

Introduction to Fullprof Suite and Sarah Representational Analysis

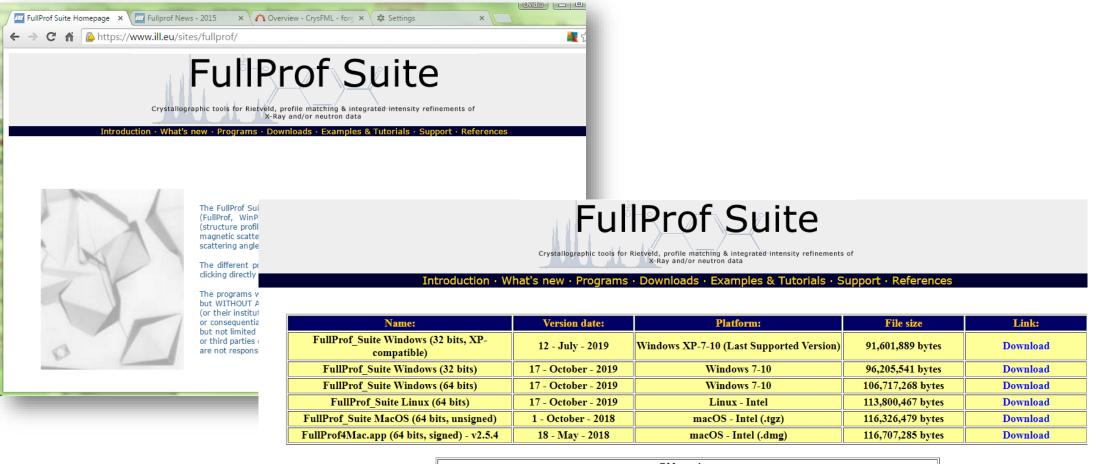
Ovidiu Garlea Neutron Scattering Division, Oak Ridge National Laboratory

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Where to download FullProf Suite

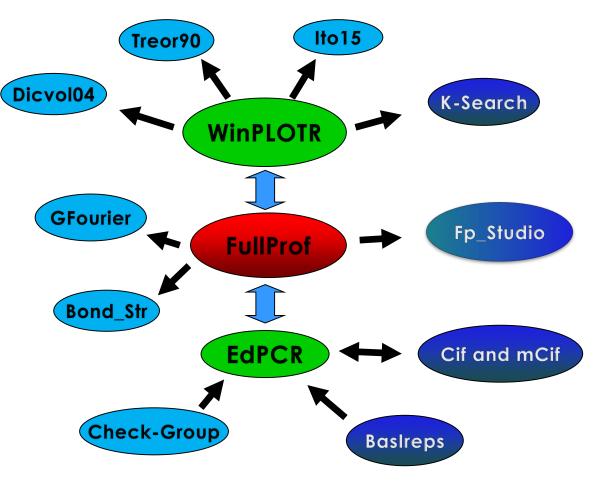
http://www.ill.eu/sites/fullprof/



	Old versions	
Windows	Linux	macOS

What is the FullProf Suite

A set of crystallographic programs (FullProf, WinPLOTR, EdPCR, FPStudio...) developed for Rietveld analysis of neutron or X-ray powder diffraction, but with capabilities for single crystal and many other useful utilities



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Developers of FullProf Suite

Juan Rodríguez-Carvajal (ILL, France) **FullProf, CrysFML, Baslreps, ...** Javier González-Platas (ULL, Tenerife, Spain) **CrysFML, GUIs, GFourier, EdPCR**



Contributors:

Laurent Chapon & Aziz Daoud-Aladine (ISIS, U.K.) T.O.F., FP_Studio Thierry Roisnel (LCSIM, Rennes, France): WinPLOTR Oscar Baltuano (IPEN, Peru): WinPLOTR-2006 Carlos Frontera (ICMAB, Barcelona, Spain): Polarized neutrons

CrysFML: Crystallographic Fortran Modules Library - set of Fortran 95 modules developed to facilitate the design and the development of crystallographic computing programs. http://forge.ill.eu/projects/show/crysfml





WinPLOTR / WinPLOTR-2006: Visualizing powder diffraction patterns.

