	1
Γ_5	1	-1	1	-1	1	-1	1	-1
Γ_6	1	-1	1	-1	-1	1	-1	1
Γ_7	1	-1	-1	1	1	-1	-1	1
Γ_8	1	-1	-1	1	-1	1	1	-1

Step 6c: Back to the main window, save the project

Save as a new project indicating irrep in the file name.

For example, for this example, the project can be saved as **CrSbSe3_10K_Mag_G1.xml**

1

Space group: **Pnma**
Cell: a = 9.14952 b = 3.78322 c = 13.3306
a = 90.000 β = 90.000 γ = 90.000

Number of symmetry operators: 1 Number of irreps: 1

	x	y	z	u	v	w	φ
1	x	y	z	u	v	w	0.000

Number of sites: 5

Atom	x	y	z	B	occ	plot	color	R	S
1 SB	0.02915	0.25000	0.65833	0.153	1.000	<input checked="" type="checkbox"/>	■	15	1.0
2 MCR3	0.15654	0.25000	0.04386	0.118	1.000	<input checked="" type="checkbox"/>	■	14	1.0
3 SE	0.17118	0.25000	0.48383	0.120	1.000	<input checked="" type="checkbox"/>	■	8	1.0
4 SE	0.28581	0.25000	0.21378	0.129	1.000	<input checked="" type="checkbox"/>	■	8	1.0
5 SE	0.50057	0.25000	0.60810	0.136	1.000	<input checked="" type="checkbox"/>	■	8	1.0

Propagation vector: q = 0.000 0.000 0.000 +q ≠ -q

Spin	Rx	Ry	Rz	tx	ty	tz	φ
1 MCR3	0.000	0.000	0.000	0.000	0.000	0.000	0.000

2

Open the fit window by clicking this icon

Step 6d: Fix all atomic parameters

On the 'Fit' window, under the 'Atoms' tab, make sure all the atomic parameters are fixed.



	Atom	x	y	z	B	occ
A1	SB	0.02899	0.25000	0.65849	0.083	1.000
A2	MCR3	0.15728	0.25000	0.04407	0.052	1.000
A3	SE	0.17125	0.25000	0.48396	0.088	1.000
A4	SE	0.28582	0.25000	0.21381	0.080	1.000
A5	SE	0.50063	0.25000	0.60826	0.080	1.000

Scale factor and $\lambda/2$: 1.00000 0.00000

Extinction parameters:

