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Fullprof refinement of commensurate structure from CW powder diffraction data [Fullprof & Magnetic Space Groups]

Stuart Calder, ORNL

MagStr2026

Duke University July 20-24



U.S. DEPARTMENT
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Mn-pyrazinecarboxylate

This example will use Fullprof and Bilbao Crystallographic Server (BCS) <https://cryst.ehu.es/>

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- Step 5: Check the magnetic model

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PHYSICAL REVIEW MATERIALS 7, 124408 (2023)

Magnetic order in the two-dimensional metal-organic framework manganese pyrazinecarboxylate with Mn-Mn dimers

S. Calder^{1,*}, R. Baral¹, N. Narayanan,² and L. D. Sanjeewa^{2,3}

¹*Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*

²*University of Missouri Research Reactor (MURR), University of Missouri, Columbia, Missouri 65211, USA*

³*Department of Chemistry, University of Missouri, Columbia, Missouri 65211, USA*

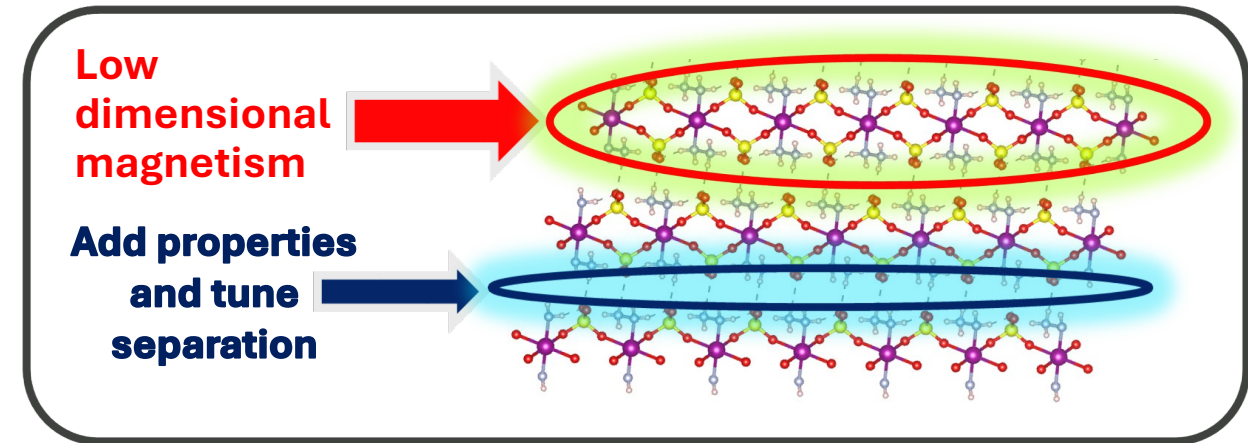
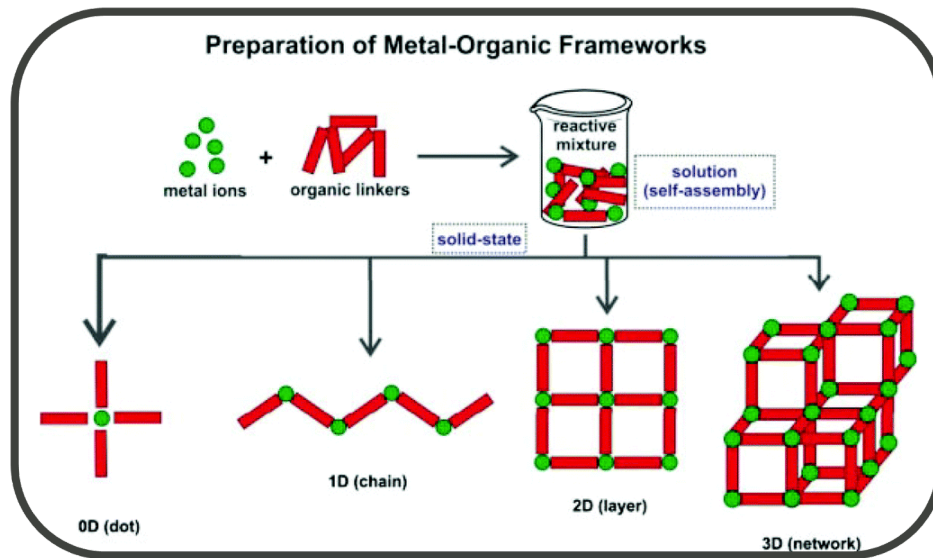
(Received 29 September 2023; revised 8 November 2023; accepted 28 November 2023; published 15 December 2023)

The magnetic properties of $[\text{Mn}(\text{pyrazinecarboxylate})_2]_n$, empirical formula $\text{C}_{10}\text{H}_6\text{MnN}_4\text{O}_4$, are investigated through susceptibility, heat capacity, and neutron scattering measurements. The structure consists of Mn-Mn dimers linked on a distorted 2D hexagonal structure. The weak out-of-plane interactions create a quasi-2D magnetic material within the larger three-dimensional metal-organic framework structure. We show that this material undergoes a two-stage magnetic transition, related to the low dimensionality of the Mn lattice. First, at 5 K, which is assigned to the initial development of short-range order in the 2D layers. This is followed by long-range order at 3.3 K. Applied field measurements reveal the potential to induce magnetic transitions in moderately small fields of ~ 2 T. Neutron powder diffraction enabled the determination of a unique magnetic space group $P2_1'/c$ (No. 14.77) at 1.5 K. This magnetic structure consists of antiferromagnetically coupled Mn-Mn dimers with spins principally along the out-of-plane a axis.

DOI: [10.1103/PhysRevMaterials.7.124408](https://doi.org/10.1103/PhysRevMaterials.7.124408)

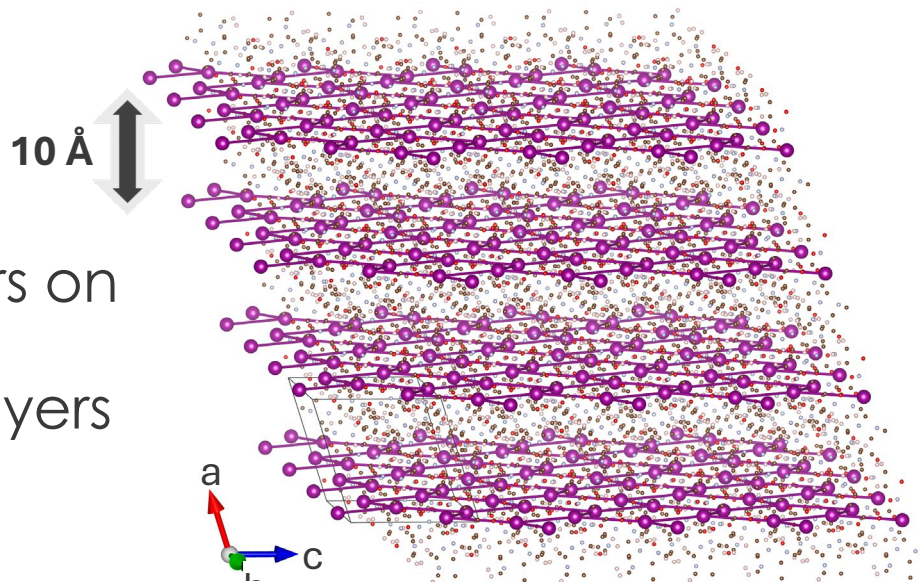
Quantum behavior by design in low dimensional Magnetic MOFs

- Magnetism largely unexplored
- Straightforward synthesis to tune low dimensional behavior.
 - Design quantum behavior on regular lattice.
 - Multifunctionality on magnetic and organic building blocks.
 - Tunable by small pressure, field, strain, light.

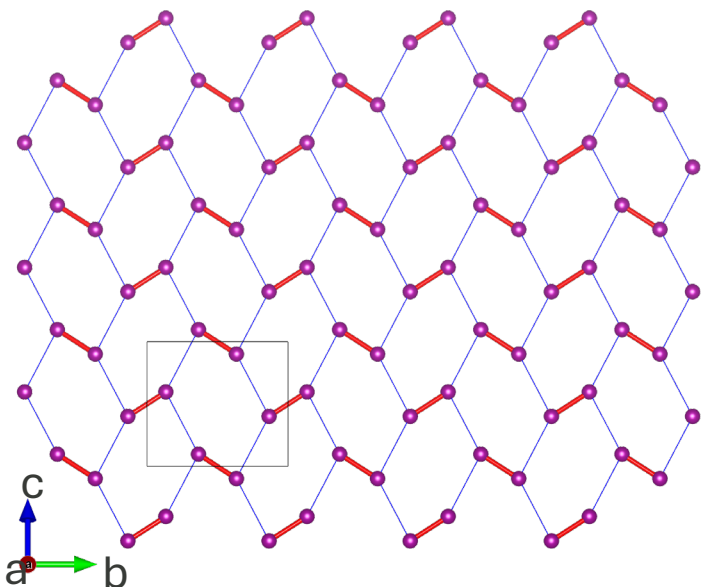


Mn-pyrazinecarboxylate ($\text{Mn}(\text{2-pzc})_2$) $\text{C}_{10}\text{H}_6\text{MnN}_4\text{O}_4$

- Well isolated 2D layers



- Mn-Mn dimers on distorted hexagonal layers



Lots of hydrogen, which creates very large background for neutron powder diffraction. Can we still determine magnetic structure?

Compound C10 H6 Mn N4 O4

Lattice type P
Space group name P21/c
Space group number 14
Setting number 1

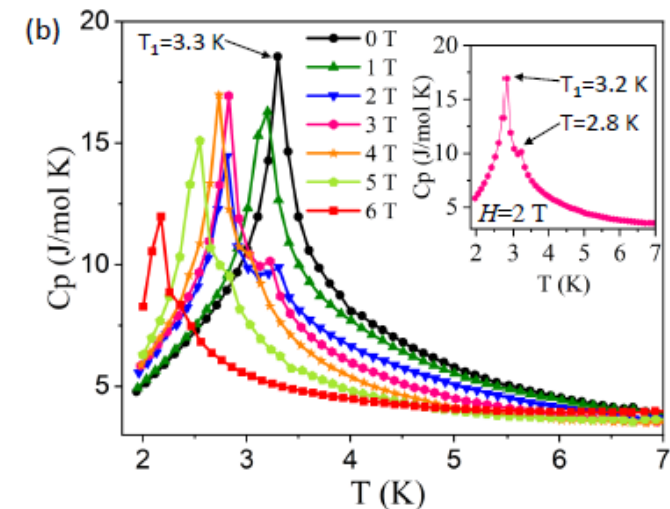
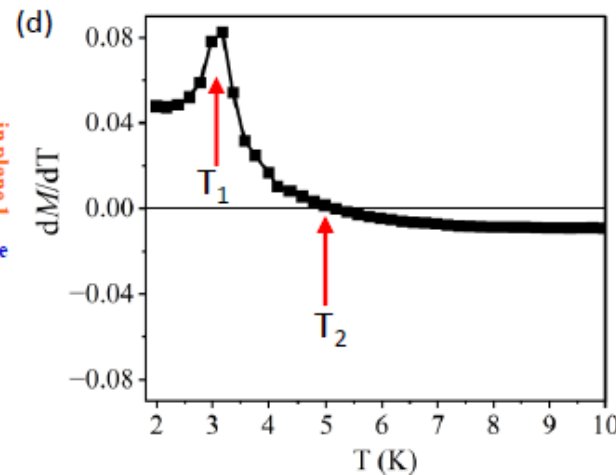
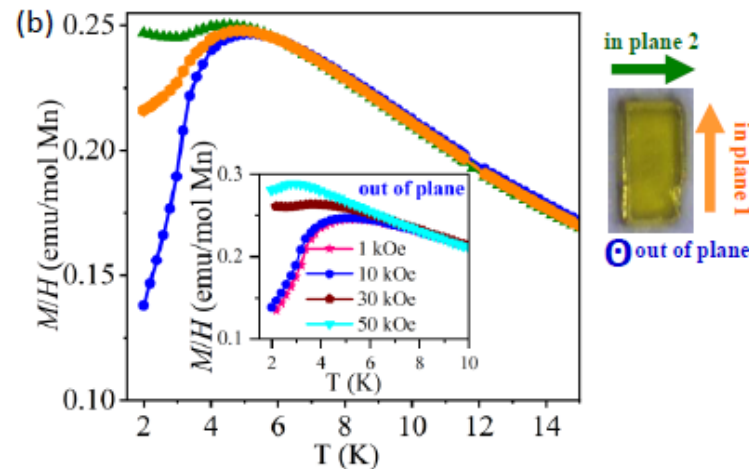
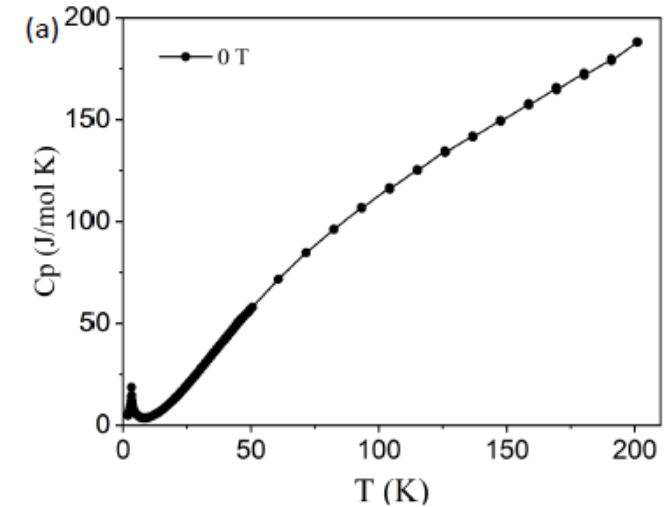
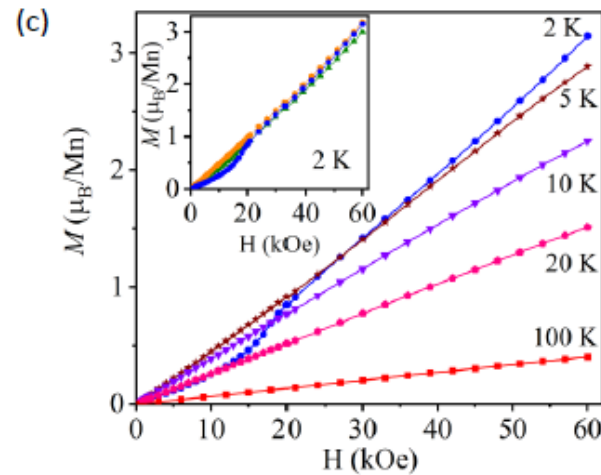
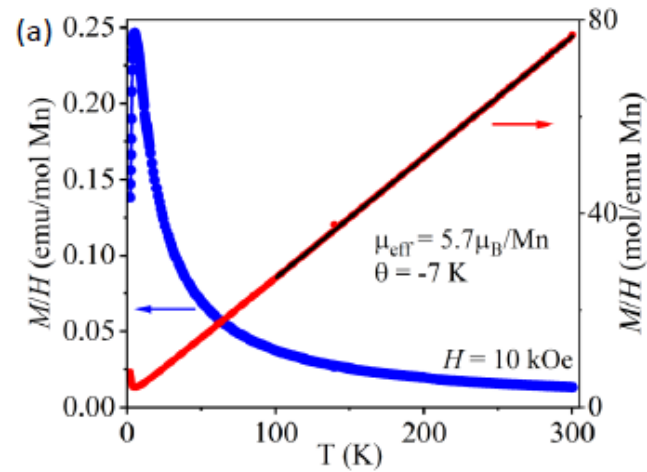
Lattice parameters
a b c alpha beta gamma
10.19000 10.90600 10.11600 90.0000 107.9600 90.0000

Structure parameters

	x	y	z	Occ.	U	Site	
Mn	0.510090		0.134260	0.598000	1.000	0.024	4e
O	0.541000		0.244300	0.426600	1.000	0.023	4e
N	0.360600		0.299100	0.562100	1.000	0.031	4e
C	0.262700		0.325100	0.619200	1.000	0.038	4e
H	0.254640		0.276940	0.691940	1.000	0.034	4e
O	0.475200		0.405900	0.287300	1.000	0.041	4e
N	0.180200		0.495900	0.472800	1.000	0.031	4e
C	0.173100		0.421500	0.573800	1.000	0.037	4e
H	0.105000		0.434840	0.615460	1.000	0.025	4e
O	0.632900	-0.009200	0.533500	1.000	1.000	0.038	4e
N	0.738100	0.176100	0.700600	1.000	1.000	0.046	4e
C	0.277700		0.468700	0.414700	1.000	0.037	4e
H	0.285650		0.517370	0.342340	1.000	0.045	4e
O	0.824800	-0.033000	0.475000	1.000	1.000	0.034	4e
N	1.018200	0.234100	0.767400	1.000	1.000	0.041	4e
C	0.367000		0.371700	0.457400	1.000	0.024	4e
C	0.471400		0.338300	0.385500	1.000	0.028	4e
C	0.796000		0.262800	0.792500	1.000	0.025	4e
H	0.742540		0.304290	0.837480	1.000	0.037	4e
C	0.933300		0.292500	0.822500	1.000	0.026	4e
H	0.968190		0.356270	0.884090	1.000	0.042	4e
C	0.960400		0.144900	0.676800	1.000	0.035	4e
H	1.015390		0.101040	0.635600	1.000	0.028	4e
C	0.823000		0.116000	0.643000	1.000	0.033	4e
C	0.758100		0.015200	0.540800	1.000	0.034	4e

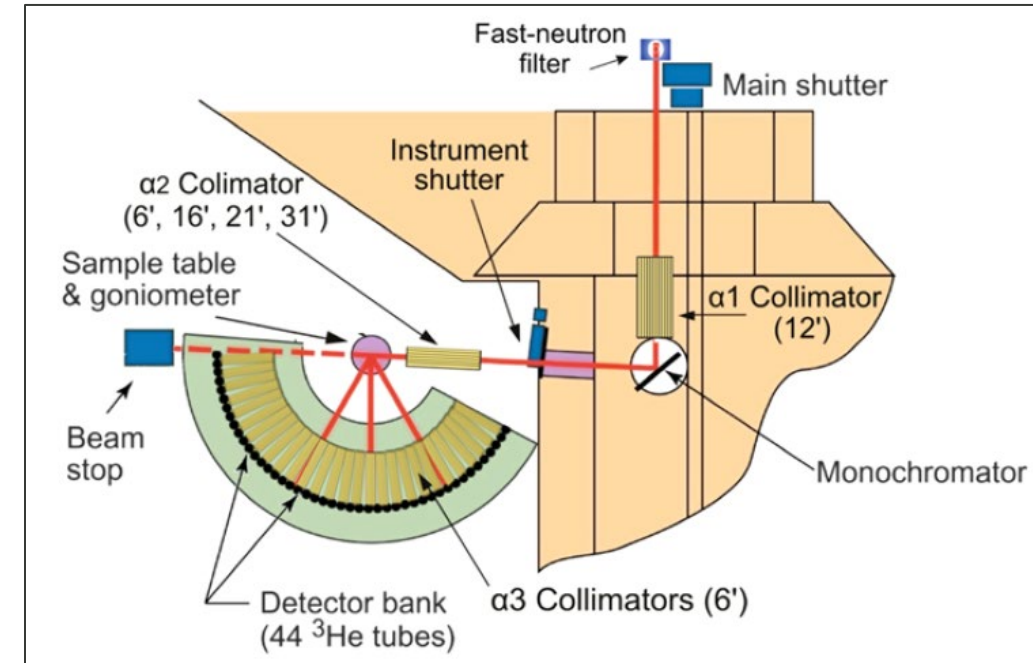
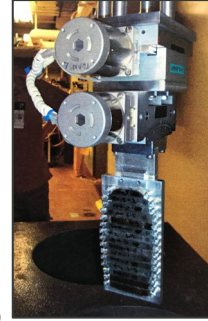
Magnetic susceptibility and heat capacity

- Two-stage transition $T_1=3.3$ K and $T_2=5$ K
- Can fit magnetic susceptibility to dimer models in interactions $J = -0.11$ meV



$\text{Cs}_2\text{Fe}_2(\text{MoO}_4)_3$: Neutron measurements on HB-2A, HFIR.

- Constant wavelength
- Germanium monochromator
 - $\sim 90^\circ$ take off angle for medium-high resolution
 - Variety of complex sample environments: 50mK, 6 Tesla, 2GPa pressure...
- Current detector is an array of 44 individual ^3He tubes
 - Low background
 - Covers $\sim 2\text{-}150^\circ$ in 2θ by scanning detector
 - **MIDAS detector upgrade coming soon!**



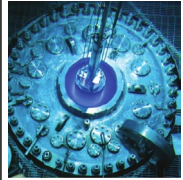
Ge(hkl)	λ (Å)	d_{max} (Å)	Q (Å $^{-1}$)	Flux (n/cm 2 s)
(113)	2.41	27.6	0.2-5.1	5×10^6
(115)	1.54	17.6	0.35-7.9	1×10^7
(117)	1.12	12.8	0.5-10.9	4×10^6



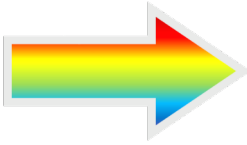
<https://neutrons.ornl.gov/powder>



A typical CS diffractometer (HFIR)



Reactor



Monochromator:

- selects λ .
- Control resolution.

Single wavelength



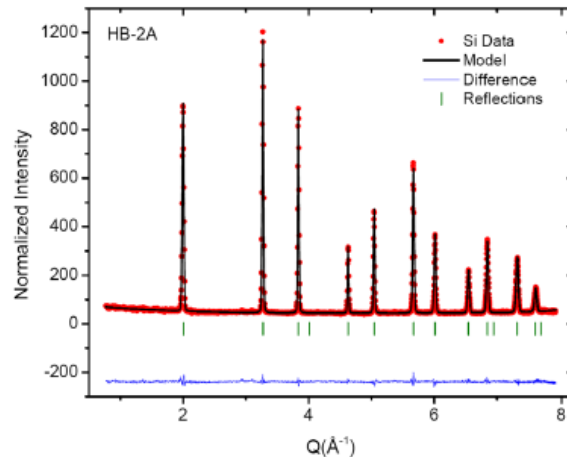
SAMPLE



Detector at 2θ measures single Q

$$\lambda = 2d \sin \theta$$

Q range limit is $4\pi/\lambda$



A typical TOF diffractometer (SNS)

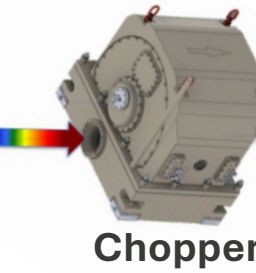
De Broglie wavelength: $\lambda = h/mv = ht/mL$

Bragg's law: $\lambda = 2d \sin \theta = \text{constant} * t$

Target



Moderator



Chopper

Multiple wavelengths



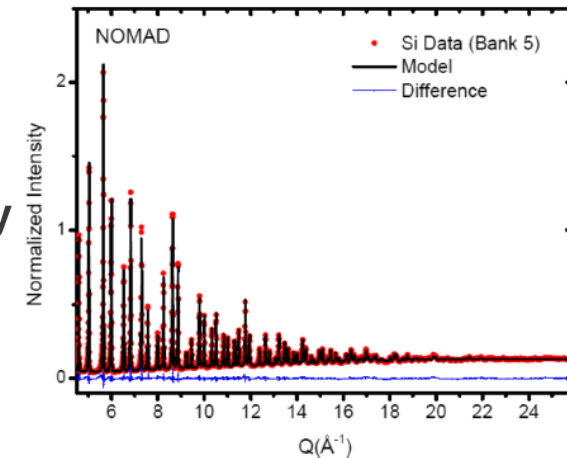
SAMPLE



Detector at 2θ measures multiple Q

Resolution depends on moderator and t, L, and 2θ

Q range determined by $\lambda_{\min}$, $\lambda_{\max}$ and 2θ



HB-2A instrument resolution and peak shape

MYRESOL.irf

This file is read only when Res≠0. The name of the file is stored in the character variable FILERES= MYRESOL.irf. All items are read in free format.

This options works, at present, only for constant wavelength type of data. The profile is assumed to be a Voigt function (Npr=7). 12 parameters or a table determine the resolution function. The parameters are $U_i, V_i, W_i, X_i, Y_i, Z_i$ ($i=1,2$ for λ_1 and λ_2)

The different types of functions are:

$$\text{Res}=1 \quad H_G^2 = (U_i \tan \theta + V_i) \tan \theta + W_i$$

$$H_L = X_i \tan \theta + \frac{Y_i}{\cos \theta} + Z_i$$

- Caglioti function describes reactor based diffractometers.
- U,V,W parameters in Fullprof.
- See paper by Hewat for definitions of U,V,W

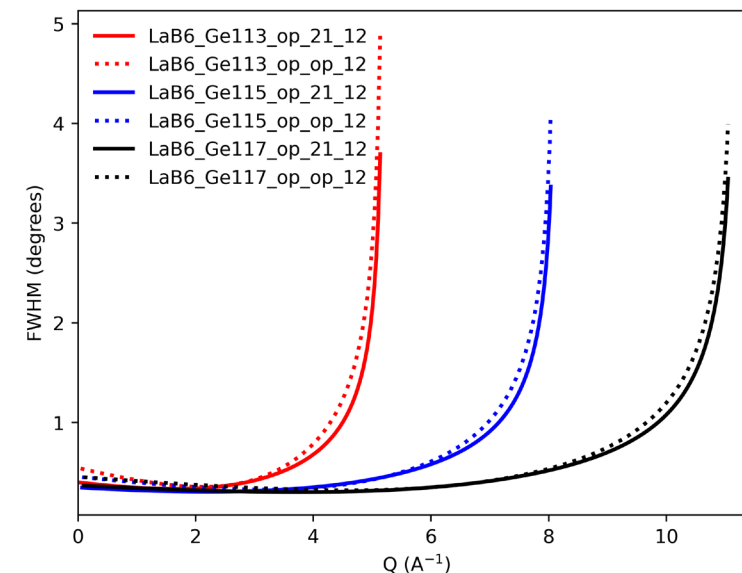
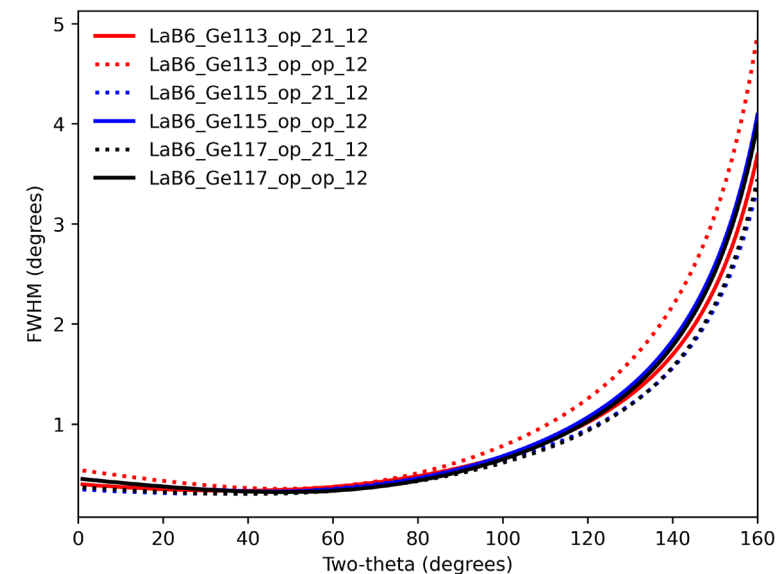
NUCLEAR INSTRUMENTS AND METHODS 127 (1975) 361-370; © NORTH-HOLLAND PUBLISHING CO.

