



July 22, 2026 | MagStr2026, Duke University

Fullprof refinement of commensurate structure from TOF data

PRESENTED BY

Danielle R. Yahne

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yahnedr@ornl.gov

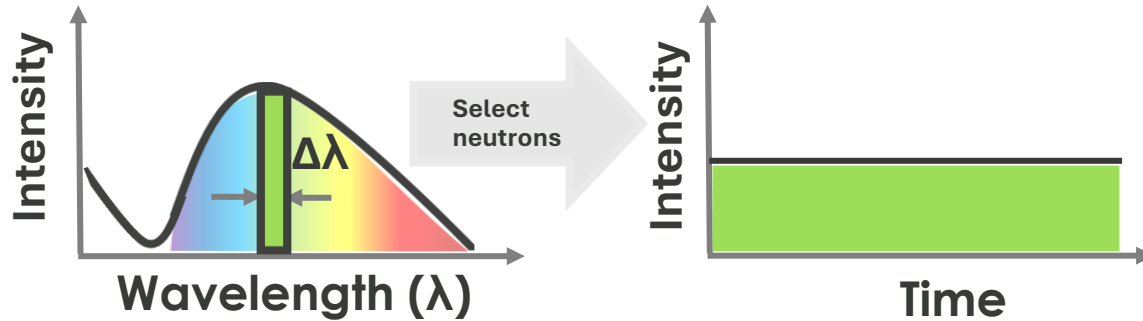
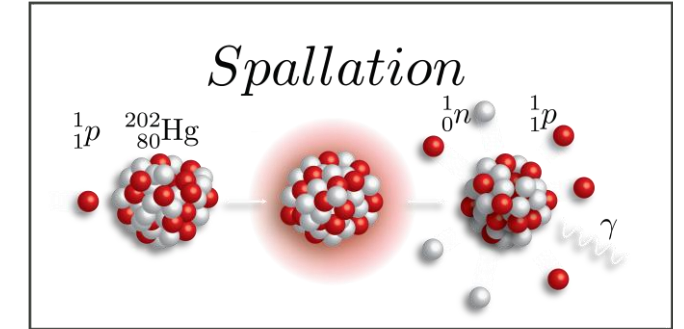
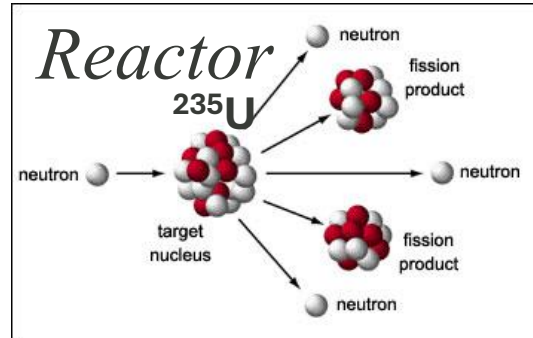
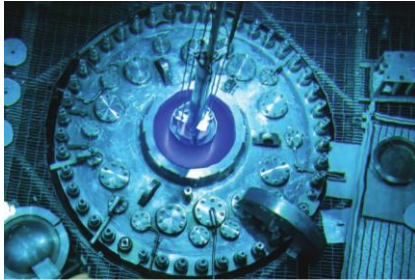


U.S. DEPARTMENT
of **ENERGY**

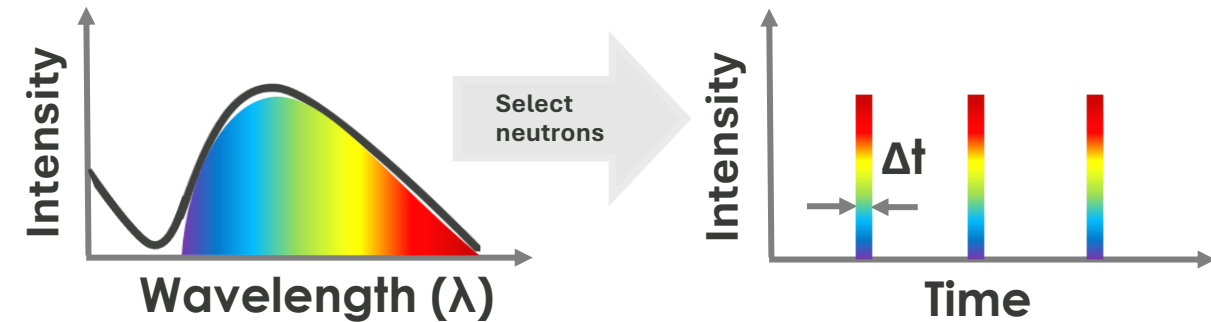
ORNL IS MANAGED BY UT-BATTELLE LLC
FOR THE US DEPARTMENT OF ENERGY



Neutron sources: Reactor (CW) and Spallation (TOF)



Small $\Delta\lambda$ used, but source on all the time



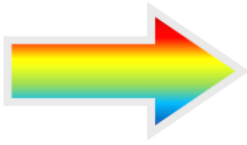
Each pulse of neutrons contains a broad spectrum of energy (λ)

Pulse of neutrons
~60 times per second

A typical CW diffractometer (HFIR)



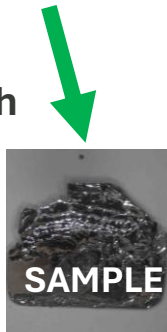
Reactor



Monochromator:

- selects λ .
- Control resolution.

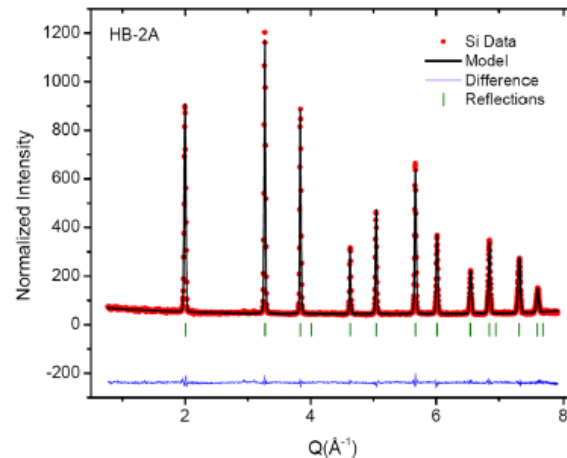
Single wavelength



Detector at 2θ measures single Q

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

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

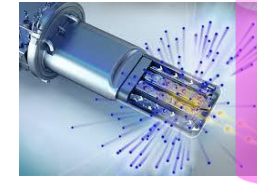


A typical TOF diffractometer (SNS)

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

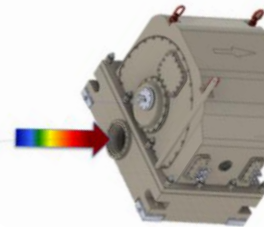
Bragg's law: $\lambda = 2d \sin \theta = \text{constant} * t$

Target



Moderator

Multiple wavelengths

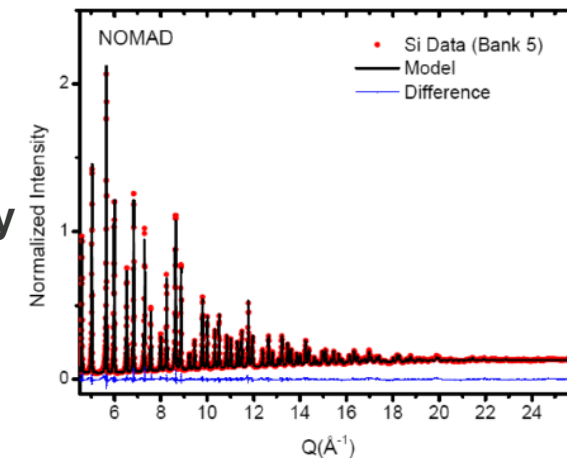


Chopper



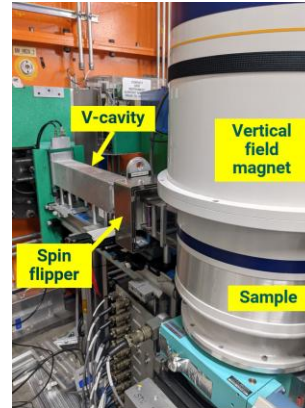
Resolution depends on moderator and t, L , and 2θ

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

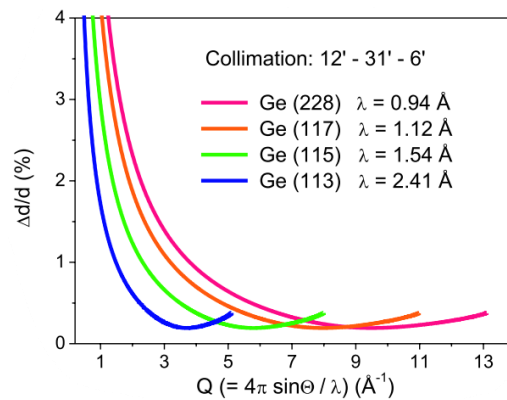
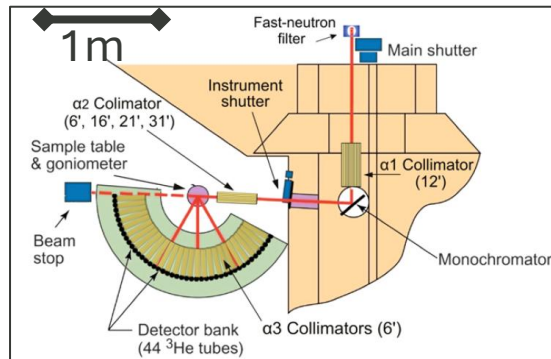


Detector at 2θ measures multiple Q

A typical CW diffractometer (HB-2A, HFIR)



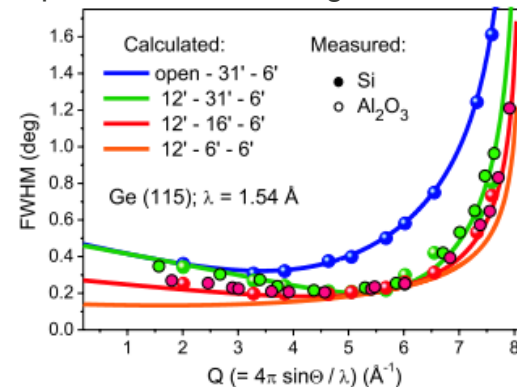
Versatile: open sample space and compact



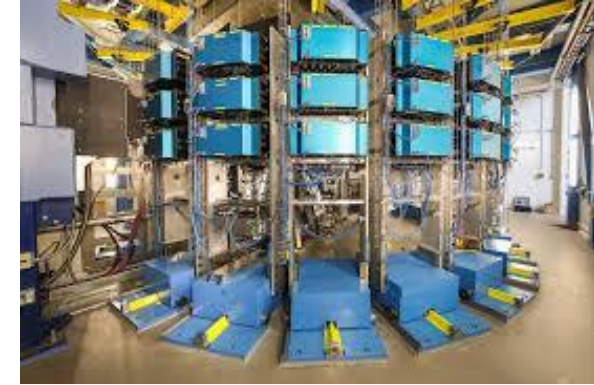
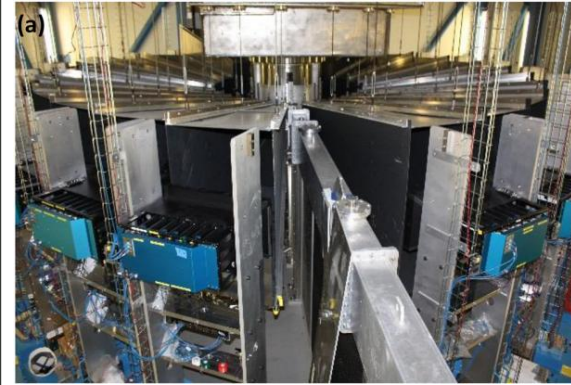
Ge(hkl)	λ (Å)	Q (Å ⁻¹)	Flux at sample (n/cm ² s)
(113)	2.41	0.2 - 5.1	5×10^6
(115)	1.54	0.35 - 7.9	1×10^7
(117)	1.12	0.5 - 10.9	4×10^6

Resolution:

best resolution $\Delta d/d$: 1×10^{-3}
Dependent on wavelengths and d



A typical TOF diffractometer (POWGEN, SNS)

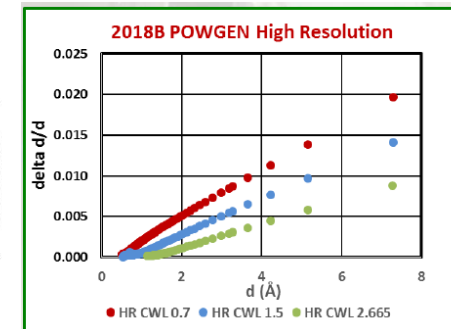
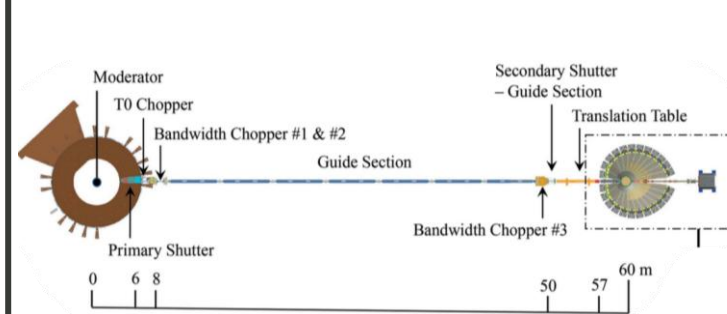


Larger, more detector coverage

Freq (Hz)	WL center	WL min	WL max	dmin	dmax	Qmin	Qmax	Bank
60	0.533	0.15	1.066	0.075	7.50	0.82	83.45	0
60	0.800	0.27	1.333	0.134	8.00	0.76	46.88	1
60	1.500	0.97	2.033	0.485	13.00	0.48	12.95	2
60	2.665	2.13	3.198	1.070	21.00	0.30	5.87	3
60	4.797	4.26	5.33	2.140	38.00	0.17	2.94	4

Resolution: best resolution $\Delta d/d$: 1×10^{-4}

Dependent on wavelengths and d



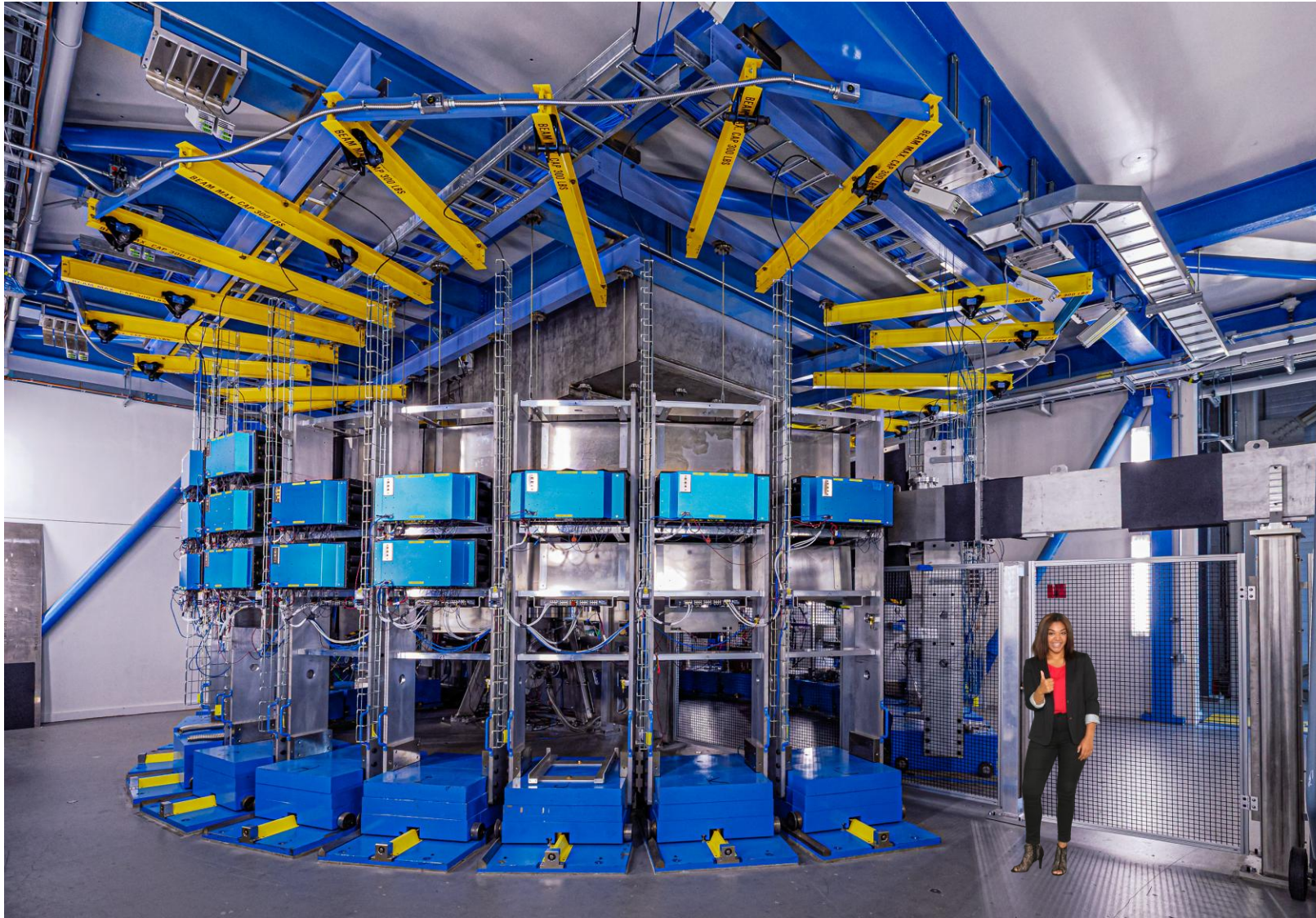
POWGEN Virtual Tour

POWGEN : High Resolution Powder Diffractometer



*"characterization of the
crystal, magnetic and
local structure of novel
polycrystalline materials"*

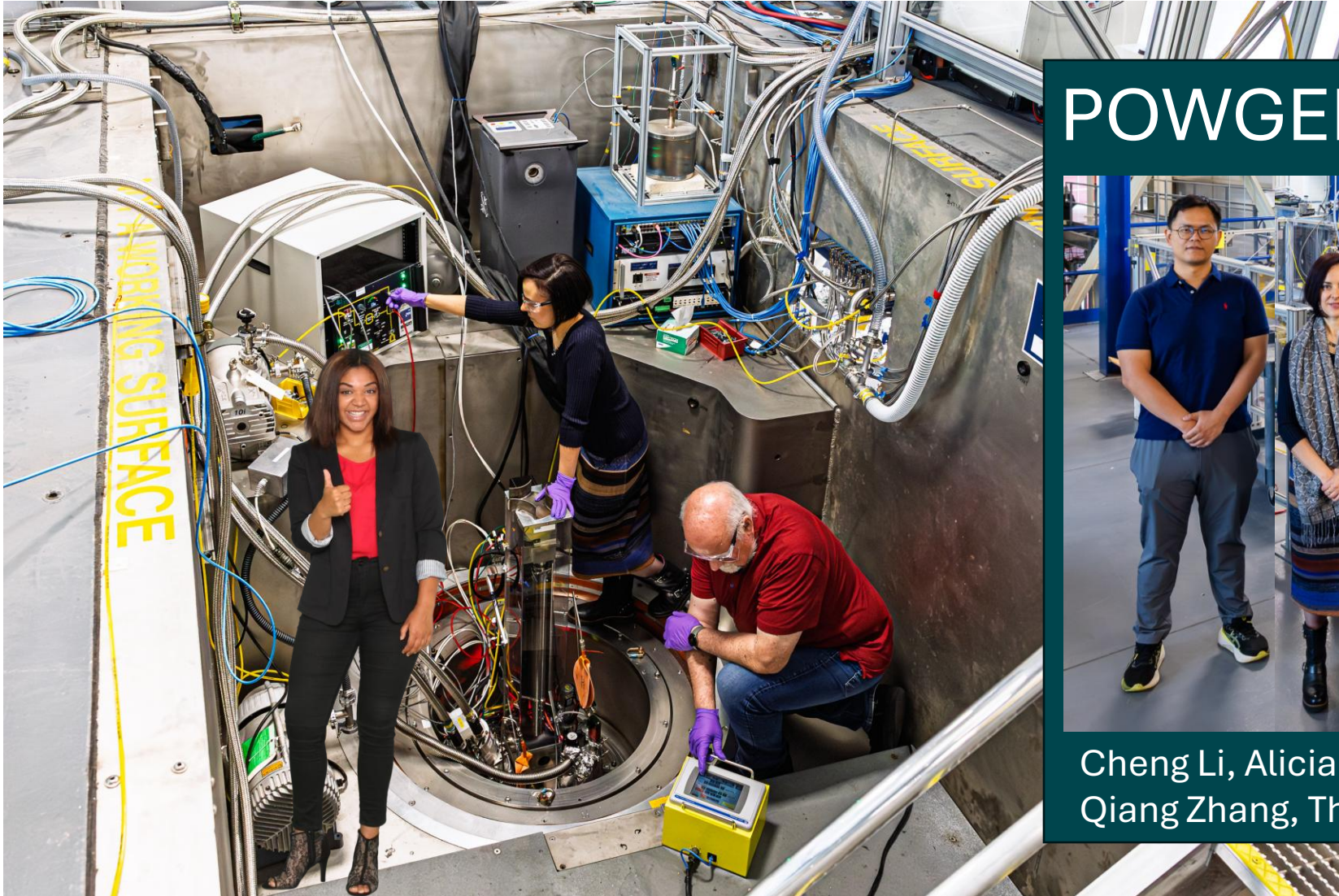
POWGEN : High Resolution Powder Diffractometer



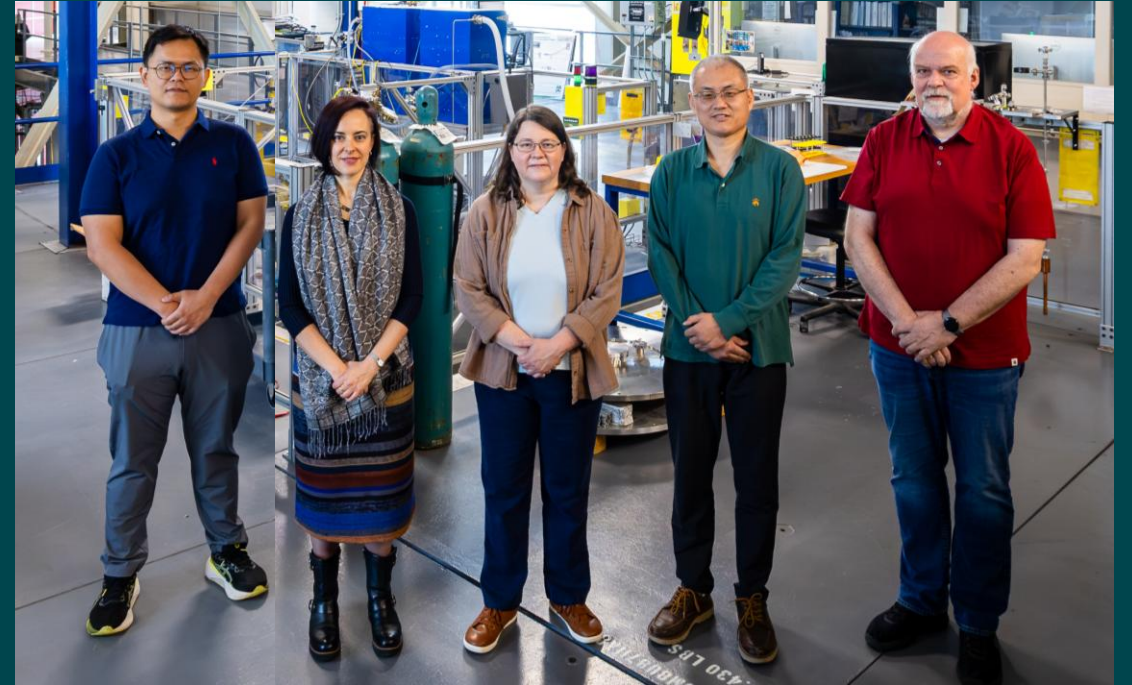
POWGEN : High Resolution Powder Diffractometer



POWGEN : High Resolution Powder Diffractometer



POWGEN Team



Cheng Li, Alicia Manjón Sanz, Melanie Kirkham,
Qiang Zhang, Thomas Proffen

POWGEN : High Resolution Powder Diffractometer

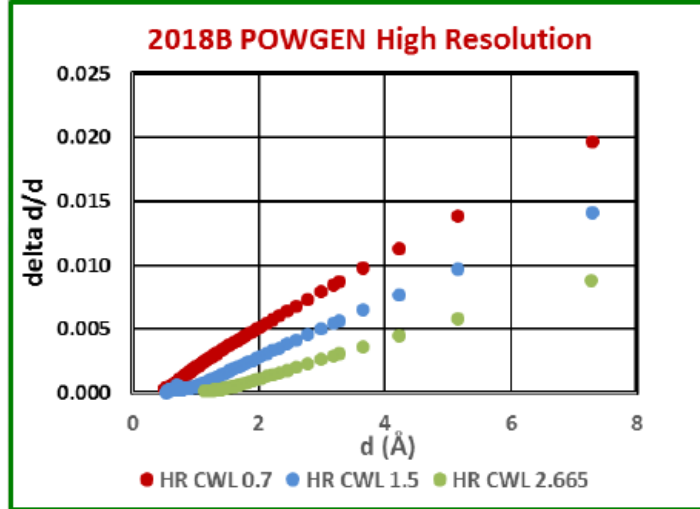
Freq (Hz)	WL center	WL min	WL max	dmin	dmax	Qmin	Qmax	Bank
60	0.533	0.15	1.066	0.075	7.50	0.82	83.45	0
60	0.800	0.27	1.333	0.134	8.00	0.76	46.88	1
60	1.500	0.97	2.033	0.485	13.00	0.48	12.95	2
60	2.665	2.13	3.198	1.070	21.00	0.30	5.87	3
60	4.797	4.26	5.33	2.140	38.00	0.17	2.94	4

$$\lambda = \frac{ht}{mL} = 2d \sin\theta$$

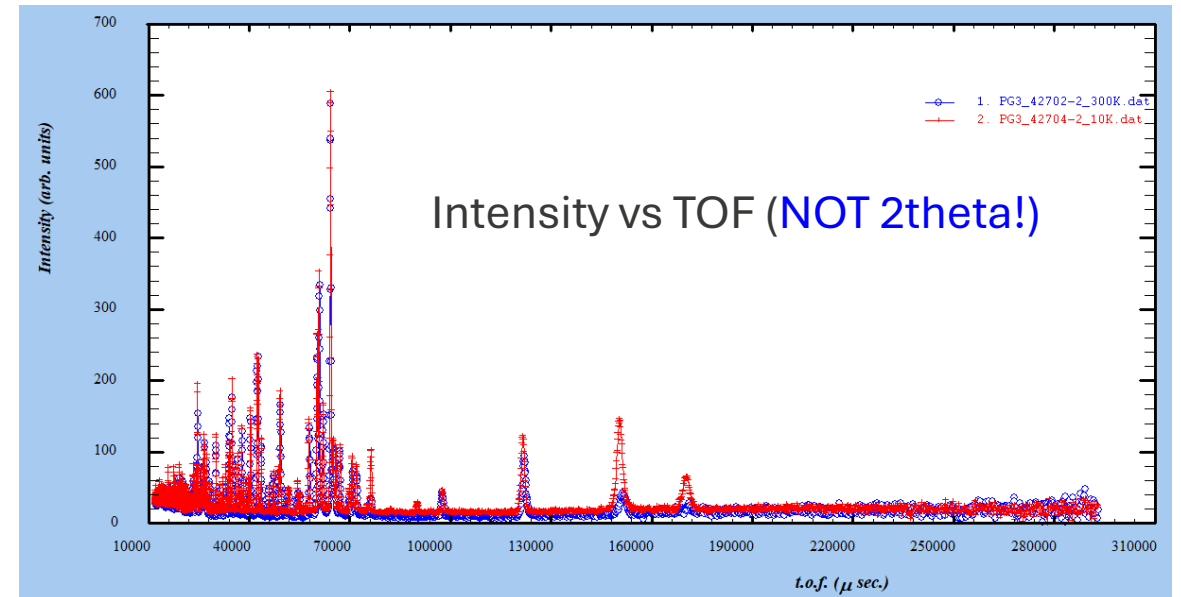
$$t.o.f. = d \frac{2mL}{h} \sin\theta$$

Known from calibration, C

Resolution: best resolution $\Delta d/d$: 1×10^{-4}



Dependent on wavelengths and d



POWGEN Peak Profile

“Convolution of back-to-back exponential with linear combination of Gaussian and Lorentzian (pseudo-Voigt)”

α : rise coefficient of exponential
– sharpness of leading TOF edge (larger = sharper)

β : decay coefficient of exponential
– sharpness of trailing TOF edge

σ : Gaussian contribution (larger = broader)

γ : Lorentzian contribution (larger = broader)