anisotropic ShelX-like model

χ_{11} χ_{12} χ_{13}
0.00000 0.00000 0.00000

χ_{22} χ_{23}
0.00000 0.00000

χ_{33}
0.00000

Becker-Coppens model

r_D : 0.000

θ_D : 0.000 Lorentzian

Step 6e: Fix all atomic parameters

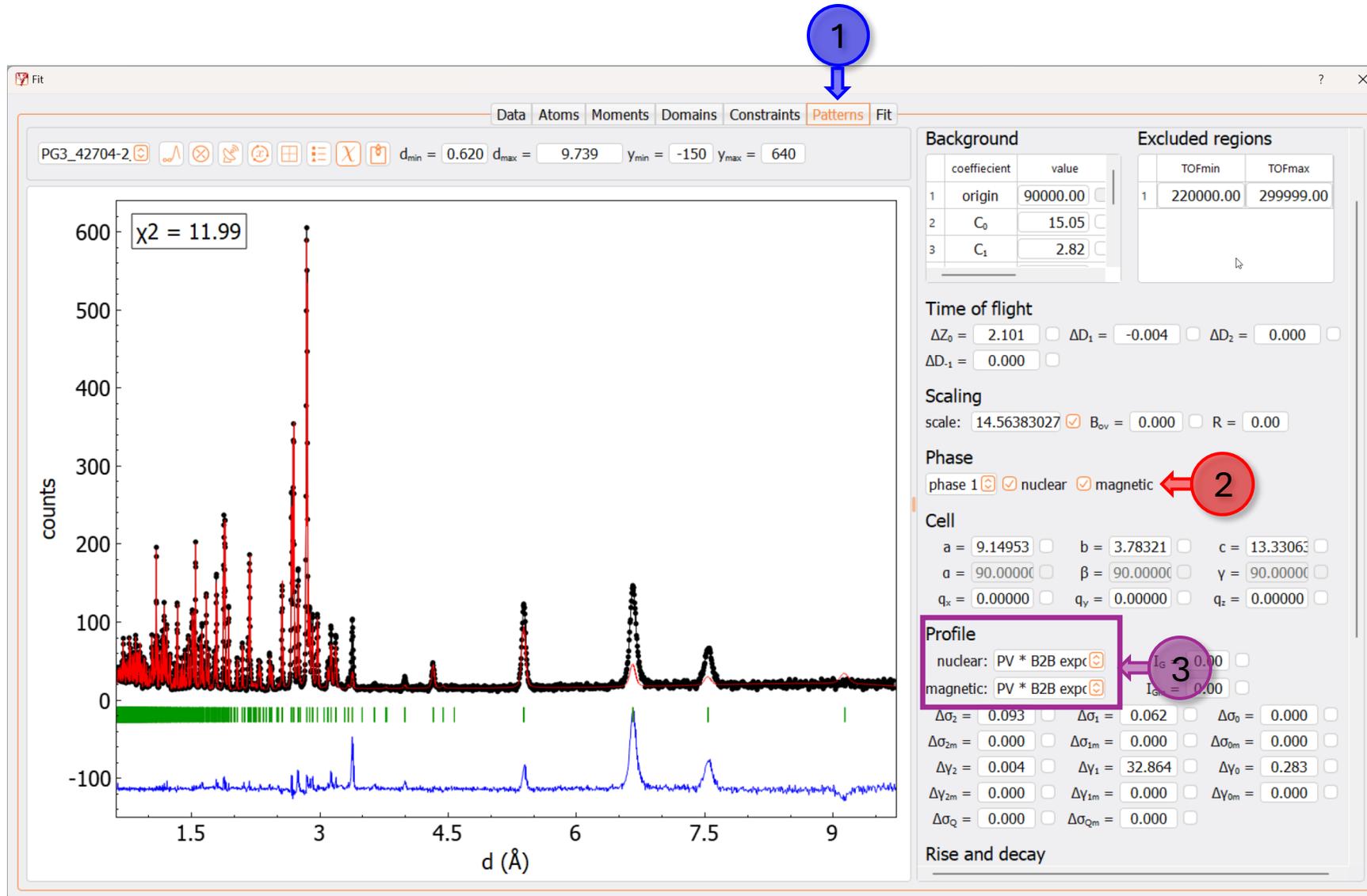
1

Spin	C1	C2	C3	C4	C5	C6	ϕ
M1 MCR3	1.000 <input checked="" type="checkbox"/>	0.000 <input type="checkbox"/>					

2

Set the coefficient of the magnetic moment to be about 1, and select it for the refinement.

Step 6f: Fix all profile parameters



Fix all parameters except the 'scale' parameter.

Also, make sure both 'nuclear' and 'magnetic' phases are active and have the same Peak profiles, 'PV * B2B exponential (Tof1)'

Step 6g: Perform fit

1

2

4

5

3

After accepting the refinement results on the 'Fit' window (keep this window open), go to the main window and click on the save button, which appends the previously saved project, **CrSbSe3_10K_Mag_G1.xml**

The fitting of magnetic peaks is rather poor with the irrep Γ_1 . We should test other irreps.

Once the convergence is reached, accept the fit results by clicking this button.

Test other irreps

Step 7a: Test all irreps by running built-in *Fit macros*

We can test each irrep one by one by selecting them in the main window of the Mag2Pol. But this can also be done much faster using the built-in fit macro 'Test irreps'.

1 Select the macro 'Test irreps'

2 Click on this arrow to run the macro

Fit

Data Atoms Moments Domains Constraints Patterns **Fit**

weight SNP: 0.000
weight intensities: 0.000
weight powder: 1.000

SNP
INT POW

Fit converged after 3 iterations
 $\chi^2 = 40457.63$
 $\chi_r^2 = 11.84$
 $R_F = 1.64$ $R_{F,mag} = 5.93$

Atoms:
SB = [0.029 0.250 0.658]
B = 0.083, occ = 1.000
MCR3 = [0.157 0.250 0.044]
B = 0.052, occ = 1.000
SE = [0.171 0.250 0.484]
B = 0.088, occ = 1.000
SE = [0.286 0.250 0.214]
B = 0.080, occ = 1.000
SE = [0.501 0.250 0.608]
B = 0.080, occ = 1.000

Magnetic moments:
MCR3: $C_1 = 1.13(7)$
 $\varphi = 0.000$
 $|\mu| = 1.13(7) \mu_B$

POWDER PARAMETERS:
scale = 14.71(2)

Polynomial background parameters:
 $C_0 = 15.050$

counts

d (Å)

View results Export results View correlations View μ -structure Export graph Undo (1) Accept