DESIGN FOR A CONVENTIONAL HIGH-RESOLUTION NEUTRON POWDER DIFFRACTOMETER

A. W. HEWAT

Institut Laue-Langevin, B.P. N° 156, 38042-Grenoble Cédex, France

Received 14 April 1975



Details of this Mn-pyrazinecarboxylate example

Neutron powder diffraction data collected at HB2A, HFIR

$\lambda = 2.41 \text{ \AA}$. Collimation: open-open-21'

Data at 20K (**MnPyz_20K.dat**) and 1.5K (**MnPyz_1p5K.dat**)

Sample in a vanadium can

Instrument resolution file: **hb2a_resolution.irf**

Crystal structure: **MnPyz.cif**

 HB2A_Ge113

 MnPyz

 MnPyz_1p5K

 MnPyz_20K

 PhysRevMaterials.7.124408

Neutron data from HB-2A

Plot the 1.5 K and 20 K data using Winplotr

Take a difference

- Convert to Q. This is the best way to report data
 - “X space” > “Q-space”. Set all to 2.41

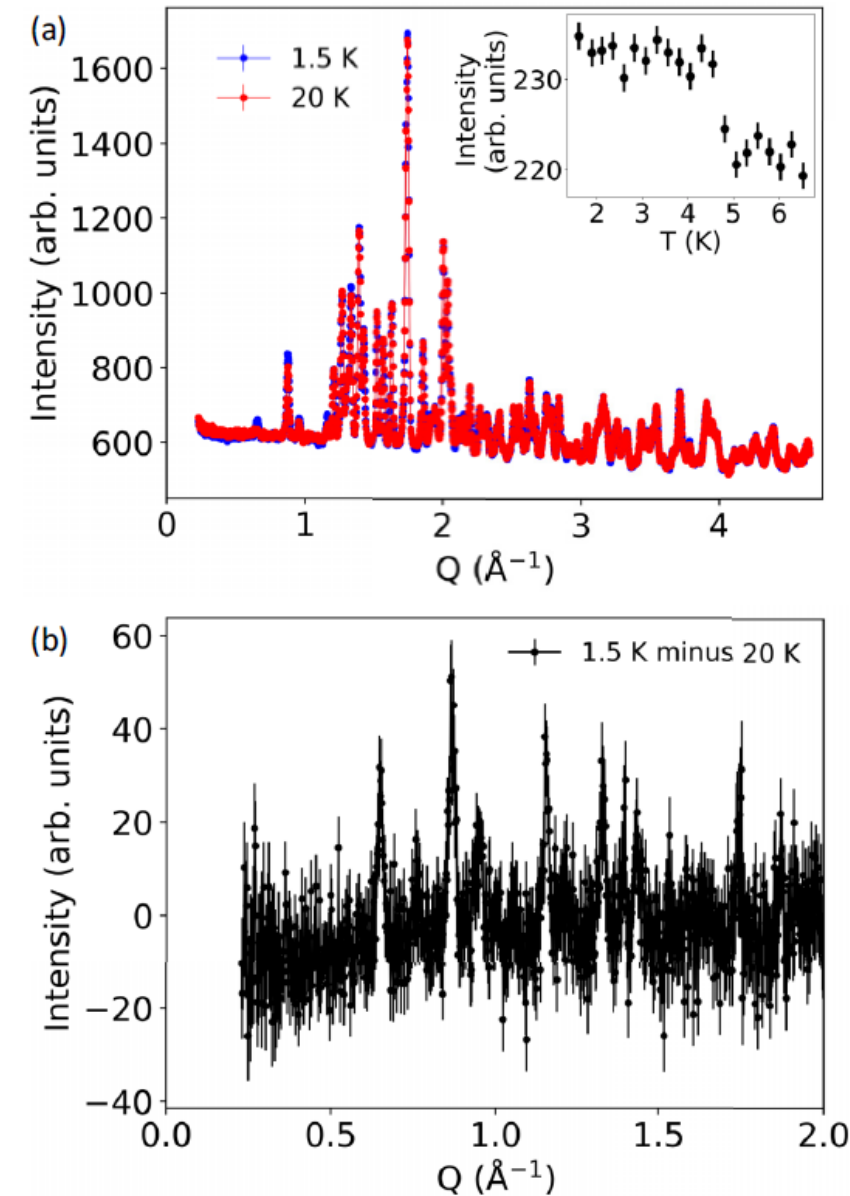
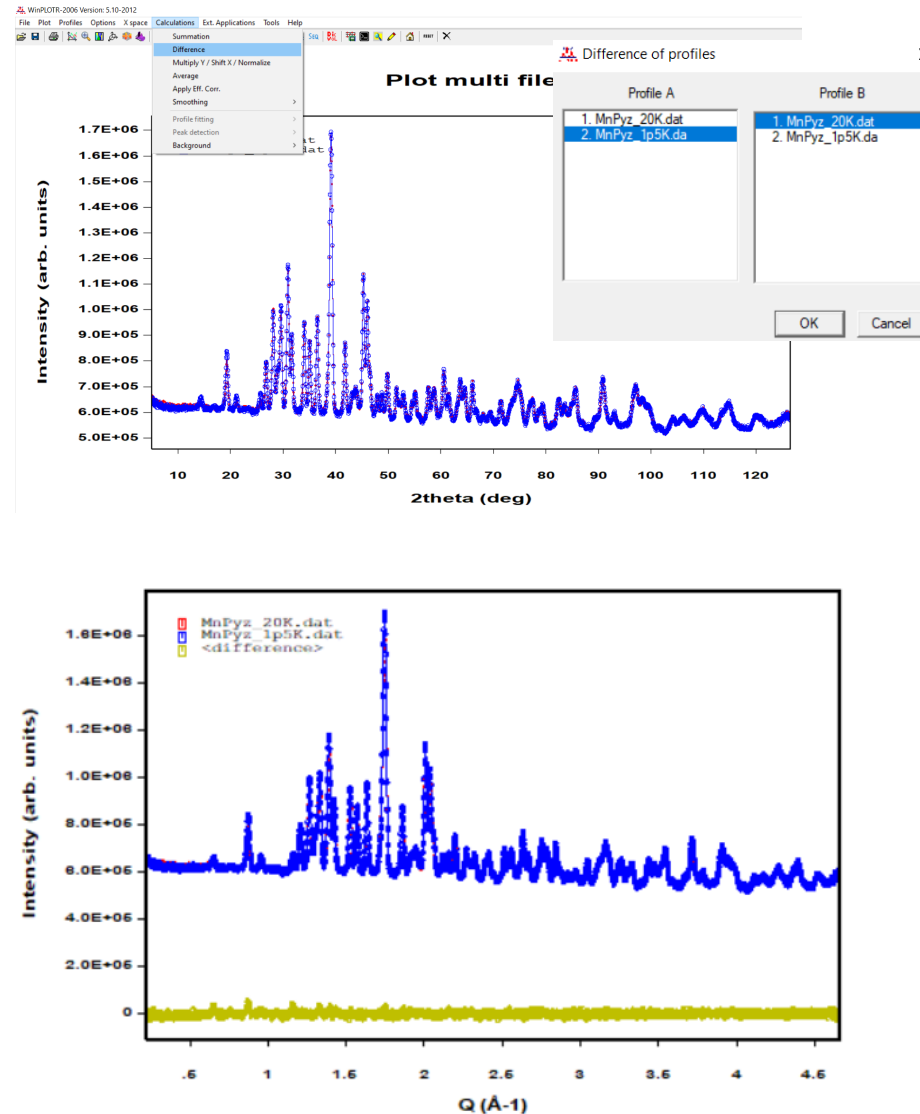


FIG. 5. (a) Neutron powder diffraction data collected at 1.5 K and 20 K. Inset: Intensity at $Q = 0.65 \text{ \AA}^{-1}$ as a function of temperature through the magnetic transition. (b) Difference of intensity at 1.5 K and 20 K in the powder diffraction data.

Mn-pyrazinecarboxylate

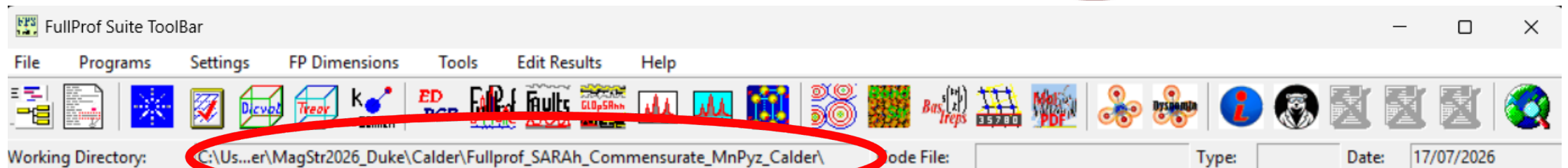
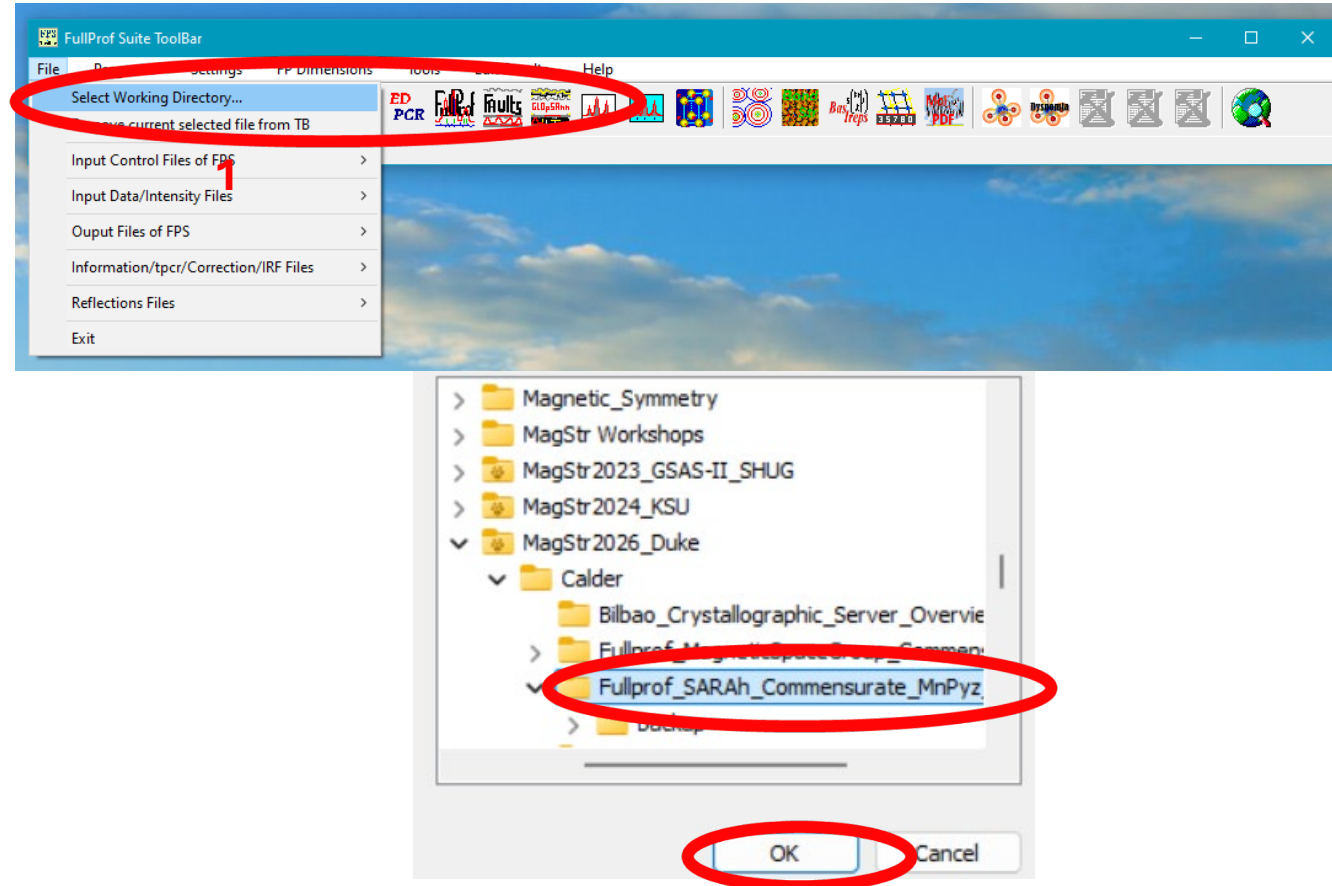
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- Step 5: Check the magnetic model

Step 1: Refine the crystal structure using FullProf

Open Fullprof Suite toolbar.

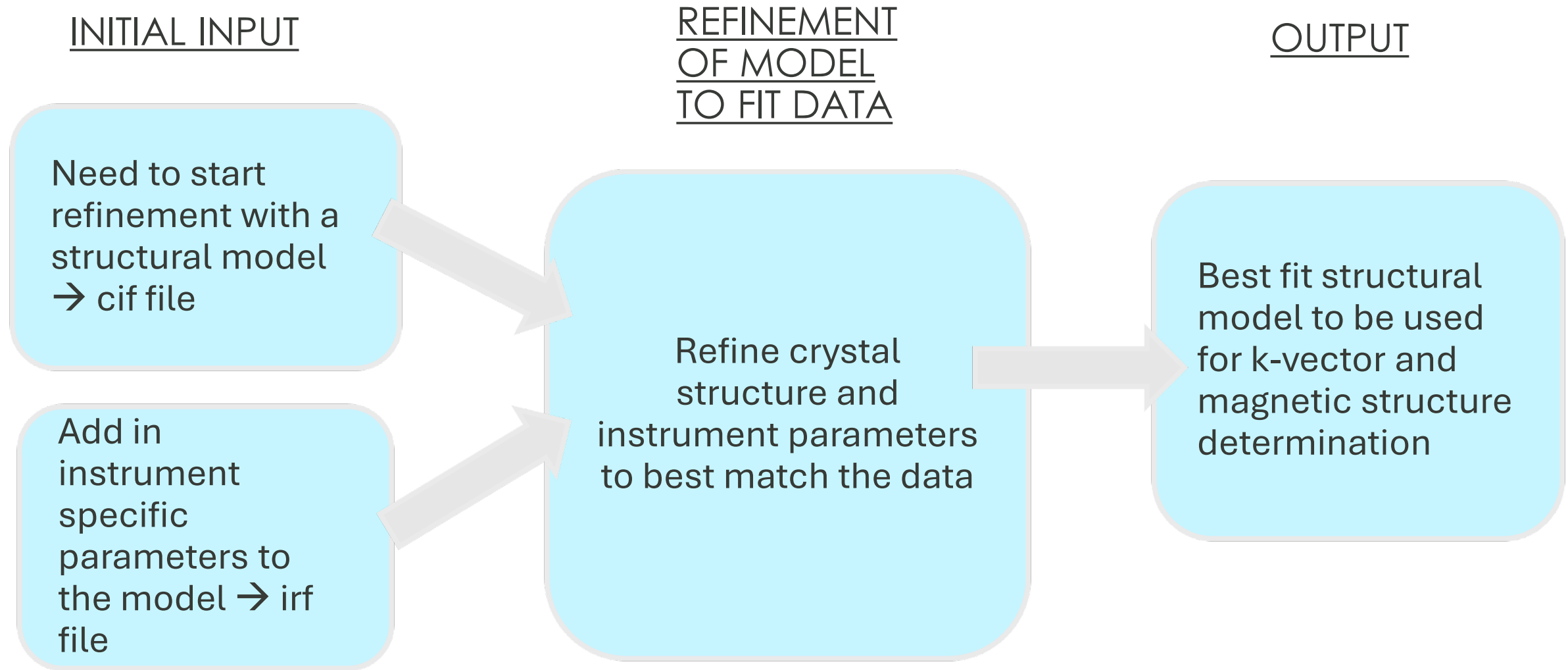
- **1.** Select working directory with data
“File>Select Working directory...”
- **2.** Browse to wherever your folder
“Fullprof_Commensurate_MnPyz_Calder” is located on your computer
and select “ok”
- **3.** Path on FP studio toolbar should
now be updated. This helps with
interacting with other features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



Step 1: Refining the crystal structure using Fullprof

- Need to start refinement with a structural model → cif file
- Add in instrument specific parameters to the model → irf file
- Get parameters close
- Then refine this model.

Step 1: Refining the crystal structure using Fullprof

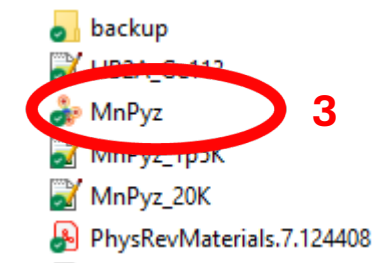
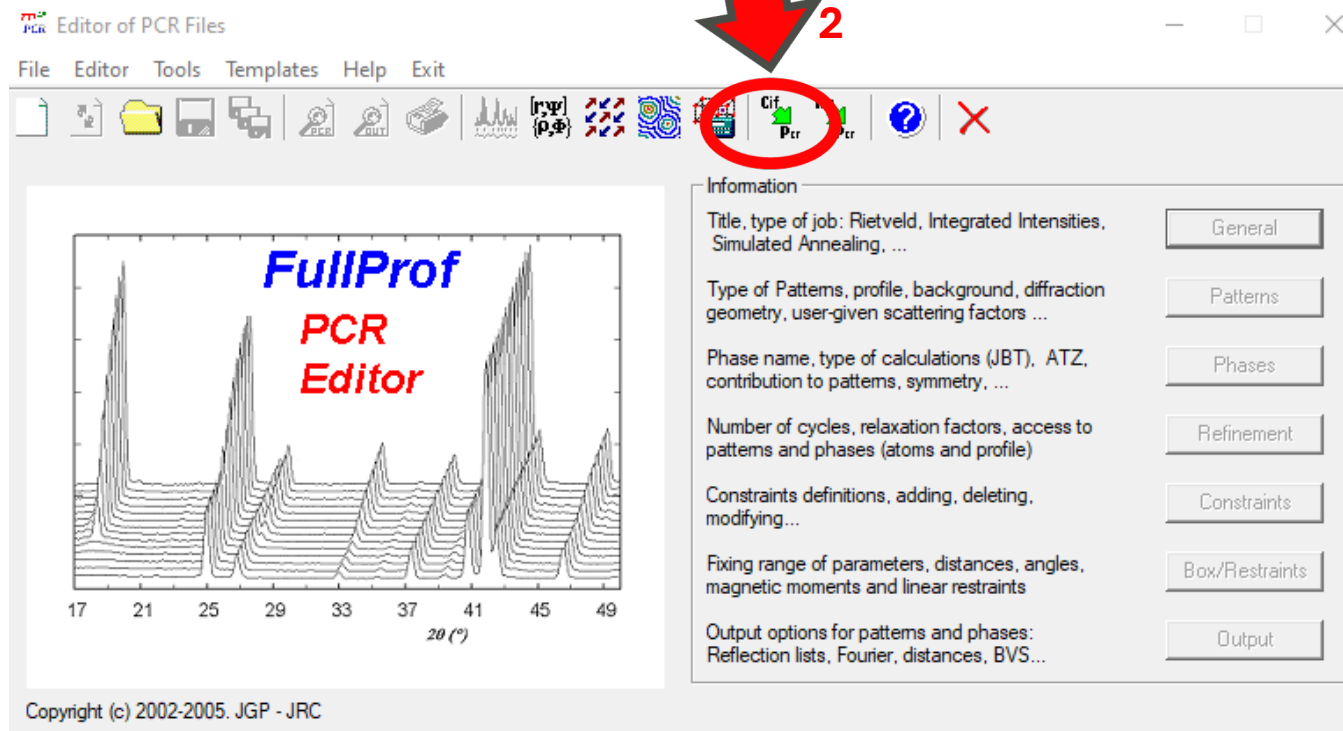
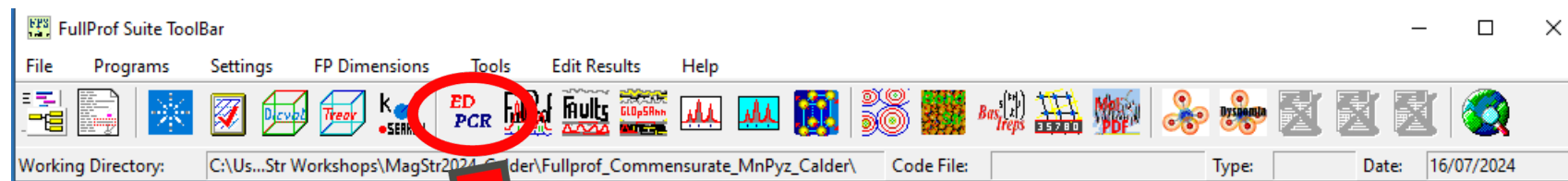


Step 1: Refine the crystal structure using FullProf

1. From FullProf Suite Toolbar open EdPCR.

2. Import crystallographic information file by clicking on “CIF→PCR”

3. Select the file “MnPyz_20K.cif”



Step 1: Refine the crystal structure using FullProf

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

1. Change “Type” to “Neutron” for constant wavelength

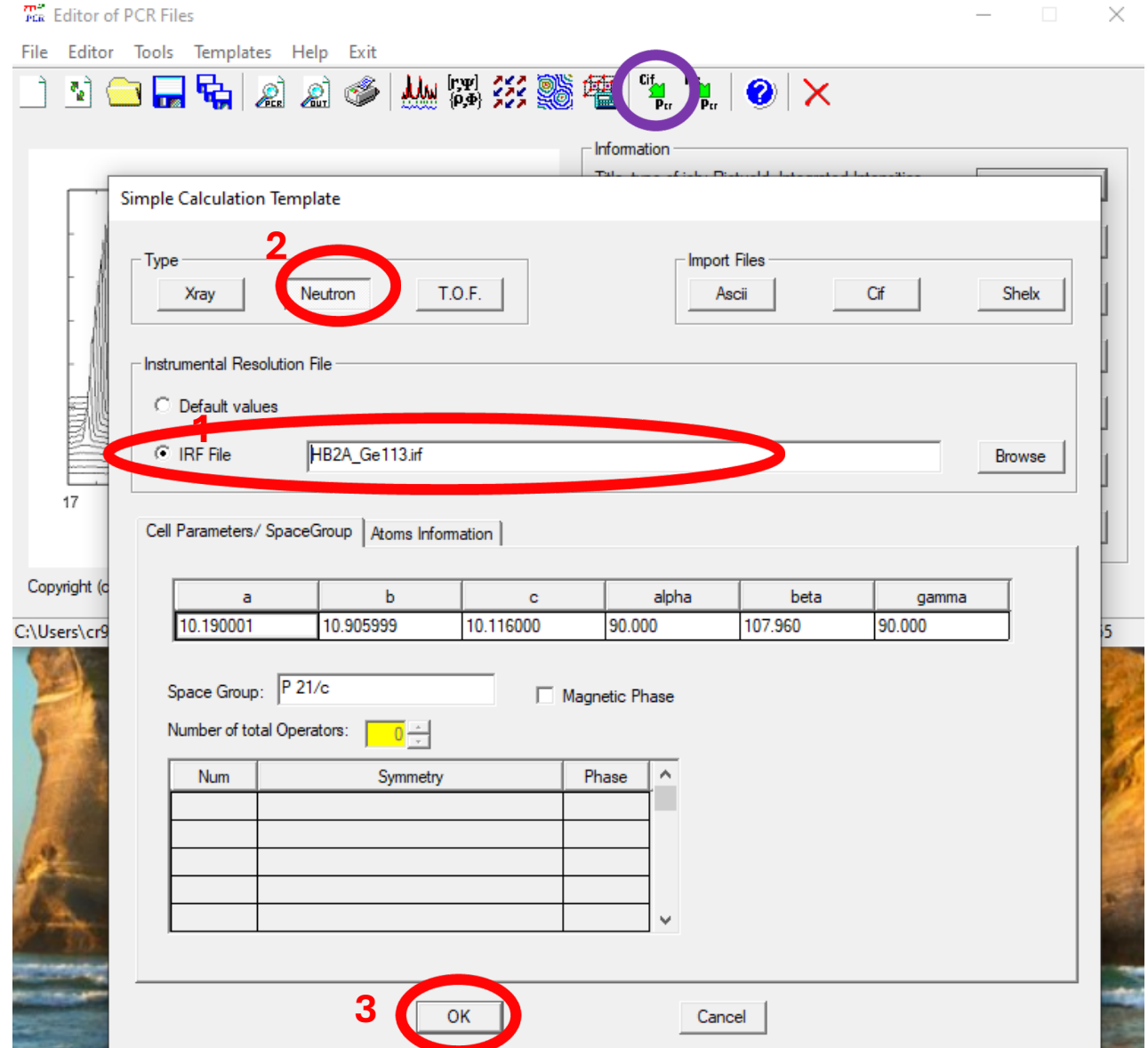
2. Load the instrument resolution file “HB2A_Ge113.irf”
(click circle and browse to file).

- *NOTE: remove the full path to just keep “HB2A_Ge113.irf”. If you don’t it could create problems later if you share file or change folders....*

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

Starting **Cell Parameters**, **Space Group** and **Atom Information** are now loaded.

Look in the tab “Atoms Information”

- Fullprof treats occupancies (Occ) in a particular way related to site multiplicities.
- **occ = site multip./general multip. Always check this has been correctly calculated after importing the .cif file.**
- In this case $\text{site}/\text{general} = 4/4 = 1$ for all atoms. So it looks straightforward. But make sure to check.

Hit “OK” to close the window

Simple Calculation Template

Type:

Import Files:

Instrumental Resolution File:
☒ Default values
☐ IRF File

Cell Parameters/ SpaceGroup **Atoms Information**

	Name	Type	X	Y	Z	B	Occ
Atom #1	Mn1	Mn	0.51009	0.13426	0.59800	0.30004	1.00000
Atom #2	O1	O	0.54100	0.24430	0.42660	0.30004	1.00000
Atom #3	N1	N	0.36060	0.29910	0.56210	0.30004	1.00000
Atom #4	C1	C	0.26270	0.32510	0.61920	0.30004	1.00000
Atom #5	H1	H	0.25464	0.27694	0.69194	0.30004	1.00000

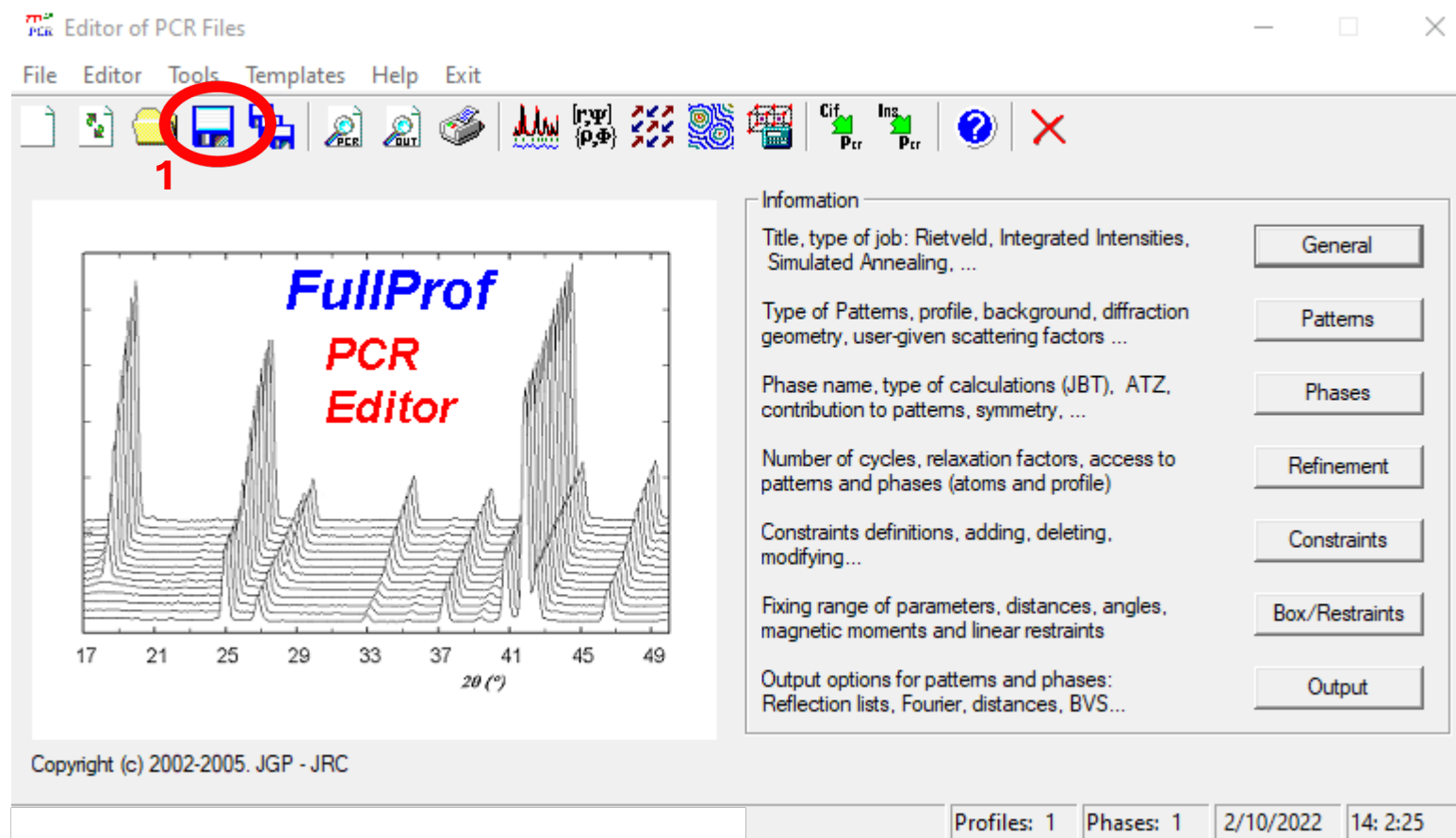
	Rx	Ry	Rz	lx	ly	lz	MPhase
Atom #1							
Atom #2							
Atom #3							
Atom #4							

When finished, hit OK

Step 1: Refine the crystal structure using FullProf

1. Save the changes.

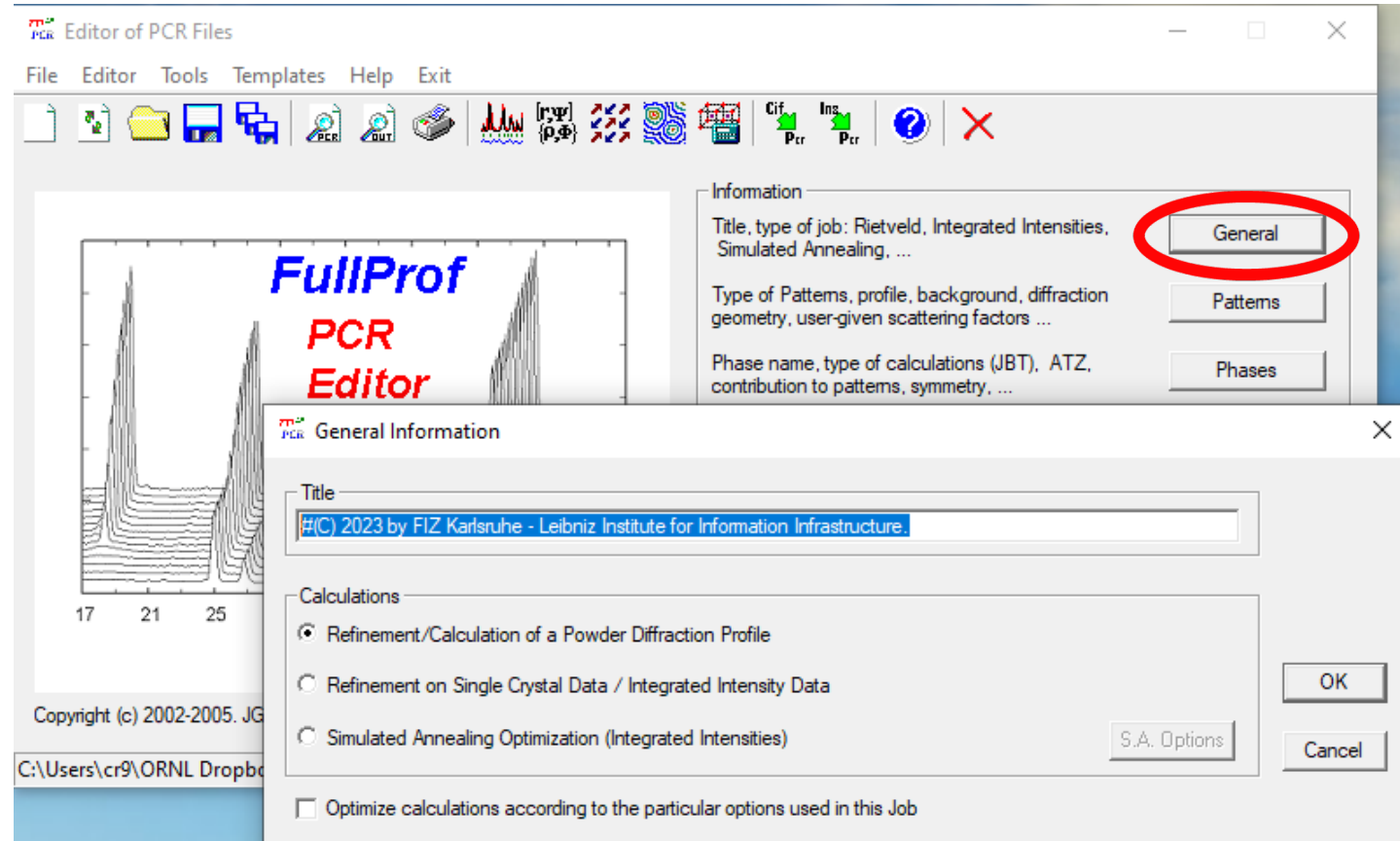
This should be done whenever changes are made in the GUI.