Fitting independent peaks (CW and TOF), interface for FullProf

FullProf : Crystal and magnetic structure refinement, powder/single crystals, polarized neutrons, multiple patterns, simulated annealing

EdPCR: Editor of the FullProf input control file

MCIF_to_PCR: Creates a PCR file with magnetic model from mcif file

GFourier and Bond_Str.: Fourier and distance/angle calculations.

K_Search: Searching propagation vectors

BasIREPS: Program for calculating basis functions of Irreducible Representations

Fp_Studio: Program for visualizing crystal and magnetic structures

Check_Group: Program for finding the space group (powders and single crystals)

Datared: Program for single crystal data reduction

GLOpSAnn: Solve crystal structures using Global Optimization with Sim. Ann.

DICVOL04, TREOR90, ITO, CrysCalc ...

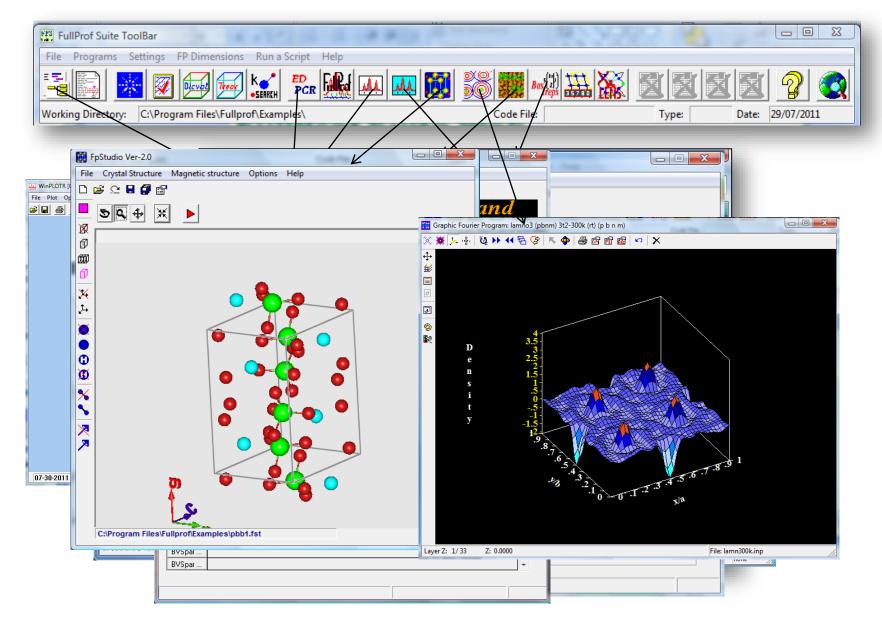
FullProf : Updates

Documented in "fp2k.inf" or... to the Fullprof homepage at "What's new"

Full Year 2019
>> 9 October 2019 : Extensive changes in the new version of FullProf concerning Simulated Annealing and Superspace.
- The current version of the FullProf program has been updated to:

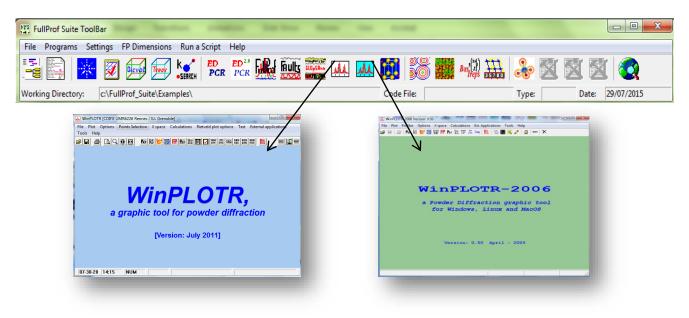
** PROGRAM FullProf.2k (Version 7.20 - Oct2019-ILL JRC) ** **********************************
 LeBail fits and Simulated annealing are now totally operable with magnetic superspace groups. Single crystal data can also be treated provided that the appropriate input integrated intensity file is given. This file is similar to the *.int file produced by a LeBail fit. The program DataRed will be modified in the near future to perform single crystal data reduction using the superspace formalism.
 Spherical coordinates for the modulation amplitudes in the superspace formalism for magnetic structures have been fully implemented. Notice that the symmetry constraints when this option is applied cannot be automatic. The best is to start a run using crystallographic components and look into the output files to see how the spherical components have been calculated and apply the appropriate constraints using refinement codewords.
- Superspace mCIFs files are now generated by FullProf. The name of these files are named as "codfile_ssgN.mcif", where "codfile" is the name of the PCR file without extension and N indicates the number of the phase. These files can be read by the program Jmol for visualizing the incommensurate magnetic structures but not by the program VESTA. The supercell option in P1 with "MULTCELL na nb nc" is still used in this case to produce a box with all magnetic moments to be visualized with VESTA. FullProf Studio files are not output because the superspace formalism has not been included in EP Studio yet

FullProf Suite ToolBar



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FullProf Suite: WinPLOTR



 \checkmark Reading the X-ray and neutron diffraction patterns

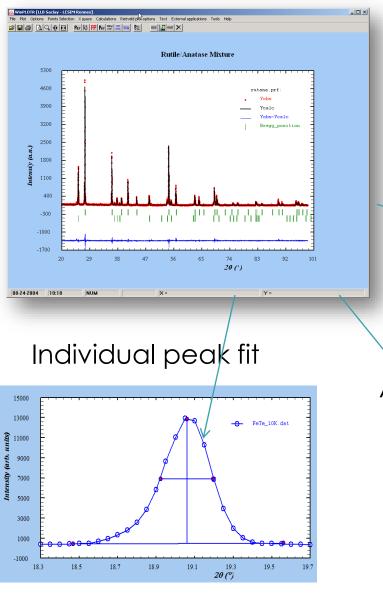
- \checkmark Automatic peak search for indexing
- ✓ Saving peaks as input for DICVOL04, Treor90, K-Search ...
- ✓ Making individual peak fit

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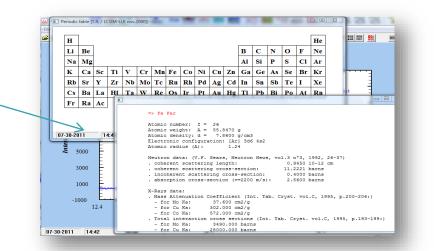
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- \checkmark Exporting a background file
- ✓ Invoking other programs of FullProf Suite

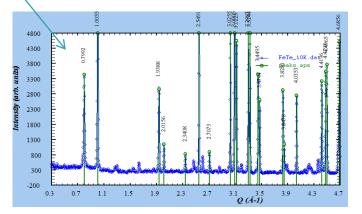
FullProf Suite: WinPLOTR



Access to other programs: (e.g., periodic table of elements, space groups info, molecular weight and unit cell volume calculation ...)