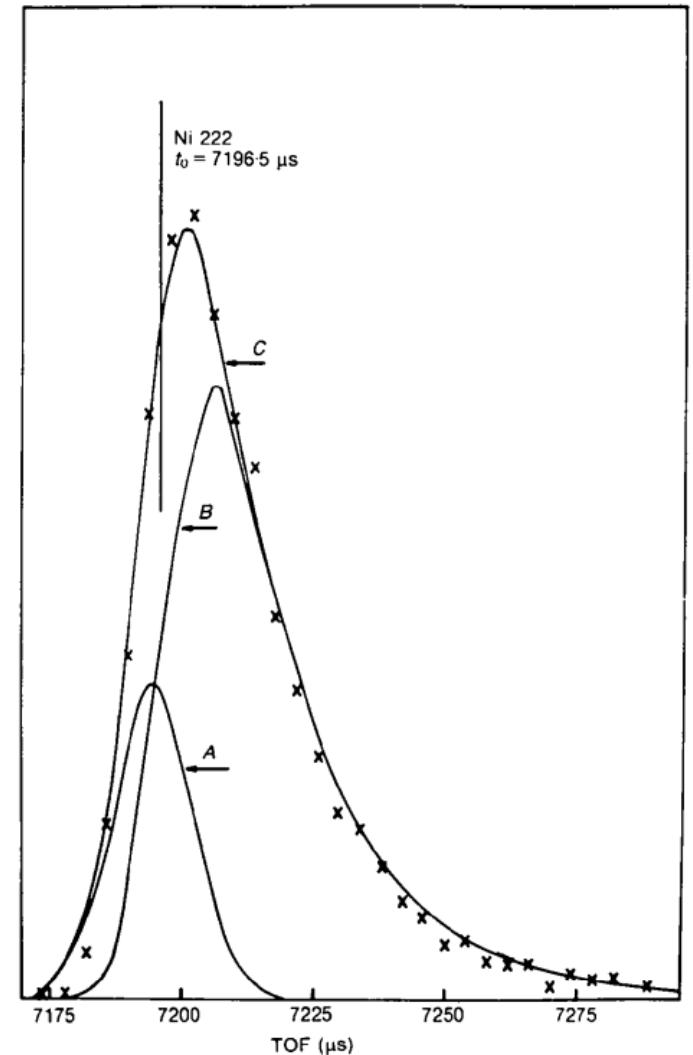
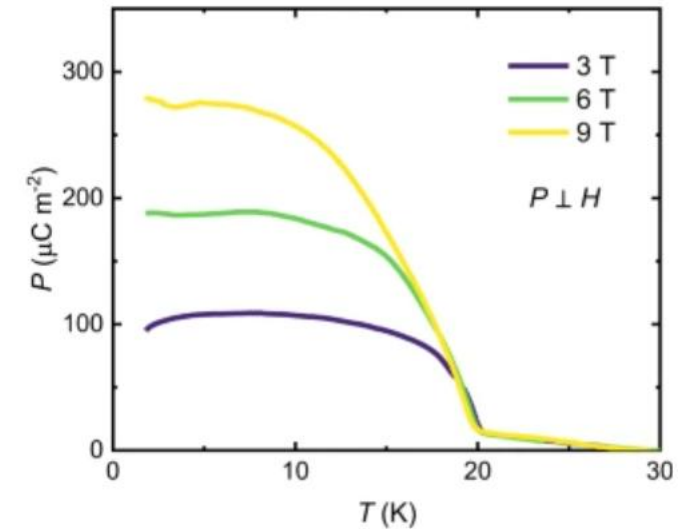
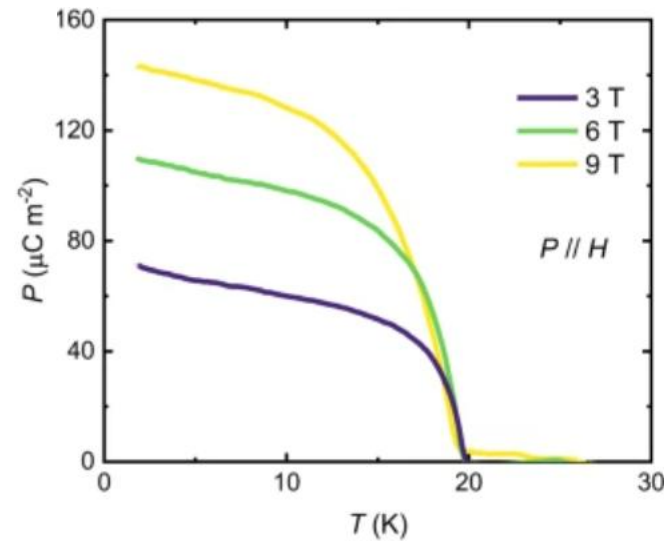
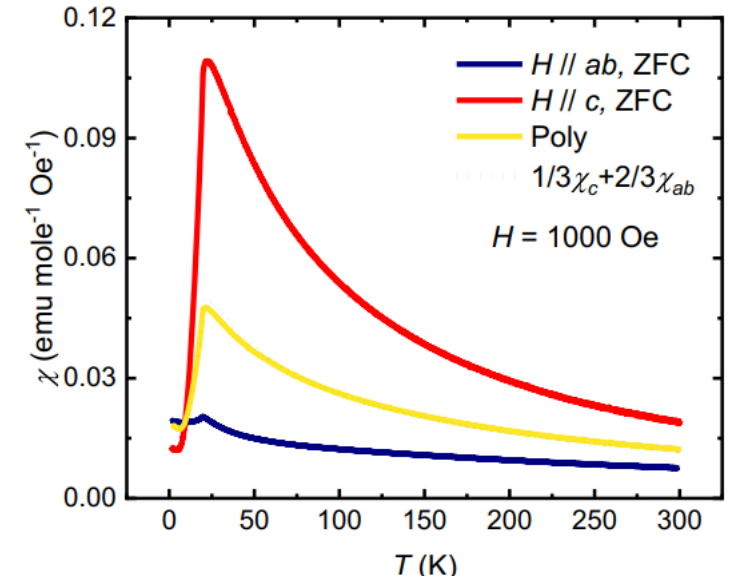
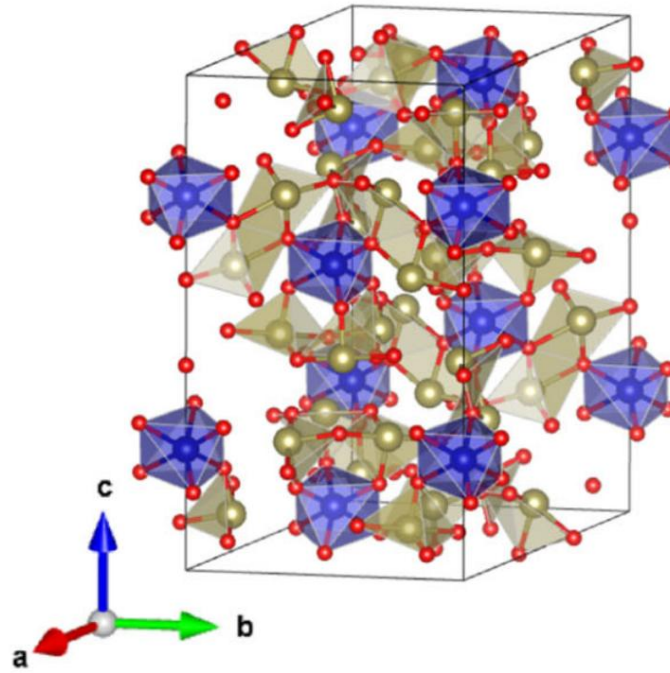
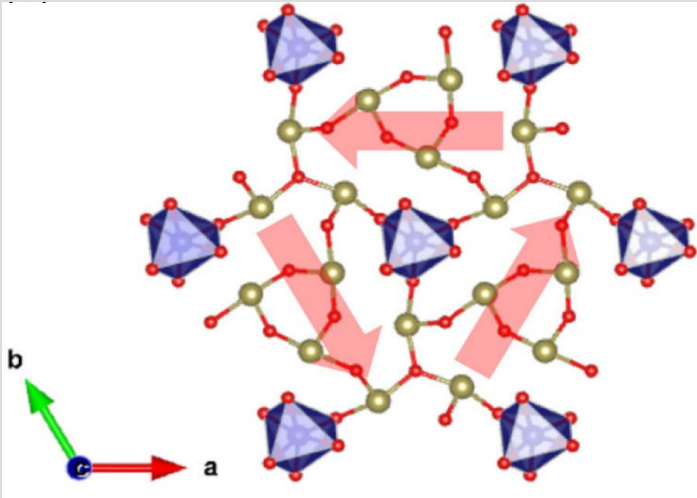


Fig. 1. The observed and calculated Ni 222 diffraction line profile from the BSS. Curve A is calculated from first term of equation (13), curve B is calculated from second term, curve C is sum of A and B; $\times$ observed values; the vertical line is the refined position of the Ni 222 reflection.

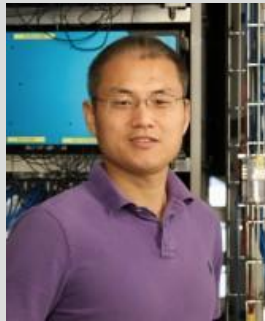
Magnetoelectricity in Co-based collinear AFM



Xianghan Xu,

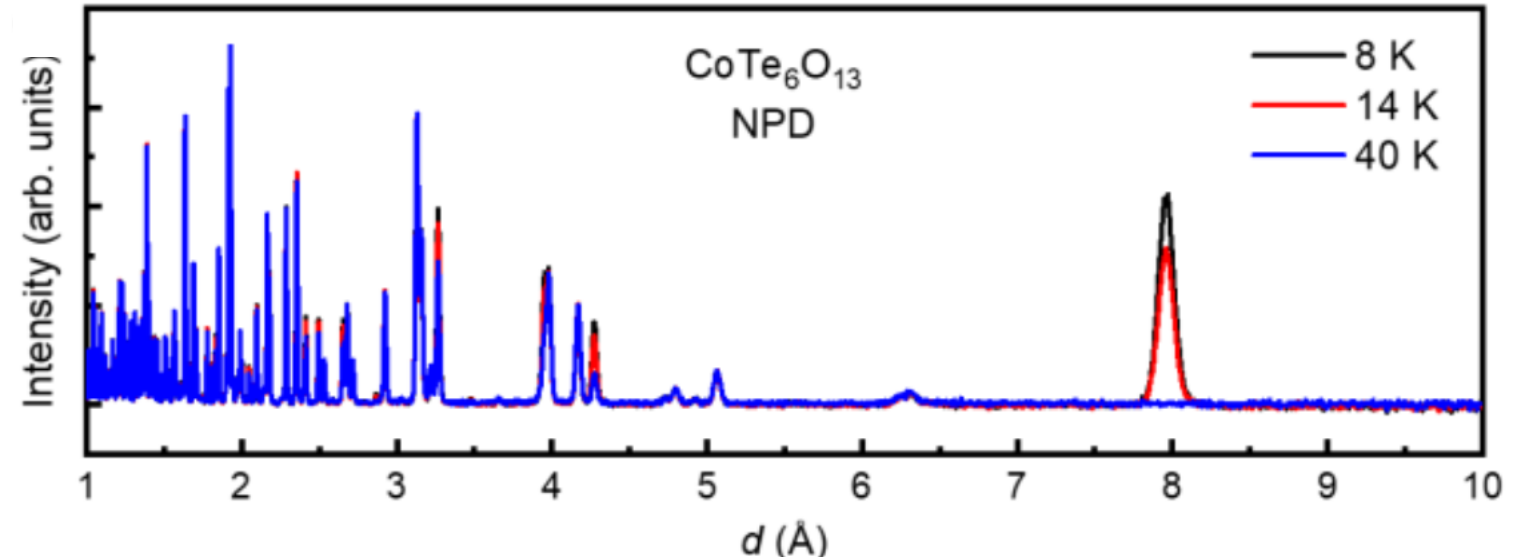
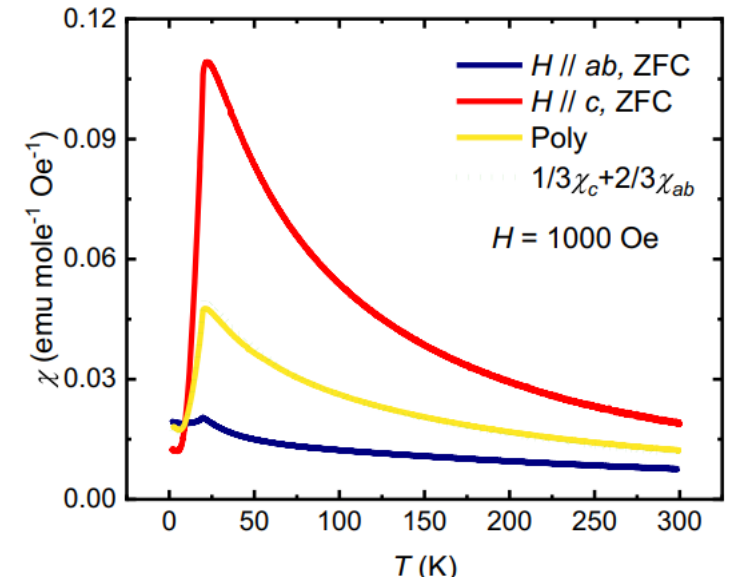
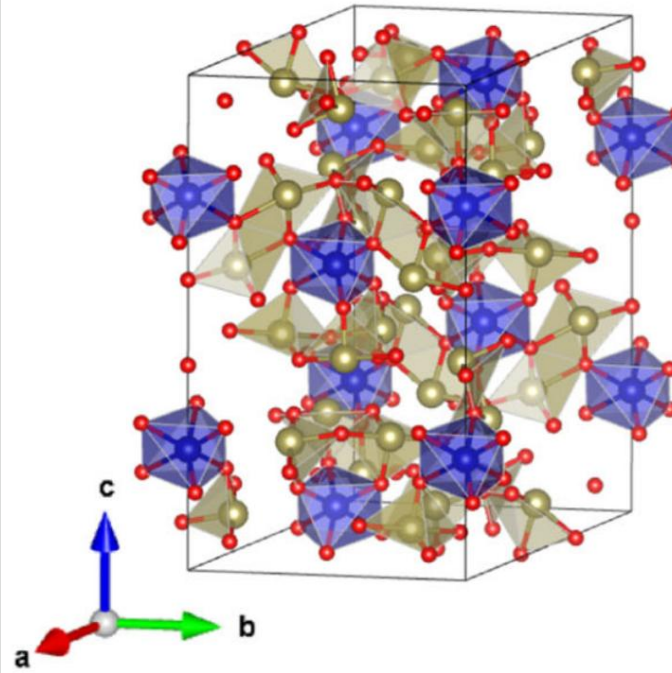
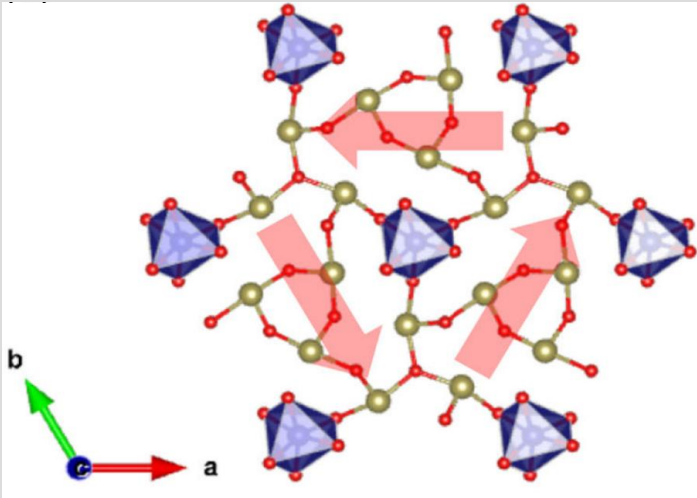


Bob Cava,



Qiang Zhang

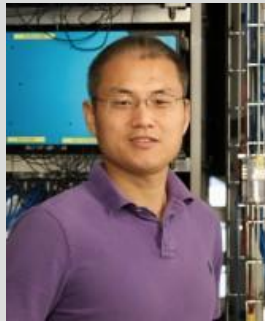
Magnetoelectricity in Co-based collinear AFM



Xianghan Xu,



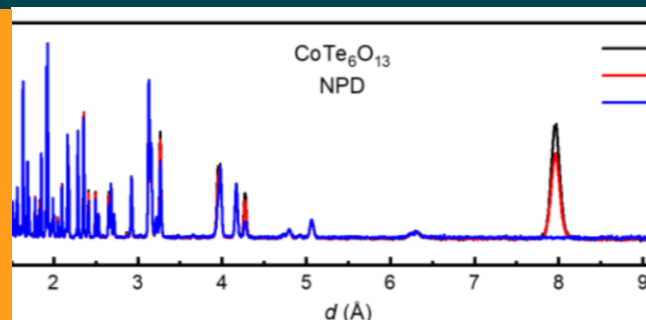
Bob Cava,



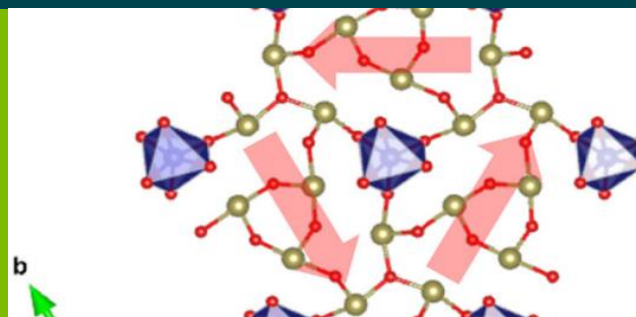
Qiang Zhang

We will need...

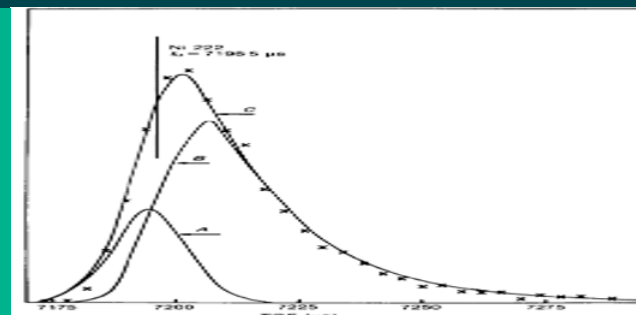
Data
(40 K, 8 K)



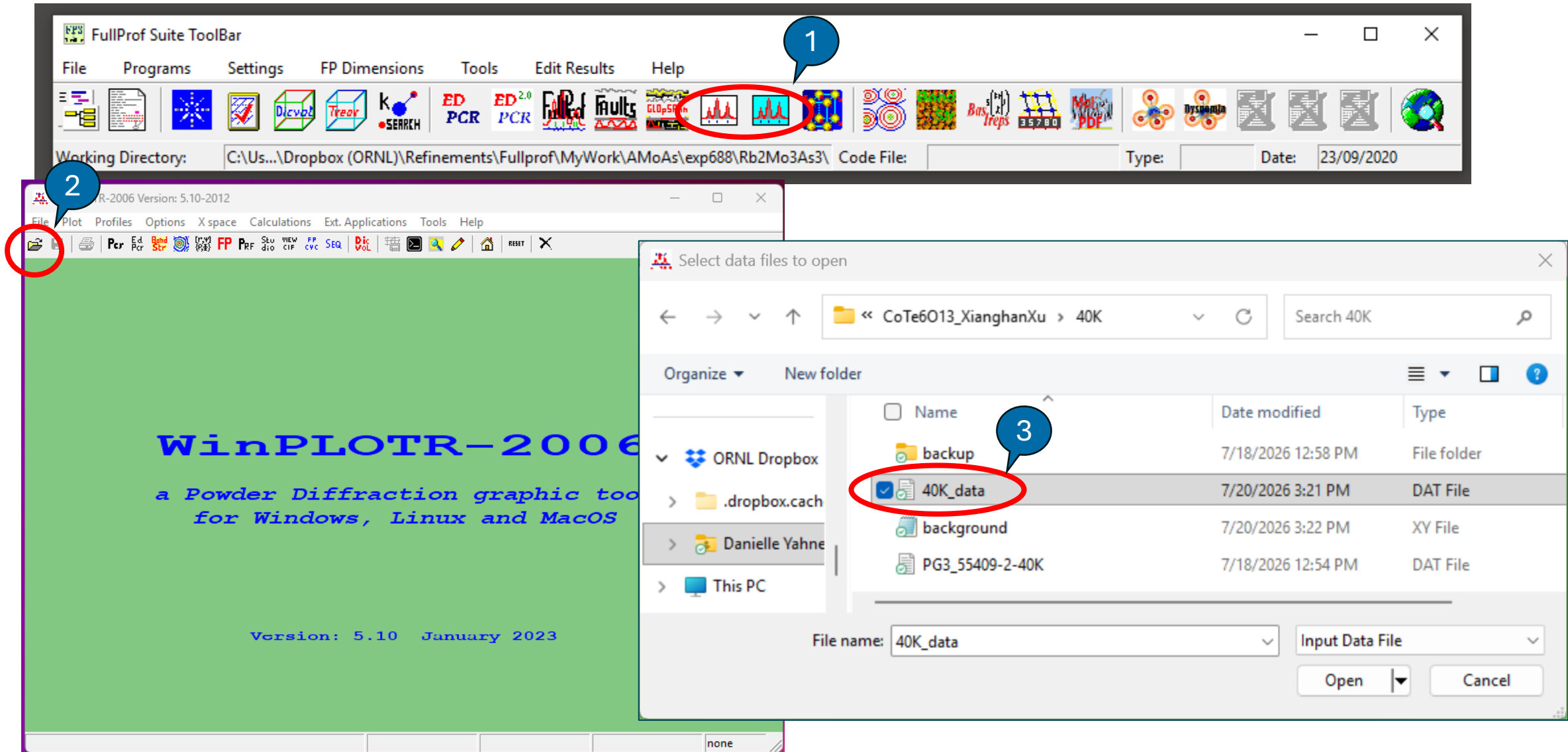
CIF



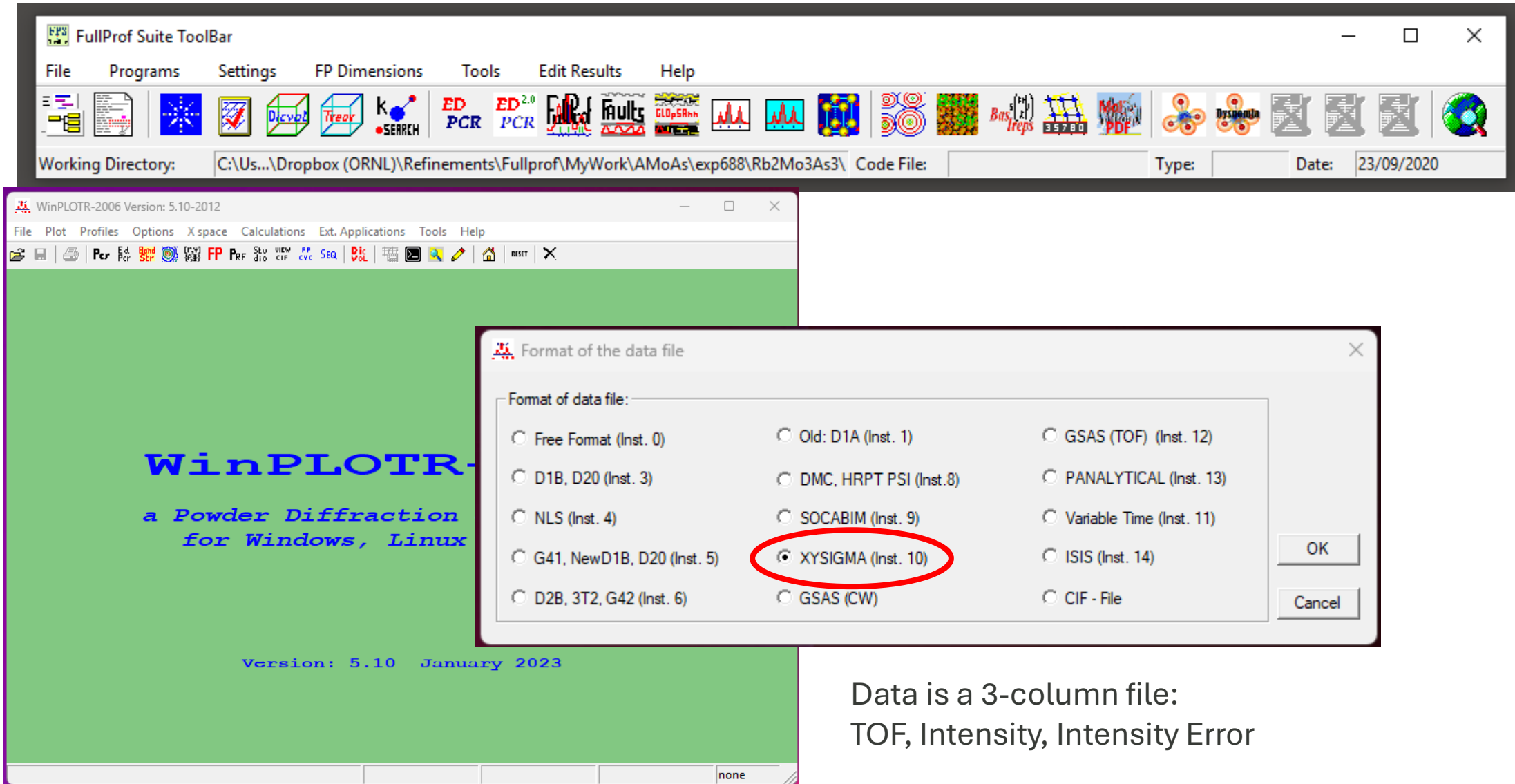
Inst.
Resolution
File



Plot the data

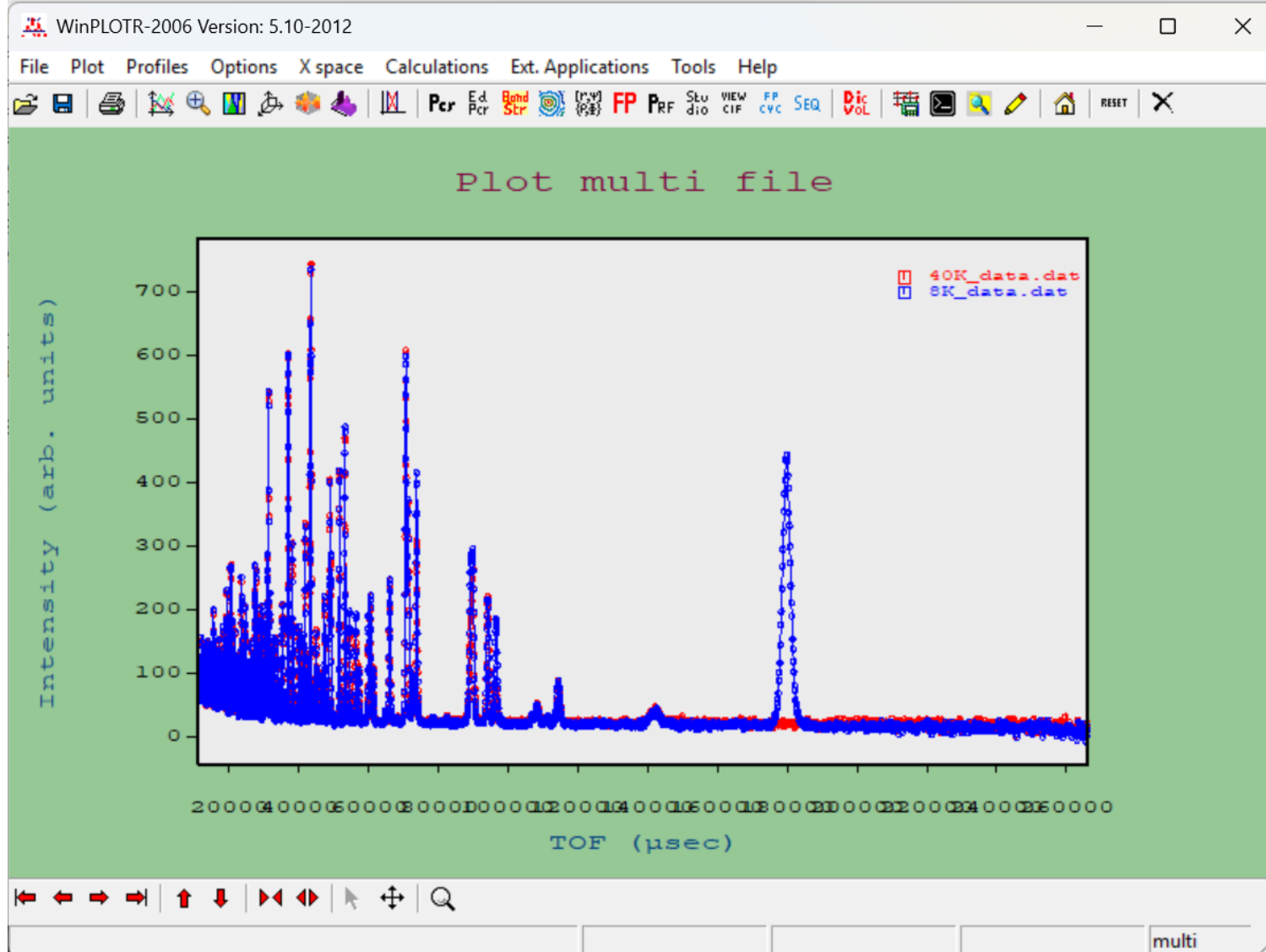


Plot the data

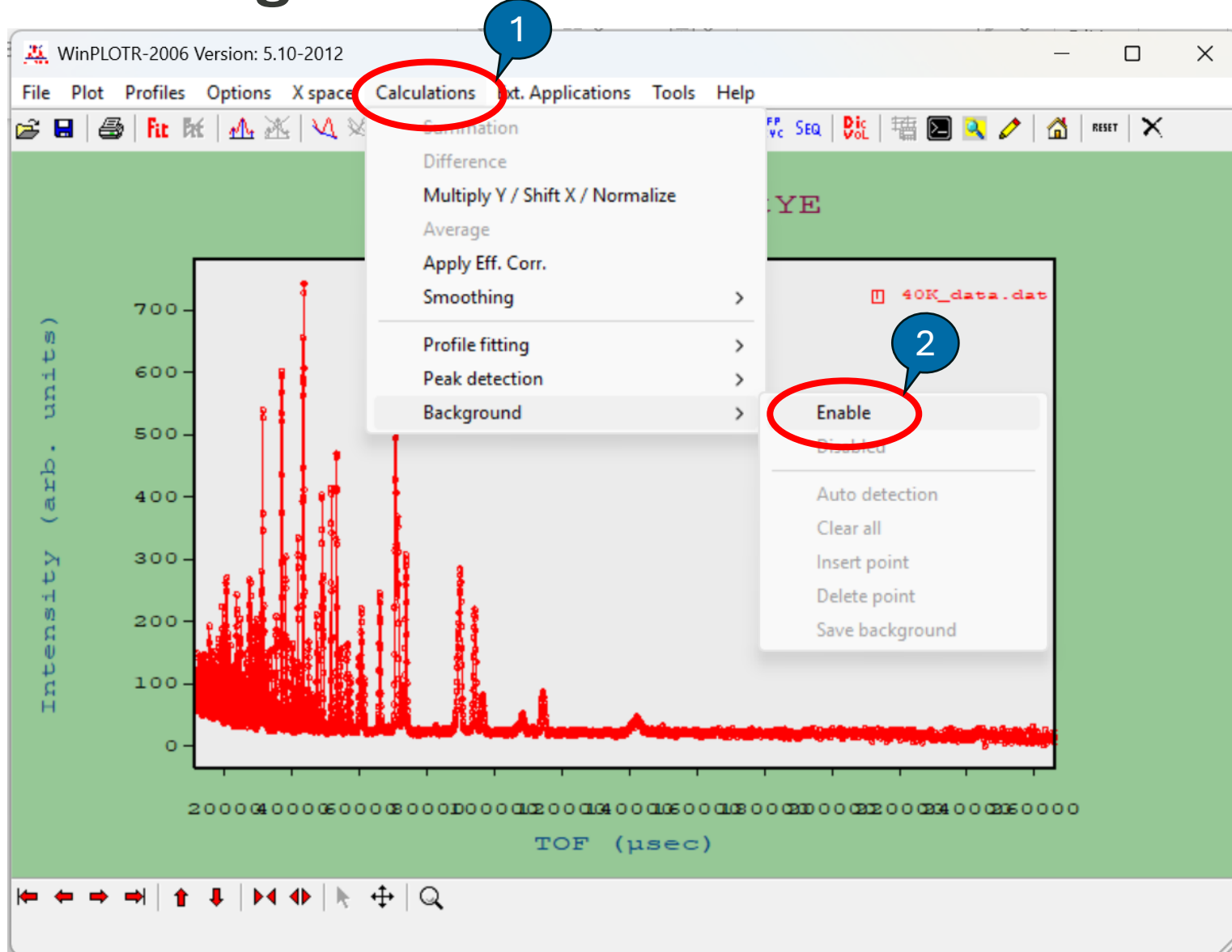


Data is a 3-column file:
TOF, Intensity, Intensity Error

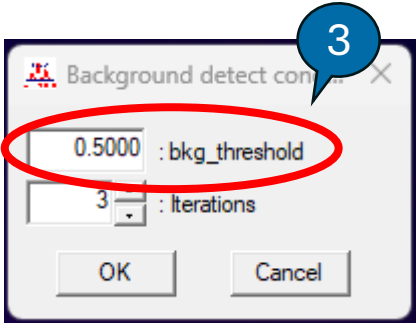
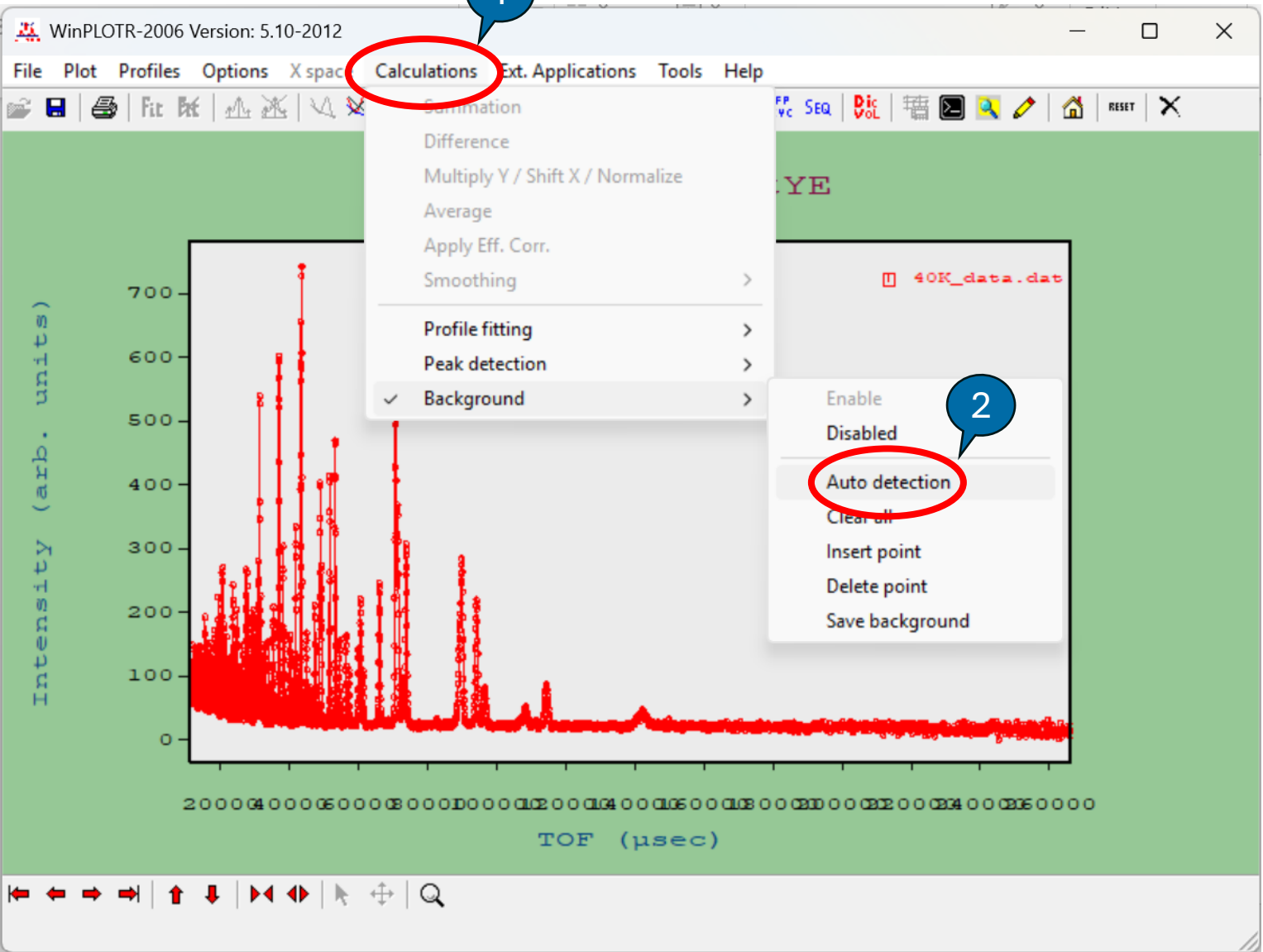
Plot the data