Step 1: Refine the crystal structure using FullProf

- “**General**” tab has refinement of powder data as default. This is what we’ll do in this example.
- Can edit title as wanted.

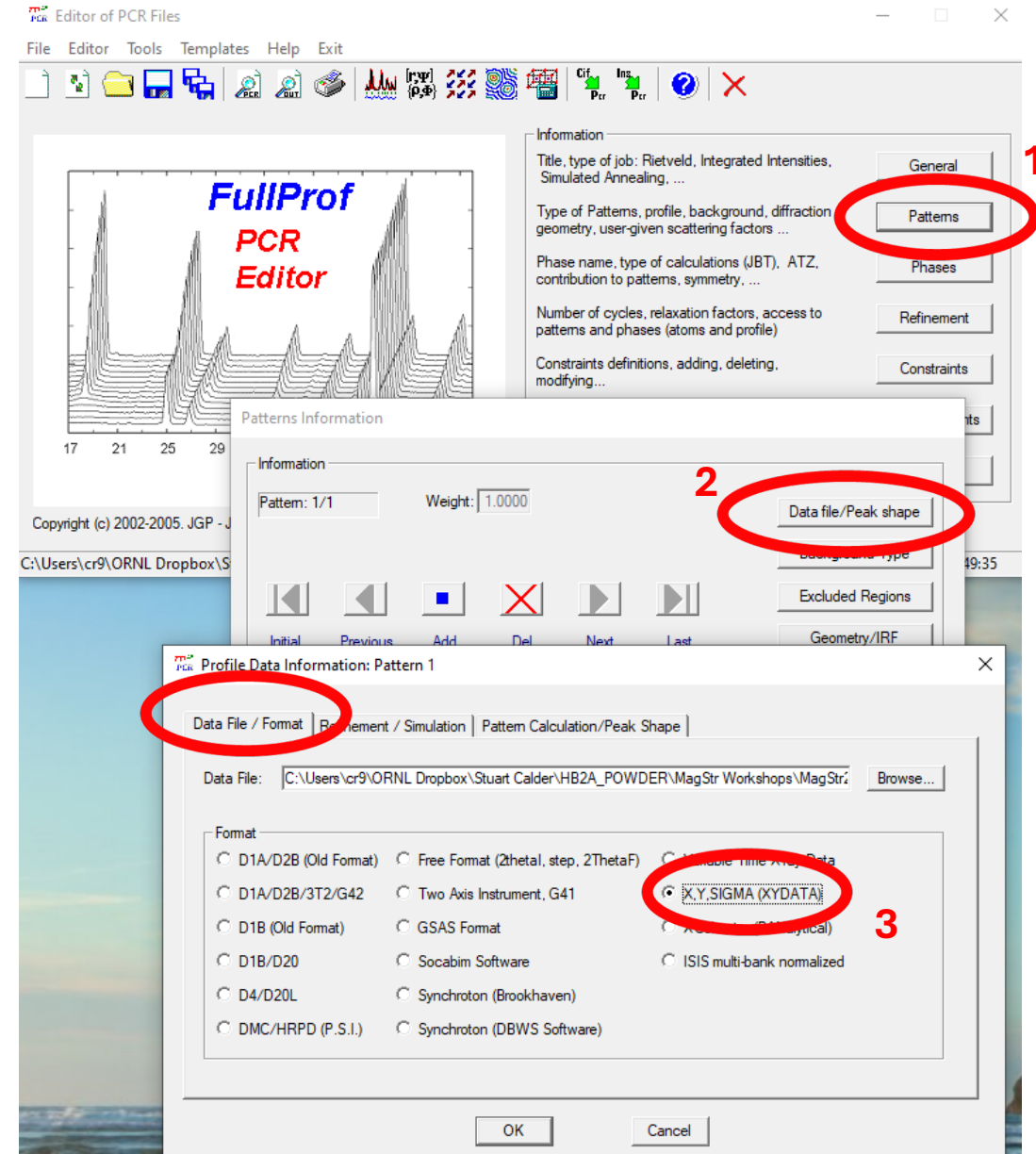
For powder refinements we don’t need to edit this tab



Step 1: Refine the crystal structure using FullProf

1. “Patterns” tab
2. Select the format of the data file Fullprof should refine.
3. Patterns → Data file/Peak Shape → X,Y,SIGMA (XYDATA)

Data format from HB-2A is simply three columns with two-theta, Intensity, Intensity Error

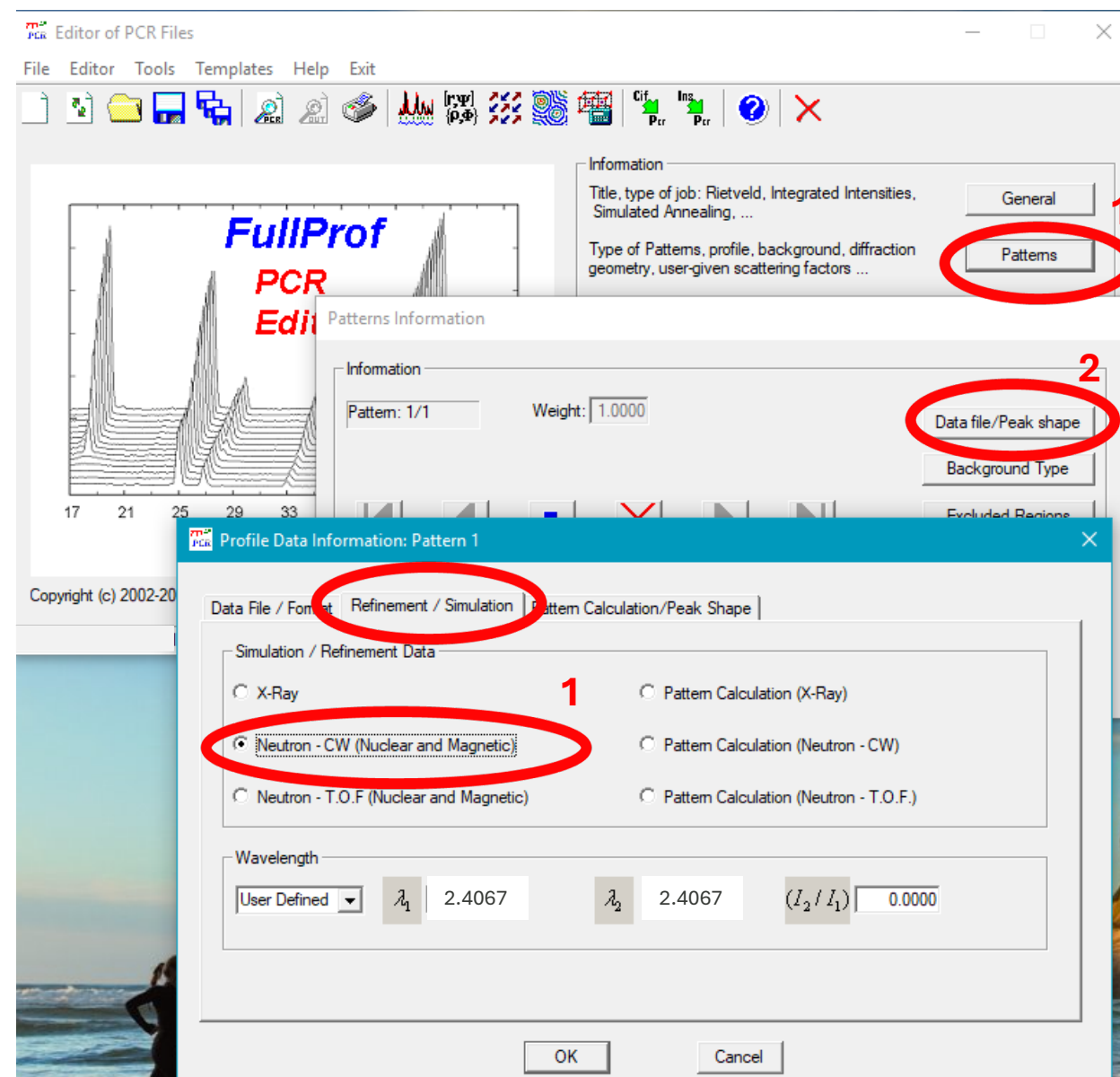


Step 1: Refine the crystal structure using FullProf

Patterns → Data file/Peak Shape
→ Refinement/Simulation

[1] Select Neutron – CW

Wavelength is already set by irf file,
2.4067 in this example.

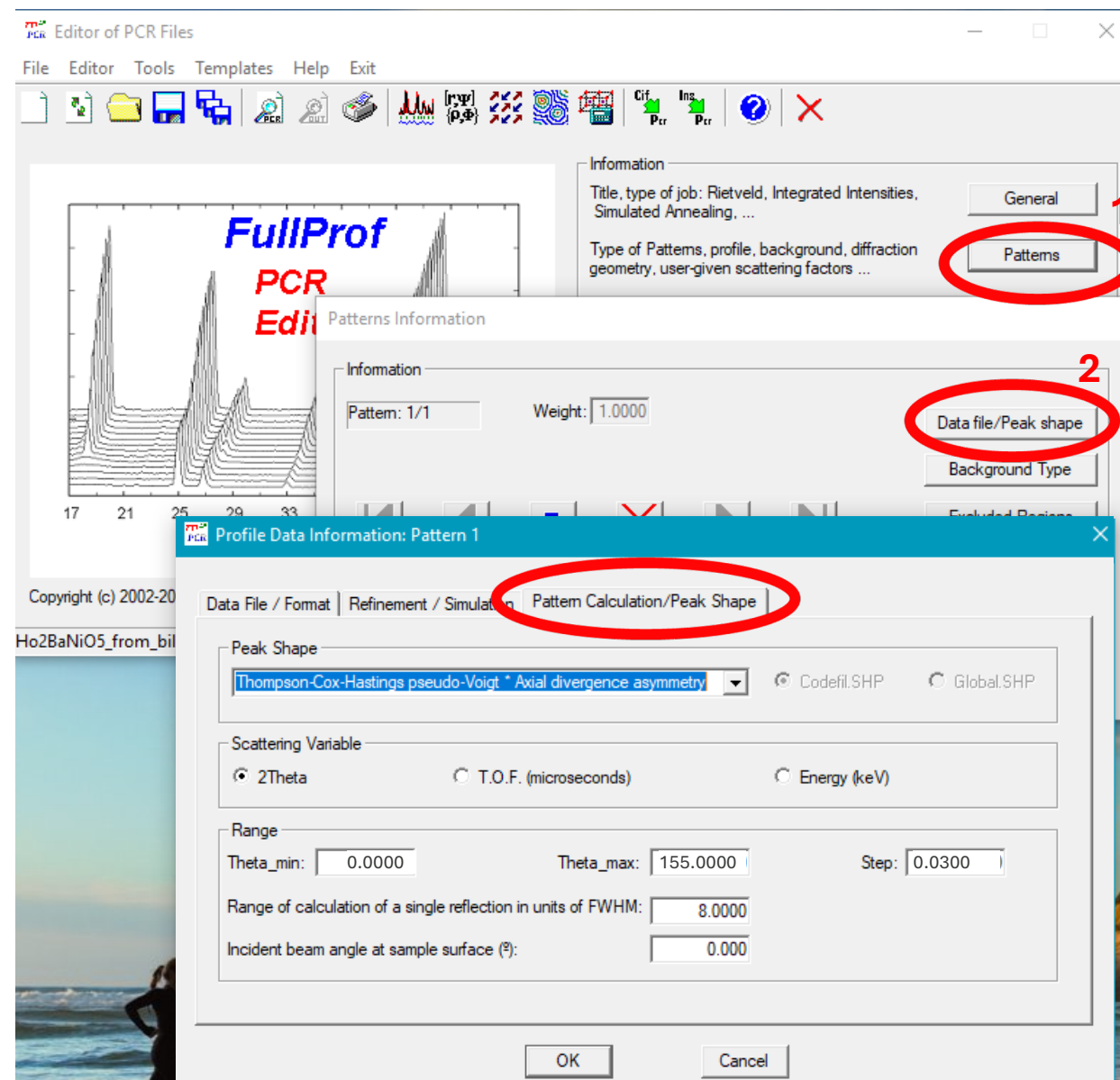


Step 1: Refine the crystal structure using FullProf

Check final tab:

Patterns → Data file/Peak Shape → Pattern Calculation/Peak Shape

Peak shape is already loaded correctly from irf file.



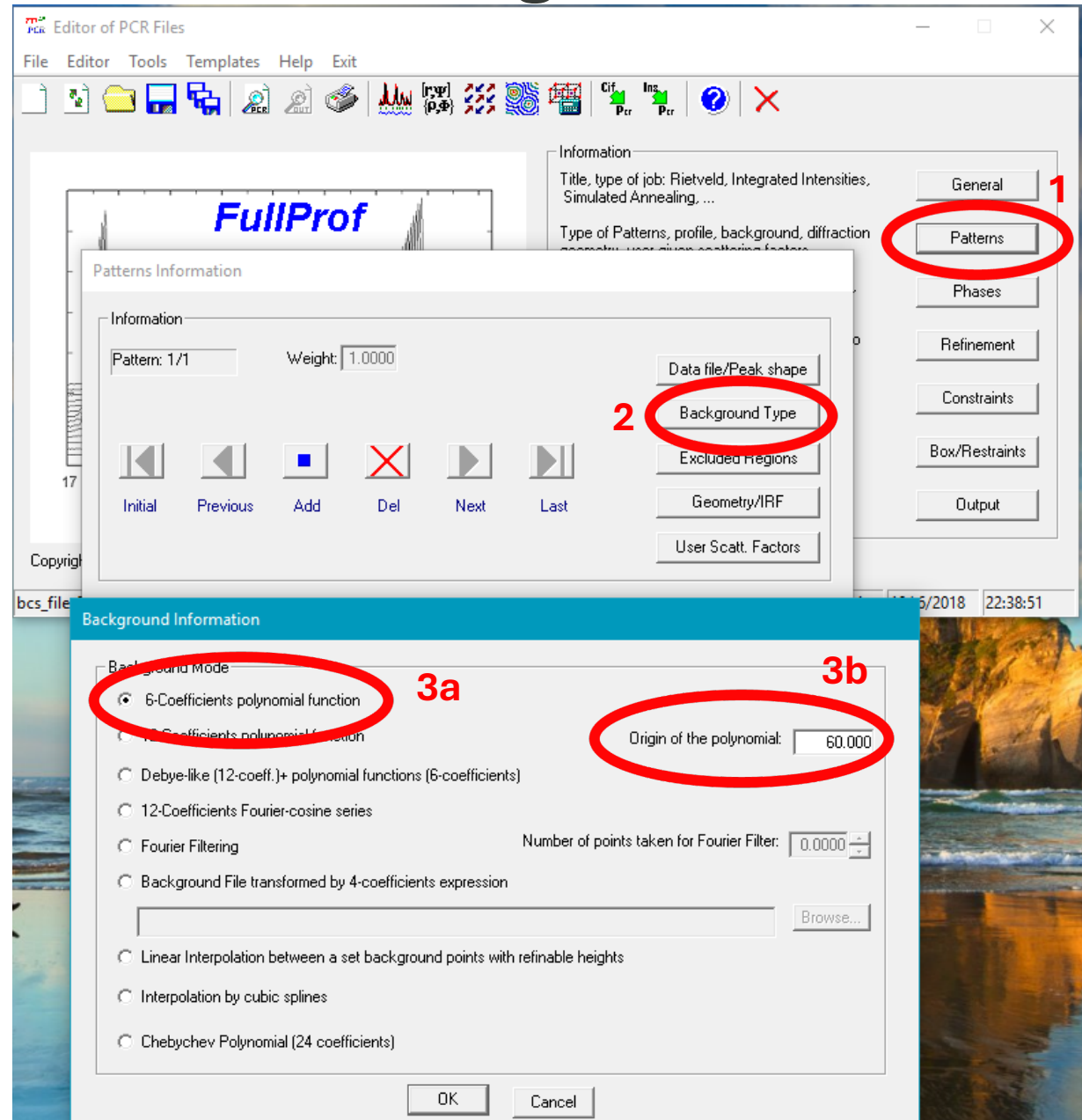
Step 1: Refine the crystal structure using FullProf

Move to next tab down to select background type

Patterns → Background Type Check “6-coefficient”

Put origin of polynomial at 60 for this example.

Background on HB-2A typically low and featureless so can be captured by simple function.



Step 1: Refine the crystal structure using FullProf

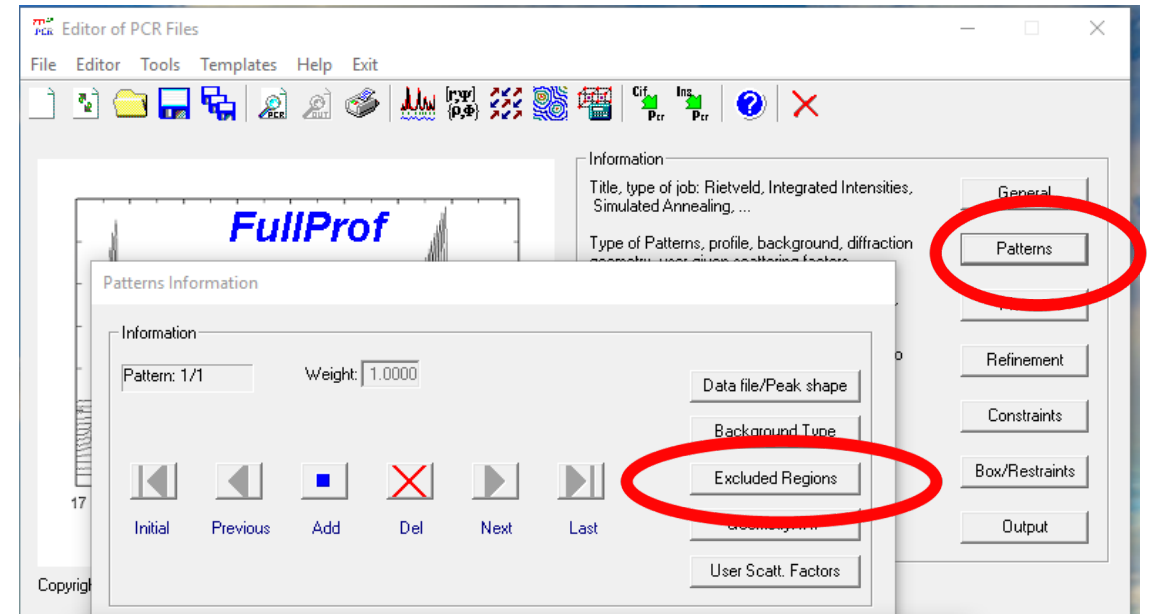
Exclude regions in the data?

We will not exclude any regions of the data

Use with care, but can cut out background.

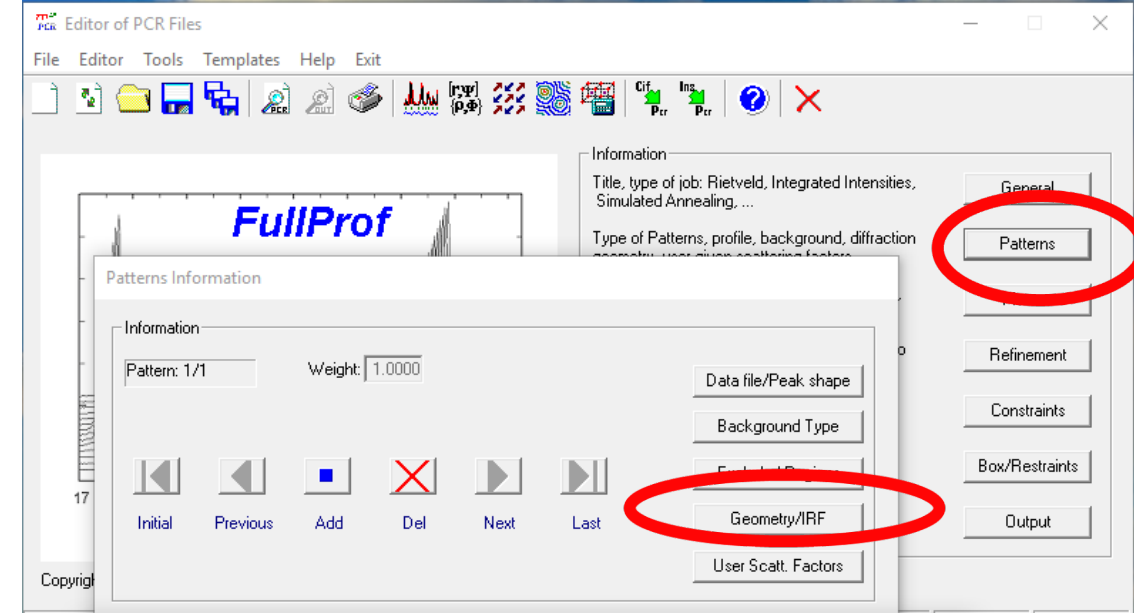
Allow focus of refinement on different regions, e.g. only low Q

Quick way to remove peaks from sample holder or can → but should try to fit these if possible!

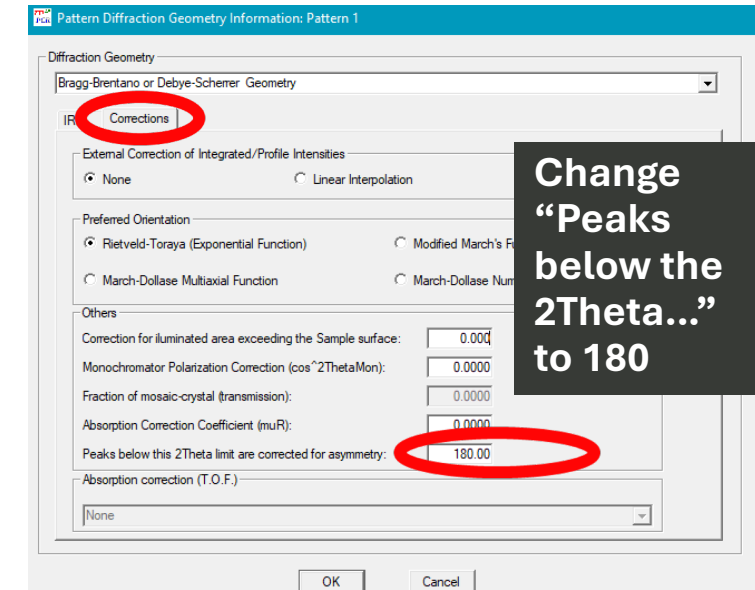
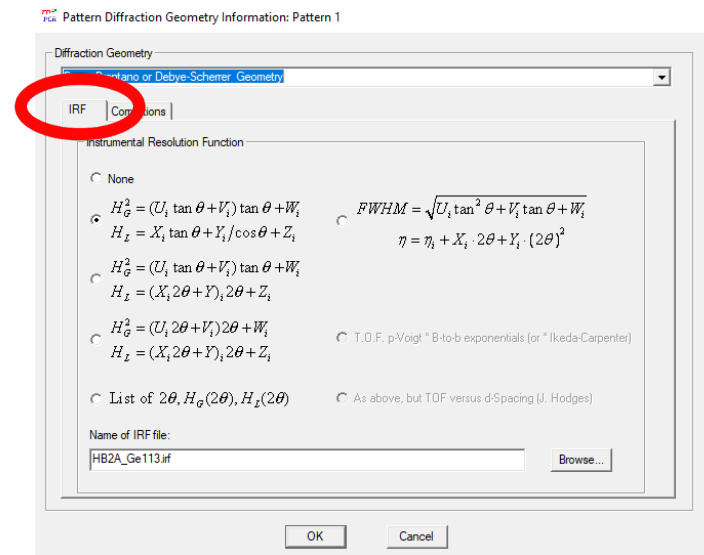


Step 1: Refine the crystal structure using FullProf

- Geometry/IRF
Populated by irf file.
- Corrections: the instrument layout gives asymmetric peaks, particularly at low angle. These can be corrected.
Change “Peaks below this 2Theta limit are corrected for asymmetry” to 180. Forgetting to do this, then refining the asymmetry parameters is a common error!



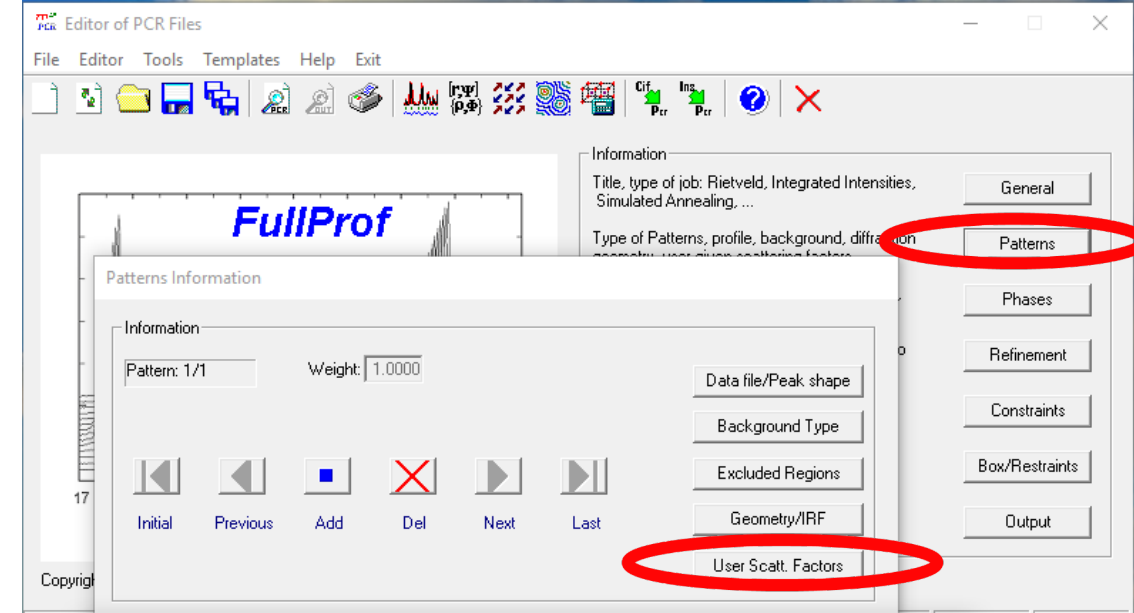
- Can correct for absorption if needed. “muR” is mu (absorption) multiplied by sample radius. Can find mu at NIST website
<https://www.ncnr.nist.gov/resources/activation/>



Step 1: Refine the crystal structure using FullProf

No further editing should be needed of the remaining “Patterns” tabs:

- User Scatt. Factors
This can be used to add e.g. a form factor that isn't tabulated



If the magnetic ion does not have form factor tables tabulated, or you want to test a non-standard form factor, this can be added here. One example would be for 5d ions, such as Ir, Os, etc.