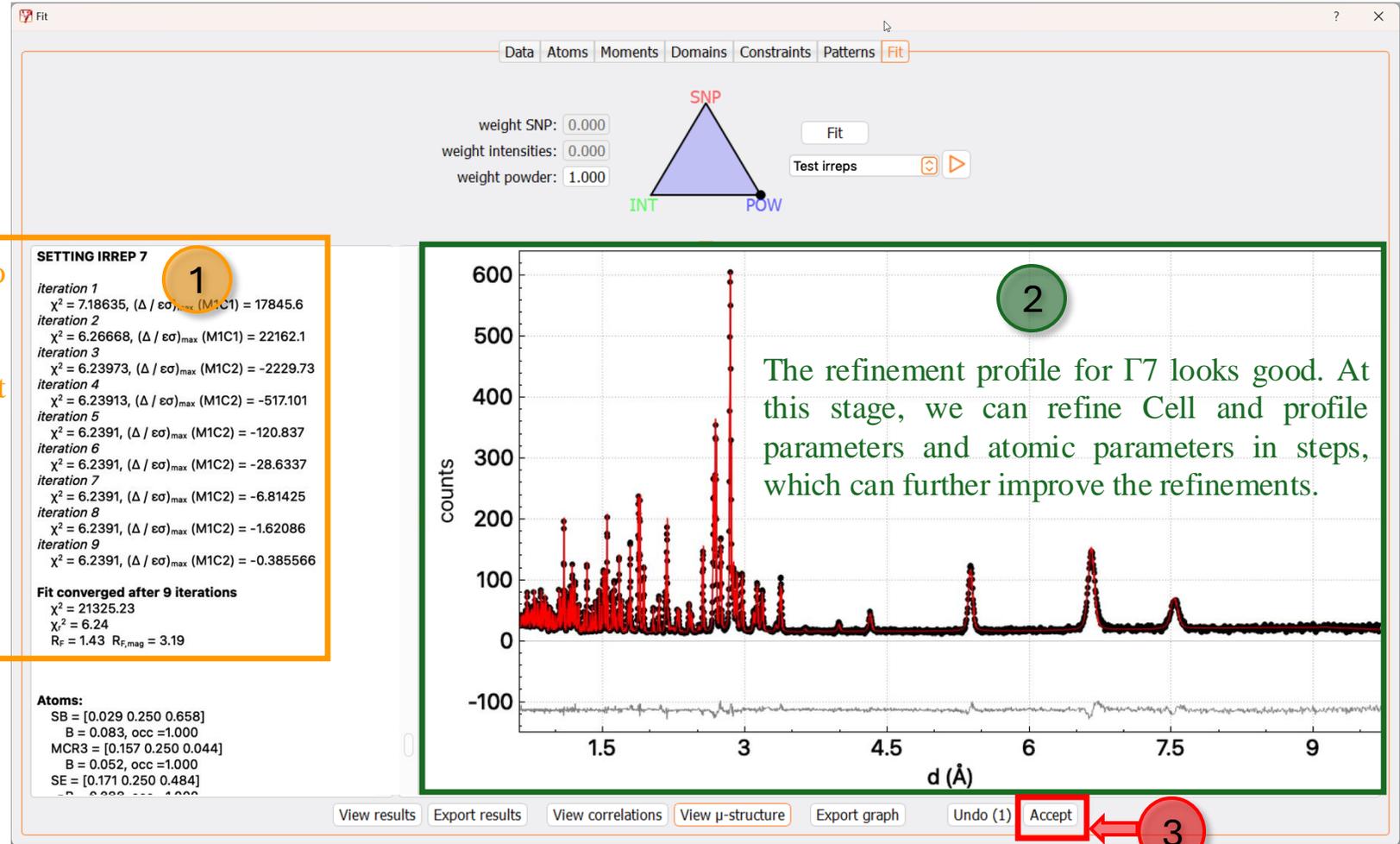
Step 7b: The macro 'Test irrep' ends with the best irrep model

The macro 'Test irreps' goes through all irreps and, at the end, reverts to the refinement of the best fitting irreps.

For the current example, the macro tested all 8 irreps.

In the end, it went back to the best model irrep, $\Gamma 7$

For this model at this stage, $\chi^2 = 6.24$, $R_{F, mag} = 3.19$



Important note:

The gamma notation between different programs may not match, so it is always a good idea to report the unambiguous, 'basis vectors'.

For example, $\Gamma 3$ in the SARAh program is equivalent to $\Gamma 7$ on Mag2Pol

Once the final refinement of the irrep model is satisfactory, accept and transfer the fit results to the main window by clicking on the 'Accept' button.