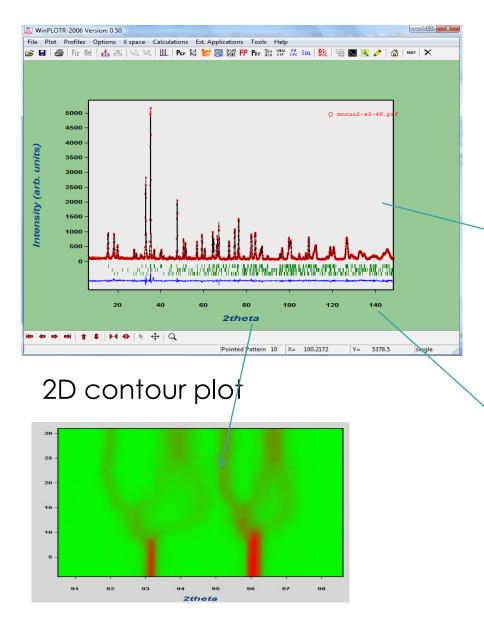
Automatic peak & background search



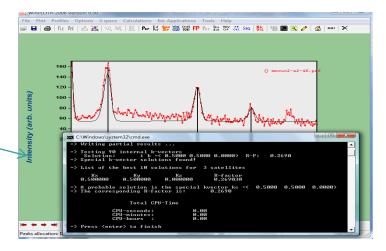
Magnetic Structure Workshop, ORNL, October 2019

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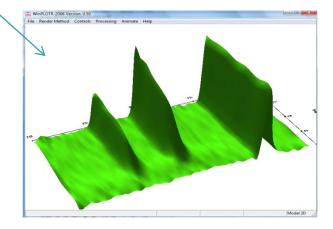
FullProf Suite: WinPLOTR-2006



Search for the magnetic propagation vector (k-search)



3D surface plot



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FullProf program

Features :

- Multiple data sets: simultaneous treatment of several powder diffraction patterns (constant wavelength X-rays & neutrons, TOF neutron, energy dispersive X-rays)
- Combined treatment of single crystal and powder data
- > Automatic mode for handling refinement codes and symmetry constraints
- Rigid body refinements + distances and angles restraints
- Special form factors
- > The treatment of micro-structural effects
- Sequential refinement



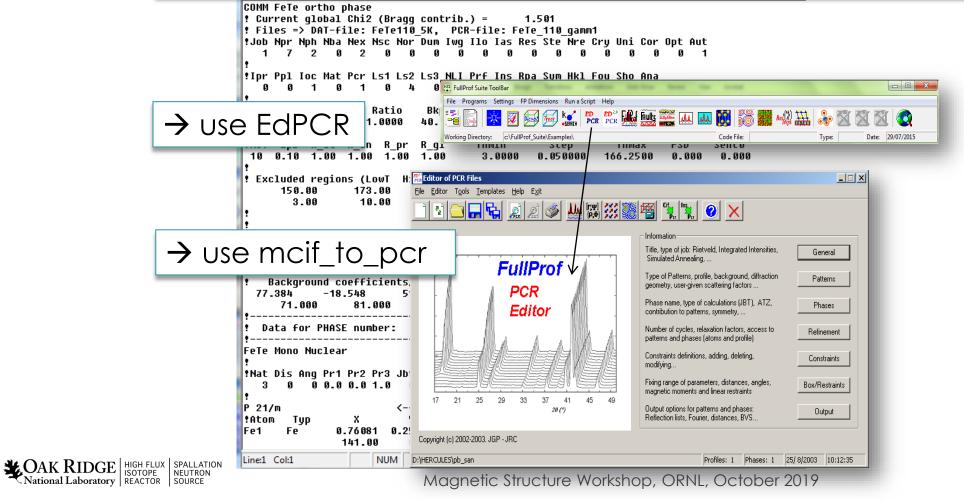
FullProf: How to create the PCR file



PCR file
 Many variables and options
 Complex to handle

\rightarrow Copy an existing PCR-file and modify it, or

al EdDCD Test Edites (CAlleses) Adaptinistentes (Deslates) fate



Steps for magnetic structure determination

- I. Well defined crystallographic structure
- II. Determine the propagation vector(s)FP_Suite: k-Search