Step 1: Refine the crystal structure using FullProf

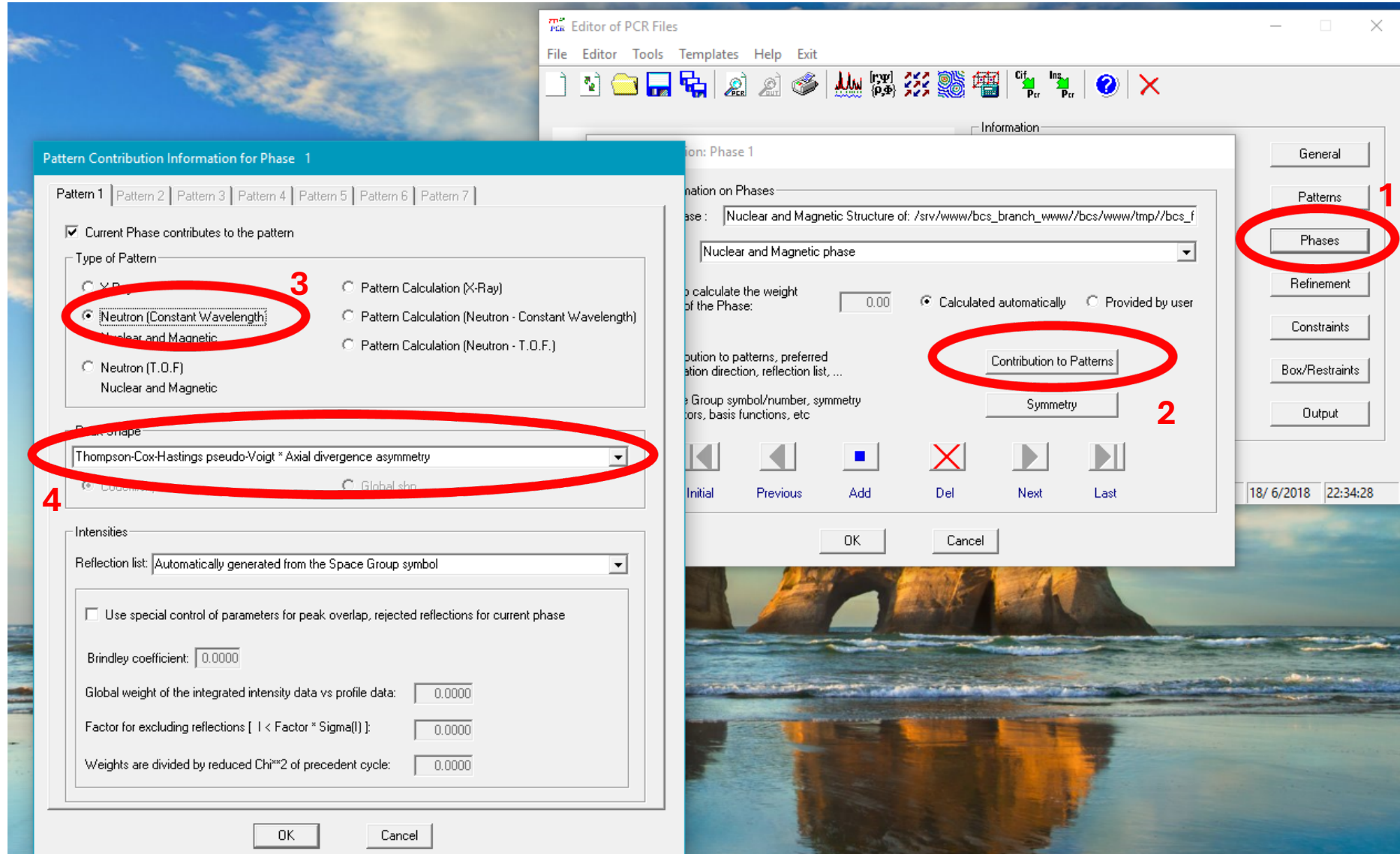
PHASES tab

Make phase contribute to refinement.

[1] Phases → [2] Contribution to Patterns → [3] Neutron (constant wavelength)

Set peak shape to “*Thompson-Cox-Hastings pseudo-Voigt*”

Can do a simulation or refinement with data. Select which one here.



Step 1: Refine the crystal structure using FullProf

REFINEMENT tab:

Setting starting values for refinements

Starting background value of 600000 (check data)

Editor of PCR Files

File Editor Tools Templates Help Exit

Information

Title, type of job: Rietveld, Integrated Intensities.

General

Patterns

Phases

Refinement

Constraints

Box/Restrains

Output

Refinement Information

Cycles of Refinement: 1

Stop Criterium of Coverage

Forced Termination when shifts < 0.02 x E.S.D.

Others: None

Relaxation Factors for Shifts

Atomic 1.00 Anisotropic 1.00 Profile 1.00 Global 1.00

Reflections ordering

☒ Only at the first cycle ☐ Each cycle

☐ Bragg R-Factor excluding reflections limiting excluded regions

Pattern 1 Pattern 2 Pattern 3 Pattern 4 Pattern 5 Pattern 6

Phase 1 Phase 2 Phase 3 Phase 4 Phase 5 Phase 6

Refinement weighting model

Background

Instrumental

Micro-Absorption

Factor of number of data points: 0

6 Coefficients Polynomial Background: Pattern 1

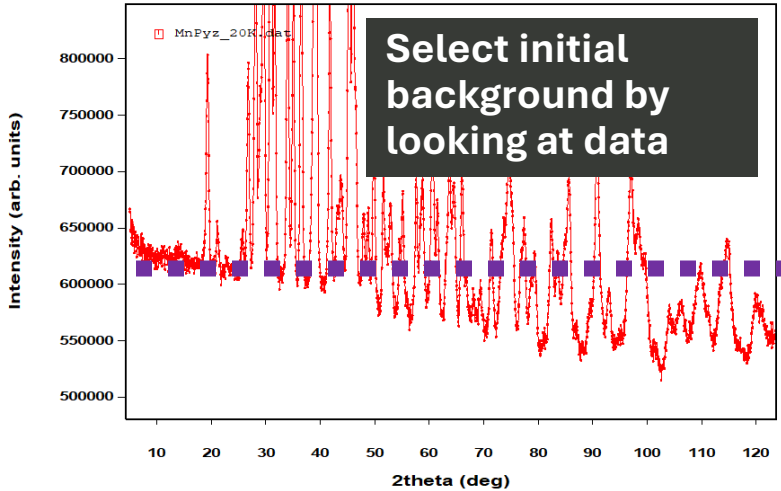
	d_0	d_1	d_2	d_3	d_4	d_5
Coefficients	600000	0.0000	0.0000	0.0000	0.0000	0.0000
	d_6	d_7	d_8	d_9	d_10	d_11
Coefficients						
	d_12	d_13	d_14	d_15	d_16	d_17
Coefficients						
	d_18	d_19	d_20	d_21	d_22	d_23
Coefficients						

Refine All

Fix All

Cancel

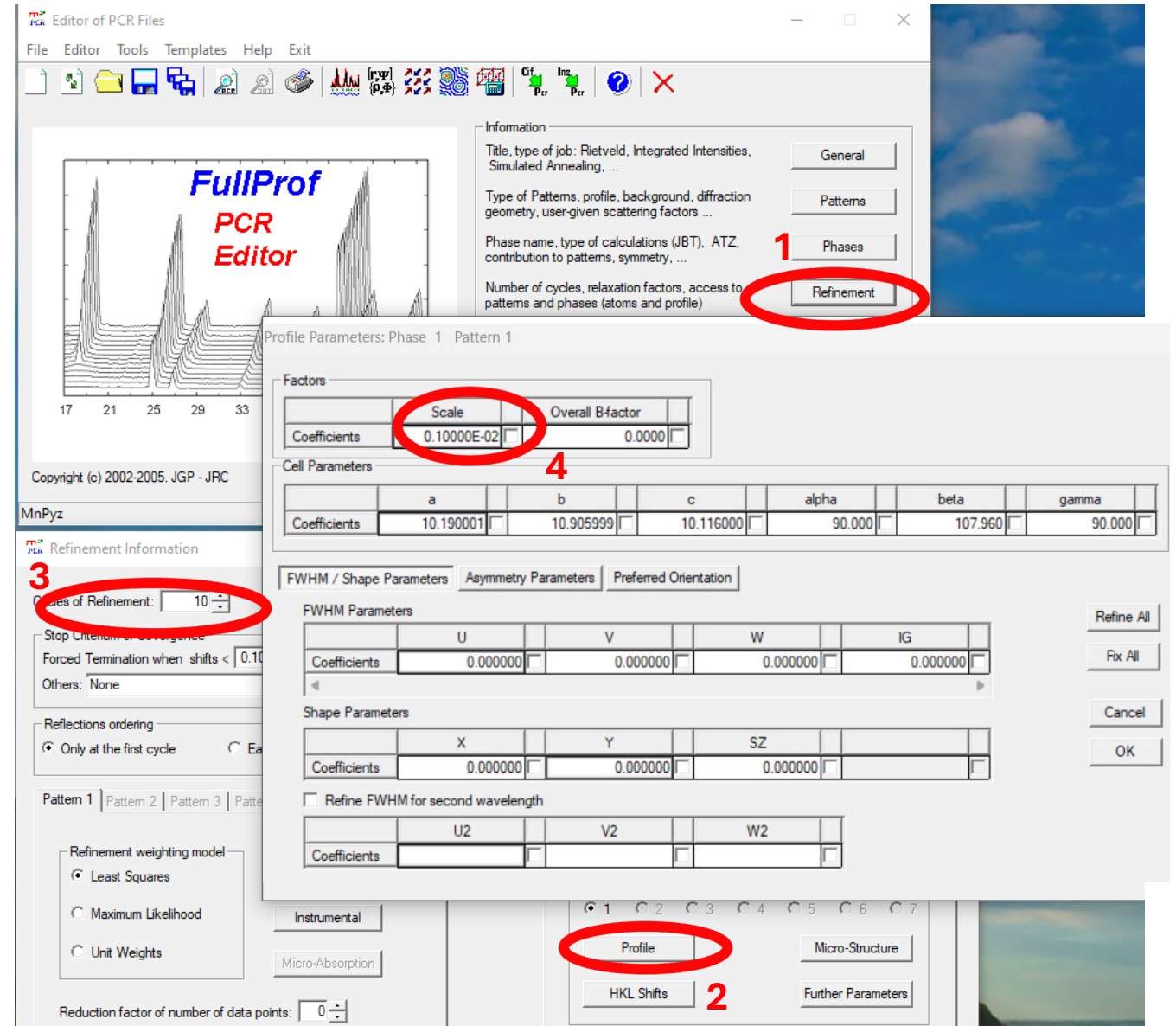
OK



Step 1: Refine the crystal structure using FullProf

1. Select “Refinement” tab again.
Update “Cycle of Refinement” to 10
2. From “Refinement” tab select:
Refinement>Profile
3. Change number of cycle refinement will run to 10
4. Scale is a default value
NOTE: You usually have to try different values by hand before refining (see next slides).

Notice U, V, W, X show zero.
BUT, the values are being read from the .irf file. So if we refine these then they add on to the irf values.



Crystal structure has been added. Instrument parameters added. We have checked background.

BEFORE setting anything to vary (refine), run the refinement with nothing refining.

This lets you see how close you are and if things have to be manually changed or if it is close enough to try a refinement

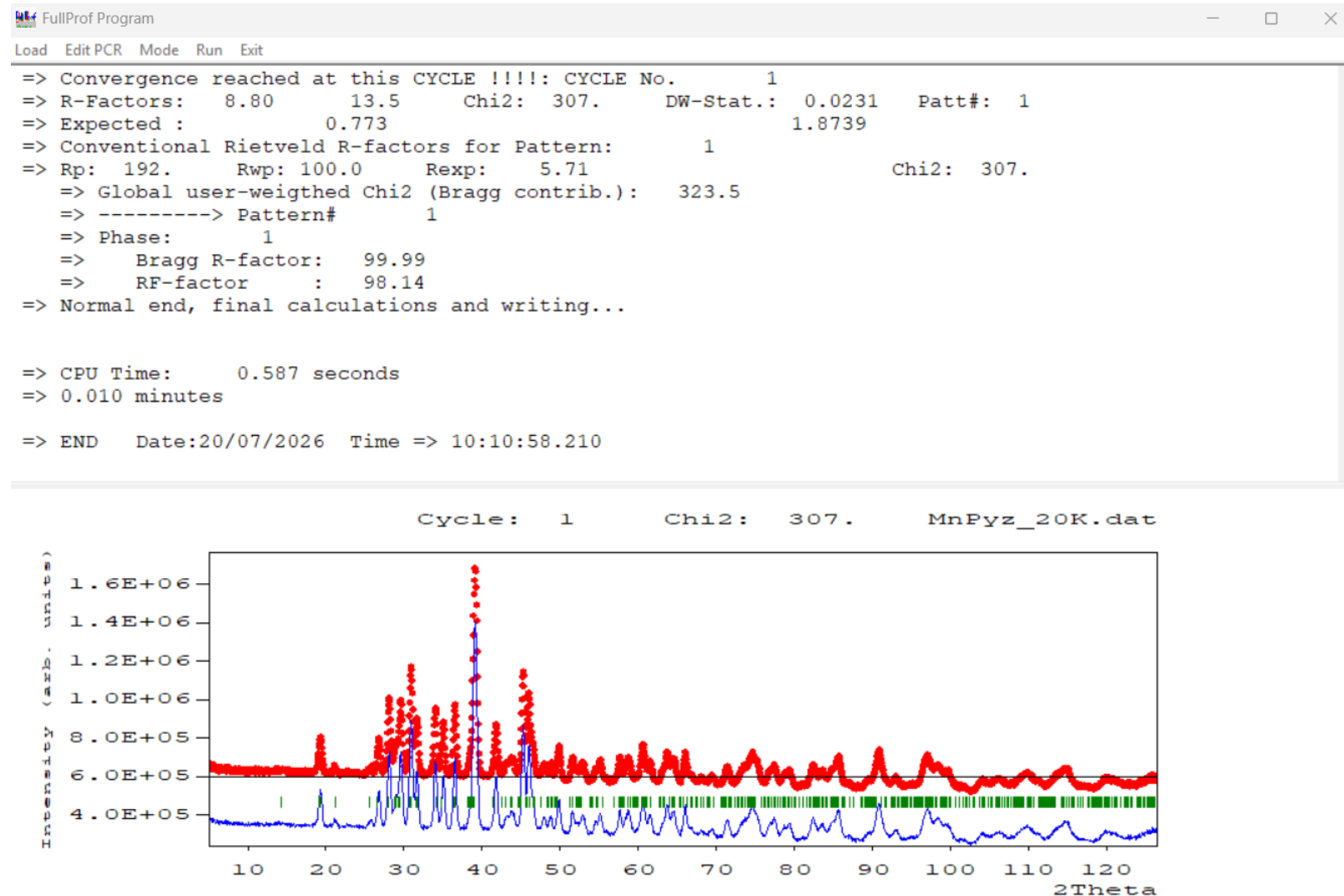
Step 1: Refine the crystal structure using FullProf

The model just shows a flat line.

This indicates the scale is not correct.

The default scale is 0.1×10^{-2} , which is too low for the data scale we have.

Increase this manually to get it close to the data.



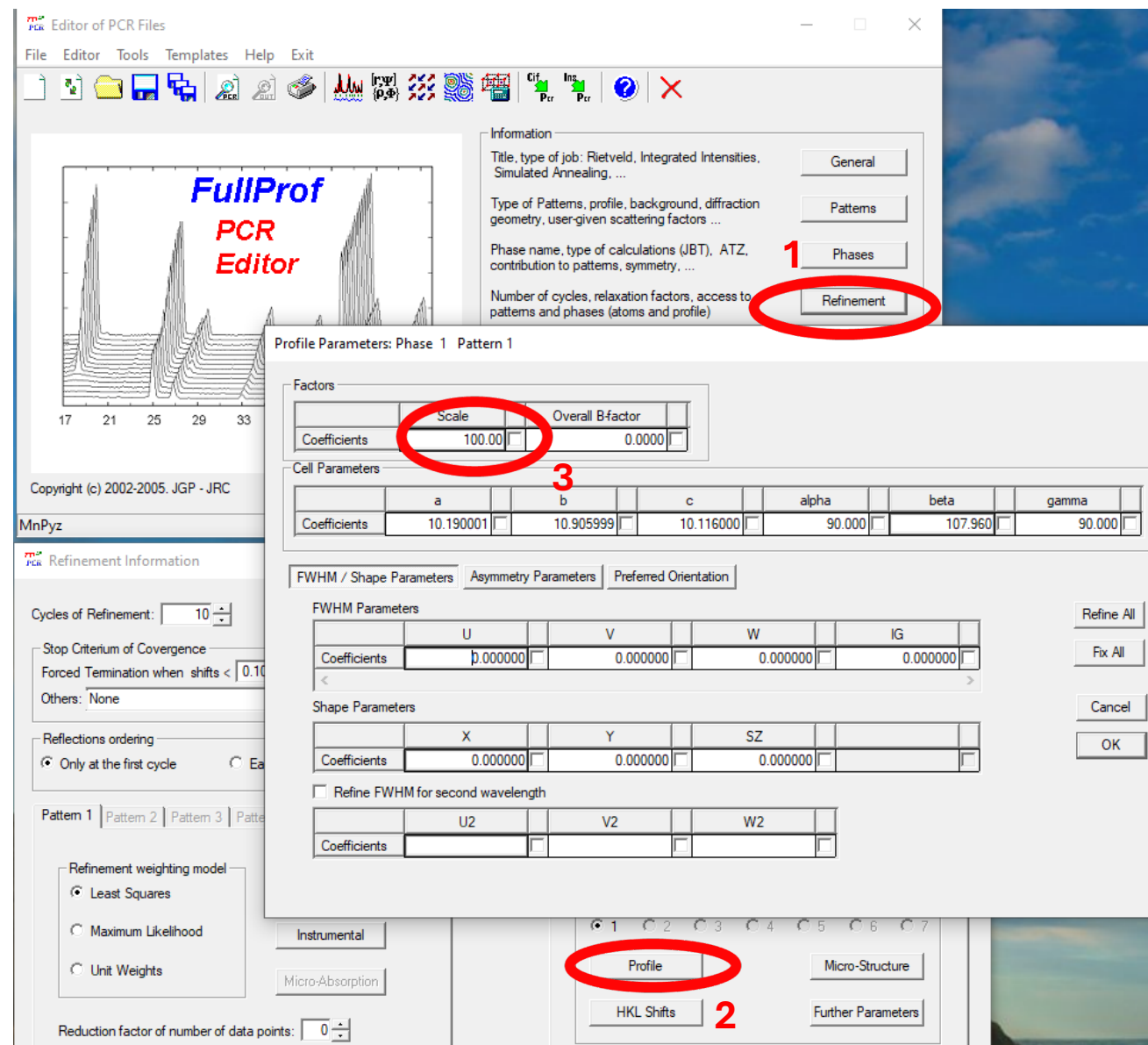
Step 1: Refine the crystal structure using FullProf

1. Select “Refinement” tab again.
Update “Cycle of Refinement” to 10

2. From “Refinement” tab select:
Refinement>Profile

3. Change scale to **100.0**

NOTE: This is a guess, you may have to try different values by hand before refining.



**Re-run refinement, again with
nothing refining**

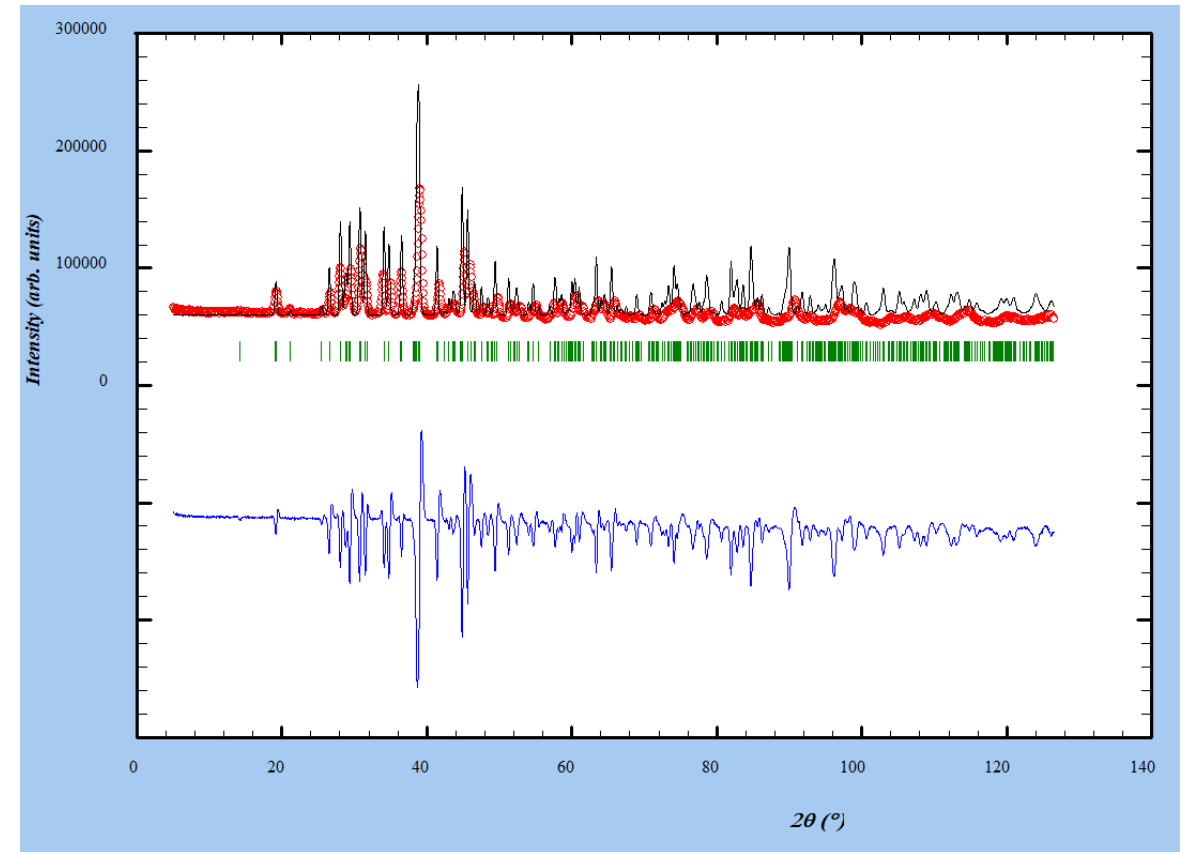
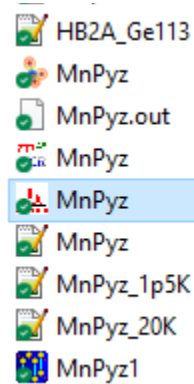
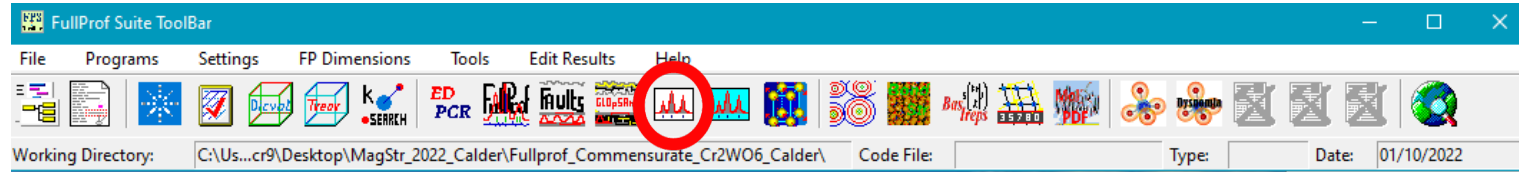
Step 1: Refine the crystal structure using FullProf

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: Always refine lattice constants before peak shape parameters.



The model and the data look “close enough” to start refining. We can now turn of parameters to refine to try to get the model and data to match.

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*)

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
Coefficients	100.00 ☒
	Overall B-factor
	0.0000 ☐

Cell Parameters											
	a		b		c		alpha		beta		gamma
Coefficients	10.190001 ☒		10.905999 ☒		10.116000 ☒		90.000 ☐		107.960 ☒		90.000 ☐

FWHM / Shape Parameters Asymmetry Parameters Preferred Orientation

FWHM Parameters							
	U		V		W		IG
Coefficients	0.000000 ☐		0.000000 ☐		0.000000 ☐		0.000000 ☐

< >

Shape Parameters

Refine All Fix All Cancel

6 Coefficients Polynomial Background: Pattern 1

	d_0		d_1		d_2		d_3		d_4		d_5
Coefficients	0.60000E+06 ☒		0.0000 ☒		0.0000 ☒		0.0000 ☒		0.0000 ☒		0.0000 ☒

	d_6		d_7		d_8		d_9		d_10		d_11

Refine All Fix All

Instrumental Parameters Refinement: Pattern 1

2_Theta							
	Zero		Displacement		Transparency		Wavelength
Coefficients	0.000000 ☒		0.000000 ☐		0.000000 ☐		0.000000 ☐

Refine All Fix All Cancel OK

```

PCr Editor of PCR Files
File Editor Tools Templates Help Exit


=====
! COMM # =
! Current global chi2 (Bragg contrib.) = 31.11
! Files => DAT-file: MnPyZ_20K.dat, PCR-file: MnPyZ
! Job Npr Nph Nba Nex Nsc Nor Dum Iwg Ilo Ias Res Ste Nre Cry Uni Cor Opt Aut
! 1 7 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 1
!
! Resolution file for Pattern# 1
HB2A_Gel13.irf
!Ipr Ppl Ioc Mat Pcr Ls1 Ls2 Ls3 NLI Prf Ins Rpa Sym Hk1 Fou Sho Ana
! 0 0 1 0 1 0 1 0 4 0 0 3 10 0 0 0 0 0 0 0 0 0
!
! Lambda1 Lambda2 Ratio Bkpos wdt Cthm muR Asylin Rpolarz 2nd-muR -> Patt# 1
! 2.406700 2.406700 0.00000 60.000 8.000 0.0000 0.0000 180.00 0.0000 0.0000
!
! NCY Eps Rat R_an R_pr R_g1 Thmin Step Thmax PSD Sent0
! 10 0.10 1.00 1.00 1.00 1.00 5.0250 0.050015 126.5250 0.000 0.000
!
! 12 !Number of refined parameters
!
! Zero Code Syscos Code Sysin Code Lambda Code MORE ->Patt# 1
! 0.01378 21.0 0.00000 0.0 0.00000 0.0 0.00000 0.00 0
! Background coefficients/codes for Pattern# 1 (Polynomial of 6th degree)
! 584587.750 -135909.203 -14207.162 182859.891 8940.036 -96032.844
! 31.00 41.00 51.00 61.00 71.00 81.00
!
! Data for PHASE number: 1 ==> Current R_bragg for Pattern# 1: 19.5855
!
=====
! Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nvk Npr More
! 25 0 0 0.0 0.0 1.0 0 0 0 0 0 1204.481 0 7 0
!
! P 21/c <-Space group symbol
! Atom Typ X Y Z Occ In Fin N_t Spc /Codes
Mn1 Mn 0.51009 0.13426 0.59800 0.30004 1.00000 0 0 0 0
O1 O 0.54100 0.24430 0.42660 0.30004 1.00000 0 0 0 0
N1 N 0.36060 0.29910 0.56210 0.30004 1.00000 0 0 0 0
C1 C 0.26270 0.32510 0.61920 0.30004 1.00000 0 0 0 0
H1 H 0.25464 0.27694 0.69194 0.30004 1.00000 0 0 0 0
O2 O 0.47520 0.40590 0.28730 0.30004 1.00000 0 0 0 0
N2 N 0.18020 0.49590 0.47280 0.30004 1.00000 0 0 0 0
C2 C 0.17310 0.42150 0.57380 0.30004 1.00000 0 0 0 0
H2 H 0.10500 0.43484 0.61546 0.30004 1.00000 0 0 0 0
O3 O 0.63290 -0.00920 0.53350 0.30004 1.00000 0 0 0 0
N3 N 0.73810 0.17610 0.70060 0.30004 1.00000 0 0 0 0
C3 C 0.27770 0.46870 0.41470 0.30004 1.00000 0 0 0 0
H3 H 0.28565 0.51737 0.34234 0.30004 1.00000 0 0 0 0
O4 O 0.82480 -0.03300 0.47500 0.30004 1.00000 0 0 0 0
N4 N 1.01820 0.23410 0.76740 0.30004 1.00000 0 0 0 0
C4 C 0.36700 0.37170 0.45740 0.30004 1.00000 0 0 0 0
C5 C 0.47140 0.33830 0.38550 0.30004 1.00000 0 0 0 0
C6 C 0.79600 0.26280 0.79250 0.30004 1.00000 0 0 0 0
H4 H 0.74254 0.30429 0.83748 0.30004 1.00000 0 0 0 0
C7 C 0.93330 0.29250 0.82250 0.30004 1.00000 0 0 0 0
H5 H 0.96819 0.35627 0.88409 0.30004 1.00000 0 0 0 0
C8 C 0.96040 0.14490 0.67680 0.30004 1.00000 0 0 0 0
H6 H 1.01539 0.10104 0.63560 0.30004 1.00000 0 0 0 0
C9 C 0.82300 0.11600 0.64300 0.30004 1.00000 0 0 0 0
ClO C 0.75810 0.01520 0.54080 0.30004 1.00000 0 0 0 0
!
!-----> Profile Parameters for Pattern # 1 ----- Phase # 1
! Scale Shap1 Str2 Str3 Strain-Model
! 49.82266 0.00000 0.00000 0.00000 0.00000 0.00000 0
! 91.00000 0.000 0.000 0.000 0.000 0.000
!
! U V W X Y GauSiz LorzSiz Size-Model
! 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0
! 0.00 0.00 alpha beta gamma # Cell Info
! 10.184688 10.811492 10.090220 90.000000 108.429535 90.000000
! 11.00000 101.00000 111.00000 0.00000 121.00000 0.00000
! Pref1 Pref2 Asy1 Asy2 Asy3 Asy4 S.L D.L
! 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
! 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
! 101.00000 101.00000 101.00000 101.00000 101.00000 101.00000 101.00000 101.00000

```

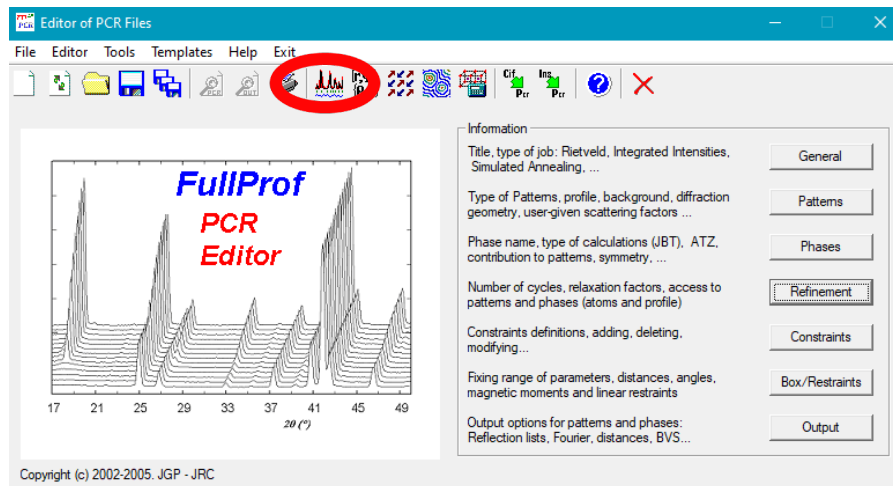
Open text with 1. [pcr and magnifying glass].