For the irrep $\Gamma 7$, at the final stage we get; $\chi^2 = 5.04$, $R_{F, mag} = 2.86$

Step 7c: Inspect the structure model and save the project

The last accepted fit results were for the irrep Γ_7 , so this project will be saved as, **CrSbSe3_10K_Mag_G7.xml**

1

The screenshot shows the Mag2Pol software interface. The main window displays a 3D structure model of CrSbSe3 in the Γ_7 setting. The model is a rectangular unit cell with axes labeled a, b, and c. The structure consists of Cr (red spheres), Sb (blue spheres), and Se (green spheres) ions. The Cr ions are shown with red arrows representing magnetic vectors. The Se ions are shown as green spheres. The Sb ions are shown as blue spheres. The structure is viewed along the c-axis. The fit results are shown in the 'Fit' window, which displays the space group Pnma, the cell parameters (a = 9.14954, b = 3.78321, c = 13.3306), and the number of symmetry operators (1) and irreps (1). The 'Atoms' window shows the following data:

Atom	x	y	z	B	occ	plot	color	R	S
1 SB	0.02897	0.25000	0.65852	0.069	1.000	<input checked="" type="checkbox"/>	blue	15	1.0
2 MCR3	0.15728	0.25000	0.04406	0.043	1.000	<input checked="" type="checkbox"/>	red	14	1.0
3 SE	0.17126	0.25000	0.48398	0.076	1.000	<input checked="" type="checkbox"/>	green	8	1.0
4 SE	0.28581	0.25000	0.21380	0.065	1.000	<input checked="" type="checkbox"/>	green	8	1.0
5 SE	0.50063	0.25000	0.60825	0.066	1.000	<input checked="" type="checkbox"/>	green	8	1.0

The 'Spins' window shows the following data:

Spin	C1	C2	C3	C4	C5	C6	ϕ
1 MCR3	2.868	0.000	0.000	0.000	0.000	0.000	0.000

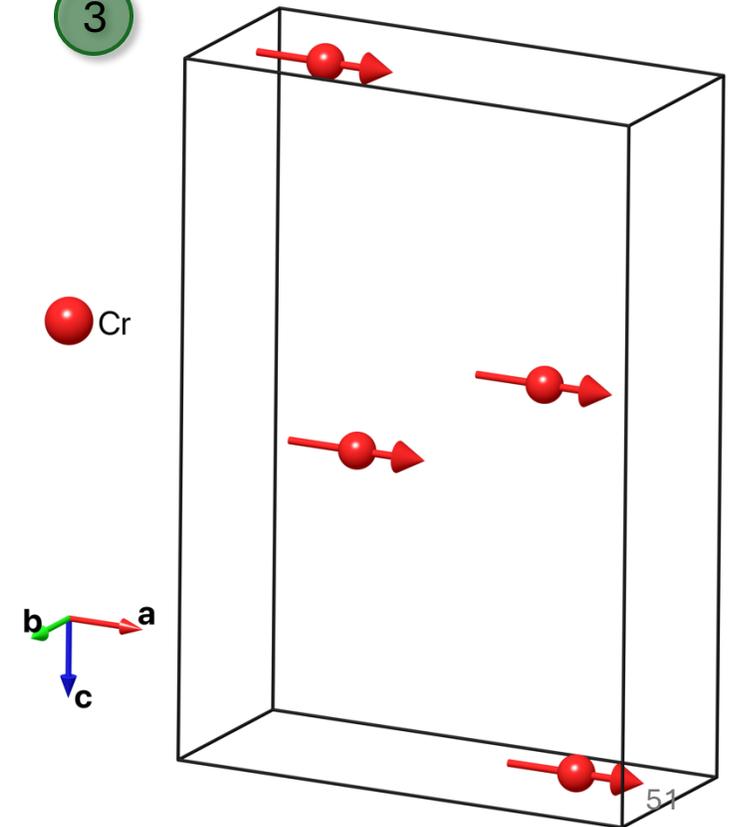
As soon as we accept the fit results of a magnetic model in the 'Fit' window, they are transferred to the main window. As we can see here, the magnetic ion in the structure model is now appended with a magnetic vector in the irrep Γ_7 setting.

2

It is possible to produce high-quality graphics (*.png) from within the Mag2Pol. Checkout the Mag2Pol manual for more details.

Here is another representation of the magnetic structure model in Γ_7 setting, produced using Mag2Pol.

3



Step 7d: Inspect full refinement results

Click this icon to open 'Sample info' window, which contains detailed information of refined Crystal structure, Magnetic structure, and Fit results. Also indicates the path and name of the current project file.