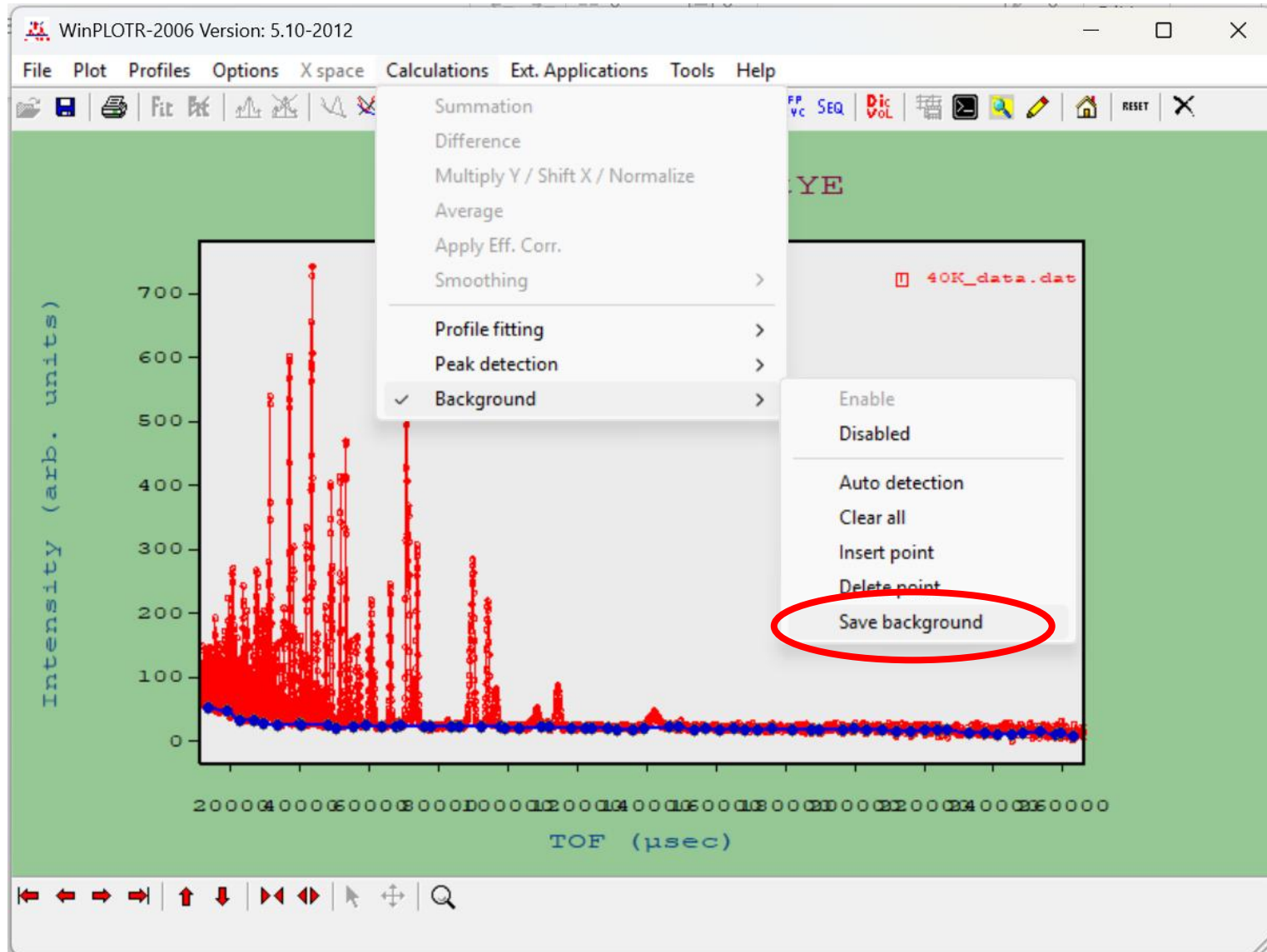
Fit background



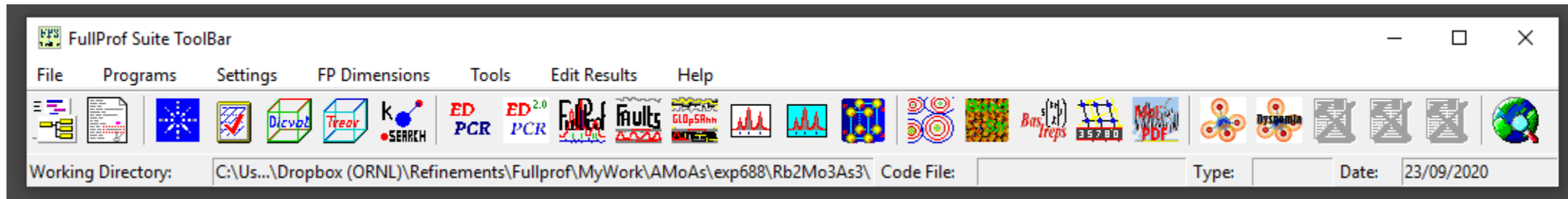
Fit background



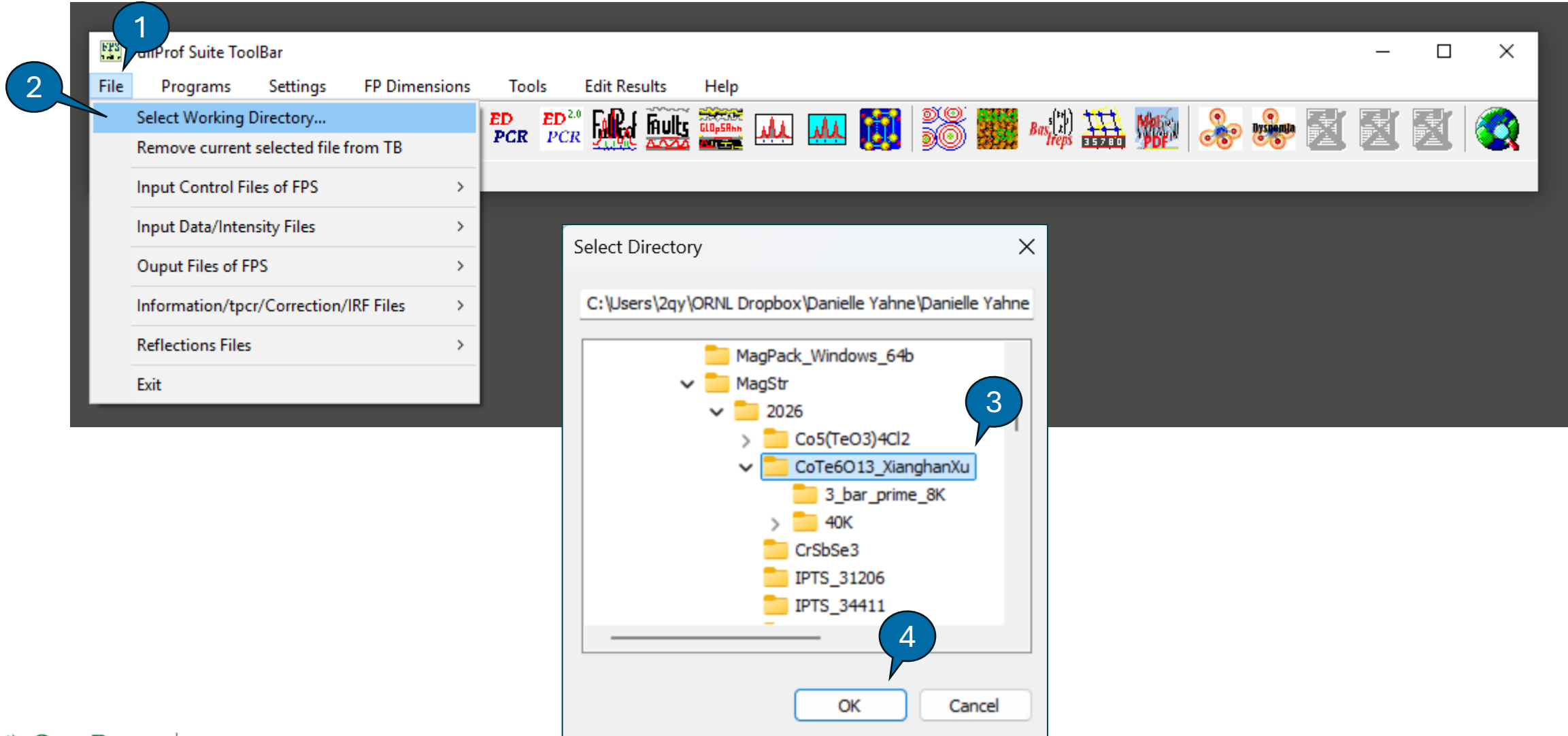
Fit background



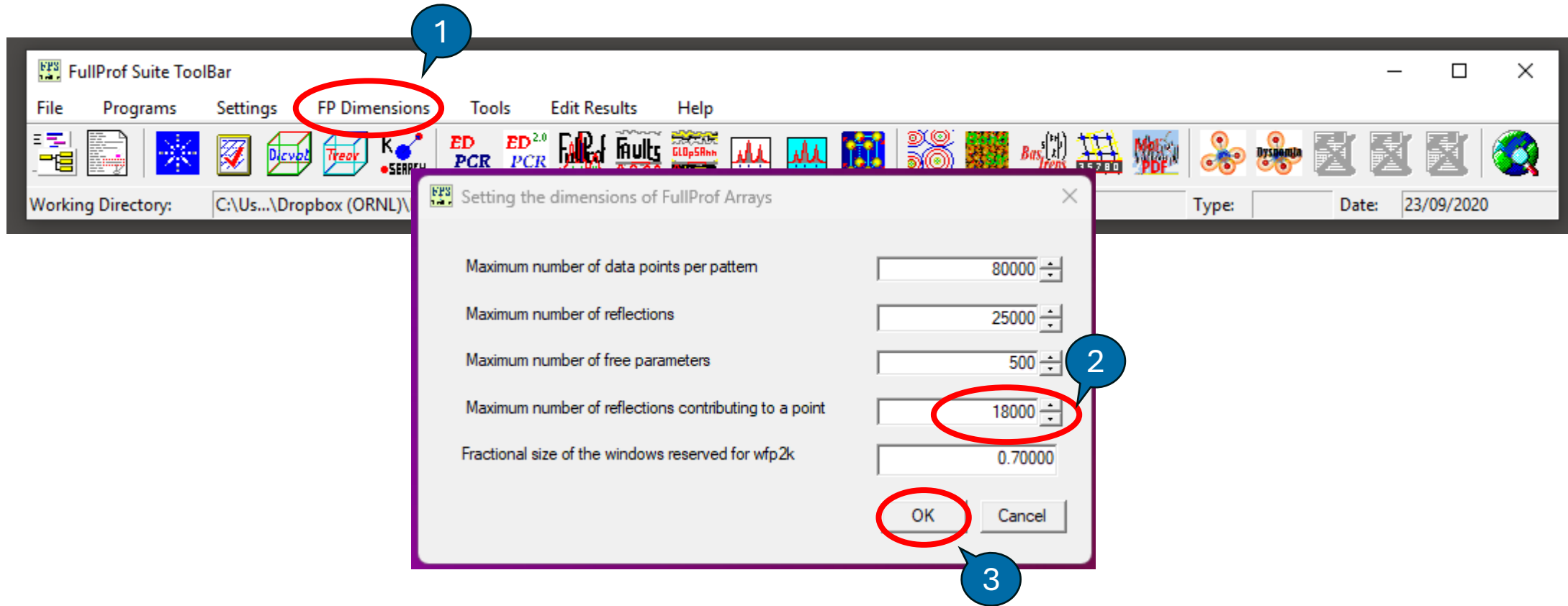
Getting started with Fullprof



Select working directory

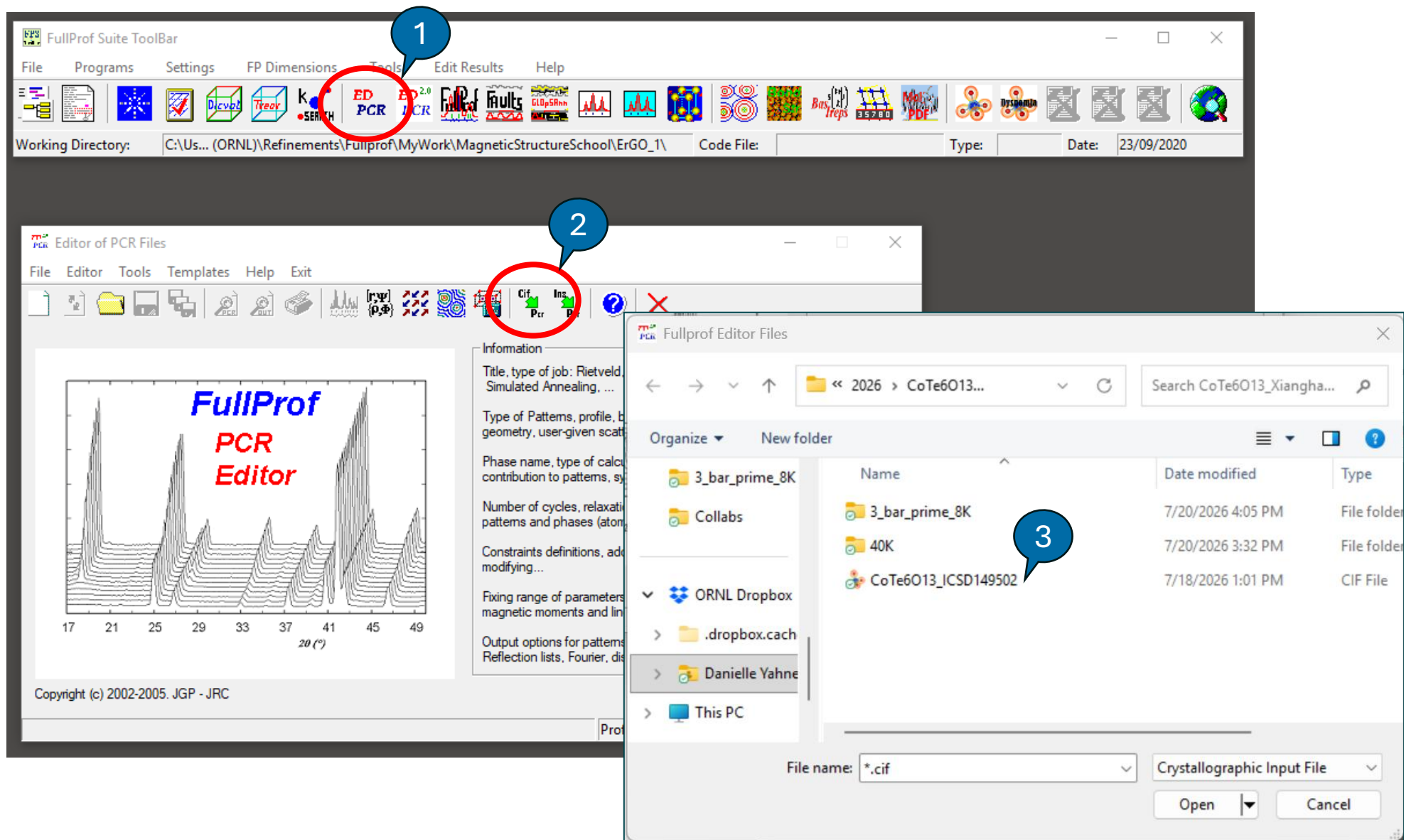


Edit FP Dimensions



Change to large number because POWGEN can detect large number of peaks

Using the PCR Editor



Importing CIF

Simple Calculation Template

Type

Xray

Neutron

T.O.F.

Import Files

Ascii

Cif

Shelx

Instrumental Resolution File

Default values

IRF File

Browse

Cell Parameters/ SpaceGroup

Atoms Information

a	b	c	alpha	beta	gamma
10.166000	10.166000	18.980999	90.000	90.000	120.000

Space Group:

R -3

☐ Magnetic Phase

Number of total Operators:

0

Num	Symmetry	Phase

OK

Cancel

Importing CIF

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	Te1	Te	0.82234	0.57097	0.73823	0.72561	1.00000
Atom #2	Te2	Te	0.60483	0.50405	0.42402	0.64508	1.00000
Atom #3	Co1	Co	0.66667	0.33333	0.57732	0.67113	0.33333
Atom #4	O1	O	0.66667	0.33333	0.74690	0.81326	0.33333
Atom #5	O2	O	0.75610	0.53690	0.64114	0.89221	1.00000

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

Site 6c
Gen. multiplicity = 18

$\text{Occ} = \text{site multiplicity} / \text{general multiplicity}$

Building PCR File

The image shows the FullProf PCR Editor software interface. The main window displays a diffraction pattern plot with the text "FullProf PCR Editor" overlaid. The plot shows multiple stacked diffraction patterns with peaks at various angles, labeled from 17 to 49 on the x-axis (2θ in degrees). The software has a menu bar (File, Editor, Tools, Templates, Help, Exit) and a toolbar with various icons. A "General" button is circled in red in the main window, with a callout bubble labeled "1".

The "General Information" dialog box is open, showing the "Title" field with the text "Descriptive Title with Sample info, maybe some experimental parameters like temperature or something". This field is circled in red, with a callout bubble labeled "2". The "Calculations" section has three radio buttons: "Refinement/Calculation of a Powder Diffraction Profile" (selected), "Refinement on Single Crystal Data / Integrated Intensity Data", and "Simulated Annealing Optimization (Integrated Intensities)". There is an "S.A. Options" button next to the third option. At the bottom, there is a checkbox "Optimize calculations according to the particular options used in this Job". The "OK" and "Cancel" buttons are at the bottom right, with a callout bubble labeled "3" near the "OK" button.

Copyright (c) 2002-2005. JGP - JRC

C:\Users\2qy\ORNL Dropbox\Danielle Yahne\Danielle Yahne's files\HB-2A\NNS_2025\MnO_Fi Profiles

Building PCR File

The image shows the FullProf PCR Editor interface. The main window displays a diffraction pattern plot with the text "FullProf PCR Editor". The "Information" panel on the right lists job details. The "Patterns Information" dialog box is open, showing "Pattern: 1/1" and "Weight: 1.0000". The "Data file/Peak shape" button is highlighted with a red circle and a blue callout labeled "2". The "Patterns" tab in the main window is also highlighted with a red circle and a blue callout labeled "1". The "Profile Data Information: Pattern 1" dialog box is open, showing the "Data File / Format" tab. The "Data File" field contains a path, and the "Format" section has "X,Y.SIGMA (XYDATA)" selected, both highlighted with red circles and blue callouts labeled "3" and "4" respectively.

FullProf
PCR
Editor

Information

Title, type of job: Rietveld, Integrated Intensities, Simulated Annealing, ...

Type of Patterns, profile, background, diffraction geometry, user-given scattering factors ...

Phase name, type of calculations (JBT), ATZ, contribution to patterns, symmetry, ...

Number of cycles, relaxation factors, access to patterns and phases (atoms and profile)

Constraints definitions, adding, deleting, ...

Patterns Information

Information

Pattern: 1/1 Weight: 1.0000

Data file/Peak shape

Background Type

Excluded Regions

Geometry/IRF

User Scatt. Factors

Initial Previous Add Del Next Last

OK Cancel

Profile Data Information: Pattern 1

Data File / Format Refinement / Simulation Pattern Calculation/Peak Shape

Data File: C:\Users\2qy\ORNL Dropbox\Danielle Yahne\Danielle Yahne's files\MagStr\2026\Ovi\Co Browse...

Format

☐ D1A/D2B (Old Format) ☐ Free Format (2theta, step, 2ThetaF) ☐ Variable Time X-ray Data

☐ D1A/D2B/3T2/G42 ☐ Two Axis Instrument, G41 ☒ X,Y.SIGMA (XYDATA)

☐ D1B (Old Format) ☐ GSAS Format ☐ X'Celerator (PANalytical)

☐ D1B/D20 ☐ Socabim Software ☐ ISIS multi-bank normalized

☐ D4/D20L ☐ Synchrotron (Brookhaven)

☐ DMC/HRPD (P.S.I.) ☐ Synchrotron (DBWS Software)

OK Cancel

Building PCR File

The image shows the FullProf PCR Editor interface. The main window displays a diffraction pattern plot with the text "FullProf PCR Editor". The "Information" panel on the right lists job details. The "Patterns Information" dialog is open, showing "Pattern: 1/1" and "Weight: 1.0000". The "Data file/Peak shape" button is highlighted with a red circle and a blue callout labeled "2". The "Patterns" tab in the main window is also highlighted with a red circle and a blue callout labeled "1". The "Profile Data Information: Pattern 1" dialog is open, showing the "Pattern Calculation/Peak Shape" tab. The "Neutron - T.O.F. (Nuclear and Magnetic)" option is selected and highlighted with a red circle and a blue callout labeled "5". The "Pattern Calculation/Peak Shape" tab is also highlighted with a red circle and a blue callout labeled "6". The "Wavelength" section shows "User Defined" and values for λ_1 , λ_2 , and (I_2 / I_1) .

FullProf
PCR
Editor

Information

Title, type of job: Rietveld, Integrated Intensities, Simulated Annealing, ...

Type of Patterns, profile, background, diffraction geometry, user-given scattering factors ...

Phase name, type of calculations (JBT), ATZ, contribution to patterns, symmetry, ...

Number of cycles, relaxation factors, access to patterns and phases (atoms and profile)

Constraints definitions, adding, deleting, ...

General

Patterns

Phases

Patterns Information

Information

Pattern: 1/1 Weight: 1.0000

Data file/Peak shape

Background Type

Excluded Regions

Geometry/IRF

User Scatt. Factors

Initial Previous Add Del Next Last

OK Cancel

Profile Data Information: Pattern 1

Data File / Format Refinement / Simulation Pattern Calculation/Peak Shape

Simulation / Refinement Data

☐ X-Ray

☐ Neutron - CW (Nuclear and Magnetic)

☒ Neutron - T.O.F. (Nuclear and Magnetic)

☐ Pattern Calculation (X-Ray)

☐ Pattern Calculation (Neutron - CW)

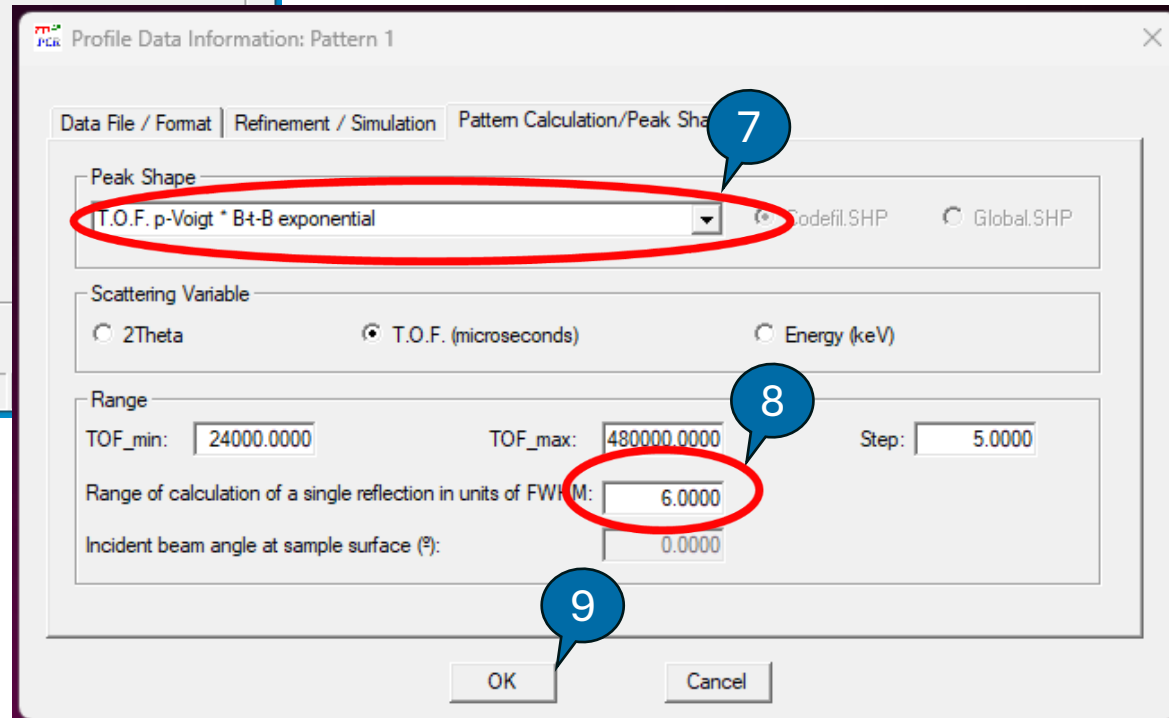
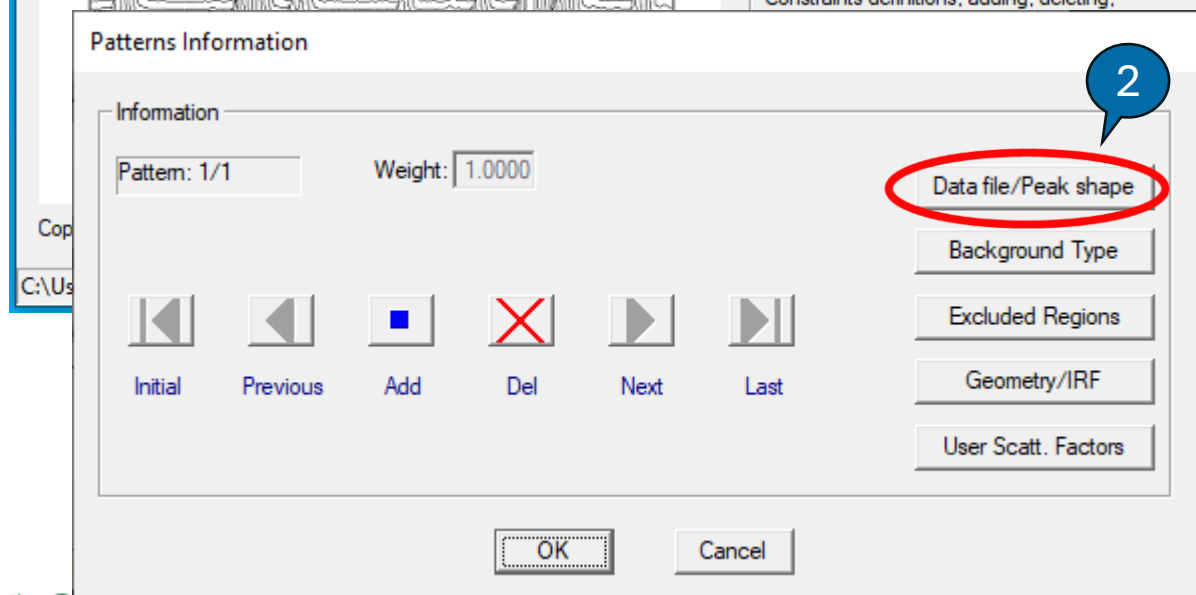
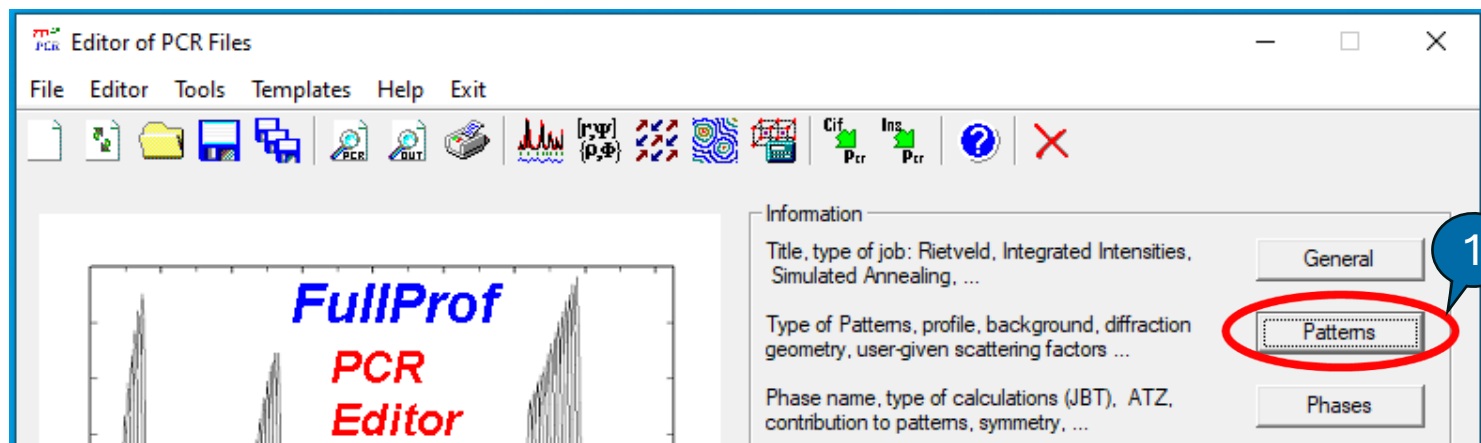
☐ Pattern Calculation (Neutron - T.O.F.)