Can quickly see and edit various things quicker than with GUI

- Anything refining has a number that ends in a 1 (e.g. 11, 21, 31, 811, 641, etc)
- The scale has a 91, so is refining.

To turn on any to refine can type a 1, then Fullprof figures out the numbering.

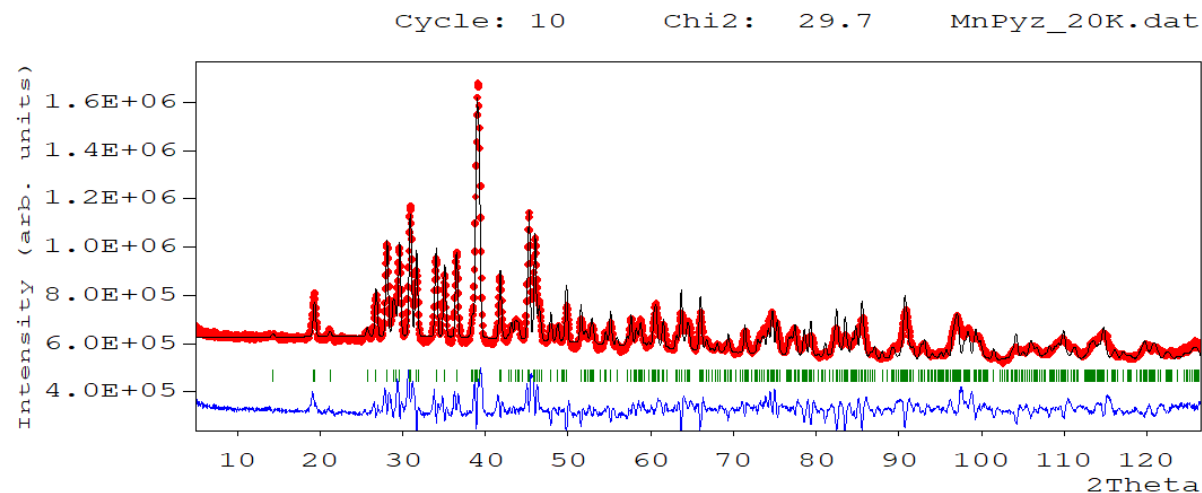
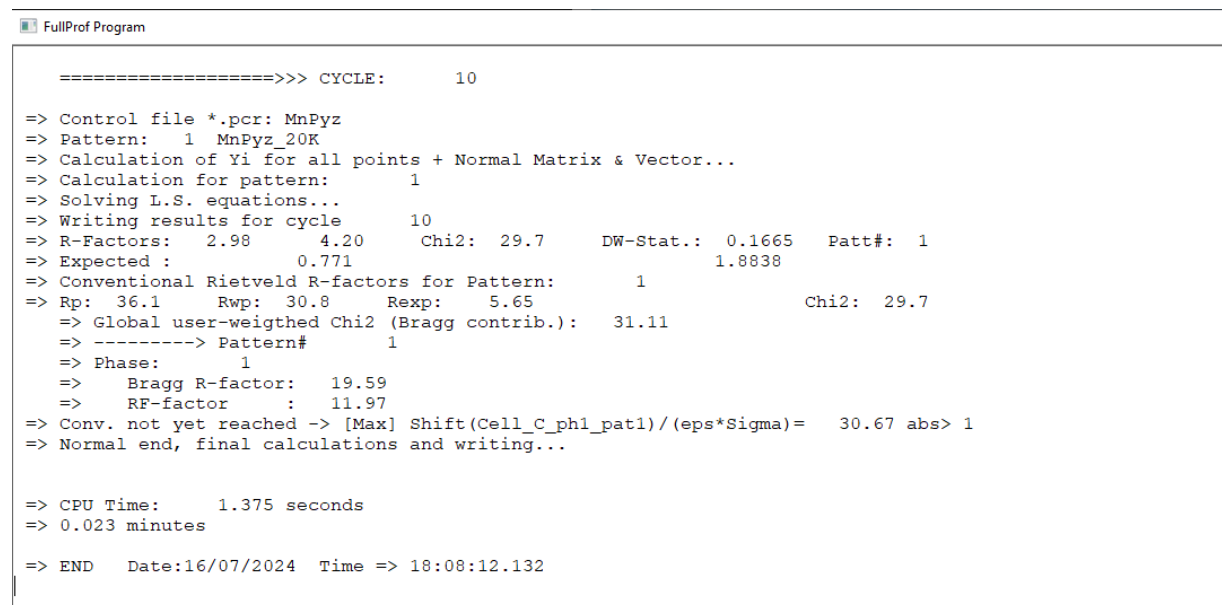
Step 1: Refine the crystal structure using FullProf



The refinement to the 20K data is closer.

Next can add in refinements to the peak shape, since the sample may add some broadening beyond the parameters loaded in with the irf file.

Peak profiles should only be run after the refinement and peak positions are close, otherwise the refinement will blow-up



Step 1: Refine the crystal structure using FullProf

Refinement → Profile → Refine U,V,W,X.

Profile Parameters: Phase 1 Pattern 1

Factors

	Scale	Overall B-factor
Coefficients	49.823 ☒	0.0000 ☐

Cell Parameters

	a	b	c	alpha	beta	gamma
Coefficients	10.184688 ☒	10.811492 ☒	10.090220 ☒	90.000 ☐	108.430 ☒	90.000 ☐

FWHM / Shape Parameters Symmetry 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

Step 1: Refine the crystal structure using FullProf

- Finally the atomic parameters can be refined. This will give a good fit and low chi values. But there are lots of variables, so care should be taken in interpreting these results for the atomic positions.

Atoms Information: Phase 1

List of Atoms

Number of Atoms:

25

	Label	Ntype	X	Y	Z	B	Occ	Therm. Fact.
Atom # 1	Mn	Mn	0.51356	0.12895	0.60217	0.30004	1.00000	Isotropic
Atom # 2	O1	O	0.54868	0.24635	0.42955	0.30004	1.00000	Isotropic
Atom # 3	N1	N	0.36244	0.30105	0.56440	0.30004	1.00000	Isotropic
Atom # 4	C1	C	0.26705	0.31210	0.62293	0.30004	1.00000	Isotropic

Anisotropic Thermal Factors / Form Factors

	B11/F1	B22/F2	B33/F3	B12/F4	B13/F5	B23/F6	F7
#							
#							
#							

Refine Positions

Refine B_iso

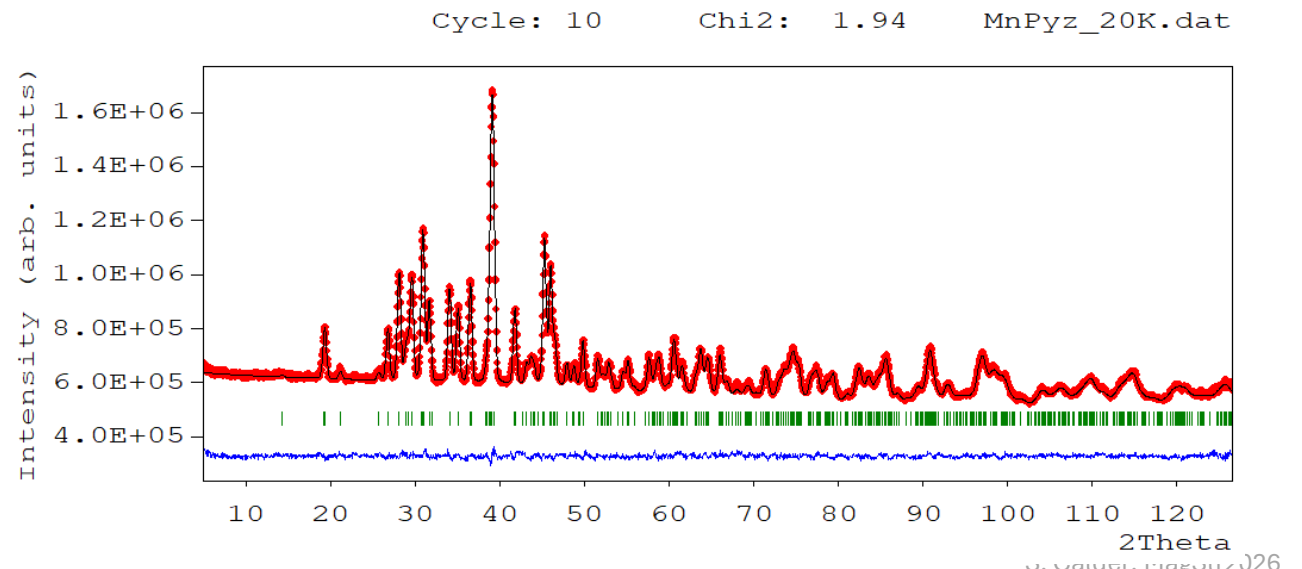
Refine B_aniso

Fix All

Cancel

OK

- Other data was collected with a shorter wavelength (1.54 Å) to cover more reflections. This is presented in the paper.



Step 1: Refine the crystal structure using FullProf

Up to now we have been refining the crystal structure at 20K, where there was no long range magnetic order.

We now want to refine the crystal structure in the magnetically ordered region (1.5K).

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 1.5 K data **FIRST TURN OFF ALL PARAMETERS.**

The peak shapes should not change with temperature since we are measuring the same sample on the same instrument!

- The lattice constants and structural parameters will vary with temperature, but the temperature change here is small. We can refine as needed.

Check in text file that nothing is refining.

[illegible]

Step 1: Refine the crystal structure using FullProf

Refine against the 1.5 K data.

NOTE: New peaks are present at low angle. These are the magnetic peaks. The structural model still captures the high angle peaks indicating there is no observable structure phase transition.

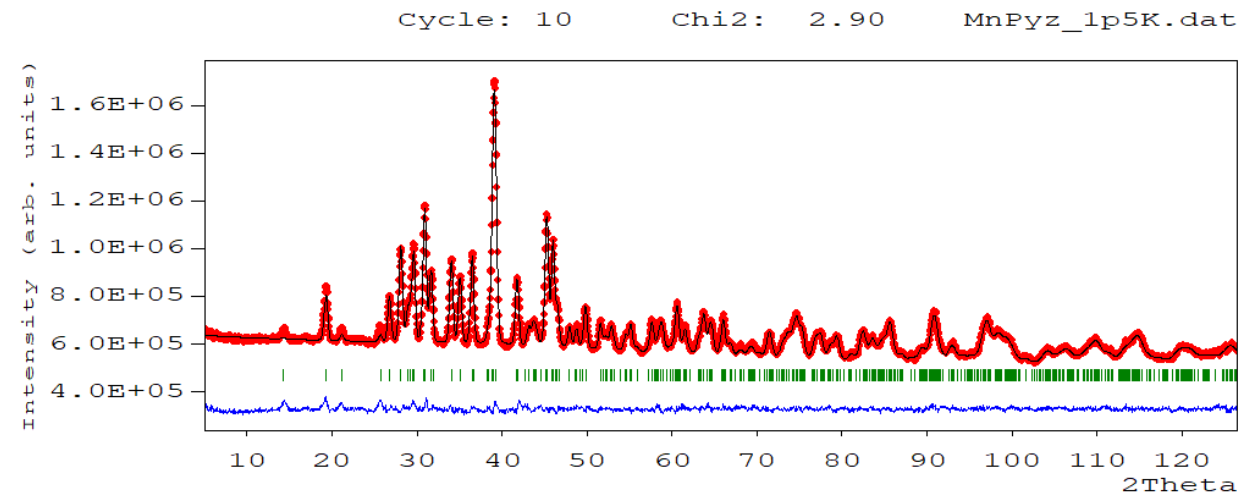
We can now use this to determine the k-vector and then magnetic structure.

```
FullProf Program
=> Expected :          0.773          1.8739
=> Conventional Rietveld R-factors for Pattern:          1
=> Rp: 8.97   Rwp: 8.31   Rexp: 4.88          Chi2: 2.90
=> Global user-weighted Chi2 (Bragg contrib.): 2.780
=> -----> Pattern#          1
=> Phase:          1
=> Bragg R-factor: 3.428
=> RF-factor      : 1.672

=> Convergence reached at this CYCLE !!!!: CYCLE No.          1
=> R-Factors: 1.02   1.32   Chi2: 2.90   DW-Stat.: 0.7071   Patt#: 1
=> Expected :          0.773          1.8739
=> Conventional Rietveld R-factors for Pattern:          1
=> Rp: 8.97   Rwp: 8.31   Rexp: 4.88          Chi2: 2.90
=> Global user-weighted Chi2 (Bragg contrib.): 3.033
=> -----> Pattern#          1
=> Phase:          1
=> Bragg R-factor: 3.428
=> RF-factor      : 1.672
=> Normal end, final calculations and writing...

=> CPU Time:      0.266 seconds
=> 0.004 minutes

=> END   Date:16/07/2024   Time => 18:27:25.873
```



Step 1: Refine the crystal structure using FullProf

The background changes slightly between 1.5 K and 20K, these parameters can be refined here or when doing the magnetic phase.

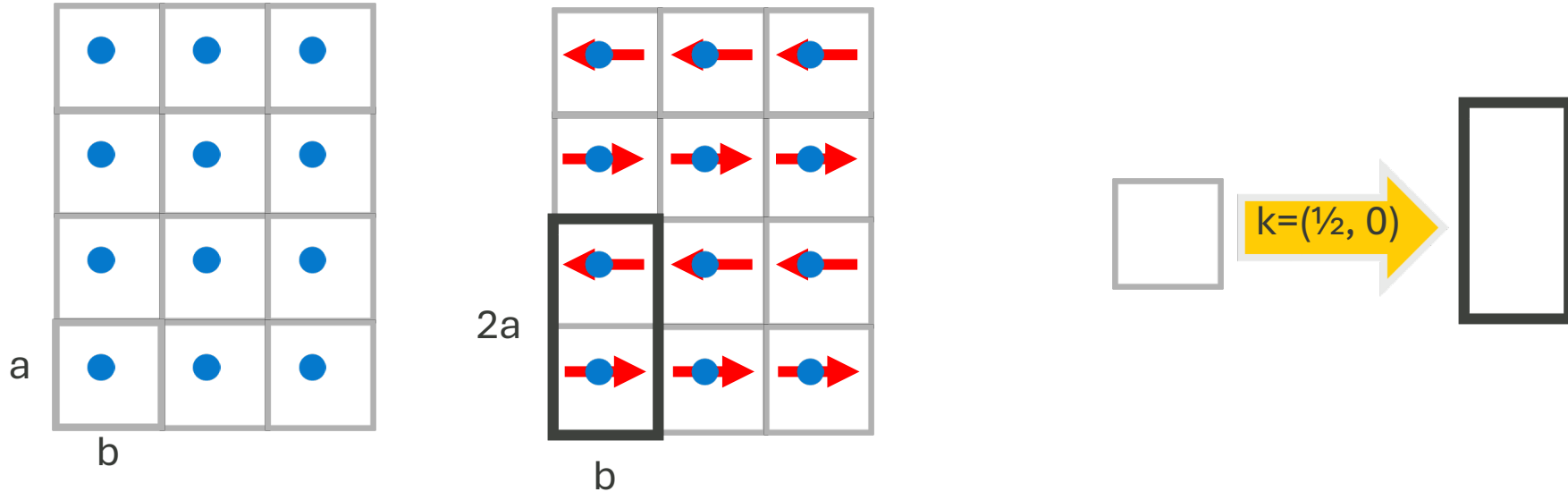
Mn-pyrazinecarboxylate

This example will use Fullprof and Bilbao Crystallographic Server (BCS) <https://cryst.ehu.es/>

- Step 0: Have a well characterized material and good background information
- 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 BCS
- Step 4: Refine the magnetic model and nuclear phase in Fullprof.
- Step 5: Check the magnetic model

Magnetic propagation vector: k-vector

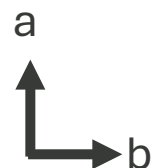
- **Crystal** and **magnetic** unit cells are not necessarily the same size.
- **k-vector** describes the relation between the crystallographic and magnetic unit cells
 - Determine with neutron diffraction



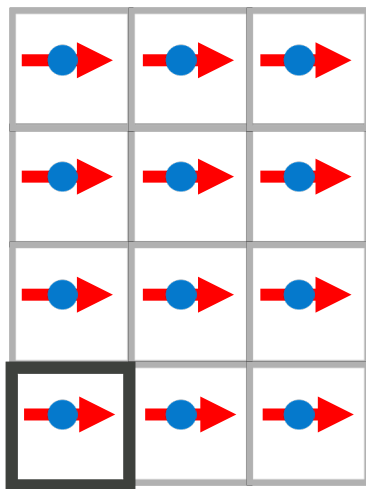
Magnetic propagation vector: k-vector

Reciprocal
space: k-vector

Real space:
crystal and
magnetic
unit cells

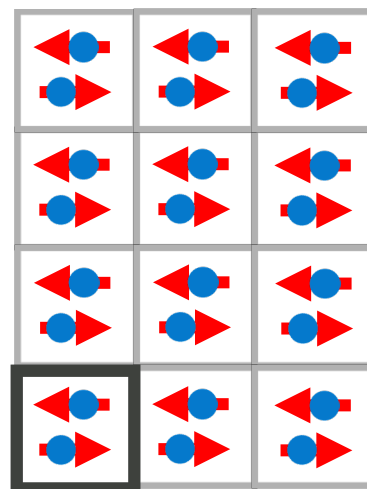


$k=(0,0)$



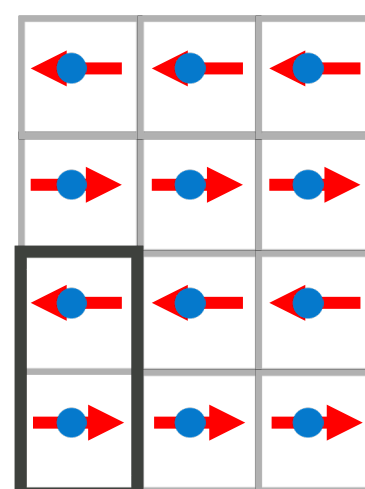
FM

$k=(0,0)$



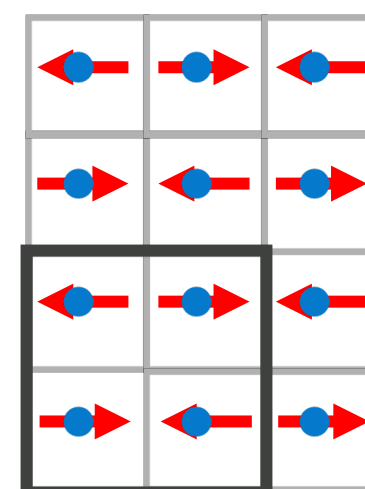
AFM

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



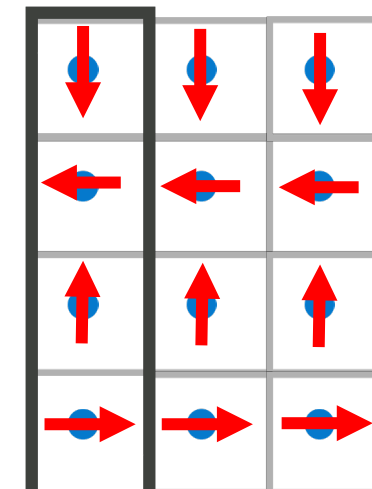
AFM

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



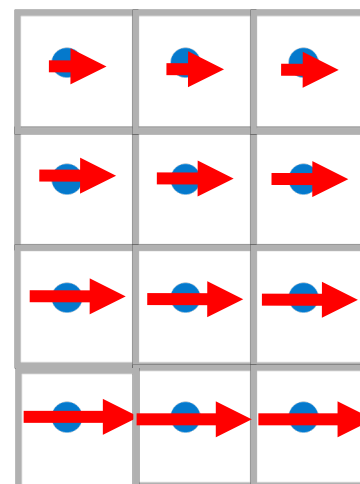
AFM

$k=(\frac{1}{4},0)$

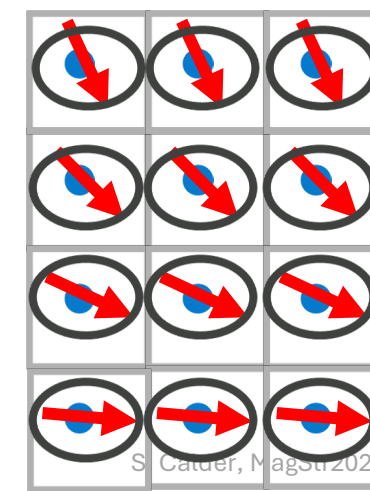


AFM

Incommensurate
spin density wave
structure with
 $k_1=(\delta,0)$



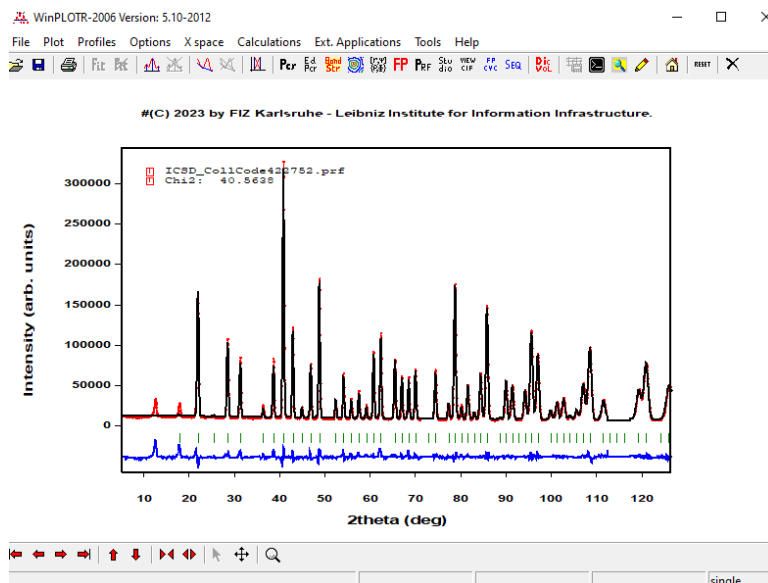
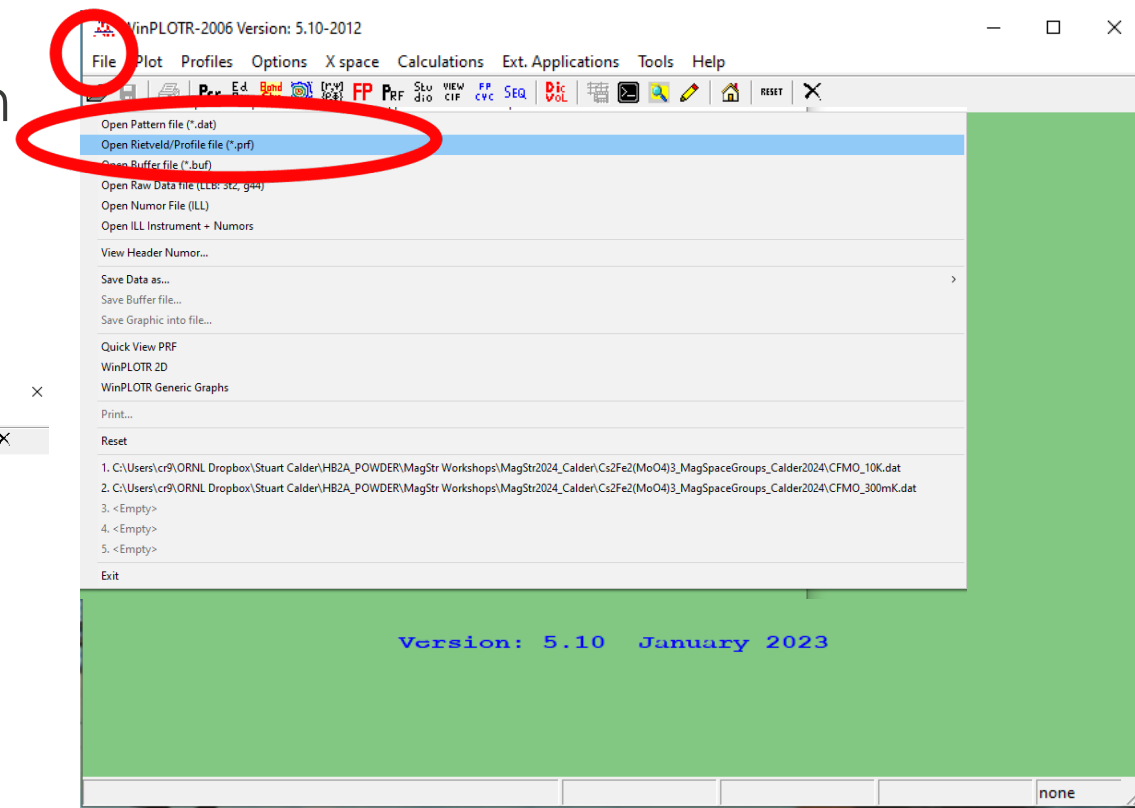
Incommensurate
Helical structure
with
 $k_1=(\delta,0)$



Determine the k-vector

WinPlotr-2006

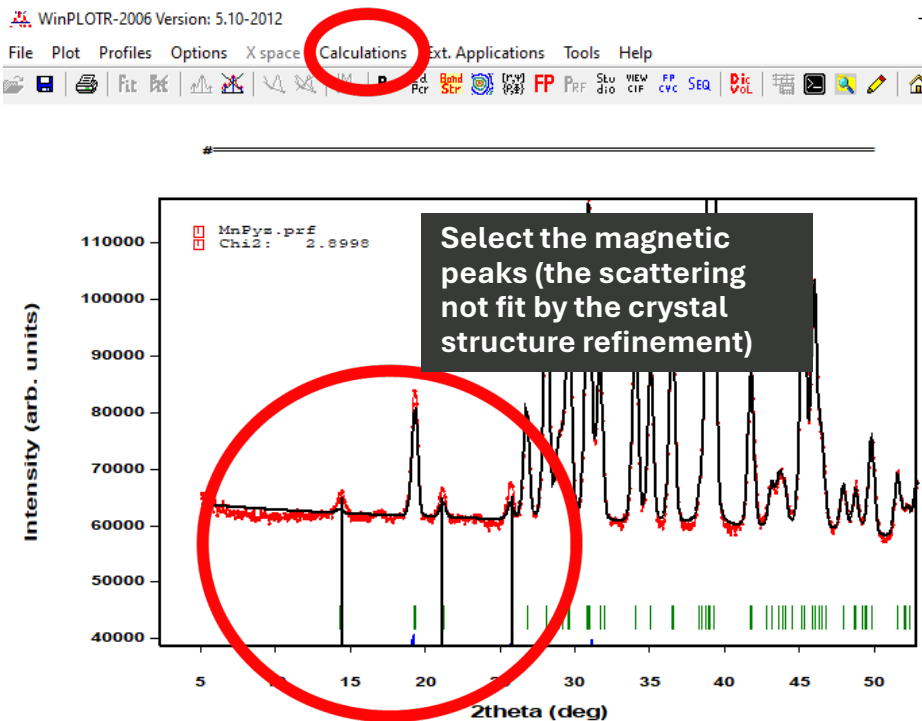
- k-search is run in WinPlotr-2006.
- Open the .prf file. Clicking on icon may open it automatically, if not follow these steps:
 - “File”>”Open Rietveld/Profile file (*.prf)”
 - Select the prf file



Determine the k-vector

Now the magnetic peaks need to be indexed to find the propagation vector that defines the magnetic unit cell.