INPUT

Peak positions of ⇐ magnetic reflections Cell parameters

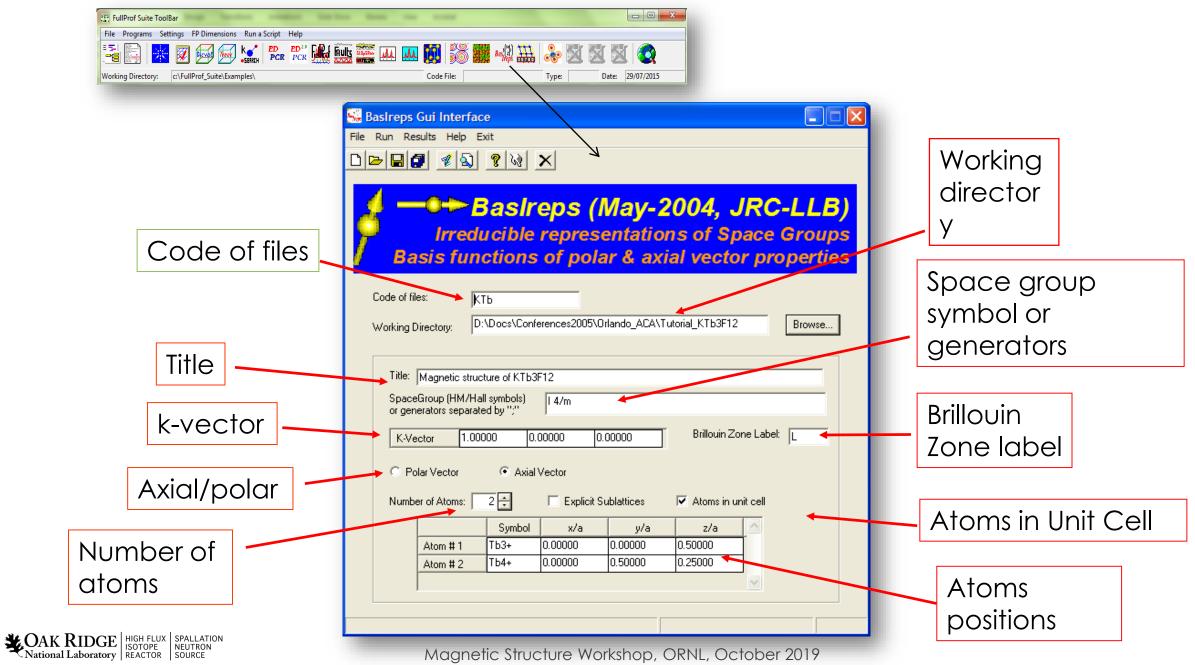
- III. Perform Symmetry Analysis FP_Suite -BasIreps, SARAh Bilbao Cryst. Server, Isodistort
- IV. Introduce and refine the magnetic phase FP_Suite: FullProf

Propagation vector
 ⇐ Space Group
 Atom positions

⇐ Atomic components of Fourier basis functions



Symmetry Analysis using Baslreps



Symmetry Analysis using Baslreps

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FullProf : Magnetic Structure Factor

magnetic moment

expanded as Fourier series

$$\mathbf{m}_{ljs} = \sum_{\{\mathbf{k}\}} \mathbf{S}_{\mathbf{k}js} \ exp\{-2\pi i \mathbf{k} \mathbf{R}_l\}$$

I : index of a direct lattice point *j* : index for a Wyckoff site (orbit) *s*: index of a sublattice of the *j*site

$$\mathbf{S}_{\mathbf{k}} = \frac{1}{2} (\mathbf{R}_{\mathbf{k}} + i\mathbf{I}_{\mathbf{k}}) \exp\{-2\pi i\phi_{\mathbf{k}}\}$$

→ Necessary condition for real moments $\mathbf{S}_{-\mathbf{k}\mathbf{j}\mathbf{s}} = \mathbf{S}_{\mathbf{k}\mathbf{j}\mathbf{s}}^{*}$

<u>The magnetic structure factor:</u>

$$\mathbf{M}(\mathbf{h}) = p \sum_{j=1}^{n} O_{j} f_{j}(\mathbf{h}) T_{j} \sum_{s} \mathbf{S}_{\mathbf{k}js} \exp\left\{2\pi i \left[(\mathbf{H} + \mathbf{k}) \{S | \mathbf{t}\}_{s} \mathbf{r}_{j} \right] \right\}$$
$$\left\{ S | \mathbf{t} \right\}_{s} \text{ Symmetry operators}$$