Wavelength

User Defined λ_1 0.0000 λ_2 0.0000 (I_2 / I_1) 0.0000

OK Cancel

Building PCR File



Building PCR File

The screenshot displays the FullProf PCR Editor software interface. The main window has a menu bar (File, Editor, Tools, Templates, Help, Exit) and a toolbar with various icons. The central area shows a plot of a diffraction pattern with the text "FullProf PCR Editor" overlaid. To the right of the plot is an "Information" panel with tabs for General, Patterns (selected), and Phases. The "Patterns" tab is circled in red and labeled with a blue circle containing the number 1. Below the main window, the "Patterns Information" dialog box is open. It has an "Information" section with "Pattern: 1/1" and "Weight: 1.0000". Below this are navigation buttons: Initial, Previous, Add, Del, Next, Last. To the right of these buttons are several tabs: Data file/Peak shape, Background Type (circled in red and labeled with a blue circle containing the number 2), Excluded Regions, Geometry/IRF, and User Scatt. Factors. At the bottom of this dialog are "OK" and "Cancel" buttons. To the right of the "Patterns Information" dialog, the "Background Information" dialog box is open. It has a "Background Mode" section with several radio button options. The option "Linear Interpolation between a set background points with refinable heights" is selected and circled in red, labeled with a blue circle containing the number 3. Other options include "6-Coefficients polynomial function", "12-Coefficients polynomial function", "Debye-like (12-coeff.)+ polynomial functions (6-coefficients)", "12-Coefficients Fourier-cosine series", "Fourier Filtering", and "Background File transformed by 4-coefficients expression". To the right of these options are input fields for "Origin of the polynomial:" (set to 40.000) and "Number of points taken for Fourier Filter:" (set to 0.0000). Below the radio button options is a "Browse..." button. At the bottom of this dialog are "OK" and "Cancel" buttons, with the "OK" button labeled with a blue circle containing the number 4.

FullProf
PCR
Editor

Information

Title, type of job: Rietveld, Integrated Intensities, Simulated Annealing, ...

Type of Patterns, profile, background, diffraction geometry, user-given scattering factors ...

Phase name, type of calculations (JBT), ATZ, contribution to patterns, symmetry, ...

Number of cycles, relaxation factors, access to patterns and phases (atoms and profile)

Constraints definitions, adding, deleting.

General

Patterns

Phases

Background Information

Background Mode

☐ 6-Coefficients polynomial function

☐ 12-Coefficients polynomial function

☐ Debye-like (12-coeff.)+ polynomial functions (6-coefficients)

☐ 12-Coefficients Fourier-cosine series

☐ Fourier Filtering

☐ Background File transformed by 4-coefficients expression

☒ Linear Interpolation between a set background points with refinable heights

☐ Interpolation by cubic splines

☐ Chebychev Polynomial (24 coefficients)

Origin of the polynomial: 40.000

Number of points taken for Fourier Filter: 0.0000

Browse...

OK

Cancel

Patterns Information

Information

Pattern: 1/1

Weight: 1.0000

Data file/Peak shape

Background Type

Excluded Regions

Geometry/IRF

User Scatt. Factors

Initial

Previous

Add

Del

Next

Last

OK

Cancel

Building PCR File

The screenshot shows the FullProf PCR Editor software interface. The main window displays a diffraction pattern with the text "FullProf PCR Editor" overlaid. The interface includes a menu bar (File, Editor, Tools, Templates, Help, Exit) and a toolbar with various icons. The "Information" panel on the right lists job details and settings. The "Patterns Information" dialog box is open, showing the "Excluded Regions" tab. A secondary "Exclude Regions: Pattern 1" dialog box is also open, showing a table of excluded regions.

Patterns Information Dialog Box:

- Information: Pattern: 1/1, Weight: 1.0000
- Buttons: Initial, Previous, Add, Del, Next, Last
- Buttons: Data file/Peak shape, Background Type, **Excluded Regions**, Geometry/IRF, User Scatt. Factors
- Buttons: OK, Cancel

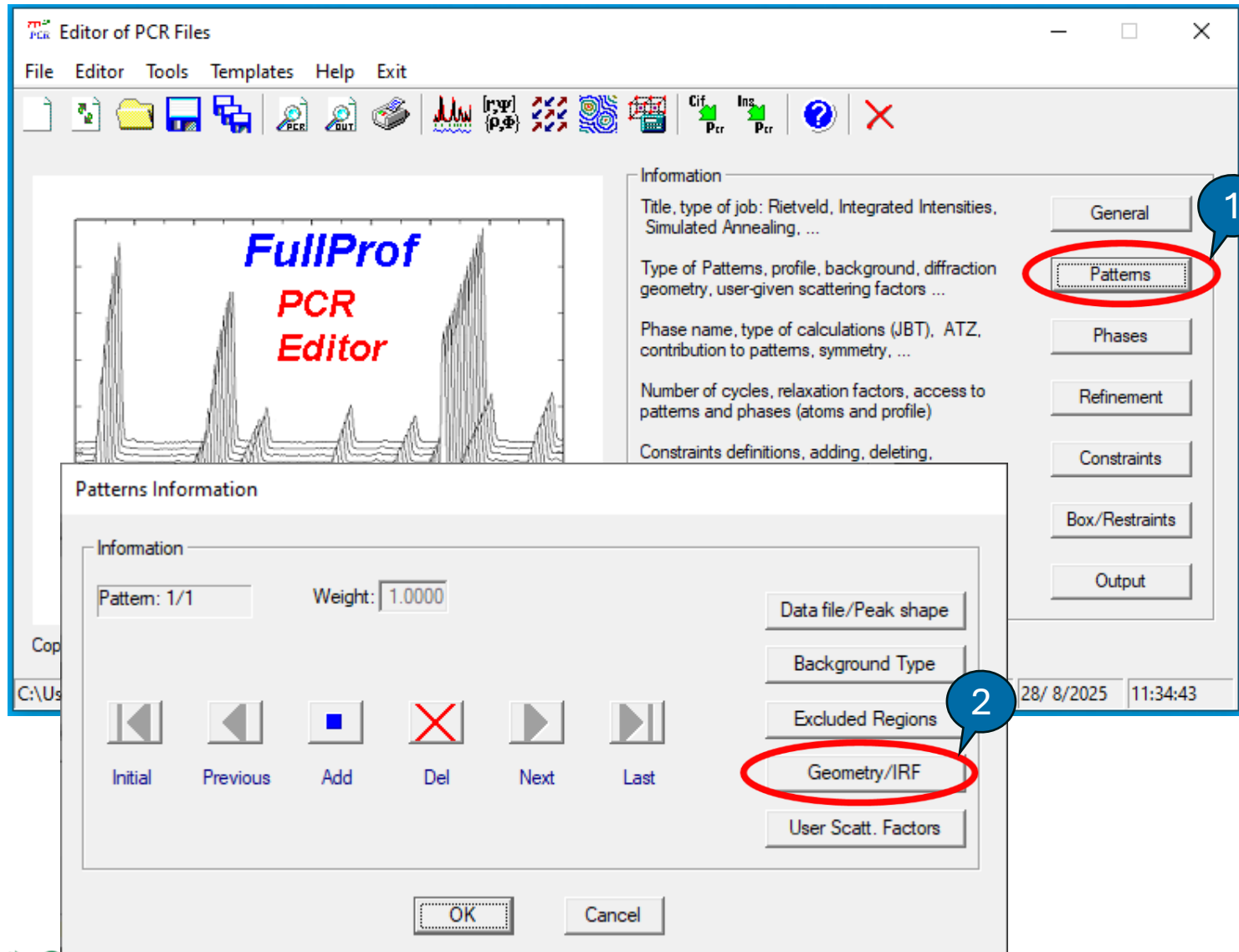
Exclude Regions: Pattern 1 Dialog Box:

- Number of excluded Regions: 1
- Table:

Region	Low bound	High bound
	0.22000E+06	0.27000E+06

Buttons: OK, Cancel

Building PCR File



Building PCR File

Pattern Diffraction Geometry Information: Pattern 1

1 **Diffraction Geometry**

Bragg-Brentano or Debye-Scherrer Geometry

IRF Corrections

Instrumental Resolution Function

☐ None

☐ $H_G^2 = (U_i \tan \theta + V_i) \tan \theta + W_i$
 $H_L = X_i \tan \theta + Y_i / \cos \theta + Z_i$
 $FWHM = \sqrt{U_i \tan^2 \theta + V_i \tan \theta + W_i}$
 $\eta = \eta_i + X_i \cdot 2\theta + Y_i \cdot (2\theta)^2$

☐ $H_G^2 = (U_i \tan \theta + V_i) \tan \theta + W_i$
 $H_L = (X_i 2\theta + Y_i) 2\theta + Z_i$

☐ $H_G^2 = (U_i 2\theta + V_i) 2\theta + W_i$
 $H_L = (X_i 2\theta + Y_i) 2\theta + Z_i$

☒ T.O.F. p-Voigt * B-to-b exponentials (or * Ikeda-Carpenter)

☐ List of $2\theta, H_G(2\theta), H_L(2\theta)$ ☐ As above, but TOF versus d-Spacing (J. Hodges)

Name of IRF file:
C:\Users\2qy\ORNL Dropbox\Danielle Yahne\Danielle Yahne's files\MagStr\2026\PG2

Browse...

2

3

4

OK Cancel

Fullprof Input Files

< > << CoTe6O13_X... > 40K Search 40K

Organize New folder

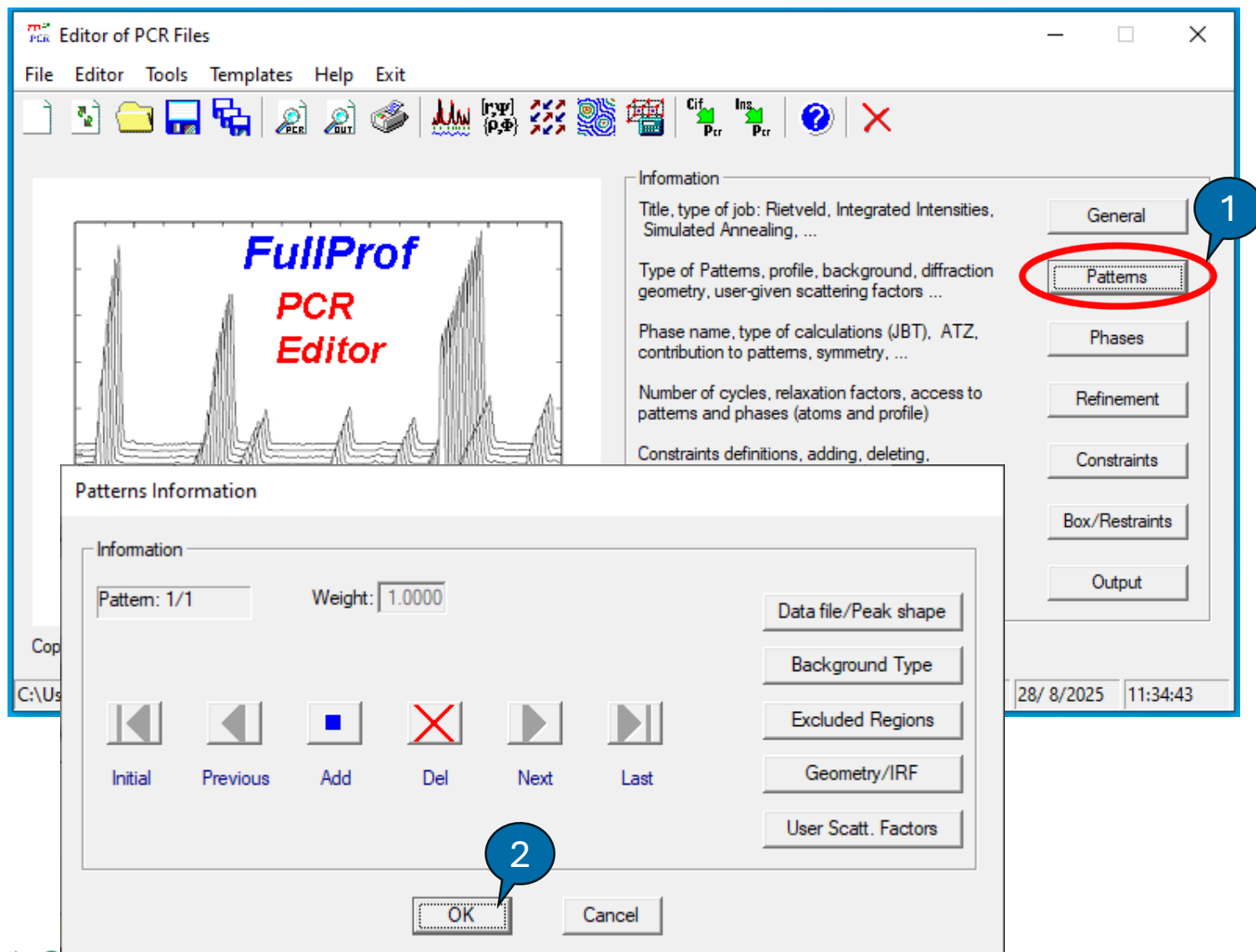
Name	Date modified	Type
3_bar_prime_8K		
CoTe6O13_Xian		
backup	7/18/2026 12:58 PM	File folder
PG2023A_HighRes_60Hz_b2_Ddep	7/18/2026 12:54 PM	IRF File

ORNL Dropbox .dropbox.cach Danielle Yahne This PC

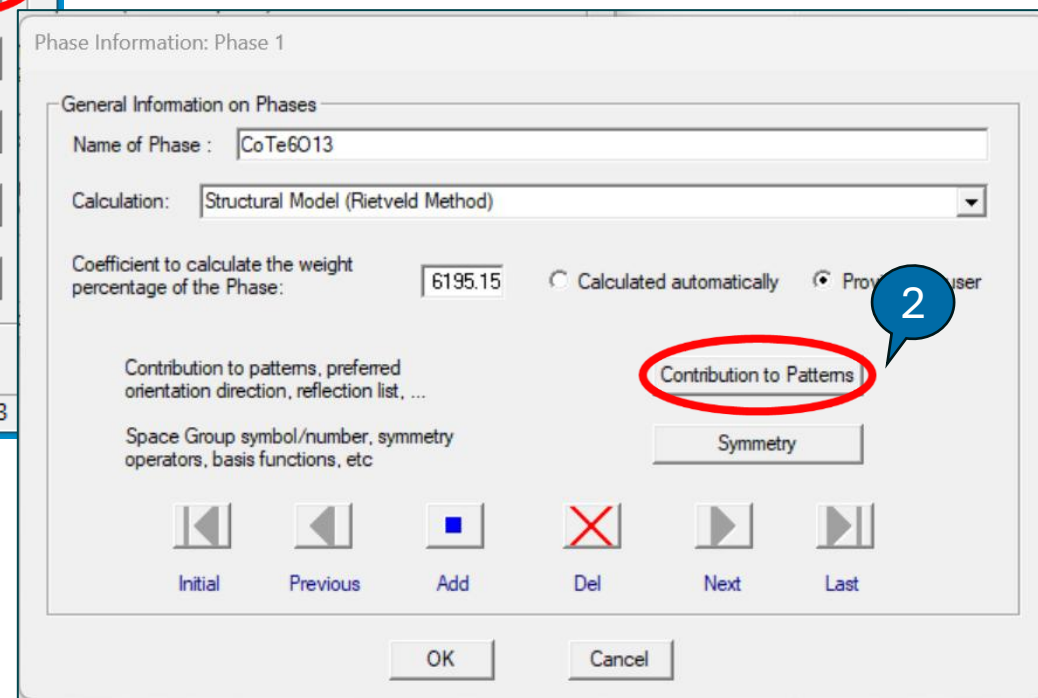
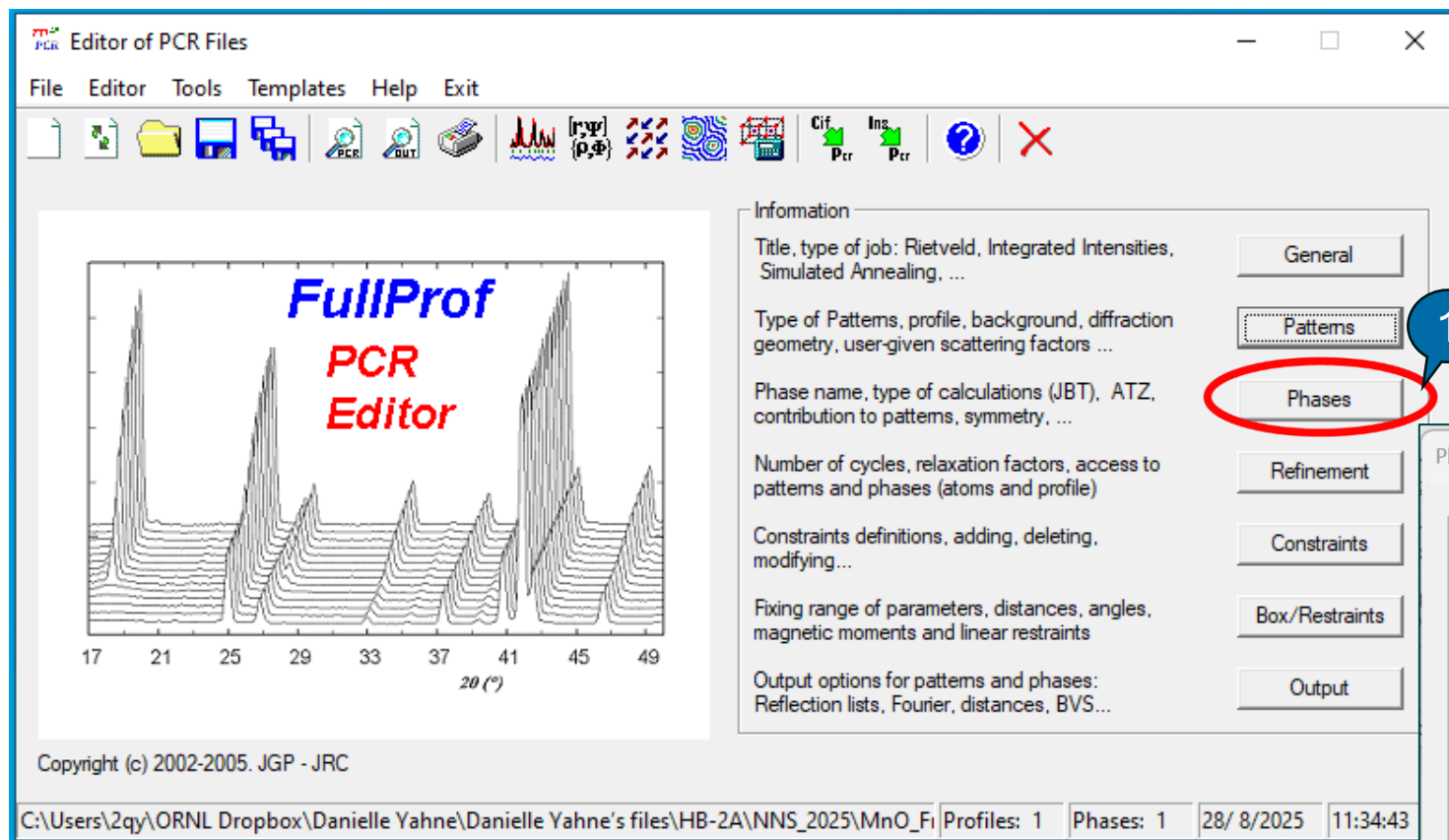
File name: PG2023A_HighRes_60Hz_b2_Ddep Instrumental Resolution File

Open Cancel

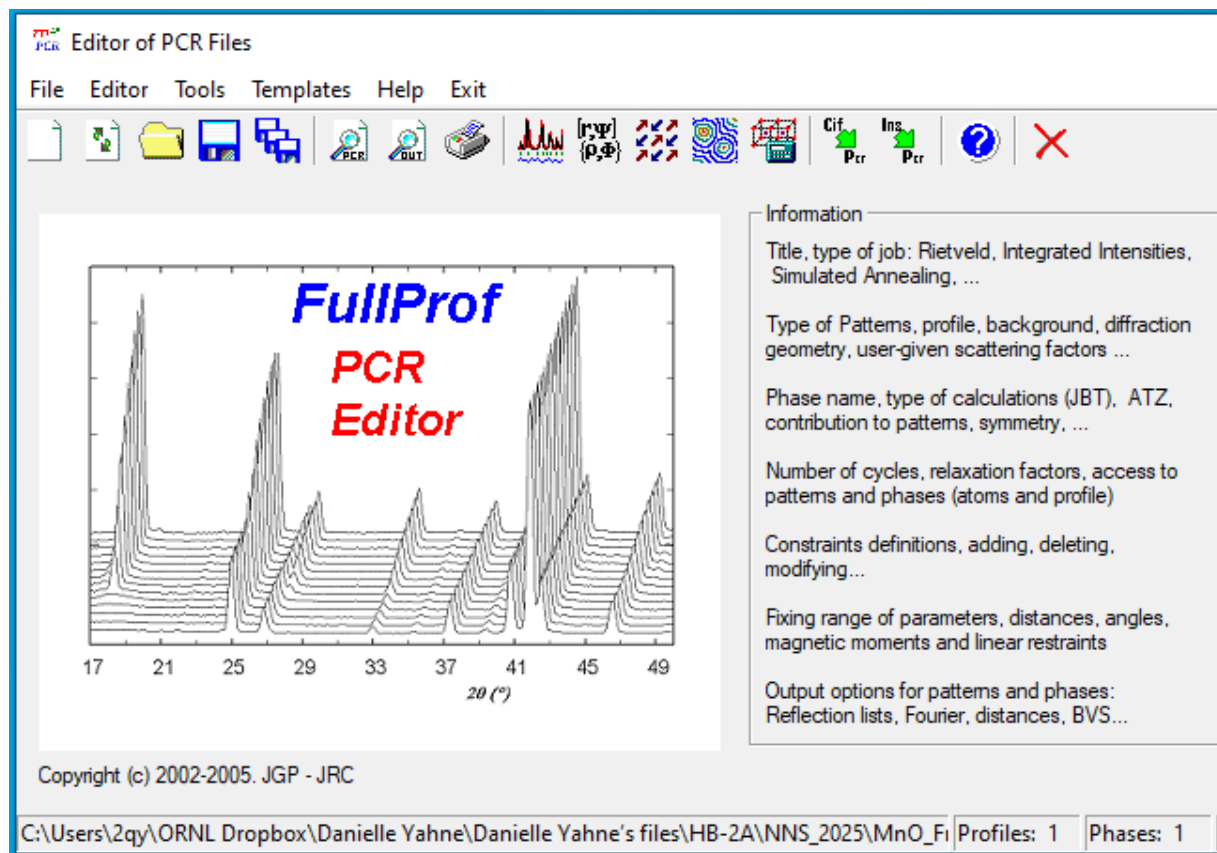
Building PCR File



Building PCR File



Building PCR File



Pattern Contribution Information for Phase 1

Pattern 1 | Pattern 2 | Pattern 3 | Pattern 4 | Pattern 5 | Pattern 6 | Pattern 7

☒ Current Phase contributes to the pattern

Type of Pattern

- ☐ X-Ray
- ☐ Neutron (Constant Wavelength) Nuclear and Magnetic
- ☒ Neutron (T.O.F) Nuclear and Magnetic
- ☐ Pattern Calculation (X-Ray)
- ☐ Pattern Calculation (Neutron - Constant Wavelength)
- ☐ Pattern Calculation (Neutron - T.O.F.)

Peak Shape

T.O.F. p-Voigt * B+t-B exponentials

Codefil.shp Global.shp

Intensities

Reflection list: Automatically generated from the Space Group symbol

☐ Use special control of parameters for peak overlap, rejected reflections for current phase

Brindley coefficient: 0.0000

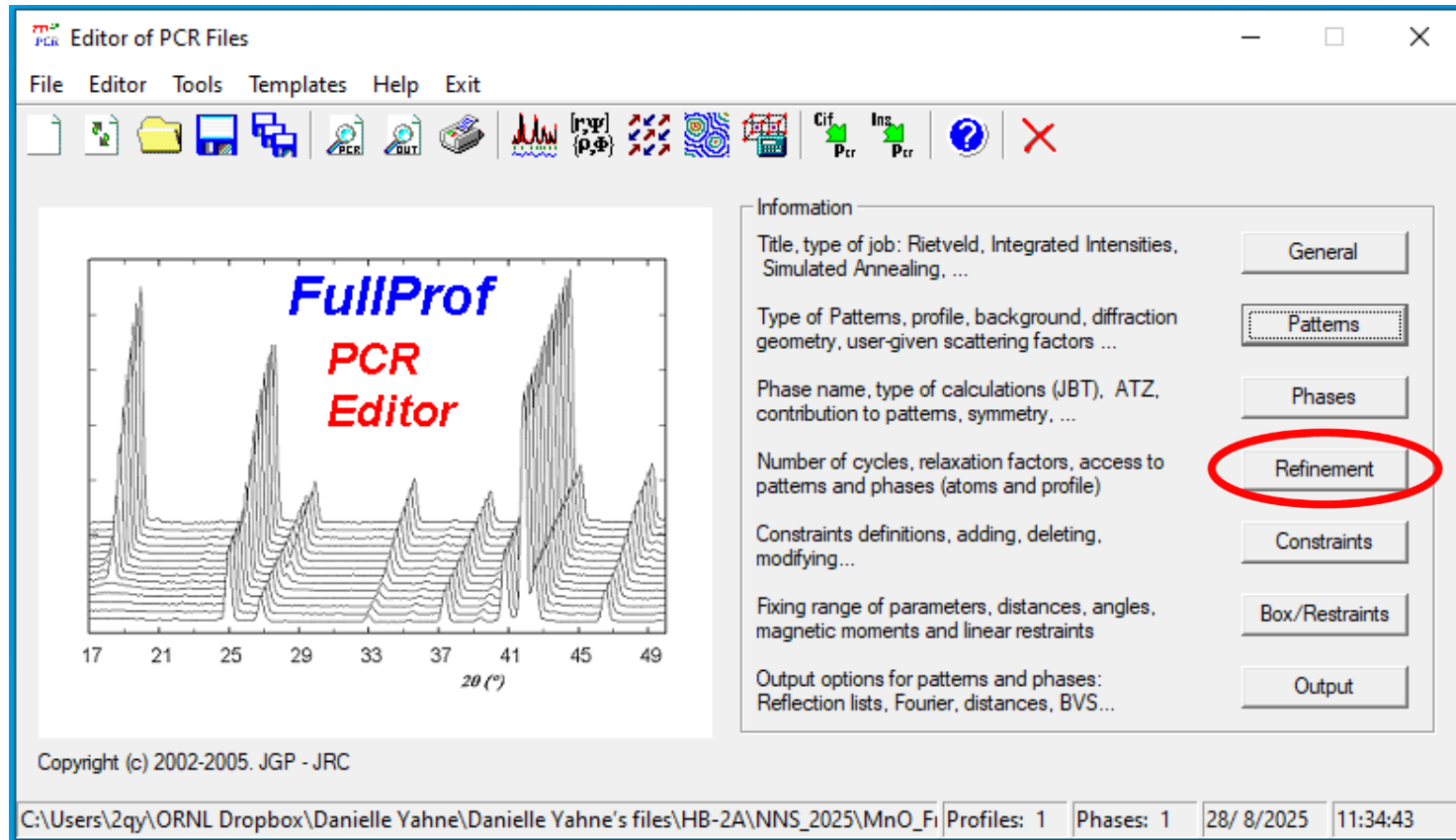
Global weight of the integrated intensity data vs profile data: 0.0000

Factor for excluding reflections [$|I| < \text{Factor} * \text{Sigma}(I)$]: 0.0000

Weights are divided by reduced χ^2 of present cycle: 0.0000

OK Cancel

Refine the nuclear structure



Refine the nuclear structure – Import background file

Refinement Information

Cycles of Refinement: 20

Stop Criterion of Coverage
Forced Termination when shifts < 0.10 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

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

Refinement weighting model
☒ Least Squares ☐ Maximum Likelihood ☐ Unit Weights
Background Instrumental Micro-Absorption

Reduction factor of number of data points: 0

OK Cancel

Phase 1 | Phase 2 | Phase 3 | Phase 4 | Phase 5

Atoms
Patterns: ☒ 1 ☐ 2 ☐ 3 ☐ 4 ☐ 5
Profile HKL Shifts Micro Absorption Further

Linear interpolation between a set of Background Points: Pattern 1

Interpolation Method
☒ Linear Interpolation ☐ Cubic Splines Interpolation

Information
Number of Points: 10

	2Theta	Counts	
1	0.000	0.000	☐
2	0.000	0.000	☐
3	0.000	0.000	☐
4	0.000	0.000	☐

Refine All Fix All **Import from Background File**

OK Cancel

Refine the nuclear structure – Import background file

The main dialog box, 'Refinement Information', contains the following settings:

- Cycles of Refinement: 20
- Stop Criterion of Coverage: Forced Termination when shifts < 0.10 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 excitation
- Pattern 1 | Pattern 2 | Pattern 3 | Pattern 4 | Pattern 5 | Pattern 6
- Refinement weighting model: ☒ Least Squares, ☐ Maximum Likelihood, ☐ Unit Weights
- Background** (highlighted in red), Instrumental, Micro-Absorption
- Reduction factor of number of data points: 0
- OK, Cancel

The inset window, 'Linear interpolation between a set of Background Points: Pattern 1', contains the following settings:

- Interpolation Method: ☒ Linear Interpolation, ☐ Cubic Splines Interpolation
- Information: Number of Points: 62
- Table:

	2Theta	Counts	
1	13517.680	52.749	☐
2	19141.094	47.987	☐
3	22786.238	32.704	☐
4	26802.139	33.314	☐

- Buttons: Refine All, Fix All, Import from Background File
- OK** (highlighted in red), Cancel

Refine scale & lattice parameters

Refinement Information

Cycles of Refinement:

Stop Criterion of Coverage
Forced Termination when shifts < x E.S.D.
Others:

Reflections ordering
☒ Only at the first cycle ☐ Each cycle

Refinement weighting model
☒ Least Squares ☐ Maximum Likelihood ☐ Unit Weights

Background
Instrumental
Micro-Absorption

Reduction factor of number of data points:

Relaxation Factors for Shifts
Atomic Anisotropic

☐ Bragg R-Factor excluding reflection

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

Phase 1 | Phase 2 | Phase 3 | Phase 4

OK Cancel

Atoms
Patterns ☒ 1 ☐ 2 ☐ 3 ☐ 4
Profile 1
HKL Shifts

Profile Parameters: Phase 1 Pattern 1

Factors

	Scale	Overall B-factor
Coefficients	5.0000 2	0.0000

Cell Parameters

	a	b	c	alpha	beta	gamma
Coefficients	10.166000 3	10.166000	18.981001	90.000	90.000	120.000

FWHM / Shape Parameters | Exponential Decay Parameters | Preferred Orientation

FWHM Parameters

	Sig_2	Sig_1	Sig_0	Z1
Coefficients	0.000000	0.000000	0.000000	0.000000

Shape Parameters

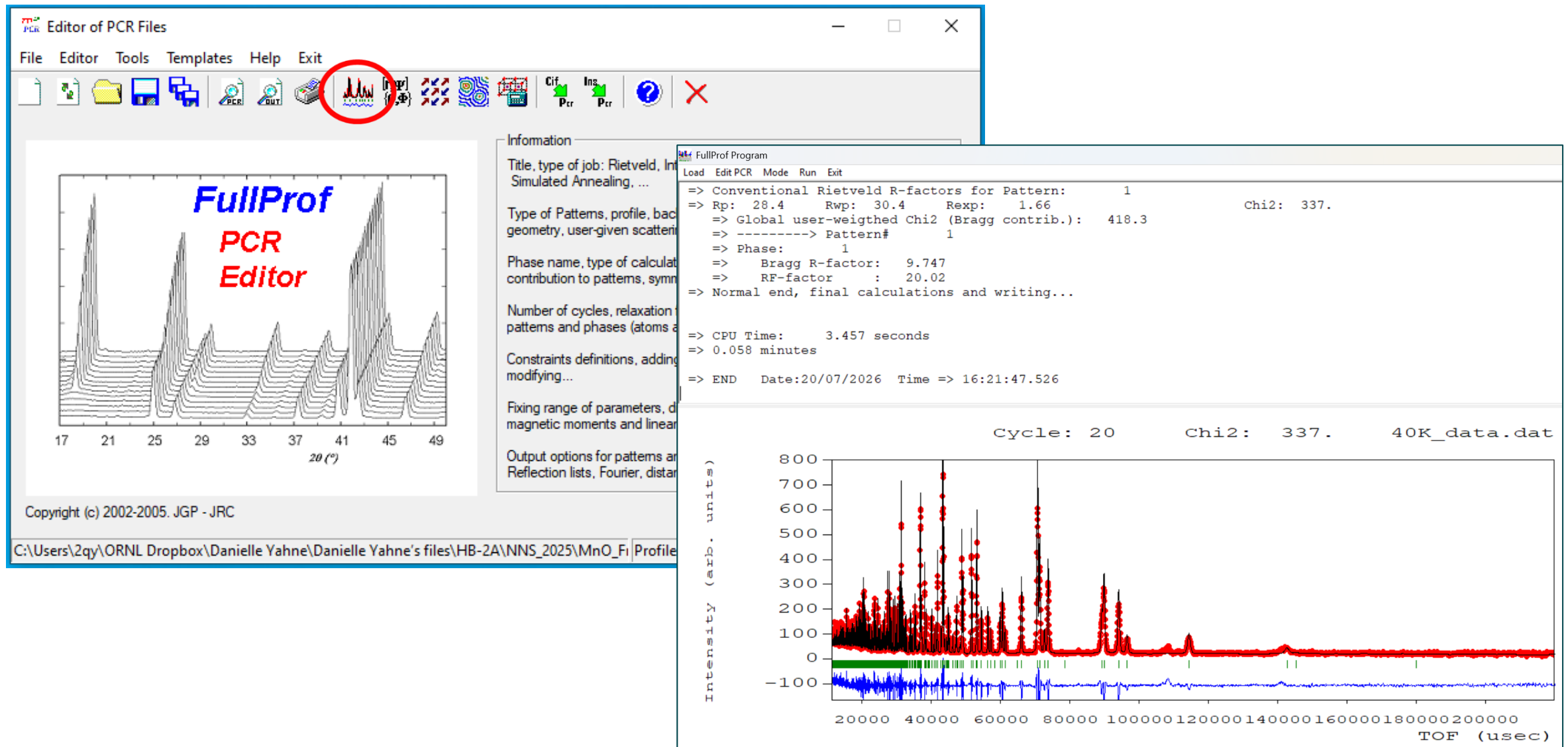
	Extinc	Abs1	Abs2
Coefficients	0.000000	0.000000	0.000000

☐ Refine FWHM for second wavelength

	U2	V2	W2
Coefficients			

Refine All
Fix All
Cancel 4
OK

Run refinement



Refine peak shape parameters

The screenshot shows the 'Refinement Information' dialog box. Callout 1 points to the 'Profile' button in the 'Patterns' section. Callout 2 points to the 'Gam_0' coefficient in the 'FWHM Parameters' table. Callout 3 points to the 'OK' button. Callout 4 points to the 'OK' button in the 'Profile Parameters' dialog. Callout 5 points to the 'OK' button in the 'Refinement Information' dialog.