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.



Input structural model, this is pulled from prf file

Input parameters for K_SEARCH

Title: #=

Lattice Type: P 21/c

Cell Parameters: 10.17611 10.80998 10.07803 90.0000 108.4390 90.0000

Tolerance (TOF/2theta): 0.300

K range (xmin, xmax, ...): 0.0 0.5 0.0 0.5 0.0 0.5

Number of Points (Na Nb Nc): 100 100 100

Wavelength (CW) / Dtt1(TOF): 2.40670

☒ Short Output ☐ Long Output ☐ No output of intermediate calculations

☒ Search only special k-vectors

OK Cancel

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

*****
*          PROGRAM K_SEARCH          *
*****
(J.R.C. ILL-January 2009)

=> The expected maximum R-factor for a solution is:      4.6089

=> Writing partial results ...

=> Testing 90 internal k-vectors
Solution:   1 k =( 0.0000 0.0000 0.0000) R-F:   0.6544
Solution:   2 k =( 0.3333 0.3333 0.0000) R-F:   1.6619
Solution:   3 k =( 0.0000 0.3333 0.3333) R-F:   1.8539
Solution:   4 k =( 0.1250 0.2500 0.0000) R-F:   1.6127
Solution:   5 k =( 0.0000 0.2500 0.1250) R-F:   2.2418
Solution:   6 k =( 0.5000 0.0000 0.1250) R-F:   1.2668
Solution:   7 k =( 0.1250 0.0000 0.5000) R-F:   1.9448
=> Special k-vector solutions found!

=> List of the best incommensurate 10 solutions for 3 satellites

      Kx       Ky       Kz       R-factor
0.000000  0.000000  0.000000  0.654422
0.500000  0.000000  0.125000  1.266762
0.125000  0.250000  0.000000  1.612743
0.333330  0.333330  0.000000  1.661932
0.000000  0.333330  0.333330  1.853868
0.125000  0.250000  0.500000  1.944756
0.500000  0.250000  0.125000  2.241826

=> The best commensurate solution is the special kvector ks =( 0.0000 0.0000 0.0000)
The corresponding R-factor is:      0.6544 to be compared with incommensurate R-factors

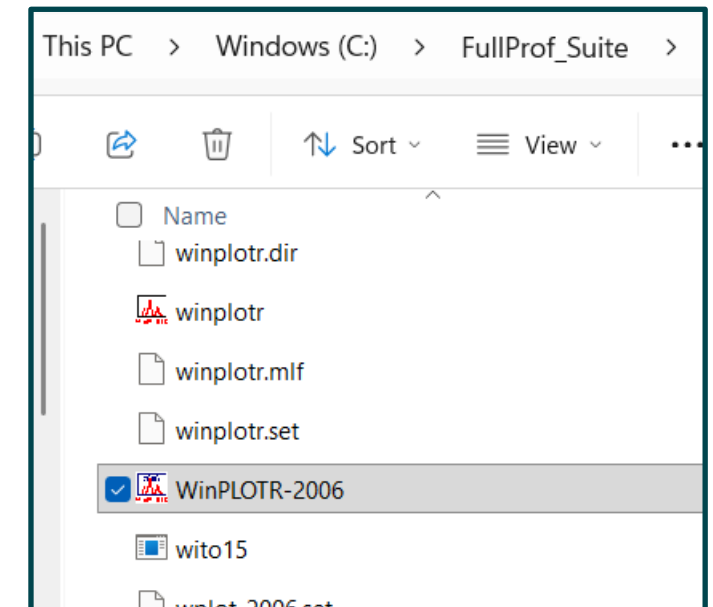
=> Powder diffraction may give wrong results even if the R-factors for the solutions are "good"
The best way to verify the solutions is to perform a full profile fitting and look for mismatches

Total CPU-Time

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

$k=(0,0,0)$

- NOTE: Depending on your set-up, k-search may not run exactly the same as on the previous slides.
 - You may not see the results shown in the black terminal when you run k-search (it might flash for a second then close)
 - Look in the folder where the .prf file is located for a “.kup” file. This can be opened with any text editor and has all the details.
- FIXES if you still cannot see the k-search results:
 - First try opening WinPlotr-2006 from the toolbar then follow previously slides.
 - If that does not work try opening WinPlotr-2006 directly from the Fullprof program location
 - Classic Fullprof is usually C:\FullProf_Suite\
 - New Fullprof is wherever you put it



- The determined k-vector is $k=000$
- With the k-vector and paramagnetic crystal structure we have all the information needed to start to determine the magnetic structure.

Mn-pyrazinecarboxylate

This example will use Fullprof and Bilbao Crystallographic Server (BCS) <https://cryst.ehu.es/>

- Step 0: Have a well characterized material and good background information
- 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 BCS**
- Step 4: Refine the magnetic space group in Fullprof.
- Step 5: Check the magnetic model

Overview of Magnetic Space Group Approach

Magnetic Space Groups

- Extension of crystallographic space groups to include spin
- Includes symmetry of all magnetic/non-magnetic atoms so can provide insights
- Incommensurate only recently added through supersymmetry description

Magnetic space groups (Shubnikov groups)

- Natural extension of the crystallographic space group description.
 - But only recently became widely used for magnetism.

1929: Heesch, introduces the antiidentity operation properties: $u^2 = 1$, $ut = tu$ for all $t \in T$

- aka time reversal group = $\{1, 1'\}$ (Z. Krist. 71, 95)

1945: Shubnikov re-introduces concept of bi-colour point groups

1951: Shubnikov describes and illustrates all of the bicolor point groups ($\rightarrow$ Shubnikov groups)

1955: Belov, Neronova, Smirnova (BNS) - first complete listing of the Shubnikov groups (Sov. Phys. Cryst 1, 487-488)

1957: Zamorzaev, group theoretical derivation of Shubnikov groups (Kristallografiya 2, 15 (Sov. Phys. Cryst., 3, 401))

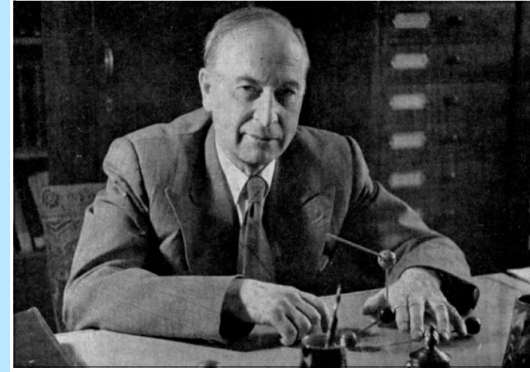
1965: Opechowski and Guccione (OG), first complete derivation and enumeration of the Shubnikov groups

2001: Litvin, corrected Opechowski-Guccione symbols (Acta Cryst. A57, 729-730)

2010: Magnetic Space Groups on computer programs (Stokes and Campbell, BYU)

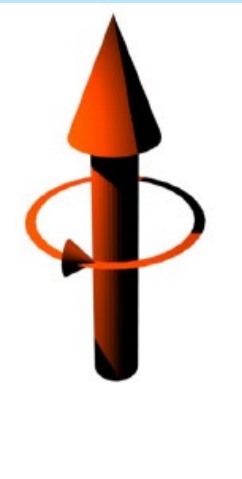
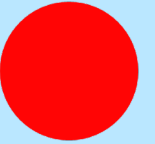
2012: Incommensurate magnetic space group approach standardized and added to software tools

Alexey Vasilyevich Shubnikov 1887-1970



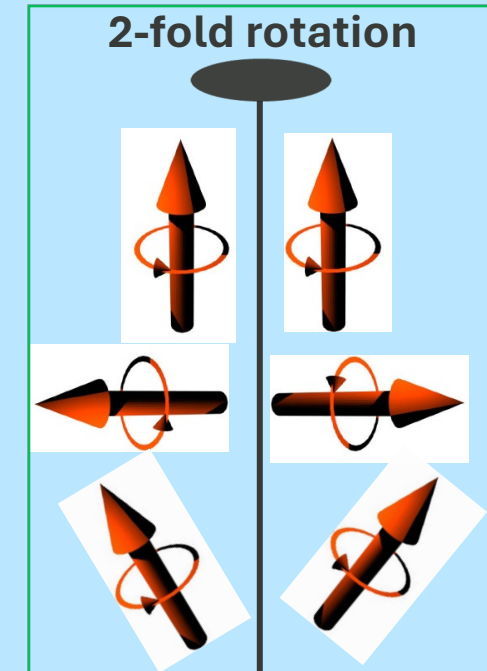
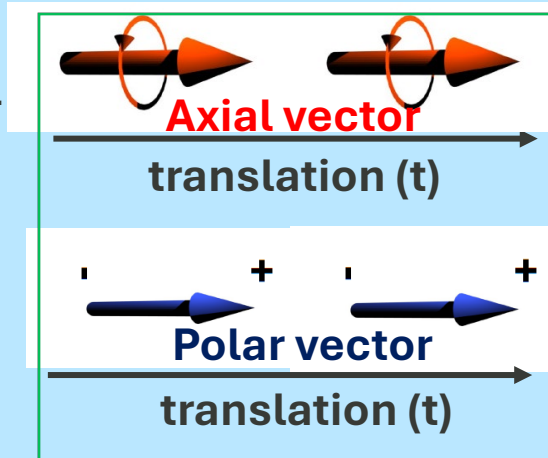
Extend Space Group Approach to include magnetism

- 230 crystallographic space groups:
 - Atoms considered as simple points at a certain location, then apply symmetry operations.
- Now add magnetic moments:
 - Underlying crystal lattice unchanged, with moments at atomic positions.
 - BUT moments are not points, they are vectors ... **axial vectors**.
 - **Location and orientation need to be considered when applying symmetry operations.**
- **Symmetry operations for crystal space groups not enough to describe magnetic structures.**

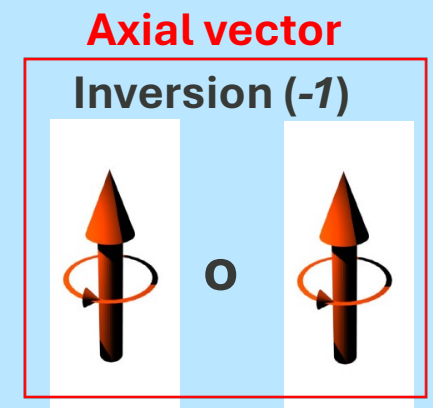
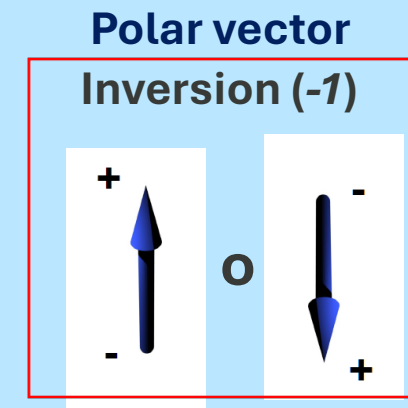
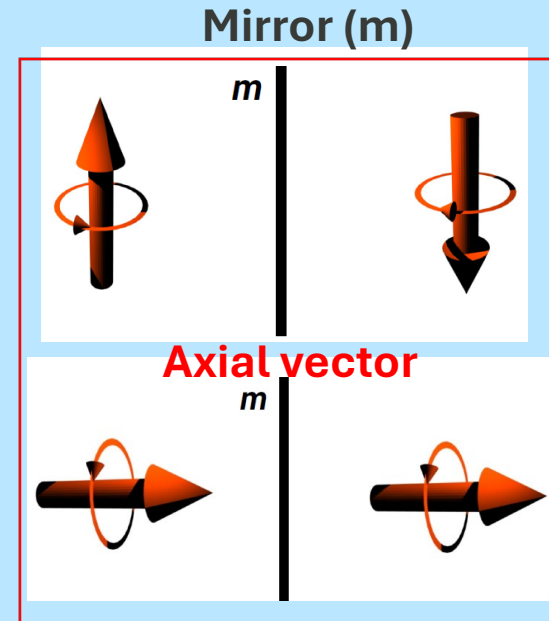
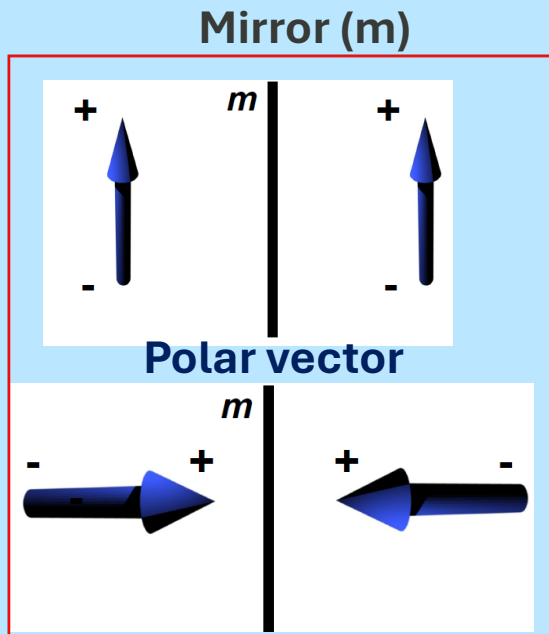


Magnetic space groups: Spins are axial vectors

- Translation (t) and 2-fold rotation are the same for axial and polar vectors.



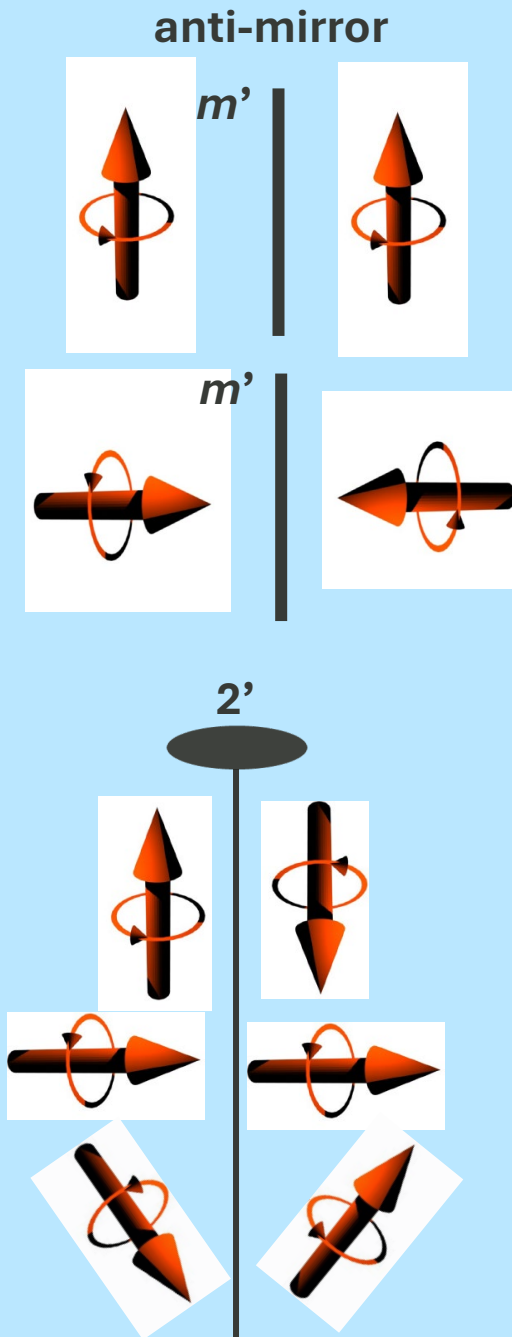
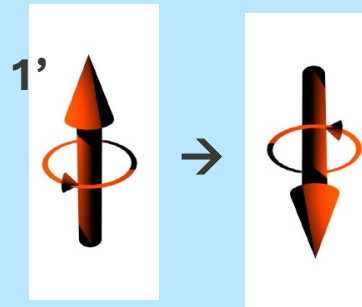
- Inversion and mirror (m) are different for axial and polar.



Magnetic space groups: Time-reversal

- To describe magnetic moments fully a new operator is added
 - Time reversal or prime ($1'$)
 - Reverses the final current loop to allow a further set of symmetry operations.
- m' (anti-mirror) behaves like polar vector
- $2'$ (anti-rotation) inverts axial vector
- t' (anti-translation)
- **All magnetic structures can be described by a combination of primed and unprimed symmetry operators**

Time reversal = spin reversal
(changes the sense of the current)



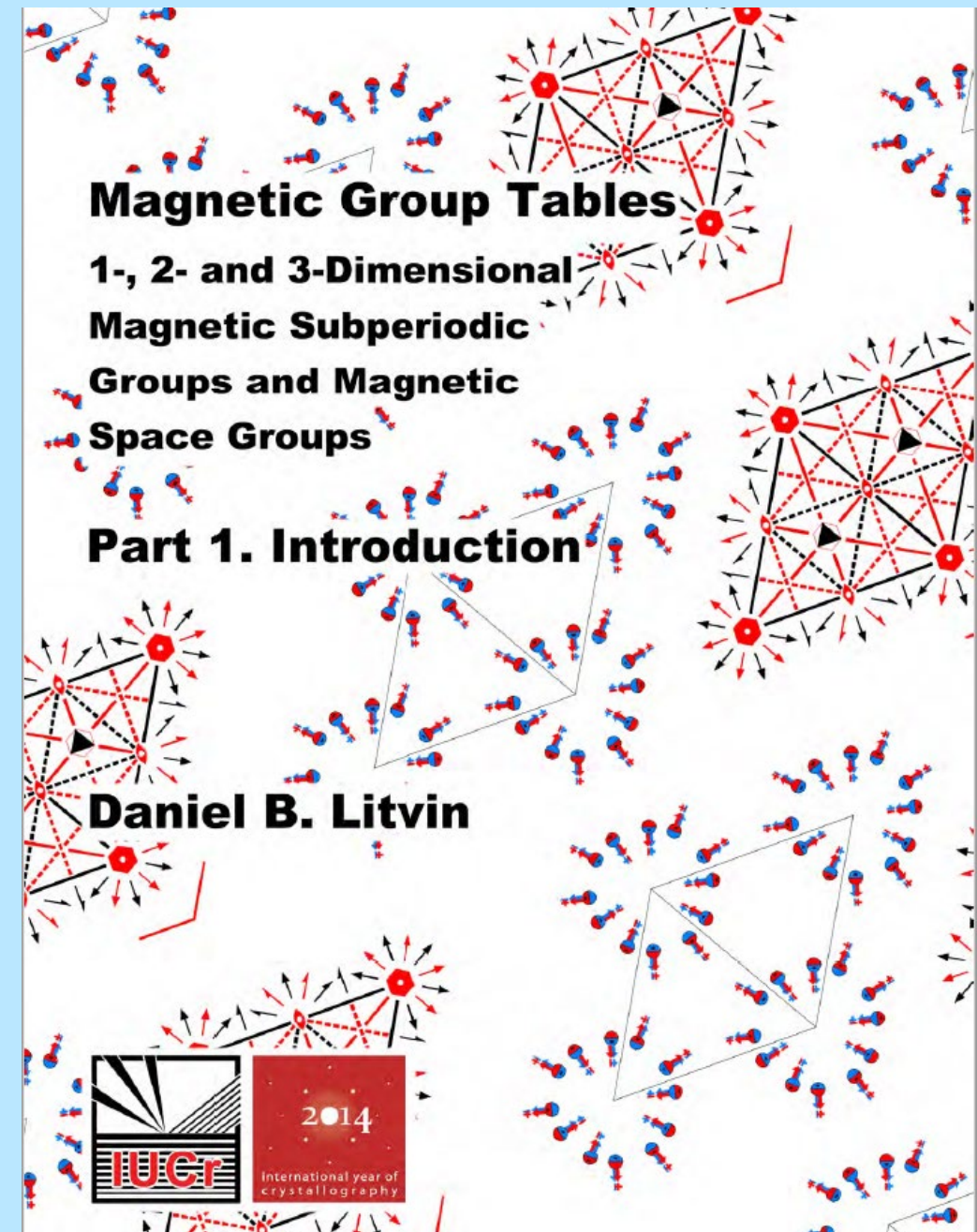
Building the magnetic space groups

- By associating the $1'$ spin operator with a color change (black to white or black to red) the magnetic symmetry theory was termed black-white symmetry.
- **The original 230 space groups are included as colorless groups and keep their standard labels**
 - e.g. *Pmmm*
- A further 230 groups are created by adding the $1'$ operator as an extra symmetry operation
 - e.g. *Pmmm1'*
 - These correspond to paramagnetic states and are termed grey (each magnetic site is both black and white = grey)
- **The remaining 1191 magnetic space groups are created by combining the $1'$ operator with one or more of the symmetry operation in each of the 230 crystallographic space groups**
 - e.g. *Pm'mm* where the mirror plane perpendicular to *a* is now an anti-mirror and the other two are unchanged.

→ Combining all possibilities leads to 1651 magnetic space groups

Magnetic space groups

- Full description of all Magnetic Space groups produced.
 - Acta Cryst A57, 729-730 (2001)
 - Acta Cryst. (2008). A64, 419-424 (2008)
- Utilized in analysis tools
 - Isodistort, Bilbao (GSAS-II), Fullprof, JANA, etc



Step 3: Create candidate magnetic models using BCS

Now the crystal structure and k-vector have been determined the magnetic structure can be found by testing model magnetic space groups.

This can be done in FullProf by creating a .mcif file from the Bilbao Crystallographic Server.

Step 3: Create candidate magnetic models using BCS

Go to the Bilbao Crystallographic Server: <http://www.cryst.ehu.es/>

Select “Magnetic Symmetry and Applications” to open the drop-down menu



Bilbao Crystallographic Server
in forthcoming schools and workshops

News:

- **New program: SPGENPOS**
06/2026: General positions of the spin point groups
- **New Article**
04/2026: Elcoro *et al.* "Automatic calculation of symmetry-adapted tensors under spin-group symmetry: STENSOR, a new tool of the Bilbao Crystallographic Server". *J. Appl. Cryst.* (2026) **59**, 640-647
- **MORPHIC EFFECTS** updates
04/2026: The magnetic-field option is now available.
- **New Article**
06/2025: Etxebarria *et al.* "Crystal tensor properties of magnetic materials with and without spin-orbit coupling. Application of spin point groups as approximate symmetries.". *Acta Cryst.* (2025) **A81**, 317-338
- **New program: MINSUP for plane groups**
06/2025: Minimal supergroups of plane groups
- **New program: CollinearSpinGroups**
05/2025: Operations of Nontrivial Collinear Spin Space Groups
- **New program: STENSOR**
04/2025: Symmetry-adapted form of crystal tensors under spin point groups
- **New Article**
04/2025: Tasci *et al.* "Computational analysis tools for magnetic structures in the Bilbao Crystallographic Server". *Acta Cryst.* (2025) **B81**

bilbao crystallographic server

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Structure Databases

Raman and Hyper-Raman scattering

Point-group symmetry

Plane-group symmetry

Double point and space groups

Step 3: Create candidate magnetic models using BCS

Then select “MAXMAGN”

Magnetic Symmetry and Applications	
Magnetic groups	
MGENPOS	General Positions of Magnetic Space Groups
MWYCKPOS	Wyckoff Positions of Magnetic Space Groups
MKVEC	The k-vector types and Brillouin zones of Magnetic Space Groups
IDENTIFY MAGNETIC GROUP	Identification of a Magnetic Space Group from a set of generators in an arbitrary setting
BNS2OG	Transformation of symmetry operations between BNS and OG settings
mCIF2PCR	Transformation from mCIF to PCR format (FullProf).
MPOINT	Magnetic Point Group Tables
MAGNEXT	Extinction Rules of Magnetic Space Groups
MAXMAGN	Maximal magnetic space groups for a given space group and a propagation vector
MAGMODELIZE	Magnetic structure models for any given magnetic symmetry
STRCONVERT	Convert & Edit Structure Data (supports the CIF, mCIF, VESTA, VASP formats -- with magnetic information where available)
k-SUBGROUPSMAG	Magnetic subgroups consistent with some given propagation vector(s) or a supercell
MAGNDATA	A collection of magnetic structures with portable cif-type files
MVISUALIZE	3D Visualization of magnetic structures with Jmol
MTENSOR	Symmetry-adapted form of crystal tensors in magnetic phases
MAGNETIC REP.	Decomposition of the magnetic representation into irreps
Get_mirreps	Irreps and order parameters in a paramagnetic space group- magnetic subgroup phase transition
Spin groups	
SPGENPOS ⚠	General positions of spin point groups
STENSOR ⚠	Symmetry-adapted form of crystal tensors under spin point groups
CollinearSpinGroups ⚠	Operations of Nontrivial Collinear Spin Space Groups

Step 3: Create candidate magnetic models using BCS

- [1] Need to have a propagation vector. This was determined using k-search in fullprof (to be (0.5,0,0.5)).
- [2] Check the box “Structure data of the paramagnetic phase will be included”. This allows you to input a .cif file.
- [3] Click submit.

MAXMAGN: Maximal magnetic space groups for a given a propagation vector and resulting magnetic structural models

MAXMAGN: Maximal magnetic space groups for a given a propagation vector and resulting magnetic structural models

MAXMAGN provides the possible magnetic space groups that can be assigned to a 1-k commensurate magnetic phase assuming that the magnetic symmetry is a maximal one. The space group of the paramagnetic phase (parent group) and the observed propagation vector are required as input. Optionally, the parent paramagnetic structure can be introduced (by hand or by a cif file). In this latter case the program provides the constrains for the different possible symmetries and cif-like files can be produced. These files permit the different alternative models to be analyzed, refined, shown graphically, transported to ab-initio codes etc., with programs as [ISODISTORT](#), [JANA2006](#), [StrConvert](#), [VESTA](#), etc. These cif-like files can also be submitted to the program [MVISUALIZE](#), which allow 3D visualization of magnetic structures with [Jmol](#). A controlled descent to lower symmetries is also possible.

This program provides an alternative to the traditional representation method for the parameterization of magnetic structures.

MAXMAGN tutorials:

Abbreviated tutorial: [download](#)
Extended tutorial: [download](#)
Last tutorial: [download](#)

Examples and further information can be found in the following paper:

J.M. Perez-Mato, S.V. Gallego, E.S. Tasci, L. Elcoro, G. de la Flor, and M.I. Aroyo
Annu. Rev. Mater. Res. (2015), **45**:13.1-13.32

which can be used to cite this program.

[2]

☒ Structure data of the paramagnetic phase will be included

☐ Non-conventional setting

Please, enter the label of the space group of the paramagnetic phase (parent group)

choose it

Please, enter the propagation vector k:

k_x

k_y

k_z

[1]

[3]

Submit

Step 3: Create candidate magnetic models using BCS

Choose .cif file (crystal structure only).

The one for this example is “MnPyz_1p5K_nuclear.cif”

Then upload the file.

Bilbao Crystallographic Server → MAXMAGN - Maximal magnetic space groups Help

Parent paramagnetic structure cif file

Option 1: Please submit a structure file (CIF format):

MnPyz_1p5K_nuclear.cif

No space group provided. The space group indicated in the cif file will be taken.

Bilbao Crystallographic Server
<https://cryst.ehu.es>

For comments, please mail to
administrador.bcs@ehu.eus

Step 3: Create candidate magnetic models using BCS

Parent phase structure data: Magnetic Atoms

The paramagnetic phase information is displayed.

- **[1]** Select the magnetic atom(s). This case Mn is the only magnetic atom and there is only one site.
- **[2]** Push Submit. This may take a few seconds to run the calculations.....