Symmetry

Space group: **Pnma**
 Cell: a = 9.14954 b = 3.78321 c = 13.3306
 $\alpha = 90.000^\circ \beta = 90.000^\circ \gamma = 90.000^\circ$

Number of symmetry operators: 1 Number of irreps: 1

	x	y	z	u	v	w	ϕ
1	x	y	z	u	v	w	0.000

Atoms

Number of sites: 5

Atom	x	y	z	B	occ	plot	color	R	S
1 SB	0.02897	0.25000	0.65852	0.069	1.000	<input checked="" type="checkbox"/>	Blue	15	1.0
2 MCR3	0.15728	0.25000	0.04406	0.043	1.000	<input checked="" type="checkbox"/>	Red	14	1.0
3 SE	0.17126	0.25000	0.48398	0.076	1.000	<input checked="" type="checkbox"/>	Green	8	1.0
4 SE	0.28581	0.25000	0.21380	0.065	1.000	<input checked="" type="checkbox"/>	Green	8	1.0
5 SE	0.50063	0.25000	0.60825	0.066	1.000	<input checked="" type="checkbox"/>	Green	8	1.0

Spins

Propagation vector: q = 0.000 0.000 0.000 +q ≠ -q

Spin	C1	C2	C3	C4	C5	C6	ϕ
1 MCR3	2.868	0.000	0.000	0.000	0.000	0.000	0.000

'Sample info' window, with the 'Crystal Structure' tab active.

Sample info (D:/OneDrive/Research/Refinement Examples/Mag2Pol/CrSbSe3_QZhang/Tutorial/CrSbSe3_10K_Mag_G7.xml)

Crystal structure | Magnetic structure | Absorption | Fit results

Chemical formula: SbCrSe₃ (Z = 4, M = 410.669 g/mol)
 Space group: Pnma
 Real lattice: a = 9.14954 Å b = 3.78321 Å c = 13.3306 Å Reciprocal lattice: a* = 0.109295 Å⁻¹ b* = 0.264326 Å⁻¹ c* = 0.0750152 Å⁻¹
 $\alpha = 90^\circ \beta = 90^\circ \gamma = 90^\circ$ $\alpha^* = 90^\circ \beta^* = 90^\circ \gamma^* = 90^\circ$
 V = 461.435 Å³ V* = 0.00216715 Å⁻³

List of atoms

	Atom	Wyckoff site	x	y	z
1.1	SB	4c	0.02897	1/4	0.65852
1.2	SB	4c	0.47103	3/4	0.15852
1.3	SB	4c	0.97103	3/4	0.34148
1.4	SB	4c	0.52897	1/4	0.84148
2.1	MCR3	4c	0.15728	1/4	0.04406
2.2	MCR3	4c	0.34272	3/4	0.54406
2.3	MCR3	4c	0.84272	3/4	0.95594
2.4	MCR3	4c	0.65728	1/4	0.45594
3.1	SE	4c	0.17126	1/4	0.48398
3.2	SE	4c	0.32874	3/4	0.98398
3.3	SE	4c	0.82874	3/4	0.51602
3.4	SE	4c	0.67126	1/4	0.01602

Step 7d: Inspect full refinement results

Mag2Pol

File Generate Structure Fit Geometry Form factors Tools View Help

Symmetry

Space group: **Pnma** Cell: a = 9.14954 b = 3.78321 c = 13.3306
 $\alpha = 90.000^\circ \beta = 90.000^\circ \gamma = 90.000^\circ$

Number of symmetry operators: 1 Number of irreps: 1

	x	y	z	u	v	w	ϕ
1	x	y	z	u	v	w	0.000

Atoms

Number of sites: 5

Atom	x	y	z	B	occ	plot	color	R	S
1 SB	0.02897	0.25000	0.65852	0.069	1.000	<input checked="" type="checkbox"/>	Blue	15	1.0
2 MCR3	0.15728	0.25000	0.04406	0.043	1.000	<input checked="" type="checkbox"/>	Red	14	1.0
3 SE	0.17126	0.25000	0.48398	0.076	1.000	<input checked="" type="checkbox"/>	Green	8	1.0
4 SE	0.28581	0.25000	0.21380	0.065	1.000	<input checked="" type="checkbox"/>	Green	8	1.0
5 SE	0.50063	0.25000	0.60825	0.066	1.000	<input checked="" type="checkbox"/>	Green	8	1.0

Spins

Propagation vector: $q = (0.000, 0.000, 0.000)$ +q ≠ -q

Spin	C1	C2	C3	C4	C5	C6	ϕ
1 MCR3	2.868	0.000	0.000	0.000	0.000	0.000	0.000

Box: a: 0.00 - 1.00 b: 0.00 - 1.00 c: 0.00 - 1.00 Domain: 1 Phase: 1
 View along: custom Rotation axis: 0 0 1 direct Step (°): 5 Zoom: 43

‘Magnetic structure’ tab information of magnetic model used in the last refinements.