Refinement Information

Cycles of Refinement: 20

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

Refinement weighting model
☒ Least Squares
☐ Maximum Likelihood
☐ Unit Weights

Background
Instrumental
Micro-Absorption

Reduction factor of number of data points: 0

Relaxation Factors for Shifts
Atomic: 1.00 Anisotropic: 1.00

Bragg R-Factor excluding reflections

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

Phase 1 | Phase 2 | Phase 3 | Phase 4

Atoms
Patterns
☒ 1 ☐ 2 ☐ 3 ☐ 4

Profile
HKL Shifts

OK Cancel

Profile Parameters: Phase 1 Pattern 1

Factors

	Scale	Overall B-factor
Coefficients	2.4761	0.0000

Cell Parameters

	a	b	c	alpha	beta	gamma
Coefficients	10.127993	10.127993	18.945887	90.000	90.000	120.000

FWHM / Shape Parameters Exponential Decay Parameters Preferred Orientation

FWHM Parameters

	Gam_2	Gam_1	Gam_0	Gam_2
Coefficients	0.000	0.000	0.000	0.000000

Shape Parameters

	Extinc	Abs1	Abs2
Coefficients	0.000000	0.000000	0.000000

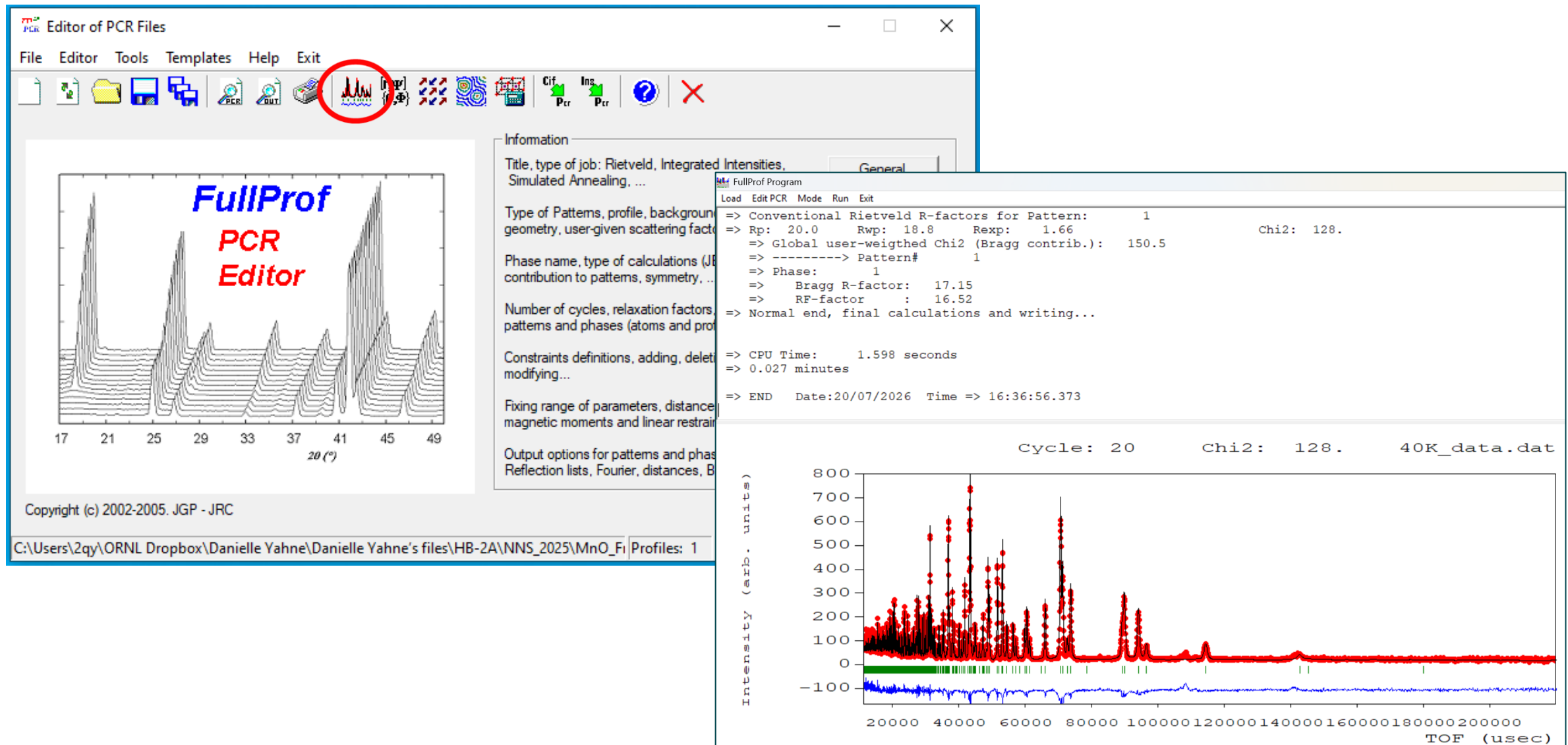
☐ Refine FWHM for second wavelength

	U2	V2	W2
Coefficients			

Refine All
Fix All
Cancel
OK

Lorentz function mainly represents the broadening of the peak shape from the sample

Run refinement



Refine atomic positions

Refinement Information

Cycles of Refinement:

Stop Criterion of Coverage
Forced Termination when shifts < x E.S.D.
Others:

Relaxation Factors for Shifts
Atomic Anisotropic Profile Global

Reflections ordering
☒ Only at the first cycle ☐ Each cycle

☐ Bragg R-Factor excluding reflections

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

Refinement weighting model
☒ Least Squares ☐ Maximum Likelihood ☐ Unit Weights

Background Instrumental Micro-Absorption

Reduction factor of number of data points:

OK Cancel

Phase 1 | Phase 2 | Phase 3

Atoms Profile HKL Shifts

Patterns
☒ 1 ☐ 2 ☐ 3

Atoms Information: Phase 1

List of Atoms
Number of Atoms:

	Label	Ntyp	X	Y	Z	B	Occ	Therm. Fact.
Atom # 1	Te1	Te	0.82234	0.57097	0.73823	0.72561	1.00000	Isotropic
Atom # 2	Te2	Te	0.60483	0.50405	0.42402	0.64508	1.00000	Isotropic
Atom # 3	Co1	Co	0.66667	0.33333	0.57732	0.67113	0.33333	Isotropic
Atom # 4	O1	O	0.66667	0.33333	0.74690	0.81326	0.33333	Isotropic

Anisotropic Thermal Factors / Form Factors

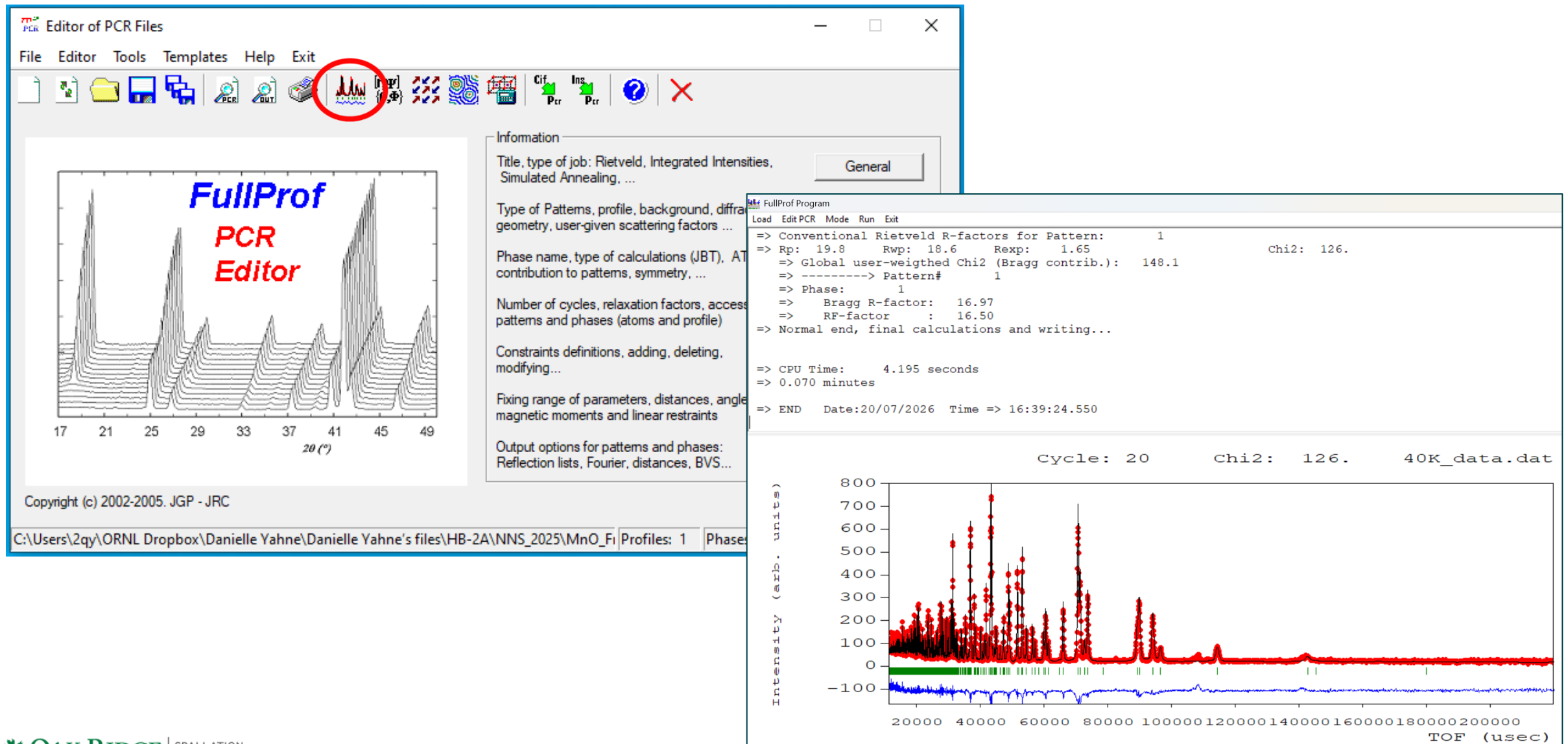
	B11/F1	B22/F2	B33/F3	B12/F4	B13/F5	B23/F6	F7
#							
#							
#							
#							

Special Form Factors

	SASH-Type	Matrix	j=1	j=2	j=3	N. Coeff.	Indices	#1	#2	#3	#4	#5	#6
#	Spherical												
	Spherical												
	Spherical												

Refine Positions Refine B_iso Refine B_aniso Fix All Cancel OK

Run refinement



Refine isotropic thermal parameters

Refinement Information

Cycles of Refinement:

Stop Criterion of Coverage
Forced Termination when shifts < x E.S.D.
Others:

Relaxation Factors for Shifts
Atomic Anisotropic Profile Global

Reflections ordering
☒ Only at the first cycle ☐ Each cycle

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

Refinement weighting model
☒ Least Squares ☐ Maximum Likelihood ☐ Unit Weights

Background

Reduction factor of number of data points:

OK Cancel

Bragg R-Factor excluding reflections

Phase 1 | Phase 2 | Phase 3

Atoms

Patterns
☒ 1 ☐ 2 ☐ 3

Profile
HKL Shifts

Make sure you check the results!
Sometimes B refines negative, which is not physical.

Atoms Information: Phase 1

List of Atoms
Number of Atoms:

	Label	Ntyp	X	Y	Z	B	Occ	Therm. Fact.
Atom # 1	Te1	Te	0.82234	0.57097	0.73823	0.72561	1.00000	Isotropic
Atom # 2	Te2	Te	0.60483	0.50405	0.42402	0.64508	1.00000	Isotropic
Atom # 3	Co1	Co	0.66667	0.33333	0.57732	0.67113	0.33333	Isotropic
Atom # 4	O1	O	0.66667	0.33333	0.74690	0.81326	0.33333	Isotropic

Anisotropic Thermal Factors / Form Factors

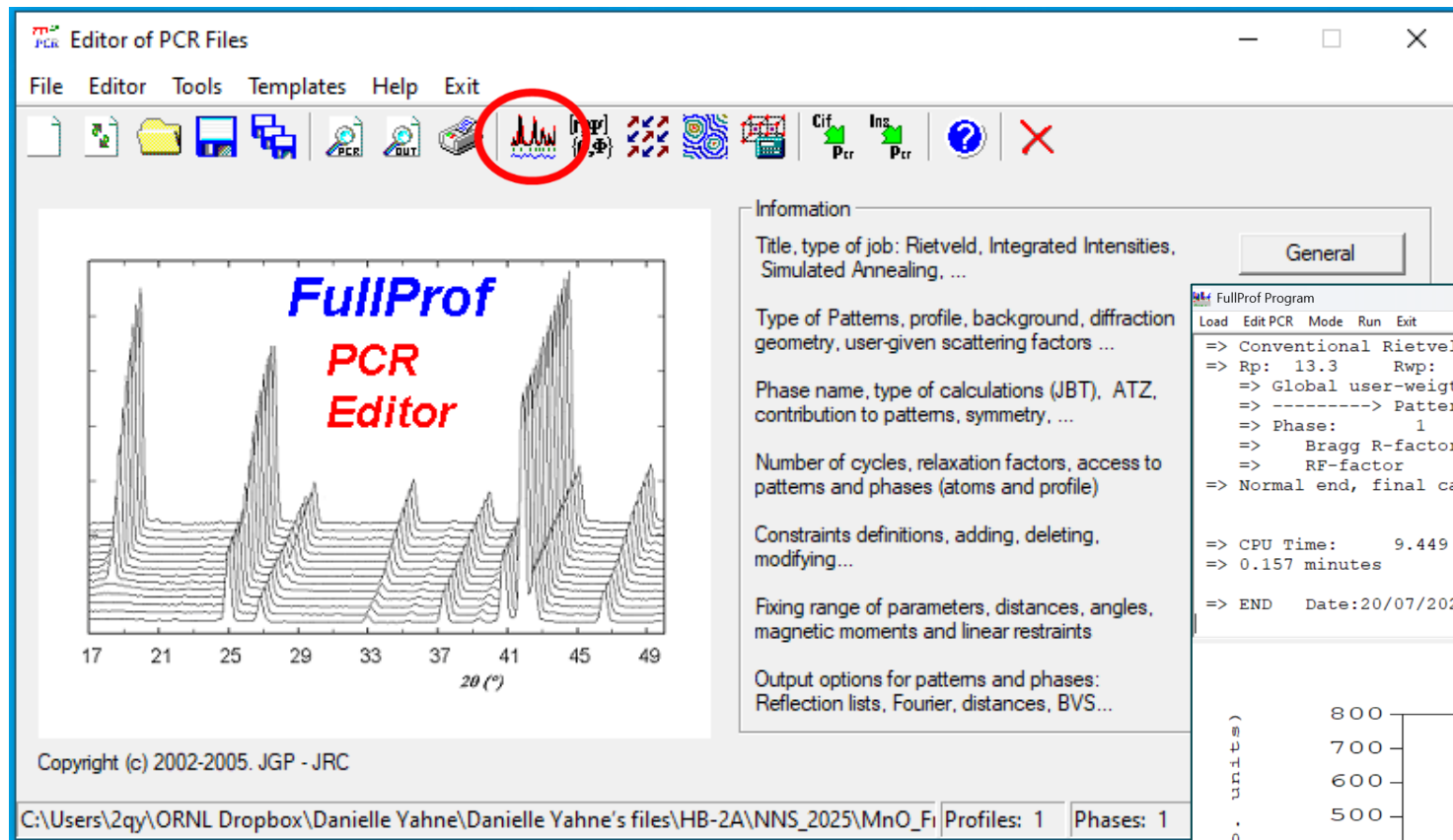
	B11/F1	B22/F2	B33/F3	B12/F4	B13/F5	B23/F6	F7
#							
#							
#							
#							

Special Form Factors

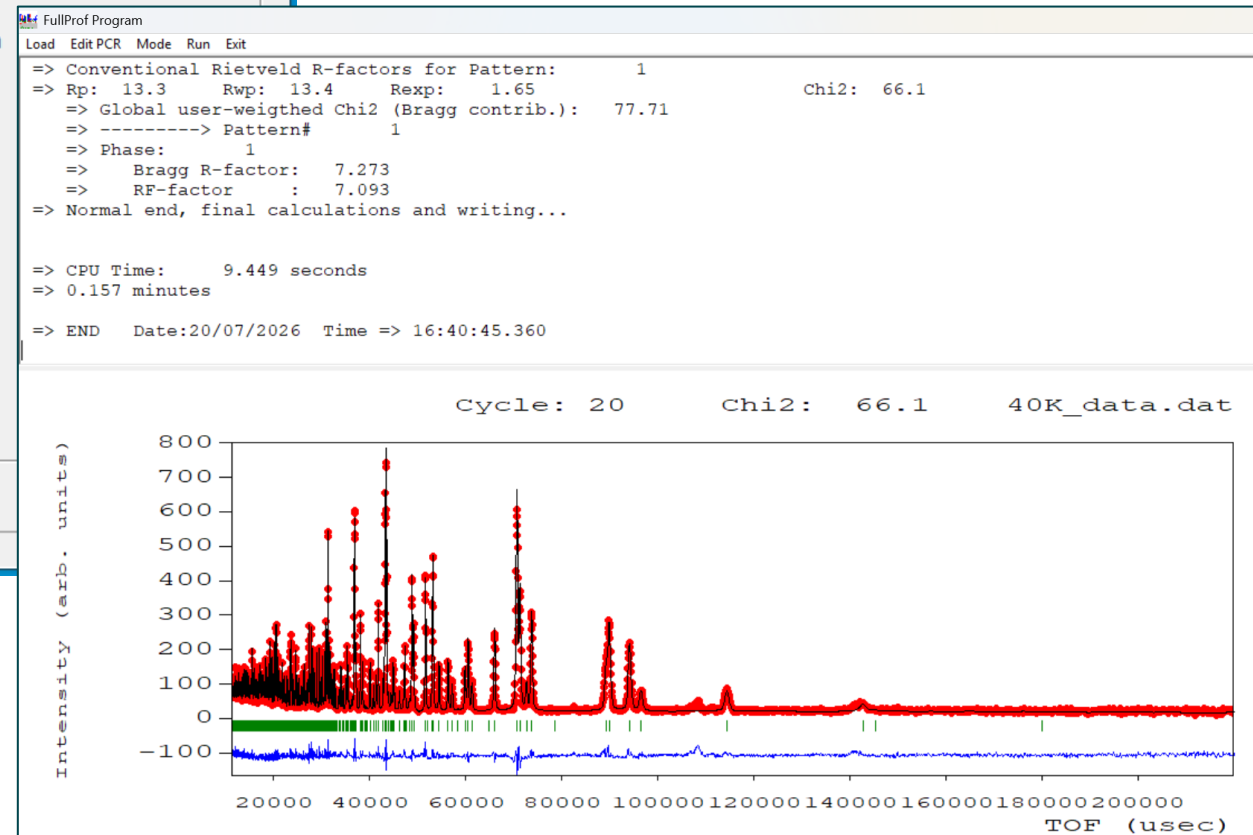
	SASH-Type	Matrix	j=1	j=2	j=3	N. Coeff.	Indices	#1	#2	#3	#4	#5	#6
#	Spherical												
	Spherical												
	Spherical												

Refine Positions
Refine B_iso
Refine B_aniso
Fix All
Cancel
OK

Run refinement



Make sure you check the results!
Sometimes B refines negative,
which is not physical.



Save refinement as & refine nuclear structure at 8 K

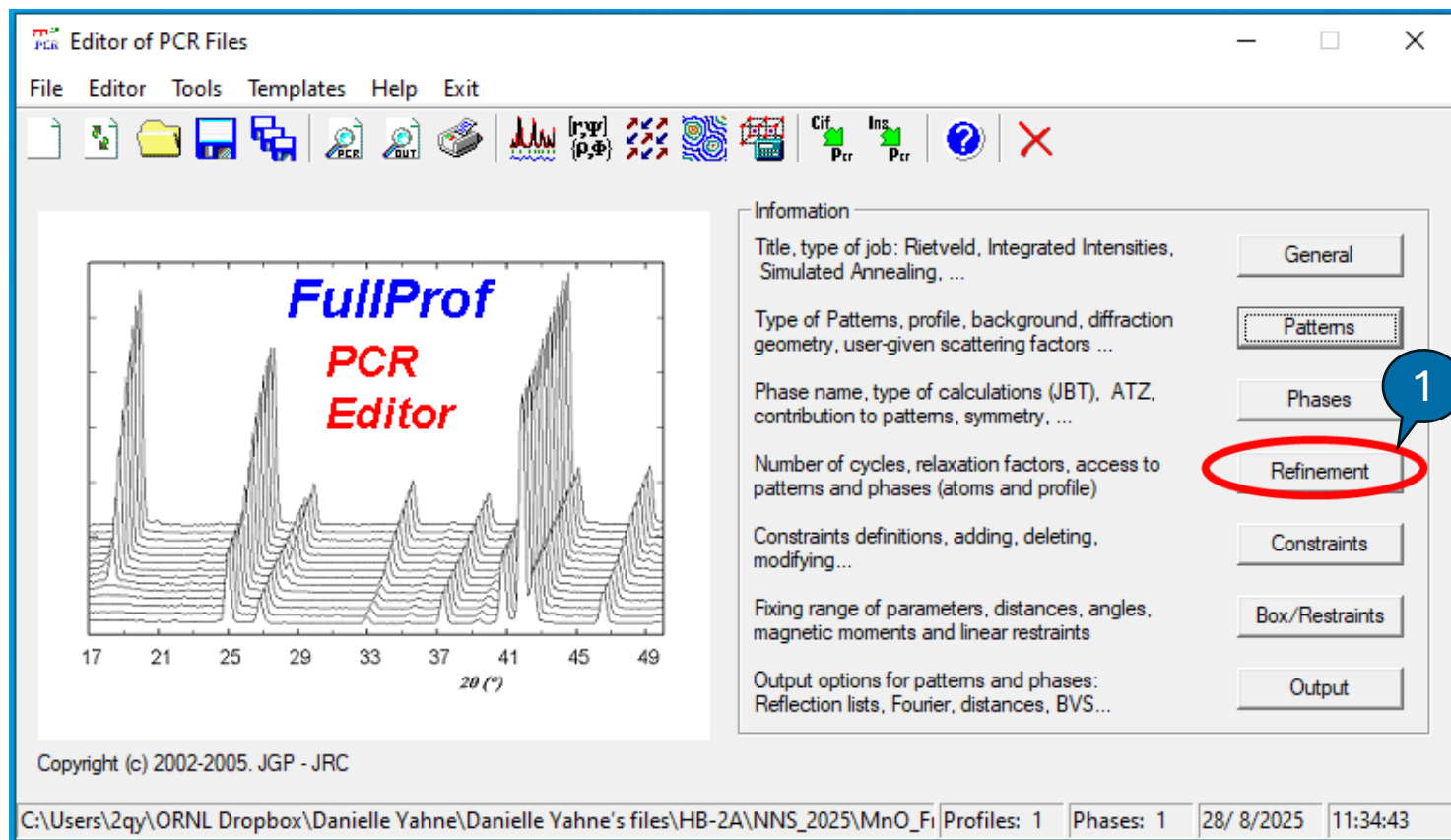
The image shows the FullProf PCR Editor interface with four numbered callouts indicating the steps to save and refine a nuclear structure at 8 K:

- 1**: The 'Save' icon in the toolbar (represented by a floppy disk) is circled in red.
- 2**: The 'Save' button in the 'Fullprof Files (PCR)' dialog box is circled in red.
- 3**: The 'General' tab in the sidebar is circled in red.
- 4**: The 'Refinement' radio button in the 'General Information' dialog box is selected.

The 'Fullprof Files (PCR)' dialog box shows the file name 'CoTe6O13_8K' and the save type 'Fullprof Input File'. The 'General Information' dialog box shows the title 'CoTe6O13 8K' and the 'Refinement' option selected under 'Calculations'.

The main window displays a plot of intensity versus 2θ (°) with the text 'FullProf PCR Editor' overlaid. The status bar at the bottom shows the file path: 'C:\Users\2qy\ORNL Dropbox\Danielle Yahne\Danielle Yahne's files\HB-2A\NNS_2025\MnO_Fi', and the number of profiles and phases: 'Profiles: 1 Phases: 1'.

Save refinement as & refine nuclear structure at 8 K



Refine nuclear structure at 8 K

Refinement Information

Cycles of Refinement:

Stop Criterion of Coverage
Forced Termination when shifts < x E.S.D.
Others:

Relaxation Factors for Shifts
Atomic Anisotropic Profile Global

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

Refinement weighting model
☒ Least Squares ☐ Maximum Likelihood ☐ Unit Weights
☒ Background ☐ Instrumental ☐ Micro-Absorption

Reduction factor of number of data points:

OK Cancel

Atoms
Patterns
☒ 1 ☐ 2 ☐ 3 ☐ 4 ☐ 5
Profile
HKL Shifts

Linear interpolation between a set of Background Points: Pattern 1

Interpolation Method
☒ Linear Interpolation ☐ Cubic Splines Interpolation

Information
Number of Points:

	2Theta	Counts	
1	13517.680	52.607	☐
2	19141.094	48.569	☐
3	22768.027	32.707	☐
4	26802.139		☐

Refine All Fix All

☒ Import from Background File

OK Cancel

Importing Background File

File Explorer: CoTe6O13_XianghanXu > 3_bar_prime_8K

Name	Date modified	Type	Size
3_bar_prime_8K			
CoTe6O13_Xian			
backup	7/20/2026 4:05 PM	File folder	
BG_8K	7/20/2026 4:04 PM	BGR File	3 KB

File name: BG_8K Background Input File

Open Cancel

Refine nuclear structure at 8 K

Refinement Information

Cycles of Refinement:

Stop Criterion of Coverage
Forced Termination when shifts < x E.S.D.
Others:

Relaxation Factors for Shifts
Atomic Anisotropic Profile Global

Reflections ordering
☒ Only at the first cycle ☐ Each cycle ☐ Bragg R-Factor excluding reflections

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

Refinement weighting model
☒ Least Squares ☐ Maximum Likelihood ☐ Unit Weights
Background Instrumental Micro-Absorption

Reduction factor of number of data points:

OK Cancel

Phase 1 | Phase 2 | Phase 3 | Phase 4

Atoms
Patterns ☒ 1 ☐ 2 ☐ 3 ☐ 4
Profile
HKL Shifts

Only refine lattice parameters – keep scale & peak shape parameters *fixed*

Profile Parameters: Phase 1 Pattern 1

Factors

	Scale	Overall B-factor
Coefficients	2.3414	0.0000

Cell Parameters

	a	b	c	alpha	beta	gamma
Coefficients	10.127827	10.127827	18.947807	90.000	90.000	120.000

FWHM / Shape Parameters Exponential Decay Parameters Preferred Orientation

FWHM Parameters

	Gam_2	Gam_1	Gam_0	Gam_2
Coefficients	5.767	10.078	0.000000	0.000000

Shape Parameters

	Extinc	Abs1	Abs2
Coefficients	0.000000	0.000000	0.000000

☐ Refine FWHM for second wavelength

	U2	V2	W2
Coefficients			

Refine All Fix All Cancel OK

Refine nuclear structure at 8 K

Refinement Information

Cycles of Refinement:

Stop Criterion of Coverage
Forced Termination when shifts < x E.S.D.
Others:

Relaxation Factors for Shifts
Atomic Anisotropic Profile Global

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

Refinement weighting model
☒ Least Squares ☐ Maximum Likelihood ☐ Unit Weights

Background Instrumental Micro-Absorption

Reduction factor of number of data points:

OK Cancel

Phase 1 | Phase 2 | Phase 3 | Phase 4

Atoms

Patterns
☒ 1 ☐ 2 ☐ 3 ☐ 4

Profile HKL Shifts

Can also refine atomic positions and thermal parameters

Atoms Information: Phase 1

List of Atoms
Number of Atoms:

	Label	Ntyp	X	Y	Z	B	Occ	Therm. Fact.
Atom # 1	Te1	Te	0.82310	0.57135	0.73814	0.27775	1.00000	Isotropic
Atom # 2	Te2	Te	0.60479	0.50442	0.42382	0.25680	1.00000	Isotropic
Atom # 3	Co1	Co	0.66667	0.33333	0.57739	0.50000	0.33333	Isotropic
Atom # 4	O1	O	0.66667	0.33333	0.74674	0.48272	0.33333	Isotropic

Anisotropic Thermal Factors / Form Factors

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

Special Form Factors

	SASH-Type	Matrix	j=1	j=2	j=3	N. Coeff.	Indices	#1	#2	#3	#4	#5	#6
#	Spherical												
	Spherical												
	Spherical												

Refine Positions
Refine B_iso
Refine B_aniso
Fix All
Cancel
OK

Refine nuclear structure at 8 K

FullProf
PCR
Editor

Information

Title, type of job: Rietveld, Integrated Intensities, Simulated Annealing, ...