Parent space group: $P2_1/c$ (No. 14)

Lattice parameters (Angstroms and degrees): a=10.17610, b=10.81000, c=10.07800, alpha=90.000000, beta=108.439003, gamma=90.000000

Atoms: Please select the magnetic ones

[1]

N	Atom name	Atom type	Wyckoff Position	Coordinates	Magnetic?
1	Mn1	Mn	4e	0.51356 0.12895 0.60217	☒
2	O1	O	4e	0.54868 0.24635 0.42955	☐
3	N1	N	4e	0.36244 0.30105 0.56440	☐
4	C1	C	4e	0.26705 0.31210 0.62293	☐
5	H1	H	4e	0.24226 0.24571 0.66885	☐
6	O2	O	4e	0.47150 0.40957 0.28321	☐
7	N2	N	4e	0.17238 0.49489 0.47494	☐
8	C2	C	4e	0.15921 0.40664 0.56866	☐
9	H2	H	4e	0.10169 0.42860 0.62270	☐
10	O3	O	4e	0.63589 -0.00640 0.53074	☐
11	N3	N	4e	0.73160 0.18010 0.70183	☐
12	C3	C	4e	0.27027 0.46870 0.41733	☐
13	H3	H	4e	0.27886 0.53942 0.33280	☐
14	O4	O	4e	0.80942 -0.02700 0.47011	☐
15	N4	N	4e	1.02037 0.23074 0.77219	☐
16	C4	C	4e	0.37122 0.39433 0.46301	☐
17	C5	C	4e	0.48774 0.34148 0.39952	☐
18	C6	C	4e	0.81776 0.26713 0.79909	☐
19	H4	H	4e	0.72837 0.31267 0.85696	☐
20	C7	C	4e	0.93956 0.27897 0.83592	☐
21	H5	H	4e	0.96853 0.33513 0.91943	☐
22	C8	C	4e	0.97946 0.13864 0.67951	☐
23	H6	H	4e	1.03201 0.08974 0.64397	☐
24	C9	C	4e	0.82851 0.11546 0.64167	☐
25	C10	C	4e	0.75618 0.02305 0.54995	☐

[2]

Submit

Step 3: Create candidate magnetic models using BCS

Maximal magnetic space groups for the parent space group $P2_1/c$
(No. 14) and the propagation vector $\mathbf{k} = (0, 0, 0)$

Maximal subgroups which allow non-zero magnetic moments for at least one atom are coloured

N	Group (BNS)	Transformation matrix	General positions	Properties	Magnetic structure
1	$P2_1'/c'$ (#14.79) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
2	$P2_1/c'$ (#14.78) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
3	$P2_1'/c$ (#14.77) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
4	$P2_1/c$ (#14.75) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show

The possible magnetic space groups are displayed in grey

To view magnetic structure and export mcif file click on “Show” in last column.

Step 3: Create candidate magnetic models using BCS **Check #1**

N	Group (BNS)	Transformation matrix	General positions	Properties	Magnetic structure
1	<i>P</i> 2 ₁ /c' (#14.79) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
2	<i>P</i> 2 ₁ /c' (#14.78) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
3	<i>P</i> 2 ₁ /c (#14.77) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
4	<i>P</i> 2 ₁ /c (#14.75) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show

Magnetic Structure

Selected magnetic space group: 1- *P*2₁/c' (#14.79)

Setting of the parent group

Parent space group *P*2₁/c (No. 14)

Lattice parameters: a=10.19000, b=10.90600, c=10.11600, alpha=90.000000, beta=107.960, gamma=90.000000

[Go to setting standard (a, b, c ; 0, 0, 0)]
[Go to an alternative setting]

Export data to MCIF file/Visualize Go to a subgroup

Only Ho can contribute to magnetic structure.

Spins only allowed along x, y, z

Atomic positions, Wyckoff positions and Magnetic Moments

N	Atom	New WP	Multiplicity	Magnetic moment	Values of M _x , M _y , M _z
1	Mn1 Mn 0.51009 0.13426 0.59800	(x,y,z m _x ,m _y ,m _z) (-x,y+1/2,-z+1/2 m _x ,-m _y ,m _z) (-x,-y,-z m _x ,m _y ,m _z) (x,-y+1/2,z+1/2 m _x ,-m _y ,m _z)	4	(M _x ,M _y ,M _z)	M _x = 0.00000 M _y = 0.00000 M _z = 0.00000
2	O1 O 0.54100 0.24430 0.42660	(x,y,z m _x ,m _y ,m _z) (-x,y+1/2,-z+1/2 m _x ,-m _y ,m _z) (-x,-y,-z m _x ,m _y ,m _z) (x,-y+1/2,z+1/2 m _x ,-m _y ,m _z)	4	-	-
3	N1 N 0.36060 0.29910 0.56210	(x,y,z m _x ,m _y ,m _z) (-x,y+1/2,-z+1/2 m _x ,-m _y ,m _z) (-x,-y,-z m _x ,m _y ,m _z) (x,-y+1/2,z+1/2 m _x ,-m _y ,m _z)	4	-	-
4	C1 C 0.26270 0.32510 0.61920	(x,y,z m _x ,m _y ,m _z) (-x,y+1/2,-z+1/2 m _x ,-m _y ,m _z) (-x,-y,-z m _x ,m _y ,m _z) (x,-y+1/2,z+1/2 m _x ,-m _y ,m _z)	4	-	-

Step 3: Create candidate magnetic models using BCS **Check #2**

N	Group (BNS)	Transformation matrix	General positions	Properties	Magnetic structure
1	<i>P2₁/c'</i> (#14.79) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
2	<i>P2₁/c'</i> (#14.78) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
3	<i>P2₁/c</i> (#14.77) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
4	<i>P2₁/c</i> (#14.75) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show

Magnetic Structure

Selected magnetic space group: 2- *P2₁/c'* (#14.78)

Setting of the parent group

Parent space group *P2₁/c* (No. 14)

Lattice parameters: a=10.19000, b=10.90600, c=10.11600, alpha=90.000000, beta=107.960, gamma=90.000000

[Go to setting standard (a, b, c ; 0, 0, 0)]
[Go to an alternative setting]

Export data to MCIF file/Visualize Go to a subgroup

Atomic positions, Wyckoff positions and Magnetic Moments

N	Atom	New WP	Multiplicity	Magnetic moment	Values of M _x , M _y , M _z
1	Mn1 Mn 0.51009 0.13426 0.59800	(x,y,z m _x ,m _y ,m _z) (-x,y+1/2,-z+1/2 -m _x ,m _y ,m _z) (-x,-y,-z -m _x ,m _y ,m _z) (x,-y+1/2,z+1/2 m _x ,m _y ,m _z)	4	(M _x ,M _y ,M _z)	M _x = 0.00000 M _y = 0.00000 M _z = 0.00000
2	O1 O 0.54100 0.24430 0.42660	(x,y,z m _x ,m _y ,m _z) (-x,y+1/2,-z+1/2 -m _x ,m _y ,m _z) (-x,-y,-z -m _x ,m _y ,m _z) (x,-y+1/2,z+1/2 m _x ,m _y ,m _z)	4	-	-
3	N1 N 0.36060 0.29910 0.56210	(x,y,z m _x ,m _y ,m _z) (-x,y+1/2,-z+1/2 -m _x ,m _y ,m _z) (-x,-y,-z -m _x ,m _y ,m _z) (x,-y+1/2,z+1/2 m _x ,m _y ,m _z)	4	-	-
4	C1 C 0.26270 0.32510 0.61920	(x,y,z m _x ,m _y ,m _z) (-x,y+1/2,-z+1/2 -m _x ,m _y ,m _z) (-x,-y,-z -m _x ,m _y ,m _z) (x,-y+1/2,z+1/2 m _x ,m _y ,m _z)	4	-	-
5	H1 H 0.85161 0.87001 0.88101	(x,y,z m _x ,m _y ,m _z) (-x,y+1/2,-z+1/2 -m _x ,m _y ,m _z)	4	-	-

Only Ho can contribute to magnetic structure.

Spins only allowed along x, y, z

Step 3: Create candidate magnetic models using BCS **Check #3**

N	Group (BNS)	Transformation matrix	General positions	Properties	Magnetic structure
1	$P2_1/c'$ (#14.79) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
2	$P2_1/c'$ (#14.78) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
3	$P2_1/c$ (#14.77) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
4	$P2_1/c$ (#14.75) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show

Magnetic Structure

Selected magnetic space group: 3- $P2_1/c$ (#14.77)

Setting of the parent group

Parent space group $P2_1/c$ (No. 14)

Lattice parameters: a=10.19000, b=10.90600, c=10.11600, alpha=90.000000, beta=107.960, gamma=90.000000

[\[Go to setting standard \(a, b, c ; 0, 0, 0\)\]](#)
[\[Go to an alternative setting\]](#)

[Export data to MCIF file/Visualize](#) [Go to a subgroup](#)

Atomic positions, Wyckoff positions and Magnetic Moments					
N	Atom	New WP	Multiplicity	Magnetic moment	Values of M_x, M_y, M_z
1	Mn1 Mn 0.51009 0.13426 0.59800	(x,y,z m_x, m_y, m_z) (-x,y+1/2,-z+1/2 $m_x, -m_y, m_z$) (-x,-y,-z $-m_x, -m_y, -m_z$) (x,-y+1/2,z+1/2 $-m_x, m_y, -m_z$)	4	(M_x, M_y, M_z)	$M_x = 0.00000$ $M_y = 0.00000$ $M_z = 0.00000$
2	O1 O 0.54100 0.24430 0.42660	(x,y,z m_x, m_y, m_z) (-x,y+1/2,-z+1/2 $m_x, -m_y, m_z$) (-x,-y,-z $-m_x, -m_y, -m_z$) (x,-y+1/2,z+1/2 $-m_x, m_y, -m_z$)	4	-	-
3	N1 N 0.36060 0.29910 0.56210	(x,y,z m_x, m_y, m_z) (-x,y+1/2,-z+1/2 $m_x, -m_y, m_z$) (-x,-y,-z $-m_x, -m_y, -m_z$) (x,-y+1/2,z+1/2 $-m_x, m_y, -m_z$)	4	-	-
4	C1 C 0.26270 0.32510 0.61920	(x,y,z m_x, m_y, m_z) (-x,y+1/2,-z+1/2 $m_x, -m_y, m_z$) (-x,-y,-z $-m_x, -m_y, -m_z$) (x,-y+1/2,z+1/2 $-m_x, m_y, -m_z$)	4	-	-

Only Ho can contribute to magnetic structure.

Spins only allowed along x, y, z

Step 3: Create candidate magnetic models using BCS **Check #4**

N	Group (BNS)	Transformation matrix	General positions	Properties	Magnetic structure
1	P2₁/c' (#14.79) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	<i>Systematic absences</i> MAGNEXT <i>Tensor properties</i> MTENSOR	Show
2	P2₁/c' (#14.78) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	<i>Systematic absences</i> MAGNEXT <i>Tensor properties</i> MTENSOR	Show
3	P2₁/c (#14.77) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	<i>Systematic absences</i> MAGNEXT <i>Tensor properties</i> MTENSOR	Show
4	P2₁/c (#14.75) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	<i>Systematic absences</i> MAGNEXT <i>Tensor properties</i> MTENSOR	Show

Only Ho can contribute to magnetic structure.

Spins only allowed along x, y, z

Magnetic Structure

Selected magnetic space group: 4- P2₁/c (#14.75)

Setting of the parent group

Parent space group P2₁/c (No. 14)

Lattice parameters: a=10.19000, b=10.90600, c=10.11600, alpha=90.000000, beta=107.960, gamma=90.000000

[Go to setting standard (a, b, c ; 0, 0, 0)]
[Go to an alternative setting]

[Export data to MCIF file/Visualize](#) [Go to a subgroup](#)

Atomic positions, Wyckoff positions and Magnetic Moments

N	Atom	New WP	Multiplicity	Magnetic moment	Values of M _x , M _y , M _z
1	Mn1 Mn 0.51009 0.13426 0.59800	(x,y,z m _x ,m _y ,m _z) (-x,y+1/2,-z+1/2 -m _x ,m _y ,m _z) (-x,-y,-z m _x ,m _y ,m _z) (x,-y+1/2,z+1/2 -m _x ,m _y ,m _z)	4	(M _x ,M _y ,M _z)	M _x = 0.00000 M _y = 0.00000 M _z = 0.00000
2	O1 O 0.54100 0.24430 0.42660	(x,y,z m _x ,m _y ,m _z) (-x,y+1/2,-z+1/2 -m _x ,m _y ,m _z) (-x,-y,-z m _x ,m _y ,m _z) (x,-y+1/2,z+1/2 -m _x ,m _y ,m _z)	4	-	-
3	N1 N 0.36060 0.29910 0.56210	(x,y,z m _x ,m _y ,m _z) (-x,y+1/2,-z+1/2 -m _x ,m _y ,m _z) (-x,-y,-z m _x ,m _y ,m _z) (x,-y+1/2,z+1/2 -m _x ,m _y ,m _z)	4	-	-
4	C1 C 0.26270 0.32510 0.61920	(x,y,z m _x ,m _y ,m _z) (-x,y+1/2,-z+1/2 -m _x ,m _y ,m _z) (-x,-y,-z m _x ,m _y ,m _z) (x,-y+1/2,z+1/2 -m _x ,m _y ,m _z)	4	-	-

Step 3: Create candidate magnetic models using BCS

- NOTE: in this MnPyz example all maximal magnetic space groups have allowed moments along x,y,z
- BUT the maximal magnetic space groups may only have allowed moments along specific directions and zero elsewhere. This can help to quickly test models.
- See the figure here from a $\text{Ho}_2\text{BaNiO}_5$ example, this magnetic space group only has spins along the b-axis for the Ho atom.
- LOOK THROUGH OTHER TUTORIAL EXAMPLES TO SEE WHAT IS POSSIBLE

$\text{Ho}_2\text{BaNiO}_5$ example

Magnetic Structure

Selected magnetic space group: 4- C_2/m (#12.63)

Setting parent-like (2a, b, 2c ; 0, 0, 0)

Parent space group $Immm$ (No. 71)

Lattice parameters: a=7.51210, b=5.73410, c=22.55500, alpha=90.00, beta=90.00, gamma=90.00

[Go to setting standard (a-c, b, 2a ; 0, 0, 1/2)]
[Go to an alternative setting]

Export data to MCIF file/Visualize Go to a subgroup

Atomic positions, Wyckoff positions and Magnetic Moments

N	Atom	New WP	Multiplicity	Magnetic moment	Values of M_x, M_y, M_z
1	Ho1 Ho 0.25000 0.00000 0.10125	(1/4,0,z 0, m_y ,0) (1/4,0,-z 0, m_y ,0) (0,1/2,z+1/4 0, m_y ,0) (0,1/2,-z+1/4 0, m_y ,0) (1/4,0,z+1/2 0,- m_y ,0) (1/4,0,-z+1/2 0,- m_y ,0) (0,1/2,z+3/4 0,- m_y ,0) (0,1/2,-z+3/4 0,- m_y ,0) (3/4,0,z 0,- m_y ,0) (3/4,0,-z 0,- m_y ,0) (1/2,1/2,z+1/4 0,- m_y ,0) (1/2,1/2,-z+1/4 0,- m_y ,0) (3/4,0,z+1/2 0, m_y ,0) (3/4,0,-z+1/2 0, m_y ,0) (1/2,1/2,z+3/4 0, m_y ,0) (1/2,1/2,-z+3/4 0, m_y ,0)	16	(0, M_y ,0)	$M_y = 0.00000$
2	Ba1 Ba 0.25000 0.50000 0.00000	(1/4,1/2,0 0, m_y ,0) (0,0,1/4 0, m_y ,0) (1/4,1/2,1/2 0,- m_y ,0) (0,0,3/4 0,- m_y ,0) (3/4,1/2,0 0,- m_y ,0) (1/2,0,1/4 0,- m_y ,0) (3/4,1/2,1/2 0, m_y ,0) (1/2,0,3/4 0, m_y ,0)	8	-	-
3	Ni1 Ni 0.00000 0.00000 0.00000	(0,0,0 0,0,0) (1/4,1/2,1/4 0,0,0) (0,0,1/2 0,0,0) (1/4,1/2,3/4 0,0,0) (1/2,0,0 0,0,0) (3/4,1/2,1/4 0,0,0) (1/2,0,1/2 0,0,0) (3/4,1/2,3/4 0,0,0)	8	(0,0,0)	-

Step 3: Create candidate magnetic models using BCS

Magnetic Structure

Selected magnetic space group: $4^- P2_1/c$ (#14.75)

Setting of the parent group

Parent space group $P2_1/c$ (No. 14)

Lattice parameters: $a=10.19000$, $b=10.90600$, $c=10.11600$, $\alpha=90.000000$, $\beta=107.960$, $\gamma=90.000000$

[Go to setting standard (a, b, c : 0, 0, 0)]
[Go to alternative setting]

Export data to MCIF file/Visualize [Go to a subgroup]

Atomic positions, Wyckoff positions and Magnetic Moments

N	Atom	New WP	Multiplicity	Magnetic moment	Values of M_x , M_y , M_z
1	Mn1 Mn 0.51009 0.13426 0.59800	(x,y,z m_x, m_y, m_z) (-x,y+1/2,-z+1/2 $-m_x, m_y, -m_z$) (-x,-y,-z m_x, m_y, m_z) (x,-y+1/2,z+1/2 $-m_x, m_y, -m_z$)	4	(M_x, M_y, M_z)	$M_x = 1.1$ $M_y = 1.2$ $M_z = 1.3$

mcCIF file of the structure

Submit this mcif file to MVisualize for 3D visualization of the structure using Jmol: [Submit to MVisualize](#)

Download mcCIF file: [bcs_file.mcif](#)
[The preview text below is non-editable, only copy-allowed]

```
#\#CIF_2.0
# Created by the Bilbao Crystallographic Server
# http://www.cryst.ehu.es
# Date: 07/07/2026 05:33:05
# MnPyz.cif

data_5y0htAoR
_audit_creation_date      2026-07-07
_audit_creation_method    "Bilbao Crystallographic Server"

_citation_journal_abbrev  ?
_citation_journal_volume  ?
_citation_page_first      ?
```

- MVisualize lets you quickly view the candidate magnetic structure.
- But we will use the downloaded mcif to fit data using fullprof.

MVisualize: 3D Visualization of magnetic structures with Jmol

MVisualize Main Page

Show/Hide File

BNS: $P 2_1/c$

Working unit cells shown: a, b, c

JSmol

Buttons: Select cell..., Toggle Parent Cell, Toggle Standard Cell, View Along Axis..., Unit Cell Info, All / Magnetic Atoms, Show/Hide Labels, Larger, Smaller, Vectors, Atoms, Window Size, Bigger, Smaller, Background Color, Toggle Quality, Center, Export PNG Image, Save PNG-3D, Save ZIP file, Show unit cell a,b,c, Add 1 cell along x, Remove 1 cell along x, Add 1 cell along y, Remove 1 cell along y, Add 1 cell along z, Remove 1 cell along z, x=1 y=1 z=1, Choose supercell, Draw bonds & polyhedra, Join, with, from 0.75 to 2.75 Å, Draw, Bonds, Polyhedra, Delete, Bonds, Polyhedra, Clear all drawings

Step 3: Create candidate magnetic models using BCS

- For this example we will choose the allowed magnetic structure $P2_1'/c$ (#14.77)
- But all should be checked to ensure the solution is uniquely correct or to determine equivalent solutions. For the paper this was done!
- If none of the maximal space groups work → go to a subgroup

Step 3: Create candidate magnetic models using BCS

N	Group (BNS)	Transformation matrix	General positions	Properties	Magnetic structure
1	$P2_1'/c$ (#14.79) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
2	$P2_1'/c$ (#14.78) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
3	$P2_1'/c$ (#14.77) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
4	$P2_1'/c$ (#14.75) Go to a subgroup	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show

- For this example we will choose the allowed magnetic structure $P2_1'/c$ (#14.77), number 3 on the list.
- But all should be checked to ensure the solution is uniquely correct or to determine equivalent solutions. For the paper this was done!
- If none of the maximal space groups work
→ go to a subgroup

Selected magnetic space group: 3- $P2_1'/c$ (#14.77)

Setting of the parent group

Parent space group $P2_1'/c$ (No. 14)

Lattice parameters: a=10.19000, b=10.90600, c=10.11600, alpha=90.000000, beta=107.960, gamma=90.000000

2. Click export/view

2. [\[Go to setting standard \(a, b, c ; 0, 0, 0\)\]](#)
[\[Go to alternative setting\]](#)
[Export data to MCIF file/Visualize](#) [Go to a subgroup](#)

1. Input values for magnetic moment

Atomic positions, Wyckoff positions and Magnetic Moments

N	Atom	New WP	Multiplicity	Magnetic moment	Values of M_x, M_y, M_z
1	Mn1 Mn 0.51009 0.13426 0.59800	(x,y,z m_x, m_y, m_z) (-x,y+1/2,-z+1/2 $m_x, -m_y, m_z$) (-x,-y,-z $-m_x, -m_y, -m_z$) (x,-y+1/2,z+1/2 $-m_x, m_y, -m_z$)	4	(M_x, M_y, M_z)	$M_x = 1.1$ $M_y = 1.2$ $M_z = 1.3$

Step 3: Create candidate magnetic models using BCS

mCIF file of the structure

Submit this mcif file to MVSUALIZE for 3D visualization of the estrutura using Jmol:

Submit to MVISUALIZE

Download mCIF file: [bcs_file.mcif](#)

~~[The preview text below is non-editable, only copy-allowed]~~

The mcif file is displayed.

This can be downloaded by clicking on “bcs_file.mcif”

We now need
to go to Step 4

```
#\#CIF_2.0
# Created by the Bilbao Crystallographic Server
# http://www.cryst.ehu.es
# Date: 08/07/2026 16:35:11
# MnPyz_1p5K_nuclear.cif

data_5y0htAoR
_audit_creation_date          2026-07-08
_audit_creation_method        "Bilbao Crystallographic Server"

_citation_journal_abbrev      ?
_citation_journal_volume      ?
_citation_page_first          ?
_citation_page_last           ?
_citation_article_id           ?
_citation_year                 ?
_citation_DOI                  ?

loop_
_citation_author_name
?

_atomic_positions_source_database_code_ICSD ?
_atomic_positions_source_other              ?

_transition_temperature ?
_experiment_temperature ?

loop_
_irrep_id
_irrep_dimension
_irrep_small_dimension
_irrep_direction_type
_irrep_action
_irrep_modes_number
_irrep_presence
```


Mn-pyrazinecarboxylate

This example will use Fullprof and Bilbao Crystallographic Server (BCS) <https://cryst.ehu.es/>

- Step 0: Have a well characterized material and good background information
- 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 BCS
- **Step 4: Refine the magnetic space group in Fullprof.**
- Step 5: Check the magnetic model

Step 4: Refine the magnetic space group in Fullprof [Create pcr]

- We have the magnetic space group information in the mcif. We now want to create the Fullprof pcr file.
- There are two ways:
 - Stay in BCS and use that
 - Load mcif directly into Fullprof

This example will use the BSC

Step 4: Refine the magnetic space group in Fullprof [Create pcr]

- Go back to the main page on server and open mCIF2PCR

bilbao crystallographic server

Contact us	About us	Publications	How to cite the server
Space-group symmetry			
Magnetic Symmetry and Applications			
Magnetic groups			
MGENPOS		General Positions of Magnetic Space Groups	
MWYCKPOS		Wyckoff Positions of Magnetic Space Groups	
MKVEC		The k-vector types and Brillouin zones of Magnetic Space Groups	
IDENTIFY MAGNETIC GROUP		Identification of a Magnetic Space Group from a set of generators in an arbitrary setting	
RNS2OG		Transformation of symmetry operations between RNS and OG settings	
mCIF2PCR		Transformation from mCIF to PCR format (FullProf).	
MAGNEXT		Extinction Rules of Magnetic Space Groups	
MAXMAGN		Maximal magnetic space groups for a given space group and a propagation vector	
MAGMODELIZE		Magnetic structure models for any given magnetic symmetry	
STRCONVERT		Convert & Edit Structure Data (supports the CIF, mCIF, VESTA, VASP formats -- with magnetic information where available)	
k-SUBGROUPSMAG		Magnetic subgroups consistent with some given propagation vector(s) or a supercell	
MAGNDATA		A collection of magnetic structures with portable cif-type files	
MVISUALIZE		3D Visualization of magnetic structures with Jmol	
MTENSOR		Symmetry-adapted form of crystal tensors in magnetic phases	
MAGNETIC REP.		Decomposition of the magnetic representation into irreps	
Get_mirreps		Irreps and order parameters in a paramagnetic space group- magnetic subgroup phase transition	
Spin groups			
SPGENPOS ⚠		General positions of spin point groups	
STENSOR ⚠		Symmetry-adapted form of crystal tensors under spin point groups	
CollinearSpinGroups ⚠		Operations of Nontrivial Collinear Spin Space Groups	

Step 4: Refine the magnetic space group in Fullprof [Create pcr]

mCIF2PCR: Transformation from mCIF to PCR format (FullProf).

mCIF_to_PCR
Given a magCIF file, it produces a PCR template that can be used as input for FullProf (the program mCIF_to_PCR (FullProf) is used). By default the provided PCR file is intended for a simulation. The file can be then modified by hand for a refinement of the model.

Choose a structure file (mCIF format):

MnPyz_BCS.mcif

[1]

[2]

[1] Choose the mcif we just created through MAXMAGN

[2] Click convert

The file has been successfully converted.

[Click to download it](#)

This will convert the file and “Click to download it” will download the .pcr file



Step 4: Refine the magnetic space group in Fullprof

- Pcr file created contains a single phase with crystal structure and magnetic ions described by a magnetic space group.
 - The initial downloaded pcr file from BCS calculates the pattern based on default values.
 - **We need to change the defaults in the .pcr file in the same way as done for the examples created from a .cif file.**
-
- **Two ways to do this:**
 - 1: Repeat step 1 to re-refine the nuclear structure by working down the Tabs in the GUI (General/Patterns/Phases/Refinement) and/or edit the text file.
 - 2: Start from the already refined nuclear pcr and do some copy and pasting.

Copy and pasting is easier and quicker, so we'll do that

Step 4: Refine the magnetic space group in Fullprof

- Start with the nuclear refinement .pcr file already done for MnPyz.
 - This was either done following all the previous steps in these slides, or as part of a separate example.
 - My pcr file is named “MnPyz_1p5K.pcr”. It is in the same folder as the data “MnPyz_1p5K.dat”

- This contains the magnetic space group details.