Sample info (D:/OneDrive/Research/Refinement Examples/Mag2Pol/CrSbSe3_QZhang_Tutorial/CrSbSe3_10K_Mag_G7.xml)

Crystal structure **Magnetic structure** Absorption Fit results

Magnetic symmetry: irrep Γ_7
 Propagation vector: $q = (0\ 0\ 0)$

List of spins for domain 1

	Spin	x	y	z	Mx	My	Mz	Sx	Sy	Sz
2.1	MCR3	0.15728	0.25	0.04406	2.87	0	0	2.87	0	0
2.2	MCR3	0.34272	0.75	0.54406	2.87	0	0	2.87	0	0
2.3	MCR3	0.84272	0.75	0.95594	2.87	0	0	2.87	0	0
2.4	MCR3	0.65728	0.25	0.45594	2.87	0	0	2.87	0	0

Step 7d: Inspect full refinement results

Mag2Pol

File Generate Structure Fit Geometry Form factors Tools View Help

Symmetry

Space group: **Pnma**

Cell: a = 9.14954 b = 3.78321 c = 13.3306

$\alpha = 90.000$ $\beta = 90.000$ $\gamma = 90.000$

Number of symmetry operators: 1 Number of irreps: 1

	x	y	z	u	v	w	ϕ
1	x	y	z	u	v	w	0.000

Atoms

Number of sites: 5

Atom	x	y	z	B	occ	plot	color	R	S
1 SB	0.02897	0.25000	0.65852	0.069	1.000	<input checked="" type="checkbox"/>	blue	15	1.0
2 MCR3	0.15728	0.25000	0.04406	0.043	1.000	<input checked="" type="checkbox"/>	red	14	1.0
3 SE	0.17126	0.25000	0.48398	0.076	1.000	<input checked="" type="checkbox"/>	green	8	1.0
4 SE	0.28581	0.25000	0.21380	0.065	1.000	<input checked="" type="checkbox"/>	green	8	1.0
5 SE	0.50063	0.25000	0.60825	0.066	1.000	<input checked="" type="checkbox"/>	green	8	1.0

Spins

Propagation vector: q = 0.000 0.000 0.000 +q -q

Spin	C1	C2	C3	C4	C5	C6	ϕ
1 MCR3	2.868	0.000	0.000	0.000	0.000	0.000	0.000

Box: a: 0.00 - 1.00 b: 0.00 - 1.00 c: 0.00 - 1.00 Domain: 1 Phase: 1

View along: custom Rotation axis: 0 0 1 direct Step (°): 5 Zoom: 43

Legend: Sb (blue), Cr (red), Se (green)

Crystal structure axes: a, b, c

The 'Fit results' tab contains detailed refinement results of last refinements.

Sample info (D:/OneDrive/Research/Refinement Examples/Mag2Pol/CrSbSe3_QZhang/Tutorial/CrSbSe3_10K_Mag_G7.xml)

Crystal structure Magnetic structure Absorption **Fit results**

Fit converged after 2 iterations

$\chi^2 = 18908.42$
 $\chi^2 = 5.04$
 $R_F = 1.41$ $R_{F,mag} = 2.86$

Atoms:

SB = [0.0290(1) 0.250 0.65852(8)]
B = 0.07(2), occ = 1.000
MCR3 = [0.1573(2) 0.250 0.0441(1)]
B = 0.04(2), occ = 1.000
SE = [0.17126(9) 0.250 0.48398(6)]
B = 0.08(1), occ = 1.000
SE = [0.28581(8) 0.250 0.21380(6)]
B = 0.06(1), occ = 1.000
SE = [0.50063(9) 0.250 0.60825(6)]
B = 0.07(1), occ = 1.000

Magnetic moments:

MCR3: $C_1 = 2.87(2)$
 $\phi = 0.000$
 $|\mu| = 2.87(2) \mu_B$

POWDER PARAMETERS:

scale = 14.50(4)

Step 7e: Export refinement results as latex tables

1

The screenshot shows the Mag2Pol software interface. The 'Tools' menu is open, and 'LaTeX export' is selected. The 'Atoms' panel shows the following data:

Atom	x	y	z	B	occ	plot	color	R	S
1 SB	0.02897	0.25000	0.65852	0.069	1.000	<input checked="" type="checkbox"/>	■	15	1.0
2 MCR3	0.15728	0.25000	0.04406	0.043	1.000	<input checked="" type="checkbox"/>	■	14	1.0
3 SE	0.17126	0.25000	0.48398	0.076	1.000	<input checked="" type="checkbox"/>	■	8	1.0
4 SE	0.28581	0.25000	0.21380	0.065	1.000	<input checked="" type="checkbox"/>	■	8	1.0
5 SE	0.50063	0.25000	0.60825	0.066	1.000	<input checked="" type="checkbox"/>	■	8	1.0

The 'Spins' panel shows the following data:

Spin	C1	C2	C3	C4	C5	C6	φ
1 MCR3	2.868	0.000	0.000	0.000	0.000	0.000	0.000

The 3D visualization shows a crystal structure with atoms Sb (blue), Cr (red), and Se (green). The axes are labeled a, b, and c.