Type of Patterns, profile, background, diffraction geometry, user-given scattering factors ...

Phase name, type of calculations (JBT), ATZ, contribution to patterns, symmetry, ...

Number of cycles, relaxation factors, access to patterns and phases (atoms and profile)

Constraints definitions, adding, deleting, modifying...

Fixing range of parameters, distances, angles, magnetic moments and linear restraints

Output options for patterns and phases: Reflection lists, Fourier, distances, BVS...

General

Patterns

Phases

Refinement

Constraints

Box/Restrains

Output

Copyright (c) 2002-2005. JGP - JRC

C:\Users\2qy\ORNL Dropbox\Danielle Yahne\Danielle Yahne's files\HB-2A\NNS_2025\MnO_F Profiles: 1 Phases: 1 28/ 8/2025 11:34:43

Output Information

PCR Input File

PCR Update: Overwrite PCR File ☒ Classical Output Format for a Single

Output Files

☐ Summary of refined parameters (RPA) ☒ Crystallographic Information File (CIF)

☐ List of Symmetry operators on file (SYM)

General Output Information Patterns Output Information Phases Output Information

Output Information File (OUT) Simulated Diffraction File (SIM) Summary Parameters File (SUM)

☐ Only Information from the last cycle is printed

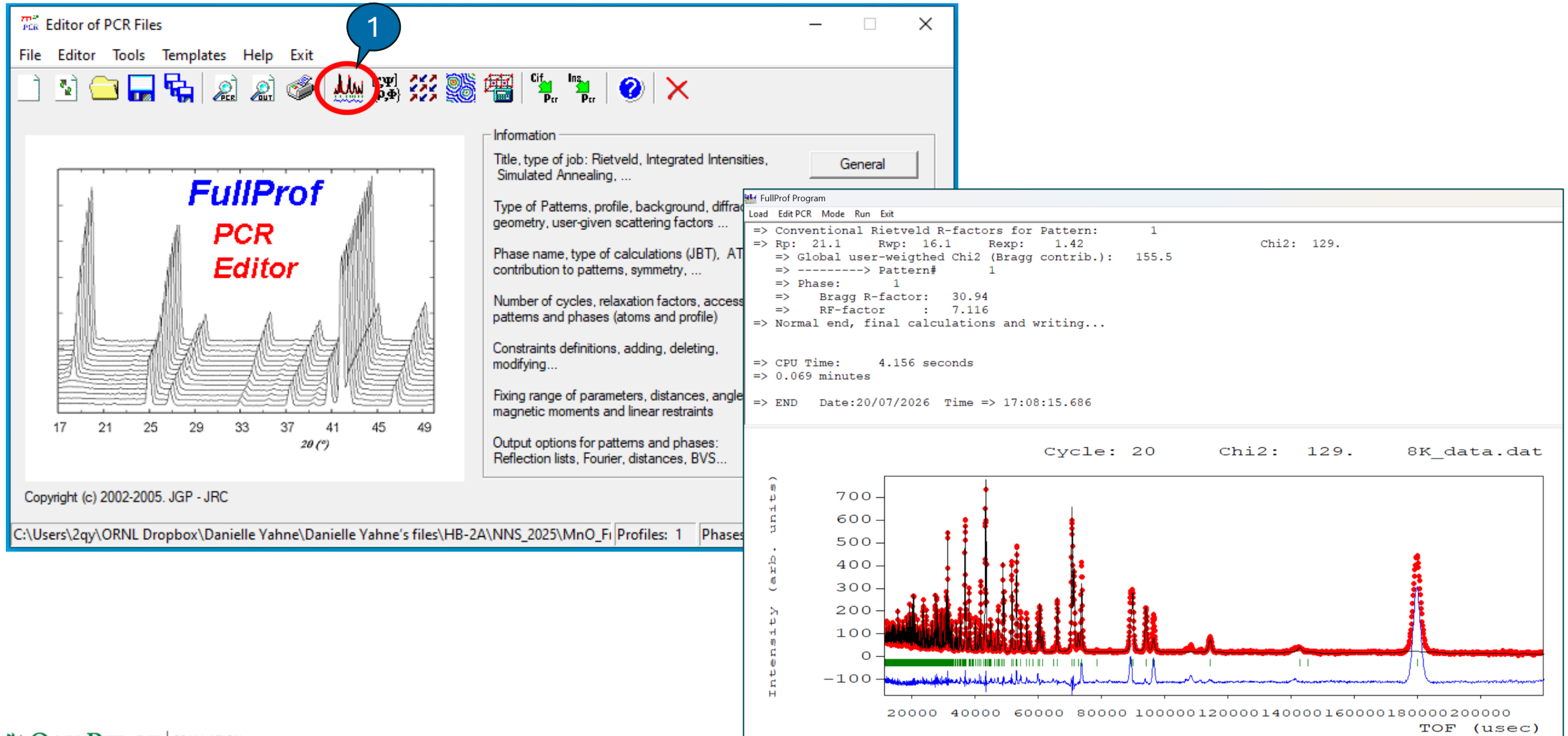
Correlation Matrix Output: None

Patterns

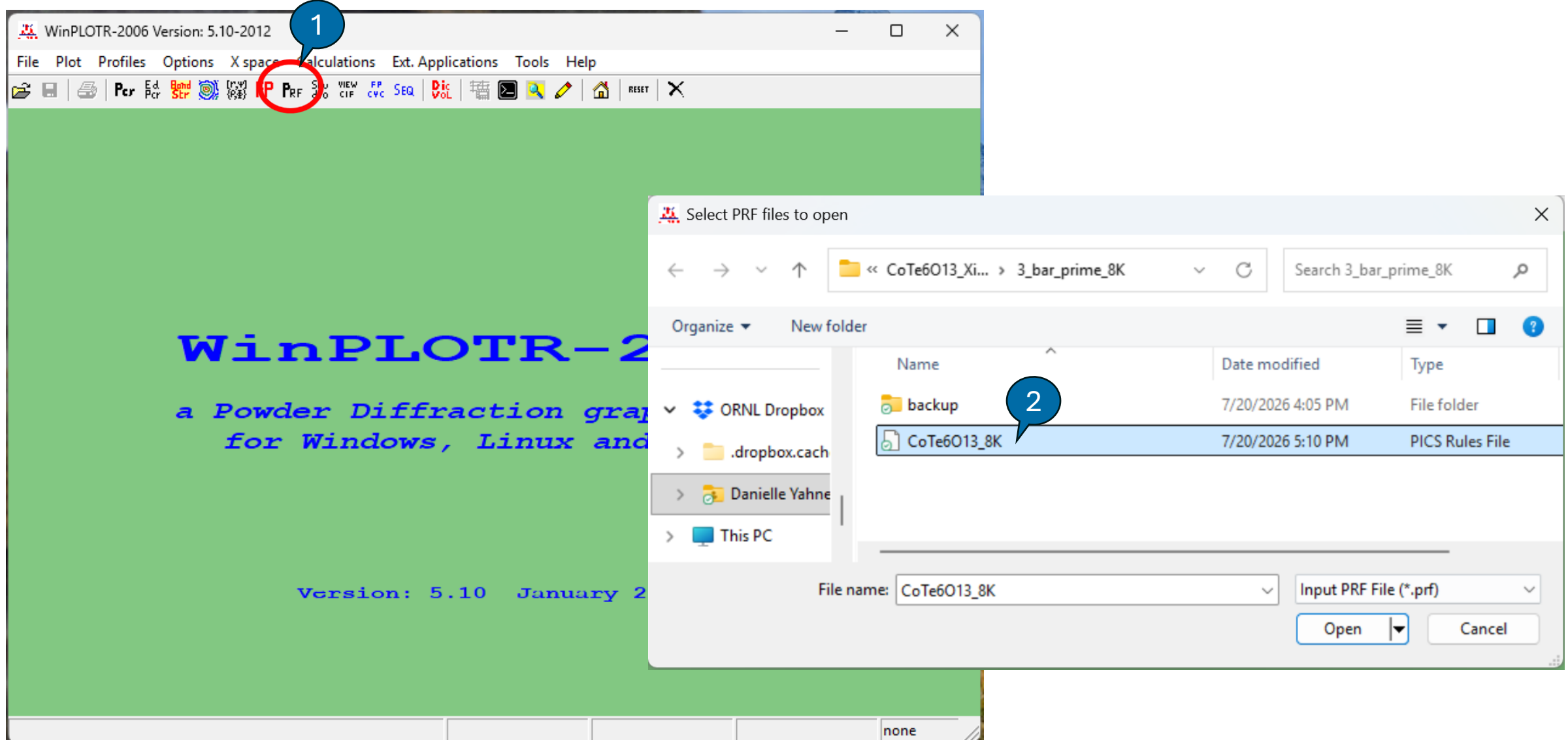
	1	-	-	-	-	-
Reflection list is written before starting cycle	☐	☐	☐	☐	☐	☐
Corrected profile intensities are written	☐	☐	☐	☐	☐	☐
Merged reflections list is written	☐	☐	☐	☐	☐	☐
Cal. and Obs. profile intensities are	☐	☐	☐	☐	☐	☐
Cal. and Obs. integrated intensities	☒	☐	☐	☐	☐	☐
List reflc. from second wavelength is	☐	☐	☐	☐	☐	☐

OK Cancel

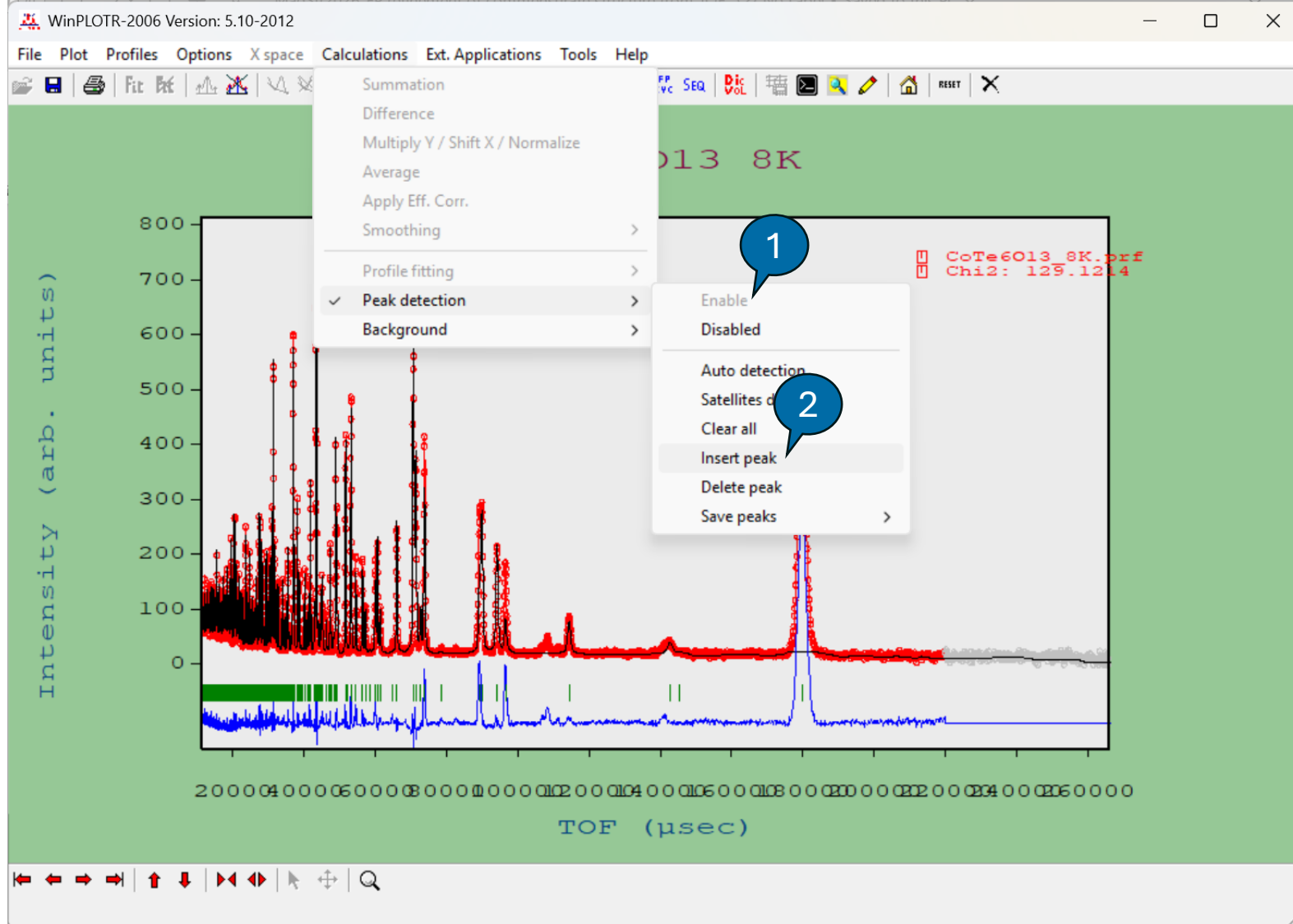
Refine nuclear structure at 8 K



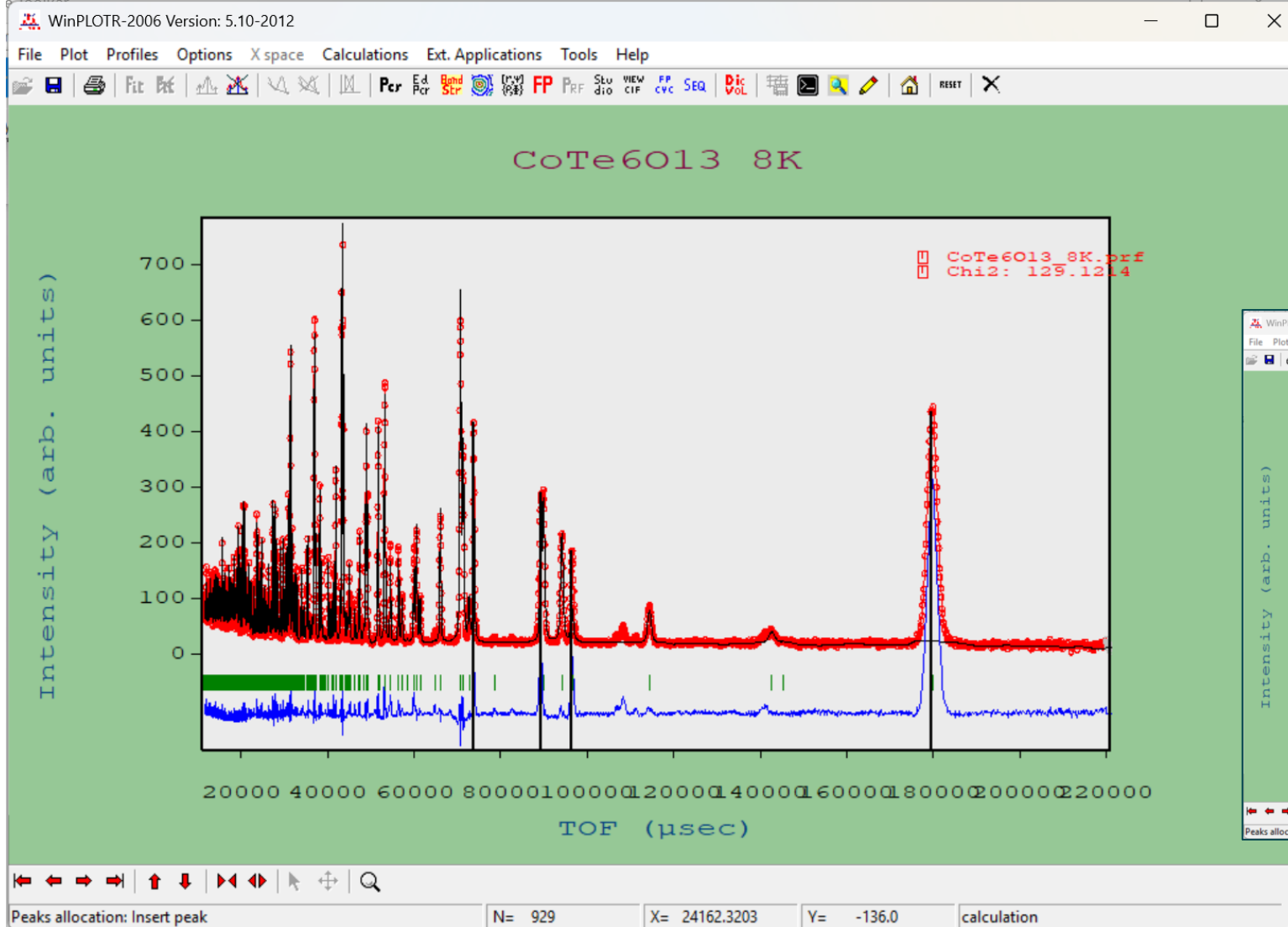
Identify magnetic peaks for k-search



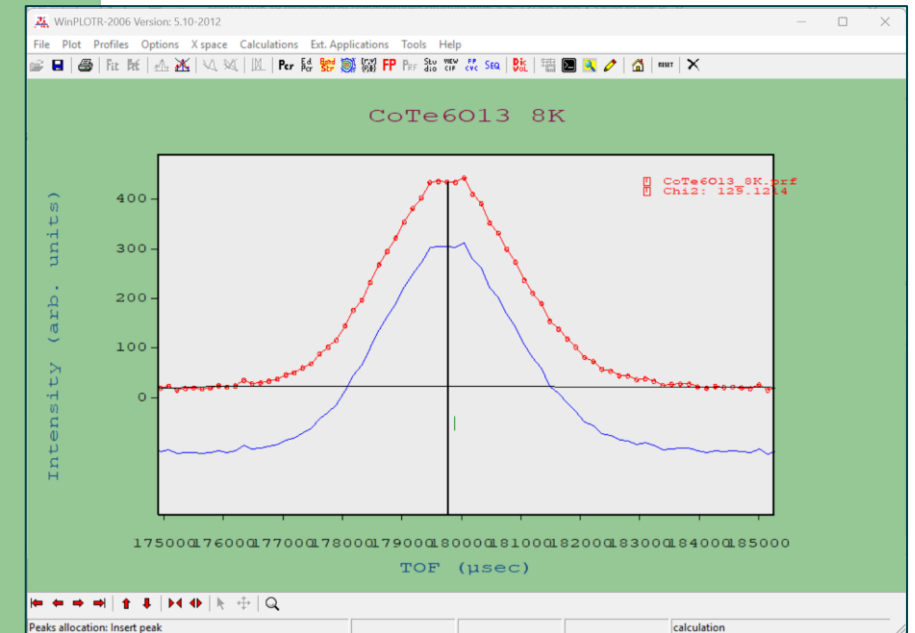
Identify magnetic peaks for k-search



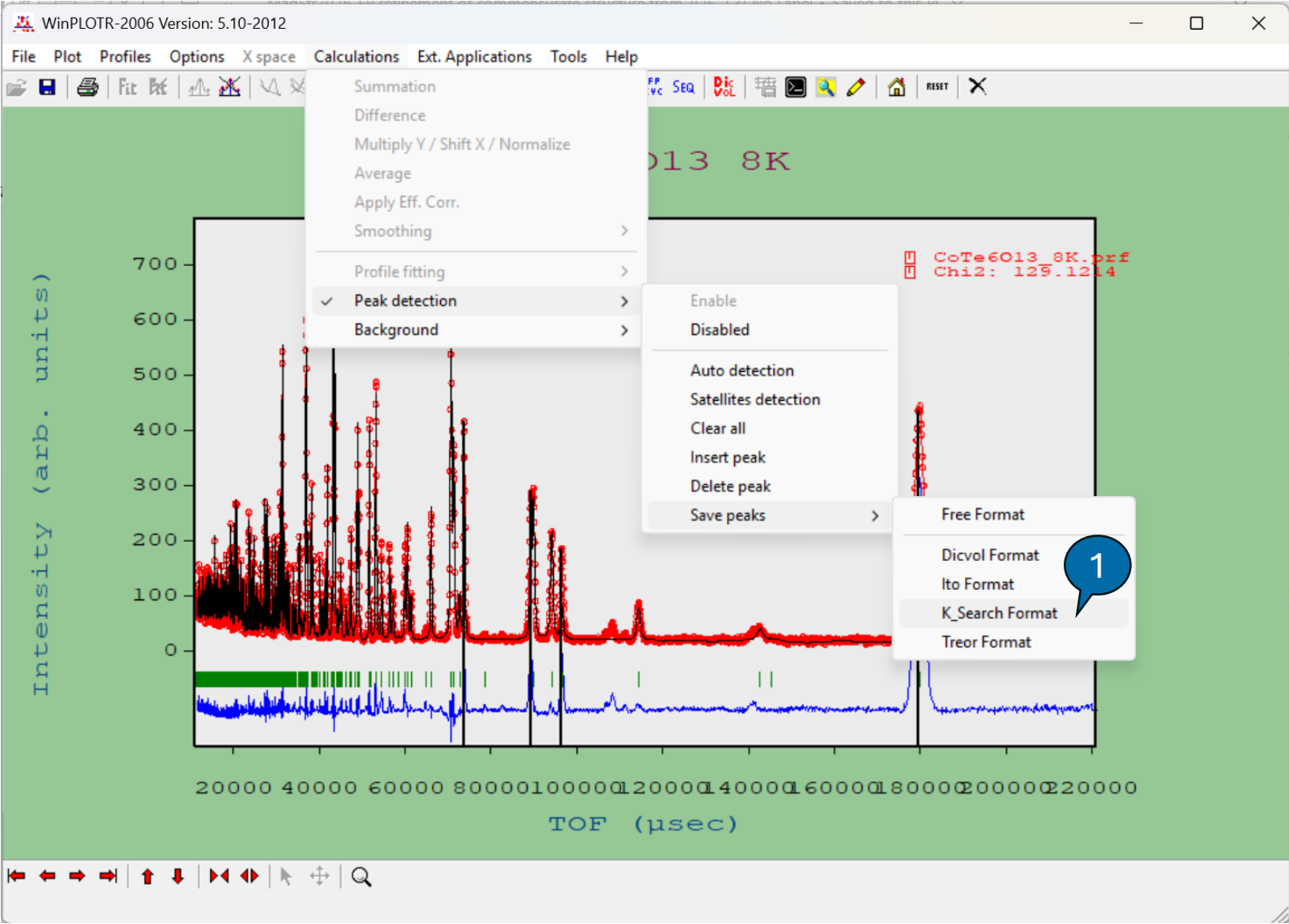
Identify magnetic peaks for k-search



Zoom in on a magnetic peak and left click in the center – repeat for clear magnetic peaks (not too many though!)



Save magnetic peaks for k-search



The figure shows the 'Input parameters for K_SEARCH' dialog box. The title is 'CoTe6013_8K Chi2:129.1214'. The 'Lattice Type' is 'R-3'. The 'Cell Parameters' are '10.12693 10.12693 18.94718 90.0000 90.0000 120.0000'. The 'Tolerance (TOF/2theta)' is '2000.00'. The 'K range (kxmin, kxmax, ...)' is '0.0 0.5 0.0 0.5 0.0 0.5'. The 'Number of Points (Na* Nb* Nc*)' is '100 100 100'. The 'Wavelength (CW) / Dtt1(TOF)' is '22591.99219'. The 'Short Output' radio button is selected. The 'Long Output' radio button is selected. The 'No output of intermediate calculations' radio button is selected. The 'Search only special k-vectors' checkbox is checked. The 'OK' and 'Cancel' buttons are at the bottom right. A blue circle with the number '2' is next to the 'OK' button.

The figure shows the 'Running K_Search' dialog box. The title is 'Running K_Search'. The question is 'Do you want to run k_Search?'. The 'Yes' and 'No' buttons are at the bottom. A blue circle with the number '3' is next to the 'Yes' button.

K-search results: $k = (0,0,0)$

```
C:\FullProf_Suite\k_search.exe X + v - □ X

=> List of the best incommensurate 10 solutions for 4 satellites

      Kx      Ky      Kz      R-factor
0.000000  0.000000  0.000000  0.114003
0.500000  0.000000  0.125000  0.306919
1.000000  0.000000  0.000000  0.753740
0.000000  1.000000  0.000000  0.753740
0.000000  0.000000  1.000000  0.753740
0.500000  0.125000  0.125000  0.799968
0.125000  0.125000  0.125000  0.966458
0.250000  0.500000  0.250000  1.061625
0.500000  0.250000  0.250000  1.062767
0.500000  0.500000  0.125000  1.168536

=> The best commensurate solution is the special kvector ks =( 0.0000 0.0000 0.0000)
=> The corresponding R-factor is:      0.1140 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:      0.02
      CPU-minutes:      0.00
      CPU-hours   :      0.00

=> Press <enter> to finish
```

Input into SARAh

SARAh – web Representational Analysis

This is the web page for a new web-based version of SARAh-Representational Analysis. Its code is inspired by the windows programme but has been entirely rewritten. It is still in a development phase and please contact me if you find problems or have suggestions. I hope that you like it; I think that it is pretty cool. One piece of advice – when you click evaluate, it will look like nothing is happening for a few seconds.

-Andrew (June 2018)



1

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

2

Propagation vector :
0 0 0

Crystallographic coordinates with each **moment carrying atom** on a separate line :
e.g. Cu2 1/2 1/2 -1/2

Co1	0.66667	0.33333	0.57732
-----	---------	---------	---------

3

4

EVALUATE

SARAh Results

$$\begin{array}{cc} \Gamma_1 & \psi_1 \\ \text{Co1} & 1) \ 0 \ 0 \ 3 \\ & 2) \ 0 \ 0 \ 3 \end{array}$$

$$\begin{array}{cc} \Gamma_2 & \psi_1 \\ \text{Co1} & 1) \ 0 \ 0 \ 3 \\ & 2) \ 0 \ 0 \ -3 \end{array}$$

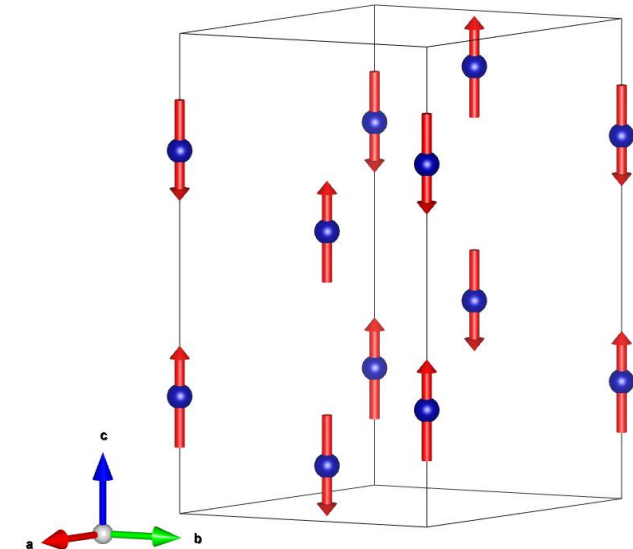
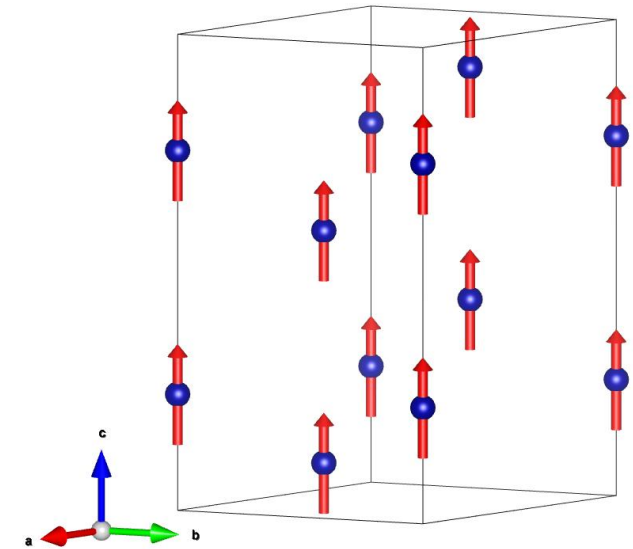
$$\begin{array}{cc} \Gamma_3 & \psi_1 \\ \text{Co1} & 1) \ 1.5-0.866025i \ -1.73205i \ 0 \\ & 2) \ 1.5-0.866025i \ -1.73205i \ 0 \end{array}$$

$$\begin{array}{cc} \Gamma_4 & \psi_1 \\ \text{Co1} & 1) \ 1.5-0.866025i \ -1.73205i \ 0 \\ & 2) \ -1.5+0.866025i \ 1.73205i \ 0 \end{array}$$

$$\begin{array}{cc} \Gamma_5 & \psi_1 \\ \text{Co1} & 1) \ 1.5+0.866025i \ 1.73205i \ 0 \\ & 2) \ 1.5+0.866025i \ 1.73205i \ 0 \end{array}$$

$$\begin{array}{cc} \Gamma_6 & \psi_1 \\ \text{Co1} & 1) \ 1.5+0.866025i \ 1.73205i \ 0 \\ & 2) \ -1.5-0.866025i \ -1.73205i \ 0 \end{array}$$

$$\Gamma_{\text{mag,Co1}} = 1 \Gamma_1^{(1)} \oplus 1 \Gamma_2^{(1)} \oplus 1 \Gamma_3^{(1)} \oplus 1 \Gamma_4^{(1)} \oplus 1 \Gamma_5^{(1)} \oplus 1 \Gamma_6^{(1)}$$



SARAh Results

$$\begin{array}{cc} \Gamma_1 & \psi_1 \\ \text{Co1} & 1) \ 0 \ 0 \ 3 \\ & 2) \ 0 \ 0 \ 3 \end{array}$$

$$\begin{array}{cc} \Gamma_2 & \psi_1 \\ \text{Co1} & 1) \ 0 \ 0 \ 3 \\ & 2) \ 0 \ 0 \ -3 \end{array}$$