Data for PHASE number: 1 ==> Current R_Bragg for Pattern# 1: 999.00

Nuclear and Magnetic Structure of: MnPyz_BCS VARY mxmymz

Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nvk Npr More
25 0 0 0.0 0.0 1.0 10 0 2 0 0 0.000 0 7 0

P2_1'/c number:14.77 <--Magnetic Space group symbol (BNS symbol & number)

Transform to standard: a,b,c;0,0,0

Parent Space Group: P2_1/c IT_number: 14

Transform from Parent: a,b,c;0,0,0

Nsym Cen N_Clat N_Ant
4 0 0 0

Symmetry operators

1 x,y,z,+1

2 -x,-y,-z,-1

3 x,-y+1/2,z+1/2,+1

4 -x,y+1/2,-z+1/2,-1

Atom	Typ	Mag	Vek	X	Y	Z	Biso	Occ	N_type	Spc
	Rx	Ry		Rz	Ix	Iy	Iz	MagPh	Line below:Codes	below:C
Mn1	MMN2	1 0	0	0.51356	0.12895	0.60217	0.00000	1.00000	1 0	#
				0.00	0.00	0.00	0.00	0.00		
	1.10000	1.20000	1.30000	0.00000	0.00000	0.00000	0.00000	0.00000	<--MagPar	
	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00		
O1	O	1 0	0	0.54868	0.24635	0.42955	0.00000	1.00000	0 0	#
				0.00	0.00	0.00	0.00	0.00		
N1	N	1 0	0	0.36244	0.30105	0.56440	0.00000	1.00000	0 0	#
				0.00	0.00	0.00	0.00	0.00		
C1	C	1 0	0	0.26705	0.31210	0.62293	0.00000	1.00000	0 0	#
				0.00	0.00	0.00	0.00	0.00		
H1	H	1 0	0	0.24226	0.24571	0.66885	0.00000	1.00000	0 0	#
				0.00	0.00	0.00	0.00	0.00		
O2	O	1 0	0	0.47150	0.40957	0.28321	0.00000	1.00000	0 0	#
				0.00	0.00	0.00	0.00	0.00		
N2	N	1 0	0	0.17238	0.49489	0.47494	0.00000	1.00000	0 0	#
				0.00	0.00	0.00	0.00	0.00		
C2	C	1 0	0	0.15921	0.40664	0.56866	0.00000	1.00000	0 0	#
				0.00	0.00	0.00	0.00	0.00		
H2	H	1 0	0	0.10169	0.42860	0.62270	0.00000	1.00000	0 0	#
				0.00	0.00	0.00	0.00	0.00		
O3	O	1 0	0	0.63589	0.99360	0.53074	0.00000	1.00000	0 0	#
				0.00	0.00	0.00	0.00	0.00		
N3	N	1 0	0	0.73160	0.18010	0.70183	0.00000	1.00000	0 0	#
				0.00	0.00	0.00	0.00	0.00		
C3	C	1 0	0	0.27027	0.46870	0.41733	0.00000	1.00000	0 0	#
				0.00	0.00	0.00	0.00	0.00		
H3	H	1 0	0	0.27886	0.53942	0.33280	0.00000	1.00000	0 0	#
				0.00	0.00	0.00	0.00	0.00		
O4	O	1 0	0	0.80942	0.97300	0.47011	0.00000	1.00000	0 0	#
				0.00	0.00	0.00	0.00	0.00		
N4	N	1 0	0	0.02037	0.23074	0.77219	0.00000	1.00000	0 0	#
				0.00	0.00	0.00	0.00	0.00		
C4	C	1 0	0	0.37122	0.39433	0.46301	0.00000	1.00000	0 0	#
				0.00	0.00	0.00	0.00	0.00		
C5	C	1 0	0	0.48774	0.34148	0.39952	0.00000	1.00000	0 0	#
				0.00	0.00	0.00	0.00	0.00		
C6	C	1 0	0	0.81776	0.26713	0.79909	0.00000	1.00000	0 0	#
				0.00	0.00	0.00	0.00	0.00		
H4	H	1 0	0	0.72837	0.31267	0.85696	0.00000	1.00000	0 0	#
				0.00	0.00	0.00	0.00	0.00		
C7	C	1 0	0	0.93956	0.27897	0.83592	0.00000	1.00000	0 0	#
				0.00	0.00	0.00	0.00	0.00		
H5	H	1 0	0	0.96853	0.33513	0.91943	0.00000	1.00000	0 0	#
				0.00	0.00	0.00	0.00	0.00		
C8	C	1 0	0	0.97946	0.13864	0.67951	0.00000	1.00000	0 0	#
				0.00	0.00	0.00	0.00	0.00		
H6	H	1 0	0	0.03201	0.08974	0.64397	0.00000	1.00000	0 0	#
				0.00	0.00	0.00	0.00	0.00		
C9	C	1 0	0	0.82851	0.11546	0.64167	0.00000	1.00000	0 0	#
				0.00	0.00	0.00	0.00	0.00		
C10	C	1 0	0	0.75618	0.02305	0.54995	0.00000	1.00000	0 0	#
				0.00	0.00	0.00	0.00	0.00		

!-----> Profile Parameters for Pattern # 1

Data for PHASE number: 1 ==> Current R_Bragg for Pattern# 1: 0.0000

Atom	Typ	X	Y	Z	Biso	Occ	In	Fin	N_t	Spc	/Codes
Mn1	Mn	0.51356	0.12895	0.60217	0.30004	1.00000	0	0	0	0	
		0.00	0.00	0.00	0.00	0.00					
O1	O	0.54868	0.24635	0.42955	0.30004	1.00000	0	0	0	0	
		0.00	0.00	0.00	0.00	0.00					
N1	N	0.36244	0.30105	0.56440	0.30004	1.00000	0	0	0	0	
		0.00	0.00	0.00	0.00	0.00					
C1	C	0.26705	0.31210	0.62293	0.30004	1.00000	0	0	0	0	
		0.00	0.00	0.00	0.00	0.00					
H1	H	0.24226	0.24571	0.66885	0.30004	1.00000	0	0	0	0	
		0.00	0.00	0.00	0.00	0.00					
O2	O	0.47150	0.40957	0.28321	0.30004	1.00000	0	0	0	0	
		0.00	0.00	0.00	0.00	0.00					
N2	N	0.17238	0.49489	0.47494	0.30004	1.00000	0	0	0	0	
		0.00	0.00	0.00	0.00	0.00					
C2	C	0.15921	0.40664	0.56866	0.30004	1.00000	0	0	0	0	
		0.00	0.00	0.00	0.00	0.00					
H2	H	0.10169	0.42860	0.62270	0.30004	1.00000	0	0	0	0	
		0.00	0.00	0.00	0.00	0.00					
O3	O	0.63589	-0.00641	0.53074	0.30004	1.00000	0	0	0	0	
		0.00	0.00	0.00	0.00	0.00					
N3	N	0.73160	0.18010	0.70183	0.30004	1.00000	0	0	0	0	
		0.00	0.00	0.00	0.00	0.00					
C3	C	0.27027	0.46870	0.41733	0.30004	1.00000	0	0	0	0	
		0.00	0.00	0.00	0.00	0.00					
H3	H	0.27886	0.53942	0.33280	0.30004	1.00000	0	0	0	0	
		0.00	0.00	0.00	0.00	0.00					
O4	O	0.80942	-0.02701	0.47011	0.30004	1.00000	0	0	0	0	
		0.00	0.00	0.00	0.00	0.00					
N4	N	1.02037	0.23074	0.77219	0.30004	1.00000	0	0	0	0	
		0.00	0.00	0.00	0.00	0.00					
C4	C	0.37122	0.39433	0.46301	0.30004	1.00000	0	0	0	0	
		0.00	0.00	0.00	0.00	0.00					
C5	C	0.48774	0.34148	0.39952	0.30004	1.00000	0	0	0	0	
		0.00	0.00	0.00	0.00	0.00					
C6	C	0.81776	0.26713	0.79909	0.30004	1.00000	0	0	0	0	
		0.00	0.00	0.00	0.00	0.00					
H4	H	0.72837	0.31267	0.85696	0.30004	1.00000	0	0	0	0	
		0.00	0.00	0.00	0.00	0.00					
C7	C	0.93956	0.27897	0.83592	0.30004	1.00000	0	0	0	0	
		0.00	0.00	0.00	0.00	0.00					
H5	H	0.96853	0.33513	0.91943	0.30004	1.00000	0	0	0	0	
		0.00	0.00	0.00	0.00	0.00					
C8	C	0.97946	0.13864	0.67951	0.30004	1.00000	0	0	0	0	
		0.00	0.00	0.00	0.00	0.00					
H6	H	1.03201	0.08974	0.64397	0.30004	1.00000	0	0	0	0	
		0.00	0.00	0.00	0.00	0.00					
C9	C	0.82851	0.11546	0.64167	0.30004	1.00000	0	0	0	0	
		0.00	0.00	0.00	0.00	0.00					
C10	C	0.75618	0.02305	0.54995	0.30004	1.00000	0	0	0	0	
		0.00	0.00	0.00	0.00	0.00					

!-----> Profile Parameters for Pattern # 1 -----> Phase # 1

Step 4: Refine the magnetic space group in Fullprof

*****NOTE: the only other place that could need to be changed is the lattice constants*****

Since the k-vector here is (0,0,0) then the original nuclear unit cell is the same size as the magnetic unit cell.

If the k-vector was non-zero then the magnetic space group takes this into account by changing the unit cell size.

e.g. for (0.5,0,0) the new magnetic space group unit cell would be 2a,b,c.

Check the value in both pcr files to see if they are different

Step 4: Refine the magnetic space group in Fullprof

The pcr file now has this line, which by default ALWAYS refines the magnetic moments. We will leave it, but if your model is not close, then it can cause problems when you run the refinements

Nuclear and Magnetic Structure of: MnPyz_BCS VARY mxmymz

Step 4: Refine the magnetic space group in Fullprof

In “Refinement” →
“atoms” input thermal
parameters (0.3).

[1,2,3]

Note that Re(x) and
Re(z) are set to refine.

This is a default in files
from mcif to pcr that we
will turn off in next
slide.

The screenshot displays the FullProf PCR Editor window. The main window shows a plot of intensity versus 2θ (degrees) with the text "FullProf PCR Editor" overlaid. The "Information" panel on the right has tabs for General, Patterns, Phases, and Refinement. The "Phases" tab is selected and circled in red, with a red "1" next to it. Below this, the "Refinement Information" panel shows "Cycles of Refinement" set to 10. The "Stop Criterion of Coverage" is set to "Forced Termination when shifts < 0.10 x E.S.D.". The "Relaxation Factors for Shifts" are set to Atomic: 1.00, Anisotropic: 1.00, Profile: 1.00, and Global: 1.00. The "Reflections ordering" is set to "Only at the first cycle". The "Atoms Information: Phase 1" panel shows a list of atoms with columns for Label, Ntype, Mag. Rot., Prog. V..., X, Y, Z, B, and Occ. The "List of Atoms" panel shows the number of atoms set to 25. The "Atoms" panel at the bottom shows the refinement parameters for Atom #1, with Re[x], Re[y], and Re[z] set to 1.10000, 1.20000, and 1.30000 respectively, all checked for refinement. The "Atoms" tab in the "Refinement Information" panel is circled in red, with a red "2" next to it.

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MnPyz_1p5K

Atoms Information: Phase 1

List of Atoms

Number of Atoms: 25

	Label	Ntype	Mag. Rot.	Prog. V...	X	Y	Z	B	Occ
Atom # 1	Mn1	MMN2	1	0	0.51356	0.12895	0.60217	0.00000	1.00000
Atom # 2	O1	O	1	0	0.54868	0.24635	0.42955	0.00000	1.00000
Atom # 3	N1	N	1	0	0.36244	0.30105	0.56440	0.00000	1.00000
Atom # 4	C1	C	1	0	0.26705	0.31210	0.62293	0.00000	1.00000

	Re[x]	Re[y]	Re[z]	Im[x]	Im[y]	Im[z]	MPhase
Atom #1	1.10000	1.20000	1.30000	0.00000	0.00000	0.00000	0.00000

Refinement Information

Cycles of Refinement: 10

Stop Criterion of Coverage

Forced Termination when shifts < 0.10 x E.S.D.

Others: None

Reflections ordering

Only at the first cycle

Each cycle

Relaxation Factors for Shifts

Atomic: 1.00 Anisotropic: 1.00 Profile: 1.00 Global: 1.00

Bragg R-Factor excluding reflections limiting excluded regions

Phase 1 Phase 2 Phase 3 Phase 4 Phase 5 Phase 6

Atoms

Prop. Vectors

Refine Positions

Refine B_iso

Refine B_aniso

Fix All

Cancel

OK

Profile

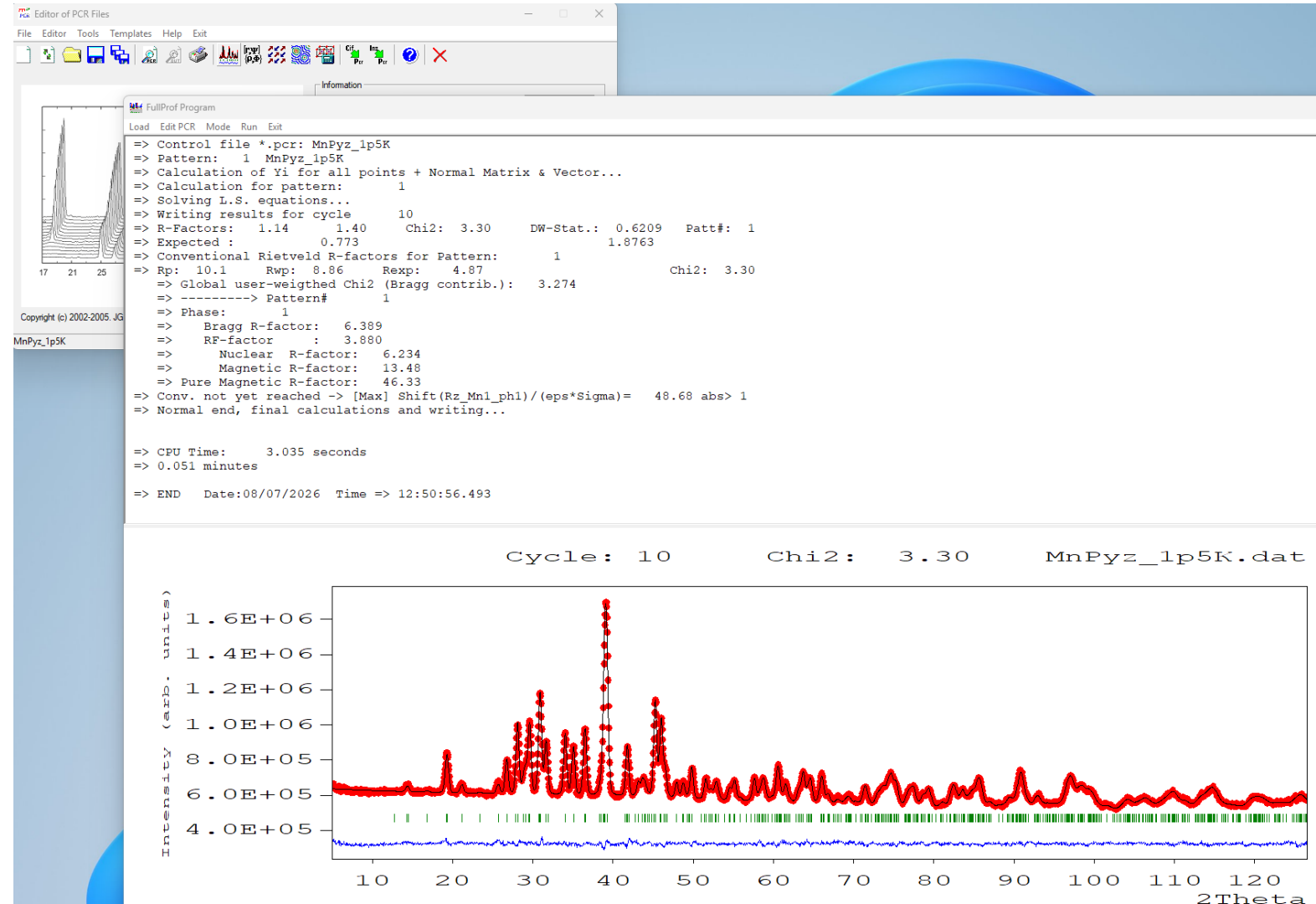
Micro-Structure

HKL Shifts

Further Parameters

Step 4: Refine the magnetic space group in Fullprof

- Since we're starting from parameters that worked already for the nuclear phase at 1.5K, then we should be close and just want to test the magnetic moments.
- Run the refinement using the 1.5K data.
- The fit works well.
- Try refining the background, lattice constants to get a slightly improved fit.



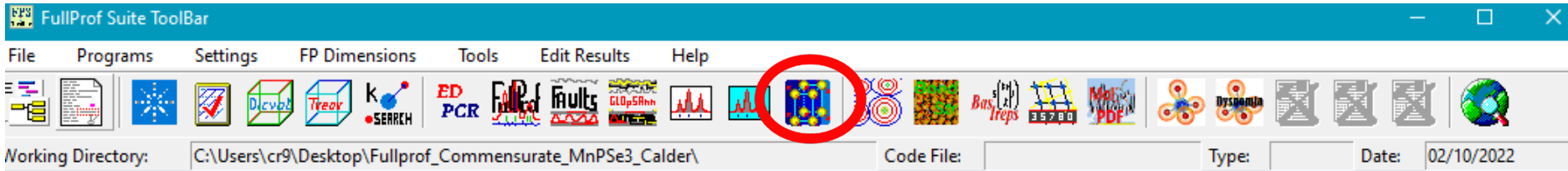
Mn-pyrazinecarboxylate

This example will use Fullprof and Bilbao Crystallographic Server (BCS) <https://cryst.ehu.es/>

- Step 0: Have a well characterized material and good background information
- 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 BCS
- Step 4: Refine the magnetic space group in Fullprof.
- **Step 5: Check the magnetic model**

Step 5: Check the magnetic model

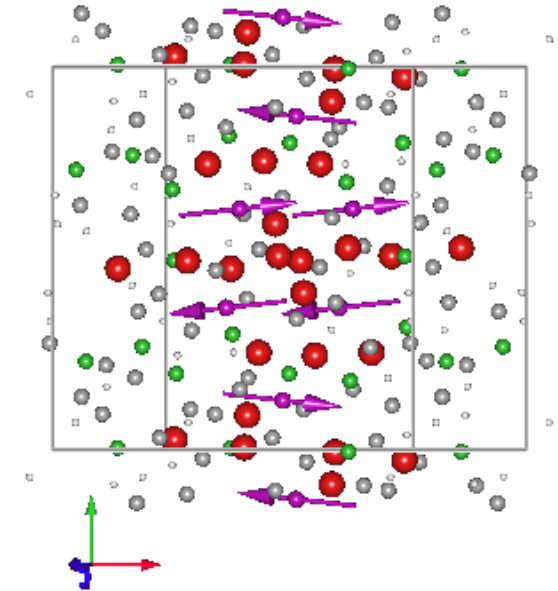
The model can be checked in FPStudio



- There is an .fst file that can be used. Open the magnetic phase
- In Fpstudio click on the drop-down menu “Magnetic Structure” and select “List magnetic moments”

MnPyz_1p5K
MnPyz_1p5K
MnPyz_1p5K.sum
MnPyz_1p5K1
MnPyz_1p5K1

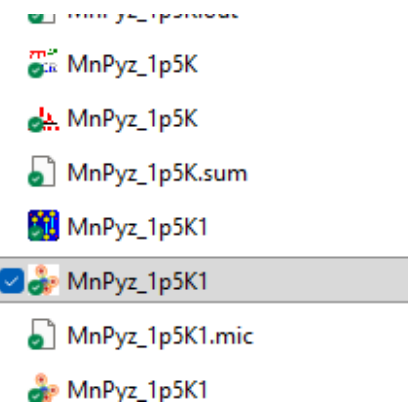
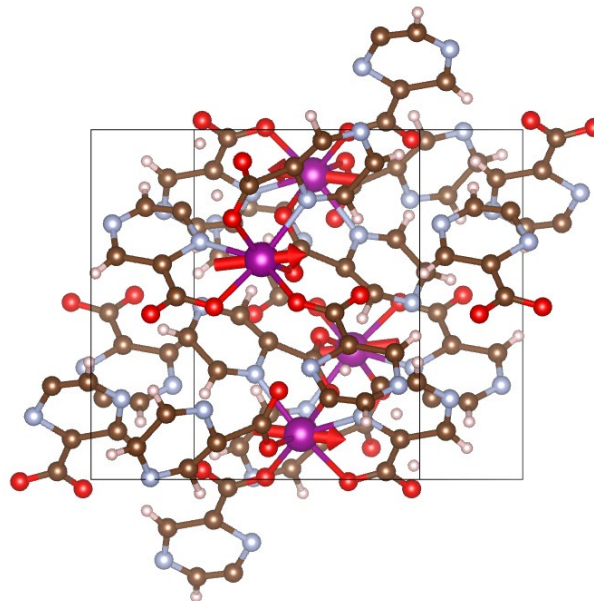
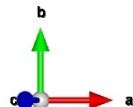
```
| Magnetic lattice type : P
unit Cell: 10.1751 10.8096 10.0768 90.0000 108.4356 90.0000
Current Box: 0 1 0 1 0 1
Magnetic k-vectors :
0.00000 0.00000 0.00000
Type of Fourier coefficients: S
Symmetry operations :
SYMM x,y,z
u,v,w,0,0
SYMM -x,-y,-z
u,-v,-w,0,0
SYMM x,-y+1/2,z+1/2
-u,v,-w,0,0
SYMM -x,y+1/2,-z+1/2
u,-v,w,0,0
Atom : Mn1 Mn
x y z Translation k MSYM m(a) m(b) m(c) Mtot
0.51356 0.12895 0.60217 ( 0, 0, 0) 1 1 3.74005 -0.37366 1.17747
( 0, 1, 0) 1 1 3.74005 -0.37366 1.17747 3.56773
( 0, 0, 0) 1 1 3.74005 -0.37366 1.17747 3.56773
0.48644 0.87105 0.39783 ( 0, -1, 0) 1 1 -3.74005 0.37366 -1.17747
( 0, 0, 0) 1 1 -3.74005 0.37366 -1.17747 3.56773
( 0, 0, 1) 1 1 -3.74005 -0.37366 -1.17747 3.56773
0.51356 0.37105 0.10217 ( 0, 0, 0) 1 1 -3.74005 -0.37366 -1.17747
( 0, 0, 1) 1 1 -3.74005 -0.37366 -1.17747 3.56773
( 0, 0, 0) 1 1 -3.74005 -0.37366 -1.17747 3.56773
0.48644 0.62895 0.89783 ( 0, 0, -1) 1 1 3.74005 0.37366 1.17747
( 0, 0, 0) 1 1 3.74005 0.37366 1.17747 3.56773
( 0, 0, 0) 1 1 3.74005 0.37366 1.17747 3.56773
```



Step 5: Check the magnetic model

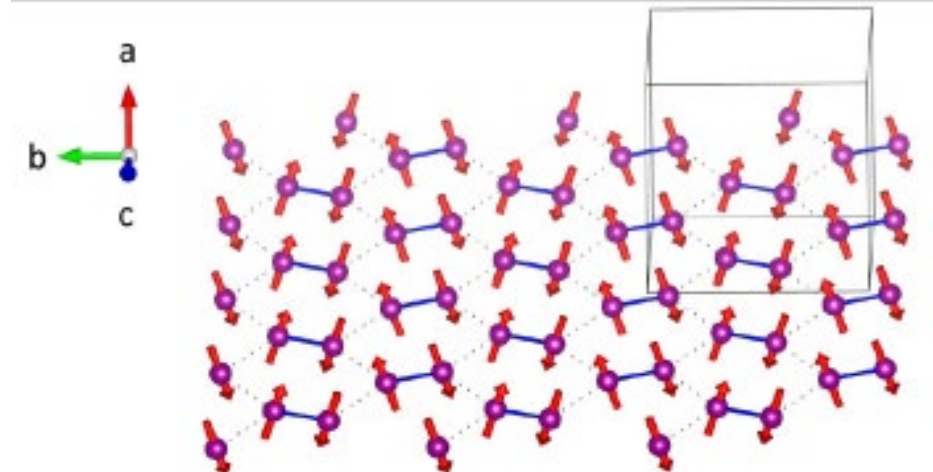
- There is also an mcif file created.
- Opening with a text editor shows the information. The magnetic moments are given at the end of the file.
- Opening with VESTA also gives this information and allows the magnetic structure to be visualized

The mcif in this case has all atoms (magnetic and non-magnetic).



```
loop_
  _atom_site_moment.label
  _atom_site_moment.crystalaxis_x
  _atom_site_moment.crystalaxis_y
  _atom_site_moment.crystalaxis_z
Mn1  3.74(7) -0.4(4)  1.2(2)

# Spherical components of magnetic moments (angles in
# degrees)
# Commented because current programs as VESTA, JMOL,
# etc. are unable to interpret them
#loop_
#  _atom_site_moment.label
#  _atom_site_moment.spherical_modulus
#  _atom_site_moment.spherical_azimuthal
#  _atom_site_moment.spherical_polar
```

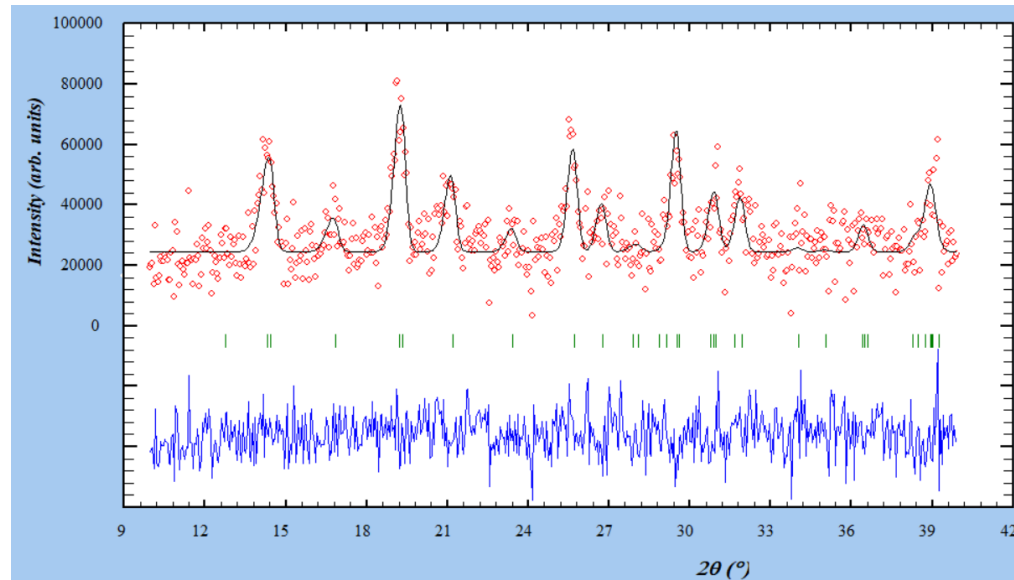


Step 5: Check the magnetic model

There is a dataset “diff_1p5Kminus20K_offset_so_no_negative_intensities.dat”. This is the difference between the 1.5 K data and the 20 K data. This can be treated as the magnetic only scattering. Use the keyword “mag_only” in the pcr file to refine only the magnetic contribution

Examples are in the backup folder. This will help to convince you of the best fit magnetic structure.

Look in the folder
\\Fullprof_MagneticSpaceGroup_Com
mensurate_MnPyz_Calder\\backup\\Mn
pyrazine_1p5Kminus20K_difference\\



Mn-pyrazinecarboxylate

Full details can be found in DOI:
[10.1103/PhysRevMaterials.7.124408](https://doi.org/10.1103/PhysRevMaterials.7.124408)

PHYSICAL REVIEW MATERIALS 7, 124408 (2023)

Magnetic order in the two-dimensional metal-organic framework manganese pyrazinecarboxylate with Mn-Mn dimers

S. Calder^{1,*}, R. Baral¹, N. Narayanan² and L. D. Sanjeewa^{2,3}

¹Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

²University of Missouri Research Reactor (MURR), University of Missouri, Columbia, Missouri 65211, USA

³Department of Chemistry, University of Missouri, Columbia, Missouri 65211, USA

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The magnetic properties of $[\text{Mn}(\text{pyrazinecarboxylate})_2]_n$, empirical formula $\text{C}_{10}\text{H}_6\text{MnN}_4\text{O}_4$, are investigated through susceptibility, heat capacity, and neutron scattering measurements. The structure consists of Mn-Mn dimers linked on a distorted 2D hexagonal structure. The weak out-of-plane interactions create a quasi-2D magnetic material within the larger three-dimensional metal-organic framework structure. We show that this material undergoes a two-stage magnetic transition, related to the low dimensionality of the Mn lattice. First, at 5 K, which is assigned to the initial development of short-range order in the 2D layers. This is followed by long-range order at 3.3 K. Applied field measurements reveal the potential to induce magnetic transitions in moderately small fields of ~ 2 T. Neutron powder diffraction enabled the determination of a unique magnetic space group $P2_1'/c$ (No. 14.77) at 1.5 K. This magnetic structure consists of antiferromagnetically coupled Mn-Mn dimers with spins principally along the out-of-plane a axis.

DOI: [10.1103/PhysRevMaterials.7.124408](https://doi.org/10.1103/PhysRevMaterials.7.124408)

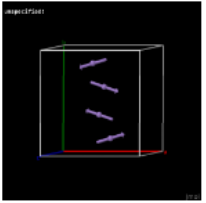
The magnetic structure is in the
MAGNDATA database

MAGNDATA: A Collection of magnetic structures with portable cif-type files Log

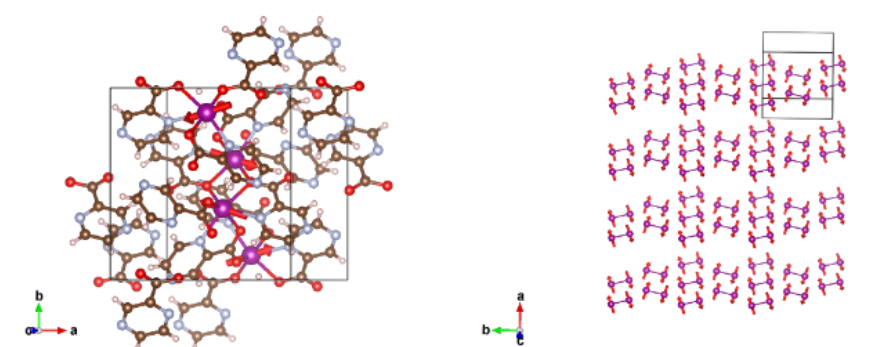
Element search (separate with space or comma): ☒ AND ☐ OR [View Full Database](#) [Advanced Search](#)

To upload any published structure click [HERE](#)

Enter the label of the structure:

 **C₁₀H₆MnN₄O₄ (#0.1010)**

[view in Jmol](#)
[Download mcif file](#)
[Download vesta file \(all atoms\)](#)
[Download vesta file \(magnetic atoms only\)](#)



Magnetic structure with all atoms Magnetic structure with only magnetic atoms

Reference: S. Calder, R. Baral, N. Narayanan, L. D. Sanjeewa, *PHYSICAL REVIEW MATERIALS* (2023) 7 124408
DOI: [10.1103/PhysRevMaterials.7.124408](https://doi.org/10.1103/PhysRevMaterials.7.124408)
Atomic positions from: Cai

Parent space group (paramagnetic phase): $P2_1/c$ (#14)
Propagation vector: k_1 (0, 0, 0)

Transition Temperature: 3.3 K
Experiment Temperature: 1.5 K

Lattice parameters of the magnetic unit cell:
10.2078(4) 10.8444(4) 10.1095(4) 90.00 108.429 90.00
Transformation from parent structure: (a,b,c,0,0,0)
[\[View matrix form\]](#)

BNS Magnetic Space Group: $P2_1'/c$ (#14.77) (standard setting)
[\[View symmetry operations\]](#)
Transformation to a standard setting: (a,b,c,0,0,0)