A variety of fit results can be copied directly in Latex format by following the menu tree:

Tools → LaTeX export

Step 7f: Export the Graphic and structure models

1

Mag2Pol

File Generate Structure Fit Geometry Form factors Tools View Help

Open Ctrl+O
Open recent
Save Ctrl+S
Save as
Import
Export
Reset
Settings
Check for updates

Cell: a = 1.14954 b = 3.78321 c = 13.3306
α = 90.000 β = 90.000 γ = 90.000
Number of irreps: 1

	X	Y	Z	u	v	w	φ
1	X	Y	Z	u	v	w	0.000

Atoms

Number of sites: 5

Atom	x	y	z	B	occ	plot	color	R	S
1 SB	0.02897	0.25000	0.65852	0.069	1.000	<input checked="" type="checkbox"/>	■	15	1.0
2 MCR3	0.15728	0.25000	0.04406	0.043	1.000	<input checked="" type="checkbox"/>	■	14	1.0
3 SE	0.17126	0.25000	0.48398	0.076	1.000	<input checked="" type="checkbox"/>	■	8	1.0
4 SE	0.28581	0.25000	0.21380	0.065	1.000	<input checked="" type="checkbox"/>	■	8	1.0
5 SE	0.50063	0.25000	0.60825	0.066	1.000	<input checked="" type="checkbox"/>	■	8	1.0

Spins

Propagation vector: q = 0.000 0.000 0.000 +q ≠ -q

Spin	C1	C2	C3	C4	C5	C6	φ
1 MCR3	2.868	0.000	0.000	0.000	0.000	0.000	0.000

Box: a: 0.00 - 1.00 b: 0.00 - 1.00 c: 0.00 - 1.00 Domain: 1 Phase: 1
View along: custom Rotation axis: 0 0 1 direct Step (°): 5 Zoom: 43

Legend:
■ Sb
■ Cr
■ Se

Coordinate system: a, b, c

The structure model can be saved as *.png (Graphic) or *.cif or *.mcif, by following the menu tree:

File→Export

Refining magnetic structure using Shubnikov groups (Magnetic space groups) instead of Irreducible representations.

Step 8a: Set up a Magnetic Space Group

One way to start this procedure is to prepare a *.mcif file on the Bilbao crystallographic server, download it, and load that *.mcif directly in Mag2Pol. The alternate starting point for this procedure would be to use the final version of the Mag2Pol project with lattice-only contribution. For this example, we will start with the saved project with lattice-only contribution, CrSbSe3_10K_Lattice.xml

1 Set up the magnetic ion

Atom	x	y	z	u	v	w	φ	color	R	S
1 MCR3	0.15728	0.25000	0.04406	0.043	1.000			red	14	1.0
3 SE	0.17126	0.25000	0.48398	0.076	1.000			green	8	1.0
4 SE	0.28581	0.25000	0.21380	0.065	1.000			green	8	1.0
5 SE	0.50063	0.25000	0.60825	0.066	1.000			green	8	1.0

Change the q-vector if necessary. Default values for this example.

2 Propagation vector $q = 0.000 \ 0.000 \ 0.000$ +q ≠ -q

Spin	C1	C2	C3	C4	C5	C6	φ
1 MCR3	2.868	0.000	0.000	0.000	0.000	0.000	0.000

3 Key board shortcut, [Ctrl + U] (on Windows) or [Cmd + U] (on Mac)

4 Click on the 'Space group tables' icon to open the new window with the same name.

5 Activate the 'Magnetic SGs' tab

6 Type the notation of an appropriate Magnetic Space Group or select it from the drop-down menu. For this example, I choose one of the allowed magnetic space groups Pnm'a'.

Space group tables window content:

Crystallographic SGs **Magnetic SGs** Magnetic SSGs Preview

Pnm'a' orthorhombic 62.447: Pnm'a'

8 operators in space group Pnm'a':

(1) $x \ y \ z + 1$	1
(2) $-x+1/2 \ -y \ z+1/2 \ -1$	$2'(0,0,1/2) \ 1/4,0,z$
(3) $-x \ y+1/2 \ -z \ -1$	$2'(0,1/2,0) \ 0,y,0$
(4) $x+1/2 \ -y+1/2 \ -z+1/2 \ +1$	$2(1/2,0,0) \ x,1/4,1/4$
(5) $-x \ -y \ -z \ +1$	$-1 \ 0,0,0$
(6) $x+1/2 \ y \ -z+1/2 \ -1$	$a' \ x,y,1/4$
(7) $x \ -y+1/2 \ z \ -1$	$m' \ x,1/4,z$
(8) $-x+1/2 \ y+1/2 \ z+1/2 \ +1$	$n(0,1/2,1/2) \ 1/4,y,z$