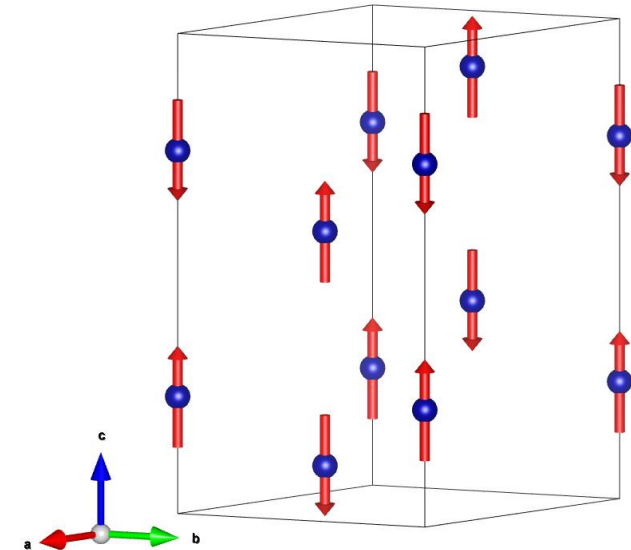
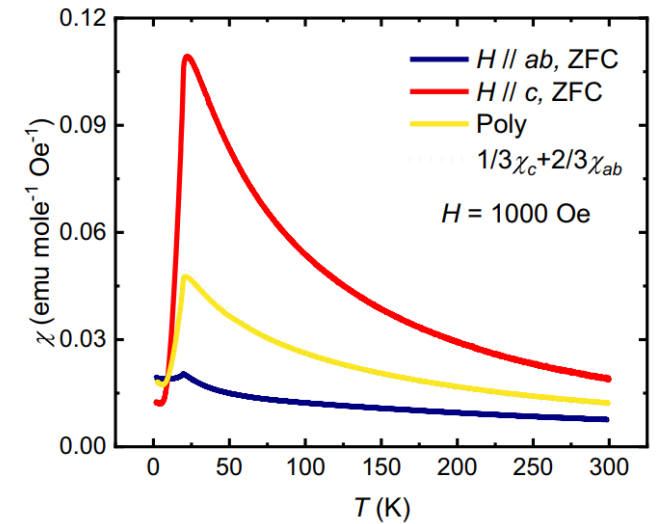
From magnetic susceptibility, Γ_2 is the most likely solution

$$\begin{array}{cc} \Gamma_3 & \psi_1 \\ \text{Co1} & 1) \ 1.5-0.866025i \ -1.73205i \ 0 \\ & 2) \ 1.5-0.866025i \ -1.73205i \ 0 \end{array}$$

$$\begin{array}{cc} \Gamma_4 & \psi_1 \\ \text{Co1} & 1) \ 1.5-0.866025i \ -1.73205i \ 0 \\ & 2) \ -1.5+0.866025i \ 1.73205i \ 0 \end{array}$$

$$\begin{array}{cc} \Gamma_5 & \psi_1 \\ \text{Co1} & 1) \ 1.5+0.866025i \ 1.73205i \ 0 \\ & 2) \ 1.5+0.866025i \ 1.73205i \ 0 \end{array}$$

$$\begin{array}{cc} \Gamma_6 & \psi_1 \\ \text{Co1} & 1) \ 1.5+0.866025i \ 1.73205i \ 0 \\ & 2) \ -1.5-0.866025i \ -1.73205i \ 0 \end{array}$$



SARAh Refine – Download Γ_1 and Γ_2

SARAh webRefine – FullProf

Three pieces of advice for using SARAh webRefine : **1.** change your browser settings to allow you to select where you save downloads (and overwrite files), **2.** when you click <evaluate>, it will look like nothing is happening for a few seconds. Look in the tab '4. Help and Strategies' for more information, **3.** if editing a pcr file creates an error, try moving your file so that its path contains no special characters: special characters and those with PHP commands, etc can fail validation c

-Andrew (February 2022)



Method 1. Conventional analysis - as projected basis vectors

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

1. powder format ▾ 2. make template pcr ▾

- ☒ Co1 $\Gamma_1 \psi_1$
- ☒ Co1 $\Gamma_2 \psi_1$
- ☐ Co1 $\Gamma_3 \psi_1$
- ☐ Co1 $\Gamma_4 \psi_1$
- ☐ Co1 $\Gamma_5 \psi_1$
- ☐ Co1 $\Gamma_6 \psi_1$

(Your browser should be set to ask for the download location so the pcr file can be overwritten. Please look in '4. Help

Submit

```
!-----> Profile Parameters for Pattern # 1
! Scale      Shape1      Bov      Str1      Str2      Str3      Strain-Model
  10.0        0.0000      0.0000      0.0000      0.0000      0.0000      0
  0.00000      0.00      0.00      0.00      0.00      0.00
!      U      V      W      X      Y      GauSiz      LorSiz      Size-Model
  0.00000      0.00000      0.00000      0.00000      0.00000      0.00000      0.00000      0
  0.00      0.00      0.00      0.00      0.00      0.00      0.00
!      a      b      c      alpha      beta      gamma
  3          3          3          90          90          90
  0.00000      0.00000      0.00000      0.00000      0.00000      0.00000

!Atom Typ Mag Vek      X      Y      Z      Biso      Occ      C1      C2      C3
! C4      C5      C6      C7      C8      C9      MagPh
Co1 MC02  1      0      0.66667  0.33333  0.57732  .30000  1.00000  0.000  0.000  0.000
      0.000  0.000  0.000  0.000  0.000  0.000  0.000  0.000  0.000  0.000
      0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00

!-----> Profile Parameters for Pattern # 1
! Scale      Shape1      Bov      Str1      Str2      Str3      Strain-Model
  10.0        0.0000      0.0000      0.0000      0.0000      0.0000      0
  0.00000      0.00      0.00      0.00      0.00      0.00
!      U      V      W      X      Y      GauSiz      LorSiz      Size-Model
  0.00000      0.00000      0.00000      0.00000      0.00000      0.00000      0.00000      0
  0.00      0.00      0.00      0.00      0.00      0.00      0.00
!      a      b      c      alpha      beta      gamma
  3          3          3          90          90          90
  0.00000      0.00000      0.00000      0.00000      0.00000      0.00000
```

Input SARAh output into 8 K Nuclear .pcr

```
CoTe6O13_8K.pcr
File Edit View

COMM CoTe6O13_8K
! Current global Chi2 (Bragg contrib.) = 154.8
! Files => DAT-file: 8K_data.dat, PCR-file: CoTe6O13_8K
! Job Npr Nph Nba Nex Nsc Nor Dum Iwg Ilo Ias Res Ste Nre Cry Uni Cor Opt
-1 9 2 62 1 0 0 0 0 0 0 5 0 0 0 1 0 0
!
02 0 0.75547 0.53766 0.64084 0.54148 1.00000 0 0 0 0
0.00 0.00 0.00 0.00 0.00
03 0 0.61392 0.47598 0.51998 0.53917 1.00000 0 0 0 0
0.00 0.00 0.00 0.00 0.00
04 0 0.79546 0.51702 0.40237 0.38343 1.00000 0 0 0 0
0.00 0.00 0.00 0.00 0.00
05 0 0.66654 0.58448 0.78246 0.53670 1.00000 0 0 0 0
0.00 0.00 0.00 0.00 0.00
!-----> Profile Parameters for Pattern # 1 -----> Phase # 1
! Scale Extinc Bov Str1 Str2 Str3 Strain-Mode
2.341364 0.0000 0.0000 0.0000 0.0000 0.0000 0
0.00000 0.00 0.00 0.00 0.00 0.00
! Sigma-2 Sigma-1 Sigma-0 Sigma-Q Iso-GStrain Iso-GSize Ani-LSize Size-Model
! Instrumental Sigma interpolated from list in IRF file (Only sample contribution is refined)
0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
0.00 0.00 0.00 0.00 0.00 0.00 0.00
! Gamma-2 Gamma-1 Gamma-0 Iso-LorStrain Iso-LorSize
! Instrumental Gamma interpolated from list in IRF file (Only sample contribution is refined)
5.7672 10.0776 0.0000 0.0000 0.0000
0.00 0.00 0.00 0.00 0.00
! a b c alpha beta gamma #Cell Info
10.126930 10.126930 18.947178 90.000000 90.000000 120.000000
11.00000 11.00000 21.00000 0.00000 0.00000 11.00000
! Pref1 Pref2 alph0 beta0 alph1 beta1 alphQ betaQ
! Instrumental alpha & beta interpolated from list in IRF file (Only shifts can be refined)
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
! Absorption correction parameters
0.00000 0.00 0.00000 0.00
! 2Th1/TOF1 2Th2/TOF2 Pattern to plot
11501.450 220000.000 1
```

Open 8 K Nuclear .pcr file, change number of phases (Nph) to 2, and copy & paste SARAh output under Phase 1 (but before 2Th1/TOF1 line)

```
Sarah_G1_G2.pcr
File Edit View

!-----> Profile Parameters for Pattern # 1 -----> Phase # 1
! Data for PHASE number: 1 ==> Current R_Bragg for Pattern # 1: 1.00
!-----> Profile Parameters for Pattern # 1 -----> Phase # 1
Template magnetic phase by SARAh - web Representational Analysis with basis vectors {1, 2}
!
! Nat Dis Mom Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nvk Npr More
1 0 0 0.0 0.0 1.0 1 0 -2 0 0 0.00 1 0 0
!
R -1 <--Space group symbol
! Nsym Cen Laue Ireps N_Bas
2 1 1 -1 2
! Real(0)-Imaginary(1) indicator for Ci
0 0
!
SYMM X, Y, Z
BASR 0 0 3. 0 0 3.
BASI 0 0 0 0 0 0
SYMM 1/3 - X, 2/3 - Y, 5/3 - Z
BASR 0 0 3. 0 0 -3.
BASI 0 0 0 0 0 0
! Atom Typ Mag Vek X Y Z Biso Occ C1 C2 C3
! C4 C5 C6 C7 C8 C9 MagPh
Co1 MC02 1 0 0.66667 0.33333 0.57732 .30000 1.00000 0.000 0.000 0.000
0.000 0.000 0.000 0.000 0.000 0.000 0.00000 0.000 0.000 0.000
0.00 0.00 0.00 0.00 0.00 0.00 0.00
!-----> Profile Parameters for Pattern # 1 -----> Phase # 1
! Scale Shape1 Bov Str1 Str2 Str3 Strain-Model
10.0 0.0000 0.0000 0.0000 0.0000 0.0000 0
0.00000 0.00 0.00 0.00 0.00 0.00
! U V W X Y GauSiz LorSiz Size-Model
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
```

Insert SARAh output phase .pcr text HERE

Copy profile parameters from nuclear phase

```

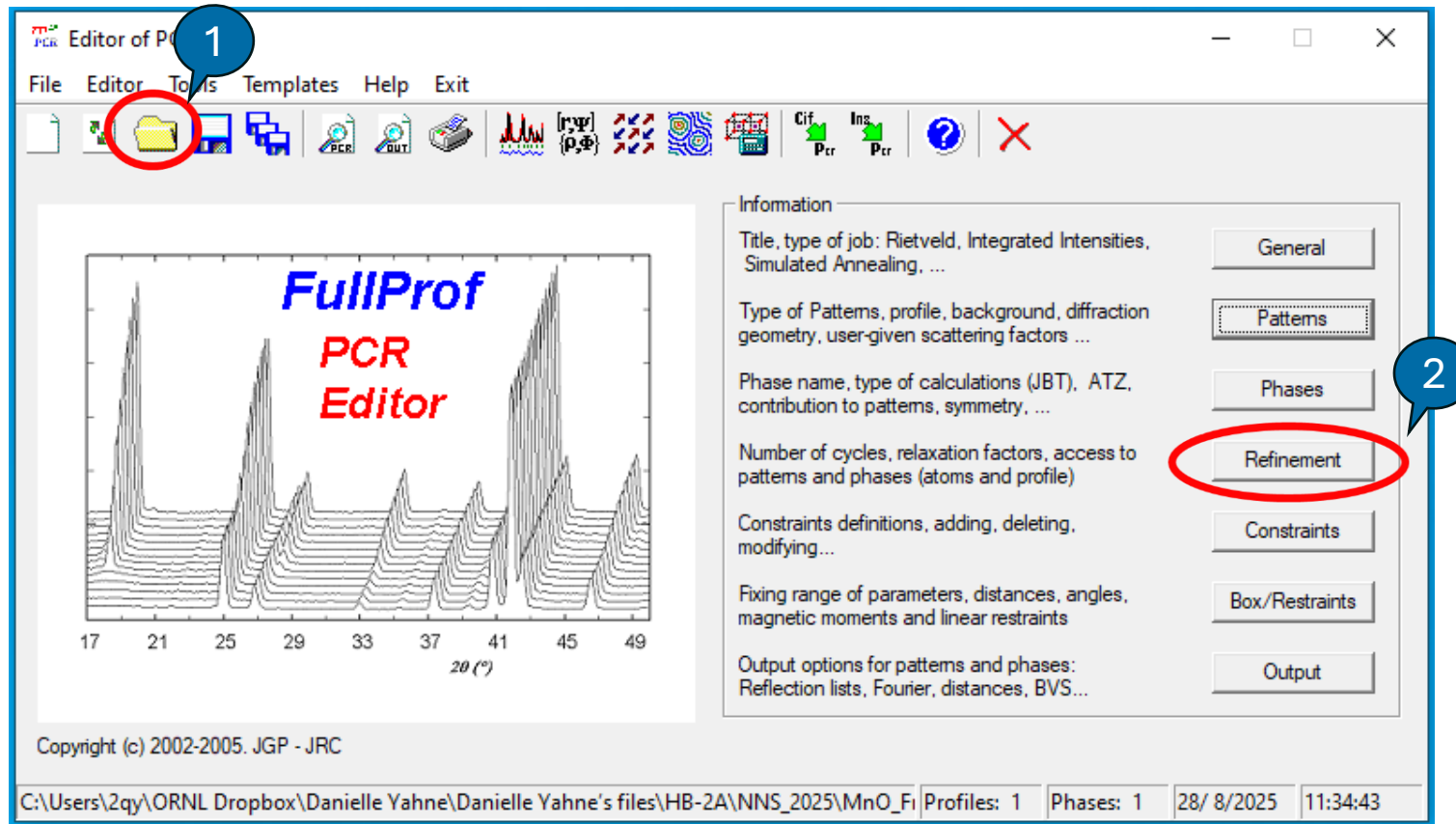
SYMM X , Y , Z
BASR 0 0 3. 0 0 3.
BASI 0 0 0 0 0 0
SYMM 1/3 - X , 2/3 - Y , 5/3 - Z
BASR 0 0 3. 0 0 -3.
BASI 0 0 0 0 0 0
!Atom Typ Mag Vek X Y Z Biso Occ C1 C2 C3
! C4 C5 C6 C7 C8 C9 MagPh
Co1 MC02 1 0 0.66667 0.33333 0.57732 .30000 1.00000 0.000 0.000 0.000
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
0.000 0.000 0.000 0.000 0.000 0.000 0.00000
0.00 0.00 0.00 0.00 0.00 0.00 0.00

!-----> Profile Parameters for Pattern # 1 -----> Phase # 1
! Scale Extinc Bov Str1 Str2 Str3 Strain-Mode
2.341364 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0
0.00000 0.00 0.00 0.00 0.00 0.00 0.00
! Sigma-2 Sigma-1 Sigma-0 Sigma-Q Iso-GStrain Iso-GSize Ani-LSize Size-Model
! Instrumental Sigma interpolated from list in IRF file (Only sample contribution is refined)
0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0
0.00 0.00 0.00 0.00 0.00 0.00 0.00
! Gamma-2 Gamma-1 Gamma-0 Iso-LorStrain Iso-LorSize
! Instrumental Gamma interpolated from list in IRF file (Only sample contribution is refined)
5.7672 10.0776 0.0000 0.0000 0.0000
0.00 0.00 0.00 0.00 0.00
! a b c alpha beta gamma #Cell Info
10.126930 10.126930 18.947178 90.000000 90.000000 120.000000
11.00000 11.00000 21.00000 0.00000 0.00000 11.00000
! Pref1 Pref2 alph0 beta0 alph1 beta1 alphQ betaQ
! Instrumental alpha & beta interpolated from list in IRF file (Only shifts can be refined)
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
!Absorption correction parameters
0.00000 0.00 0.00000 0.00 ABS: ABSCOR1 ABSCOR2
! Propagation vectors:
0. 0. 0. Propagation Vector 1
0.000000 0.000000 0.000000
! 2Th1/TOF1 2Th2/TOF2 Pattern to plot
11501.450 22000.000 1

```

Copy & paste nuclear (Phase 1)
profile parameters into
magnetic phase (Phase 2)

Reload pcr file & open refinement tab



Refinement now has 2 phases (Phase 1: Nuclear, Phase 2: Magnetic)

The screenshot shows the 'Refinement Information' dialog box with several settings. Two blue callout circles with numbers are present: circle '1' points to the 'Bragg R-Factor' checkbox, and circle '2' points to the 'Atoms' button. The 'Phase 2' tab in the 'Patterns' section is also highlighted with a red circle.

Refinement Information

Cycles of Refinement: 20

Stop Criterium of Coverage
Forced Termination when shifts < 0.10 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 limiting reflections limiting excluded regions

Pattern 1 | Pattern 2 | Pattern 3 | Pattern 4 | Pattern 5 | Pattern 6 | Pattern 7

Refinement weighting model
☒ Least Squares ☐ Maximum Likelihood ☐ Unit Weights
Background Instrumental Micro-Absorption

Reduction factor of number of data points: 0

OK Cancel

Phase 1 | **Phase 2** | Phase 3 | Phase 4 | Phase 5 | Phase 6 | Phase 7

Atoms Prop. Vectors

Patterns
☒ 1 ☐ 2 ☐ 3 ☐ 4 ☐ 5 ☐ 6 ☐ 7

Profile Micro-Structure
HKL Shifts Further Parameters

Refine C2 mixing coefficient

Refinement Information

Cycles of Refinement: 20

Stop Criterium of Coverage
Forced Termination when shifts < 0.10 x E.S.D.
Others: None

Reflections ordering
☒ Only at the first cycle ☐ Each cycle

Pattern 1 | Pattern 2 | Pattern 3 | Pattern 4 | Pattern 5

Refinement weighting model
☒ Least Squares
☐ Maximum Likelihood
☐ Unit Weights

Reduction factor of number of data points: 0

Atoms Information: Phase 2

List of Atoms
Number of Atoms: 1

	Label	Ntyp	Mag. Rot.	Prog. Vec.	X	Y	Z	B	Occ
Atom # 1	Co1	MCO2	1	0	0.66667	0.33333	0.57732	0.30000	1.00000

Rx Ry Rz lx ly lz MPhase

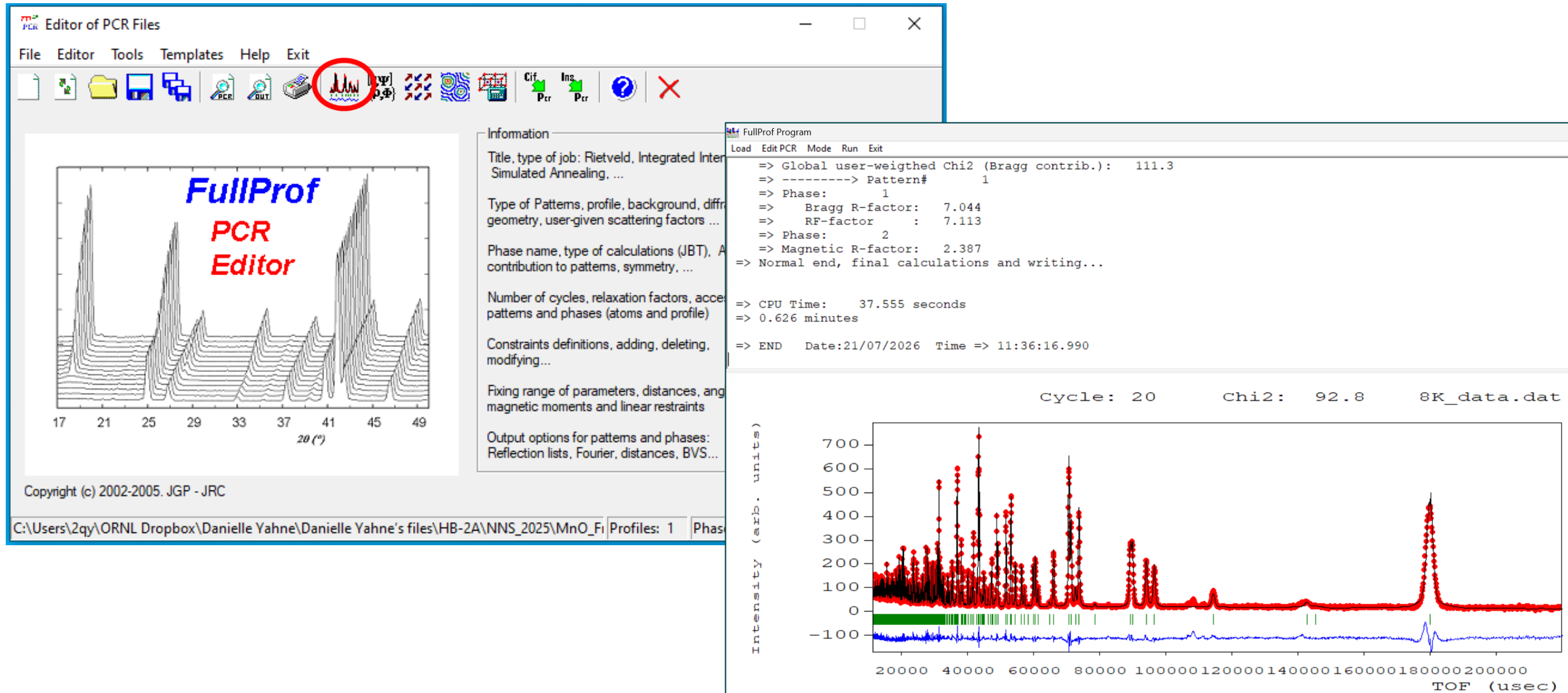
	Rx	Ry	Rz	lx	ly	lz	MPhase
Atom #1							

Basis Functions Coefficients

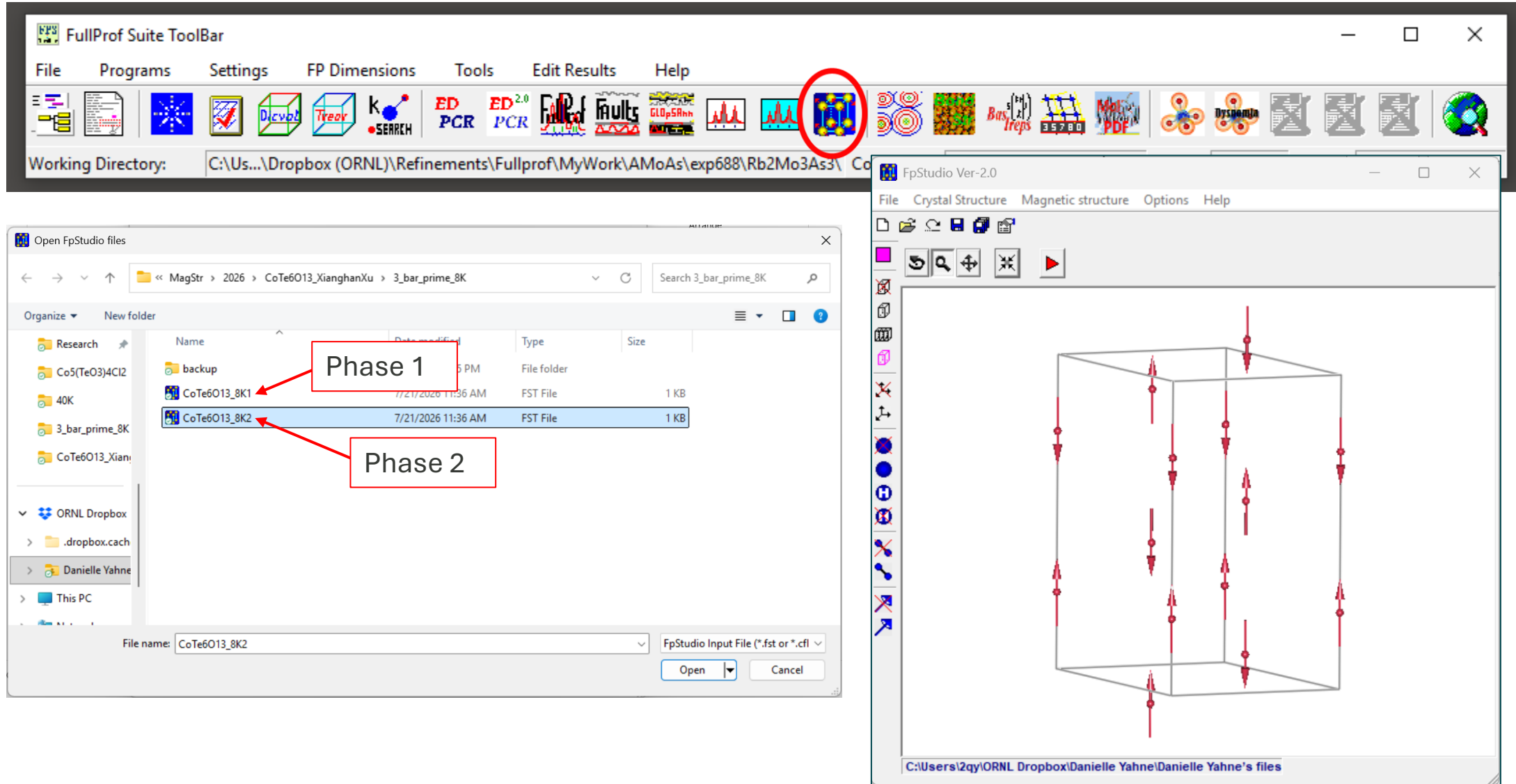
	C1	C2	C3	C4	C5	C6	C7
Atom # 1	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Refine Positions
Refine B_iso
Fix All
Cancel
OK

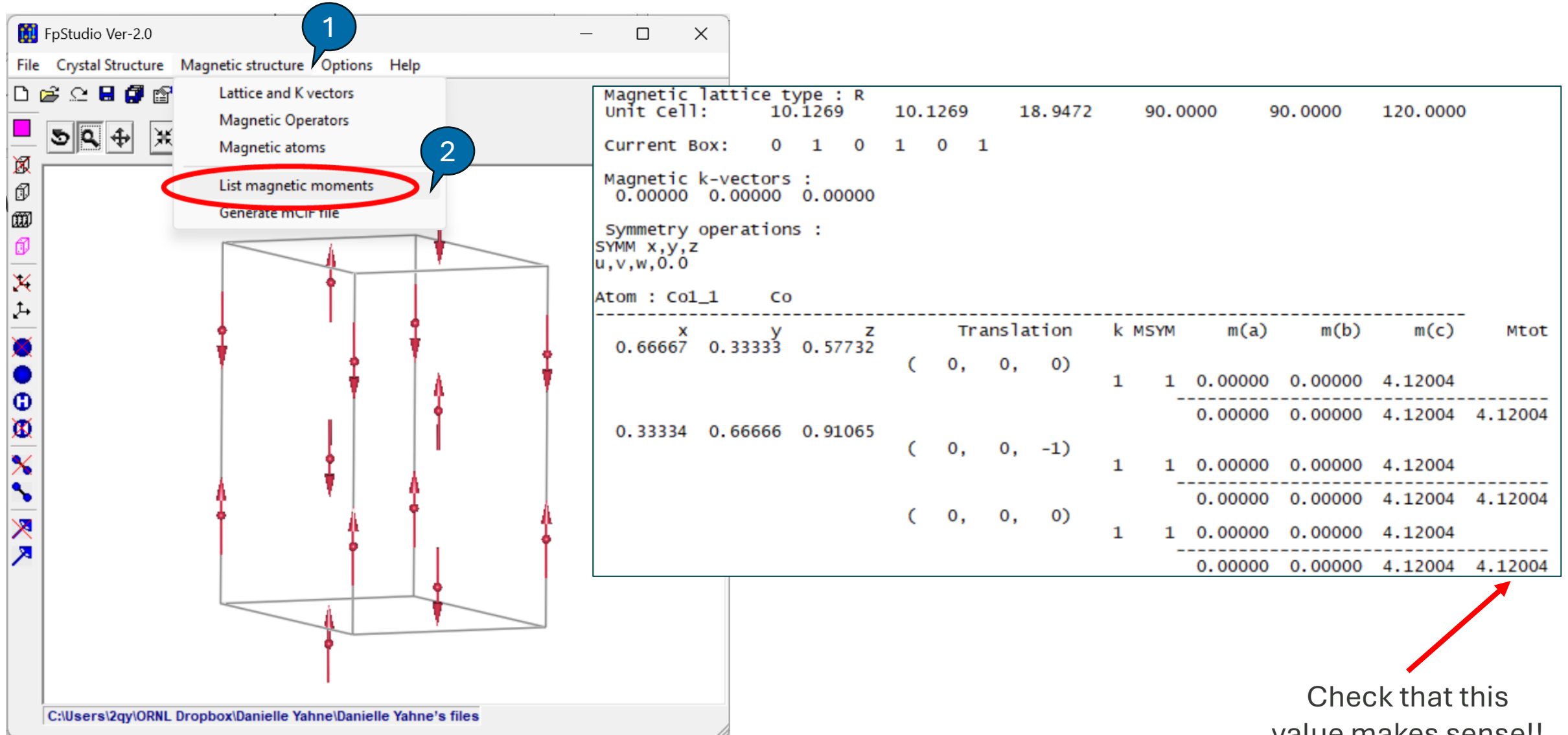
Run magnetic refinement at 8 K



Look at results with Fullprof Studio



Look at results with Fullprof Studio



Look at Fullprof Summary file

==> COEFFICIENTS OF BASIS VECTORS:

=> Real(0)-Imaginary(1) indicators of basis functions coefficients

C1:0 C2:0

Co1 C1= 0.0000(0) C2= 1.3733(196) C3= 0.0000(0)
 C4= 0.0000(0) C5= 0.0000(0) C6= 0.0000(0)
 C7= 0.0000(0) C8= 0.0000(0) C9= 0.0000(0)
 Phase/2pi= 0.0000(0)

$$\vec{m}_j = \sum_{v, \vec{k}} C_v^{\vec{k}} \vec{\psi}_{i,v}^{\vec{k}} e^{-2\pi i \vec{k} \cdot \vec{t}_{ij}}$$

Γ_2	ψ_1			
Co1	1)	0	0	3
	2)	0	0	-3

$$\vec{m}_{Co_1} = 1.3733(196) * \begin{bmatrix} 0 \\ 0 \\ 3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 4.12(6) \end{bmatrix}$$

PAUSE before we switch to Magnetic Space Groups

Alternative description of magnetic structure using MSGs

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
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)
k-SUBGROUPSMAG	Magnetic subgroups consistent with some given propagation vector
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-m

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 148

Please, enter the propagation vector k:

k_x

0

k_y

0

k_z

0

4

Submit

Input CIF & identify magnetic ion

1

Option 1: Please submit a structure file (2 format):

Choose File

No file chosen

Upload the file

Note: The space group of the cif file will supersede any previous one.