4 Wyckoff positions:

8 d $x, y, z [u, v, w]$ $-x+1/2, -y, z+1/2 [u, v, -w]$ $-x, y+1/2, -z [u, -v, w]$

Basis: (a, b, c; 0, 0, 0) Transform MSG

1	0	0	0
0	1	0	0
0	0	1	0

R =

0
0
0

t =

Step 8b: Transfer the Magnetic Space Group for the refinement

4 Save the project with an appropriate name.
For this example, CrSbSe3_10K_Pnm'a'.xml

5 Click this icon to open the 'Fit' window.

3 This is updated automatically to the selected Magnetic Space Group

Switch to the 'Preview' tab

1

2

Click on the button 'Transfer MSG'

Crystal structure

Atom	Wyckoff position	parameter	value
1 SB	4c	x	0.02897
1 SB	4c	z	0.65852
2 MCR3	4c	x	0.15728
2 MCR3	4c	z	0.04406
3 SE	4c	x	0.17126
3 SE	4c	z	0.48398
4 SE	4c	x	0.28581
4 SE	4c	z	0.21380
5 SE	4c	x	0.50063
5 SE	4c	z	0.60825

Reset parameters Reset symmetry

Step 8c: Perform the refinement using the chosen Magnetic Space Group

1

Fix all parameters except magnetic moments and scale parameter.

Also, make sure both 'nuclear' and 'magnetic' phases are active and have the same Peak profiles, '*PV * B2B exponential (Tof1)*'

2

The screenshot shows the 'Fit' software interface. At the top, there are tabs for 'Data', 'Atoms', 'Moments', 'Domains', 'Constraints', 'Patterns', and 'Fit'. The 'Fit' tab is active. Below the tabs, there are three weight input fields: 'weight SNP: 0.000', 'weight intensities: 0.000', and 'weight powder: 1.000'. To the right of these fields is a blue triangle with vertices labeled 'SNP', 'INT', and 'POW'. A red circle with the number '3' and an arrow points to the 'Fit' button. To the right of the 'Fit' button is the text 'Click on the fit button'. Below the weight fields, there is a 'POW nuclear' button. The main area of the interface is a plot of 'counts' versus 'd (Å)'. The plot shows a series of peaks, with the highest peak at approximately 2.8 Å. A red circle with the number '4' is placed over the plot. At the bottom of the interface, there are buttons for 'View results', 'Export results', 'View correlations', 'View μ-structure', 'Export graph', 'Undo (1)', and 'Accept'. On the left side of the interface, there is a text box with the number '5' and the text: 'The refinement results using the Magnetic Space Group Pnm'a' are identical to those obtained using irrep Γ7.'

Fit converged after 3 iterations
 $\chi^2 = 18906.68$
 $\chi_r^2 = 5.04$
 $R_F = 1.41$ $R_{F,mag} = 2.86$

Atoms:
SB = [0.0290(1) 0.250 0.65851(8)]
B = 0.07(2), occ = 1.000
MCR3 = [0.1573(2) 0.250 0.0441(1)]
B = 0.04(2), occ = 1.000
SE = [0.17126(9) 0.250 0.48397(6)]
B = 0.08(1), occ = 1.000
SE = [0.28581(8) 0.250 0.21380(6)]
B = 0.07(1), occ = 1.000
SE = [0.50063(9) 0.250 0.60826(6)]
B = 0.07(1), occ = 1.000

Magnetic moments:
MCR3: $C_i = 2.87(2)$
 $\phi = 0.000$
 $|\mu| = 2.87(2) \mu_B$

POWDER PARAMETERS:
scale = 14.50(4)

Polynomial background parameters:

5
The refinement results using the Magnetic Space Group Pnm'a' are identical to those obtained using irrep Γ_7 .

4
Repeat the fitting by activating more parameters in succession until all necessary parameters are refined and the fit is satisfactory, like the one here.

If you have any questions:

Regarding the experiments and data collected at the instrument POWGEN, SNS

Contact:

Qiang Zhang
SNS, Oak Ridge National Laboratory,
Knoxville, USA
Email: zhangq6@ornl.gov

Regarding Mag2Pol and need to report bugs.

Contact:

Navid Qureshi
Institute Laue Langevin,
Grenoble, France
Email: qureshi@ill.fr

Regarding this tutorial

Contact:

Naveen Kumar Chogondahalli Muniraju
Institute of Nuclear Physics, PAN
Krakow, Poland
Email: naveen.chogondahalli@ifj.edu.pl

Good luck with your next refinement project!