Option 2: Specify structure data by hand:
Space Group: C2/c (No. 15)
Lattice parameters (Angstroms and degrees):
a= b= c= alpha=90 beta=
Number of unique atomic positions:

Submit

Parent space group: R-3 (No. 148)
Lattice parameters (Angstroms and degrees): a=10.12693, b=10.12693, c=18.94720, alpha=90.0000, beta=90.0000, gamma=120.000

Atoms: Please select the magnetic ones

N	Atom name	Atom type	Wyckoff Position	Coordinates	Magnetic?
1	Te1	Te	18f	0.82273 0.57159 0.73806	☐
2	Te2	Te	18f	0.60519 0.50483 0.42380	☐
3	Co1	Co	6c	0.66667 0.33333 0.57739	☒
4	O1	O	6c	0.66667 0.33333 0.74695	☐
5	O2	O	18f	0.75547 0.53766 0.64084	☐
6	O3	O	18f	0.61392 0.47598 0.51998	☐
7	O4	O	18f	0.79546 0.51702 0.40237	☐
8	O5	O	18f	0.66654 0.58448 0.78246	☐

Submit

Maximal magnetic space groups & constraints

Maximal magnetic space groups for the parent space group $R\text{-}3$ (No. 148) 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	$R\text{-}3'$ (#148.19) 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	Co1 Co 0.00000 0.00000 0.24406	$(0,0,z \mid 0,0,m_z)$ $(0,0,-z \mid 0,0,-m_z)$ $(2/3,1/3,z+1/3 \mid 0,0,m_z)$ $(2/3,1/3,-z+1/3 \mid 0,0,-m_z)$ $(1/3,2/3,z+2/3 \mid 0,0,m_z)$ $(1/3,2/3,-z+2/3 \mid 0,0,-m_z)$	6	$(0,0,M_z)$	$M_z = 0.00000$
---	--------------------------------	---	---	-------------	-----------------

2	$R\text{-}3$ (#148.17) 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	Co1 Co 0.00000 0.00000 0.24406	$(0,0,z \mid 0,0,m_z)$ $(0,0,-z \mid 0,0,m_z)$ $(2/3,1/3,z+1/3 \mid 0,0,m_z)$ $(2/3,1/3,-z+1/3 \mid 0,0,m_z)$ $(1/3,2/3,z+2/3 \mid 0,0,m_z)$ $(1/3,2/3,-z+2/3 \mid 0,0,m_z)$	6	$(0,0,M_z)$	$M_z = 0.00000$
---	--------------------------------	--	---	-------------	-----------------

Magnetic Structure

Selected magnetic space group: 1- *R*-3' (#148.19)

Setting of the parent group

Parent space group *R*-3 (No. 148)

Lattice parameters: a=10.16600, b=10.16600, c=18.98100, alpha=90, beta=90, gamma=120



[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	Te1 Te 0.82234 0.57097 0.73823	(x,y,z m _x ,m _y ,m _z) (-y,x-y,z -m _y ,m _x -m _y ,m _z) (-x+y,-x,z -m _x +m _y ,m _x ,m _z) (-x,-y,-z -m _x ,m _y ,m _z) (y,-x+y,-z m _y ,m _x +m _y ,m _z) (x-y,x,-z m _x -m _y ,m _x ,m _z) (x+2/3,y+1/3,z+1/3 m _x ,m _y ,m _z) (-y+2/3,x-y+1/3,z+1/3 -m _y ,m _x -m _y ,m _z) (-x+y+2/3,-x+1/3,z+1/3 -m _x +m _y ,m _x ,m _z) (-x+2/3,-y+1/3,-z+1/3 -m _x ,m _y ,m _z) (y+2/3,-x+y+1/3,-z+1/3 m _y ,m _x +m _y ,m _z) (x-y+2/3,x+1/3,-z+1/3 m _x -m _y ,m _x ,m _z) (x+1/3,y+2/3,z+2/3 m _x ,m _y ,m _z) (-y+1/3,x-y+2/3,z+2/3 -m _y ,m _x -m _y ,m _z) (-x+y+1/3,-x+2/3,z+2/3 -m _x +m _y ,m _x ,m _z) (-x+1/3,-y+2/3,-z+2/3 -m _x ,m _y ,m _z) (y+1/3,-x+y+2/3,-z+2/3 m _y ,m _x +m _y ,m _z) (x-y+1/3,x+2/3,-z+2/3 m _x -m _y ,m _x ,m _z)	18	-	-
2	Te2 Te 0.60483 0.50405 0.42402	(x,y,z m _x ,m _y ,m _z) (-y,x-y,z -m _y ,m _x -m _y ,m _z) (-x+y,-x,z -m _x +m _y ,m _x ,m _z) (-x,-y,-z -m _x ,m _y ,m _z) (y,-x+y,-z m _y ,m _x +m _y ,m _z) (x-y,x,-z m _x -m _y ,m _x ,m _z) (x+2/3,y+1/3,z+1/3 m _x ,m _y ,m _z) (-y+2/3,x-y+1/3,z+1/3 -m _y ,m _x -m _y ,m _z) (-x+y+2/3,-x+1/3,z+1/3 -m _x +m _y ,m _x ,m _z) (-x+2/3,-y+1/3,-z+1/3 -m _x ,m _y ,m _z) (y+2/3,-x+y+1/3,-z+1/3 m _y ,m _x +m _y ,m _z) (x-y+2/3,x+1/3,-z+1/3 m _x -m _y ,m _x ,m _z) (x+1/3,y+2/3,z+2/3 m _x ,m _y ,m _z) (-y+1/3,x-y+2/3,z+2/3 -m _y ,m _x -m _y ,m _z) (-x+y+1/3,-x+2/3,z+2/3 -m _x +m _y ,m _x ,m _z) (-x+1/3,-y+2/3,-z+2/3 -m _x ,m _y ,m _z) (y+1/3,-x+y+2/3,-z+2/3 m _y ,m _x +m _y ,m _z) (x-y+1/3,x+2/3,-z+2/3 m _x -m _y ,m _x ,m _z)	18	-	-
3	Co1 Co 0.00000 0.00000 0.24399	(0,0,z 0,0,m _z) (0,0,-z 0,0,-m _z) (2/3,1/3,z+1/3 0,0,m _z) (2/3,1/3,-z+1/3 0,0,-m _z) (1/3,2/3,z+2/3 0,0,m _z) (1/3,2/3,-z+2/3 0,0,-m _z)	6	(0,0,M _z)	M _z = 2



Save mCIF & Visualize structure

mCIF file of the structure

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

Download mCIF 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: 21/07/2026 22:15:10
# CoTe6O13_ICSD149502.cif

data_5yOhtAoR
_audit_creation_date      2026-07-21
_audit_creation_method    "Bilbao Crystallographic Server"

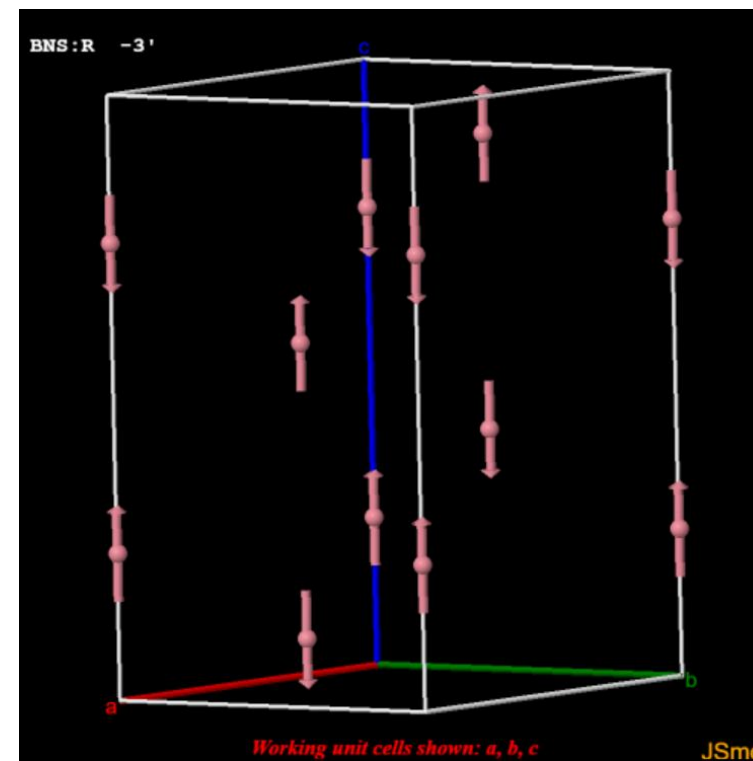
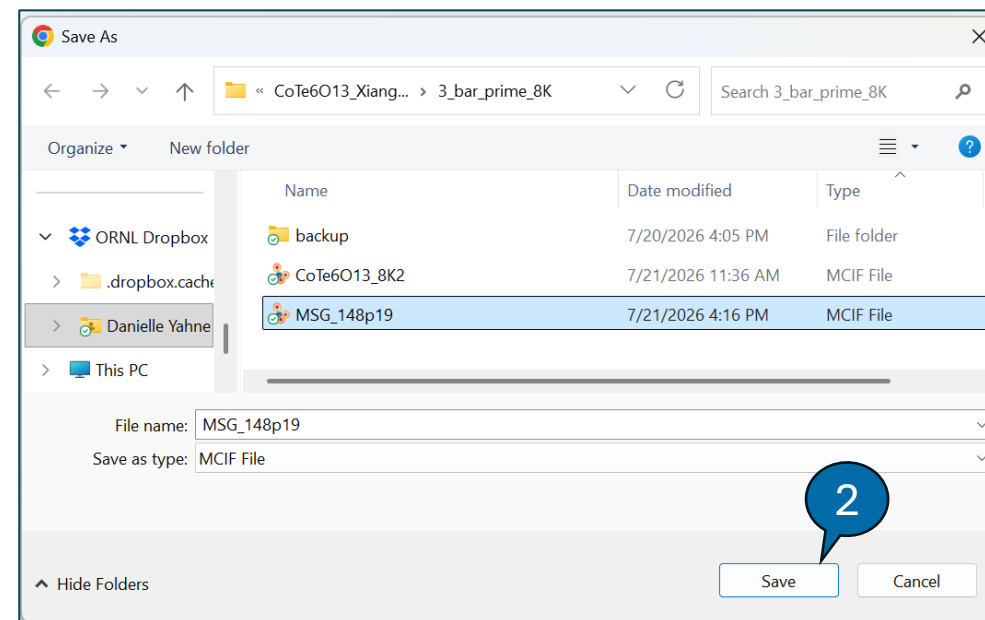
_citation_journal_abbrev  ?
_citation_journal_volume  ?
_citation_page_first      ?
_citation_page_last       ?
_citation_article_id      ?
_citation_year            ?
_citation_DOI             ?

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
? ? ? ? ? ? ?
```



Convert mCIF to PCR

bilbao crystallographic server

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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
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

Choose a structure file (mCIF format):

Choose File

MSG_148p19.mcif

Convert

The file has been successfully converted.

Click to download it

Open PCR file that we just saved

```
!-----
! Data for PHASE number: 1 ==> Current R_Bragg for Pattern# 1: 999.00
!-----
Nuclear and Magnetic Structure of: MSG_148p19 VARY mxmymz
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nvk Npr More
  8  0  0 0.0 0.0 1.0 10  0  2  0  0  0.000  0  7  0
!
R-3' number:148.19 <--Magnetic Space group symbol (BNS symbol & number)
Transform to standard: a,b,c;0,0,0
Parent Space Group: R-3 IT_number: 148
Transform from Parent: a,b,c;0,0,0
! Nsym Cen N_Clat N_Ant
  6  0  2  0
!
! Centring vectors
  0.66667 0.33333 0.33333
  0.33333 0.66667 0.66667
! Symmetry operators
  1 x,y,z,+1
  2 -x,-y,-z,-1
  3 -x+y,-x,z,+1
  4 x-y,x,-z,-1
  5 y,-x+y,-z,-1
  6 -y,x-y,z,+1
!
!Atom Typ Mag Vek X Y Z Biso Occ N_type Spc /Line below:Codes
! Rx Ry Rz Ix Iy Iz MagPh / Line below:Codes
! beta11 beta22 beta33 beta12 beta13 beta23 / Line below:Codes
Te1 Te 1 0 0.82234 0.57097 0.73823 0.00000 1.00000 0 0 #
  0.00 0.00 0.00
Te2 Te 1 0 0.60483 0.50405 0.42402 0.00000 1.00000 0 0 #
  0.00 0.00 0.00
Co1 MCO2 1 0 0.00000 0.00000 0.24399 0.00000 0.33333 1 0 #
  0.00 0.00 0.00
  0.00000 0.00000 2.00000 0.00000 0.00000 0.00000 <-MagPar
  0.00 0.00 0.00 0.00 0.00 0.00
```


Replace atomic data in 8 K fit (and save as)

```
!-----
! Data for PHASE number: 1 ==> Current R_Bragg for Pattern# 1: 999.00
!-----
Nuclear and Magnetic Structure of: MSG_148p19
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth      ATZ      Nvk Npr More
  8  0  0 0.0 0.0 1.0 10  0  2  0  0      0.000  0  7  0
!
R-3' number:148.19 <--Magnetic Space group symbol (BNS symbol & number)
Transform to standard: a,b,c;0,0,0
Parent Space Group: R-3      IT_number: 148
Transform from Parent: a,b,c;0,0,0
! Nsym Cen N_Clat N_Ant
  6  0  2  0
!
! Centring vectors
  0.66667  0.33333  0.33333
  0.33333  0.66667  0.66667
! Symmetry operators
  1 x,y,z,+1
  2 -x,-y,-z,-1
  3 -x+y,-x,z,+1
  4 x-y,x,-z,-1
  5 y,-x+y,-z,-1
  6 -y,x-y,z,+1
!
!Atom Typ Mag Vek X Y Z Biso Occ N_type Spc
! Rx Ry Rz Ix Iy Iz MagPh / Line below:Codes
! beta11 beta22 beta33 beta12 beta13 beta23 / Line below:Codes
Te1 Te 1 0 0.82234 0.57097 0.73823 0.00000 1.00000 0 0 #
      0.00 0.00 0.00 0.00 0.00 0.00
Te2 Te 1 0 0.60483 0.50405 0.42402 0.00000 1.00000 0 0 #
      0.00 0.00 0.00 0.00 0.00 0.00
Co1 MC02 1 0 0.00000 0.00000 0.24399 0.00000 0.33333 1 0 #
      0.00 0.00 0.00 0.00 0.00 0.00
      0.00000 0.00000 2.00000 0.00000 0.00000 0.00000 <-MagPar
      0.00 0.00 0.00 0.00 0.00 0.00
O1 0 1 0 0.00000 0.00000 0.41357 0.00000 0.33333 0 0 #
      0.00 0.00 0.00 0.00 0.00 0.00
O2 0 1 0 0.75610 0.53690 0.64114 0.00000 1.00000 0 0 #
      0.00 0.00 0.00 0.00 0.00 0.00
O3 0 1 0 0.61440 0.47550 0.52014 0.00000 1.00000 0 0 #
      0.00 0.00 0.00 0.00 0.00 0.00
O4 0 1 0 0.79510 0.51670 0.40240 0.00000 1.00000 0 0 #
      0.00 0.00 0.00 0.00 0.00 0.00
O5 0 1 0 0.66700 0.58560 0.78160 0.00000 1.00000 0 0 #
      0.00 0.00 0.00 0.00 0.00 0.00
```

COPY

```
! Zero_i+SHF Dtt1_i+SHF Dtt2_i+SHF Dtt_1overd_i+SHF TwoThetaBank (Only shifts are refined)
! -2.81735 22591.99219 1.30826 0.41407 90.00000
! Zero Code Dtt1 Code Dtt2 Code Dtt_1overd Code 2ThetaBank -> Patt# 1
! 0.00000 0.00 0.00000 0.00 0.00000 0.00 0.00000 0.00 90.000
!-----
! Data for PHASE number: 1 ==> Current R_Bragg for Pattern# 1: 7.0442
!-----
CoTe6013
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth      ATZ      Nvk Npr More
  8  0  0 0.0 0.0 1.0  0  0  0  0  0      6195.148  0  9  0
!
!
R -3 <--Space group symbol
!Atom Typ X Y Z Biso Occ In Fin N_t Spc /Codes
Te1 Te 0.82273 0.57159 0.73806 0.26373 1.00000 0 0 0 0
      0.00 0.00 0.00 0.00 0.00
Te2 Te 0.60519 0.50483 0.42380 0.23087 1.00000 0 0 0 0
      0.00 0.00 0.00 0.00 0.00
Co1 Co 0.66667 0.33333 0.57159 0.33333 1.00000 0 0 0 0
      0.00 0.00 0.00 0.00 0.00
O1 0 0.66667 0.33333 0.74695 0.46750 0.33333 0 0 0 0
      0.00 0.00 0.00 0.00 0.00
O2 0 0.75547 0.53766 0.64084 0.54148 1.00000 0 0 0 0
      0.00 0.00 0.00 0.00 0.00
O3 0 0.61392 0.47598 0.51998 0.53917 1.00000 0 0 0 0
      0.00 0.00 0.00 0.00 0.00
O4 0 0.79546 0.51702 0.40237 0.38343 1.00000 0 0 0 0
      0.00 0.00 0.00 0.00 0.00
O5 0 0.66654 0.58448 0.78246 0.53670 1.00000 0 0 0 0
      0.00 0.00 0.00 0.00 0.00
!-----> Profile Parameters for Pattern # 1 -----> Phase # 1
! Scale Extinc Bov Str1 Str2 Str3 Strain-Mode
  2.341364 0.0000 0.0000 0.0000 0.0000 0.0000 0
      0.00000 0.00 0.00 0.00 0.00 0.00
! Sigma-2 Sigma-1 Sigma-0 Sigma-Q Iso-GStrain Iso-GSize Ani-LSize Size-Model
! Instrumental Sigma interpolated from list in IRF file (Only sample contribution is refined)
      0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0
      0.00 0.00 0.00 0.00 0.00 0.00 0.00
! Gamma-2 Gamma-1 Gamma-0 Iso-LorStrain Iso-LorSize
! Instrumental Gamma interpolated from list in IRF file (Only sample contribution is refined)
      5.7672 10.0776 0.0000 0.0000 0.0000
      0.00 0.00 0.00 0.00 0.00
```

Load MSG PCR

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PCR
Editor

Information

Title, type of job: Rietveld, Integrated Intensities, Simulated Annealing, ...

Type of Patterns, profile, background, diffraction geometry, user-given scattering factors ...

Phase name, type of calculations (JBT), ATZ, contribution to patterns, symmetry, ...

Number of cycles, relaxation factors, access to patterns and phases (atoms and profile)

Constraints definitions, adding, deleting, modifying...

Fixing range of parameters, distances, angles, magnetic moments and linear restraints

Output options for patterns and phases: Reflection lists, Fourier, distances, BVS...

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C:\Users\2qy\ORNL Dropbox\Danielle Yahne\Danielle Yahne's files\HB-2A\NNS_2025\MnO_F | Profiles: 1 | Phases: 1 | 28/ 8/2025 | 11:34:43

Refine Mz component

Refinement Information

Cycles of Refinement:

Stop Criterion of Convergence
Forced Termination when shifts < x E.S.D.
Others:

Relaxation Factors for Shifts
Atomic Anisotropic Profile Global

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 |

Refinement weighting model
☒ Least Squares ☐ Maximum Likelihood ☐ Unit Weights

Reduction factor of number of data points:

OK

Phase 1 | Phase 2 | Phase 3 | Phase 4 | Phase 5 | Phase 6 | Phase 7 |

Atoms

Patterns
☒ 1 ☐ 2 ☐ 3 ☐ 4 ☐ 5 ☐ 6 ☐ 7

Copy Thermal parameters & refine Mz

Atoms Information: Phase 1

List of Atoms

Number of Atoms:

	Label	Ntyp	Mag. Rot.	Prog. V...	X	Y	Z	B	Occ
Atom # 1	Te1	Te	1	0	0.82234	0.57097	0.73823	0.00000	1.00000
Atom # 2	Te2	Te	1	0	0.60483	0.50405	0.42402	0.00000	1.00000
Atom # 3	Co1	MCO2	1	0	0.00000	0.00000	0.24399	0.00000	0.33333
Atom # 4	O1	O	1	0	0.00000	0.00000	0.41357	0.00000	0.33333

	Re[x]	Re[y]	Re[z]	Im[x]	Im[y]	Im[z]	MPhase
Atom #3	0.00000	0.00000	2.00000	0.00000	0.00000	0.00000	0.00000

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

Refine Positions

Refine B_iso

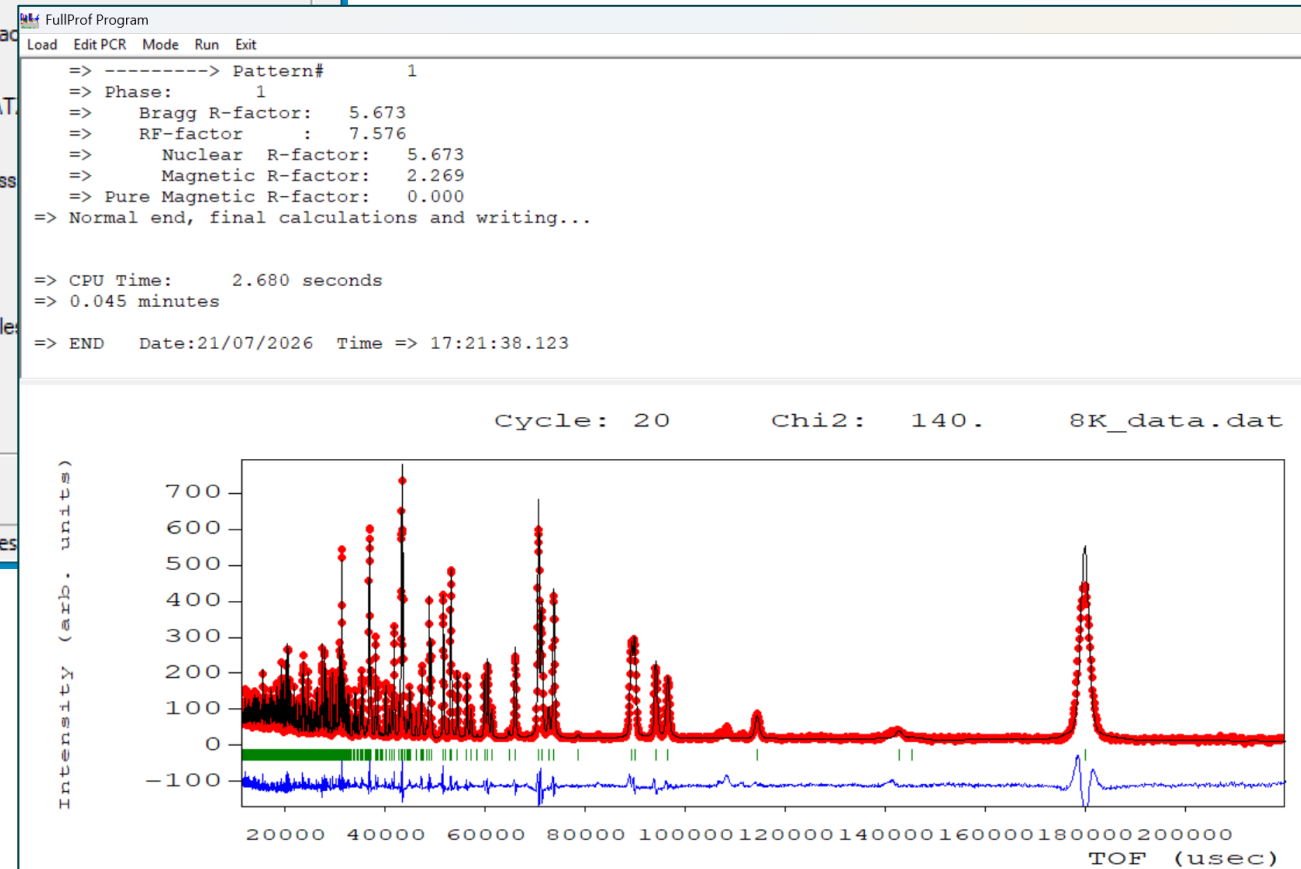
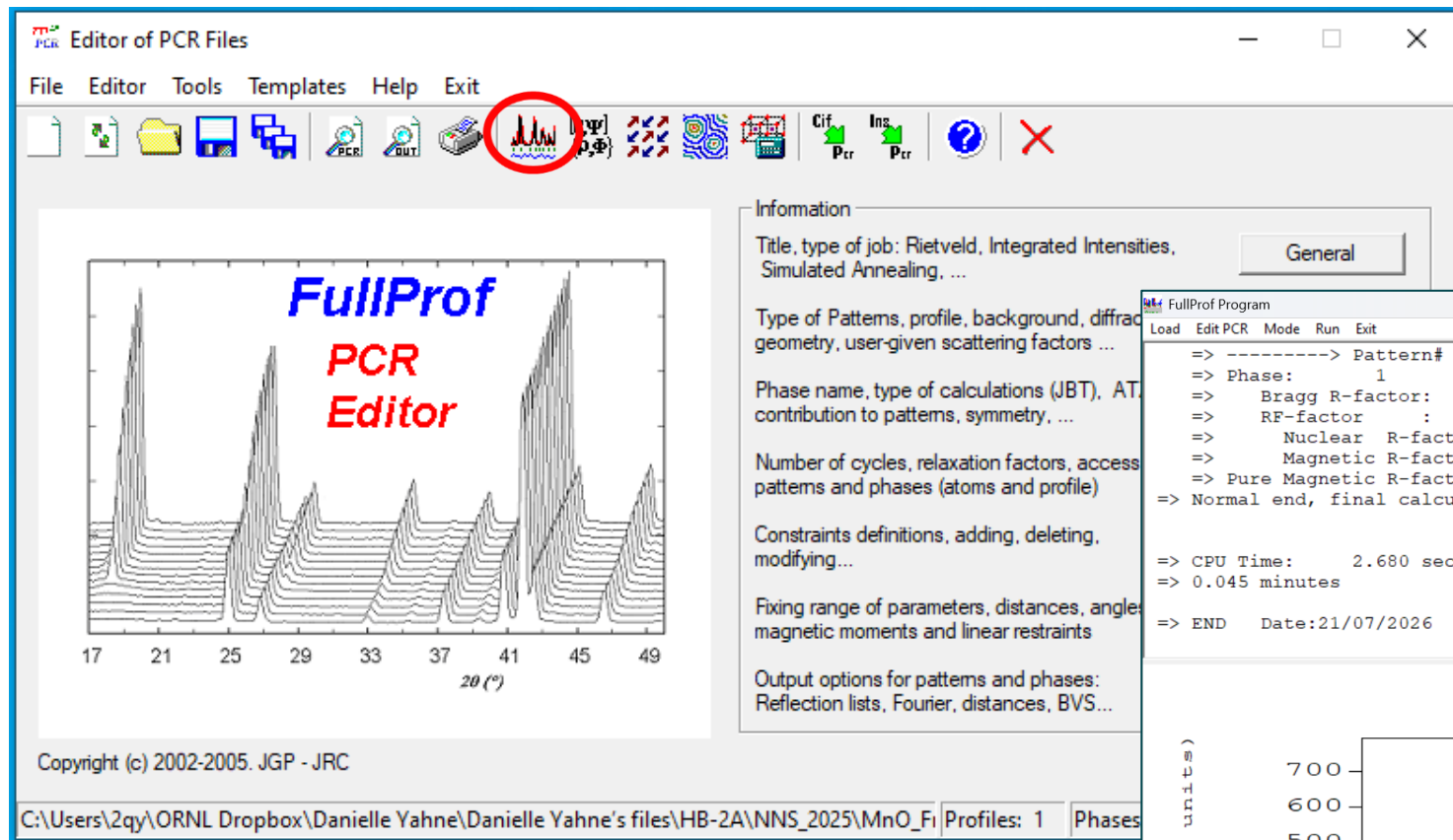
Refine B_aniso

Fix All

Cancel

OK

Run refinement

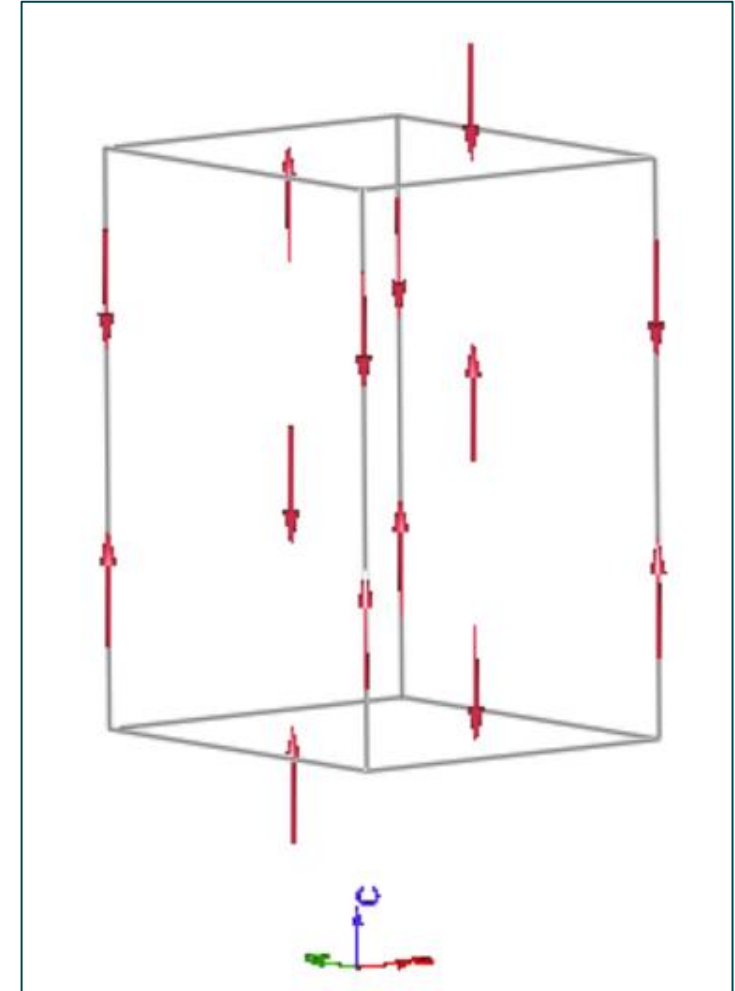


Results agree with SARAh refinement

Atom : Co1		Co											
x	y	z	Translation			k	MSYM	m(a)	m(b)	m(c)	Mtot		
0.00000	0.00000	0.24399	(	0,	0,	0)	1	1	0.00000	0.00000	3.97575		
								0.00000	0.00000	3.97575	3.97575		
			(	0,	1,	0)	1	1	0.00000	0.00000	3.97575		
								0.00000	0.00000	3.97575	3.97575		
			(	1,	0,	0)	1	1	0.00000	0.00000	3.97575		
								0.00000	0.00000	3.97575	3.97575		
			(	1,	1,	0)	1	1	0.00000	0.00000	3.97575		
								0.00000	0.00000	3.97575	3.97575		

==> MAGNETIC MOMENT PARAMETERS:

Name	Mx	sMx	My	sMy	Mz	sMz	M	sM	MPhas	sMPhas
Co1	0.000(0)		0.000(0)		3.976(93)		3.9757(939)		0.0000(0)	



Further information

nature communications



Article

<https://doi.org/10.1038/s41467-023-43858-z>

Large off-diagonal magnetoelectricity in a triangular Co^{2+} -based collinear antiferromagnet

Received: 31 March 2023

Accepted: 22 November 2023

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Check for updates

Xianghan Xu¹✉, Yiqing Hao², Shiyu Peng³, Qiang Zhang², Danrui Ni¹,
Chen Yang¹, Xi Dai³, Huibo Cao² & R. J. Cava¹✉

Magnetic toroidicity is an uncommon type of magnetic structure in solid-state materials. Here, we experimentally demonstrate that collinear spins in a material with $R\bar{3}$ lattice symmetry can host a significant magnetic toroidicity, even parallel to the ordered spins. Taking advantage of a single crystal sample of $\text{CoTe}_6\text{O}_{13}$ with an $R\bar{3}$ space group and a Co^{2+} triangular sublattice, temperature-dependent magnetic, thermodynamic, and neutron diffraction results reveal A-type antiferromagnetic order below 19.5 K, with magnetic point group $\bar{3}'$ and $\mathbf{k} = (0,0,0)$. Our symmetry analysis suggests that the missing mirror symmetry in the lattice could lead to the local spin canting for a toroidal moment along the c axis. Experimentally, we observe a large off-diagonal magnetoelectric coefficient of 41.2 ps/m that evidences the magnetic toroidicity. In addition, the paramagnetic state exhibits a large effective moment per Co^{2+} , indicating that the magnetic moment in $\text{CoTe}_6\text{O}_{13}$ has a significant orbital contribution. $\text{CoTe}_6\text{O}_{13}$ embodies an excellent opportunity for the study of next-generation functional magnetoelectric materials.