FullProf: Magnetic Structure Refinement

many different ways of treating magnetic structures

> Fourier coefficients refinement:

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- The magnetic symmetry is introduced together with explicit symmetry operators of the crystal structure.
- The refined variables are directly the components of the S_{kis} vectors.
- A relation exist between S_{kjl} and $S_{kjs} = M_{js} S_{kjl} exp \left\{-2\pi i \phi_{kj}\right\}$

> Coefficients of basis functions refinement:

• Fourier coefficients as linear combinations of the basis functions of the irreducible representation of the propagation vector group G_k

$$\mathbf{S}_{kjs} = \sum_{n\lambda} C_{n\lambda}^{\nu} \mathbf{S}_{n\lambda}^{k\nu} (js)$$

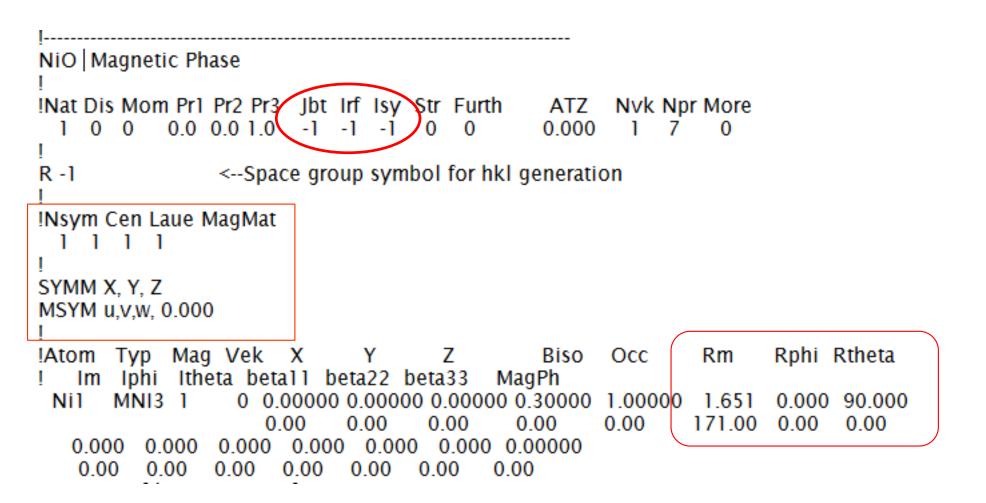
- The basis functions of the IRs are introduced together with explicit symmetry operators of the crystal structure.
- The refined variables are directly the coefficients C_1, C_2, C_3, \dots

FullProf : Symmetry operators between Fourier components (along the crystallographic axes)

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FullProf : Symmetry operators between Fourier components (Polar coordinates)



FullProf : Symmetry operators corresponding to a magnetic space group (mcif_to_pcr)

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FullProf : Basis functions coefficients (created from Sarah or BasIrep)

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BASI 0 0 0 0 0 0 0 0 0	
SYMM $-x+1, -y, z+1/2$	
BASR -1 0 0 -1 0 0 0 1	
BASI 0 0 0 0 0 0 0 0 0 0	
SYMM $-x+1/2, y+1/2, -z+1/2$	
BASR 1 0 0 0 -1 0 0 0 1	
BASI 0 0 0 0 0 0 0 0 0 0	
SYMM $x-1/2, -y+1/2, -z$	
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💥 ОАК

Magnetic situcture workshop, OkiaL, October 2017

FullProf : using Amplimodes (mcif to pcr – Isotropy)

Data for PHASE number: 1 ==> Current R Bragg for Pattern# 1: 0 AMPLIMODES for FullProf FIX xyz !Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nvk Npr More 0 0.0 0.0 1.0 1000.0 0 7 4 0 -6 2 0 1 0 P4/mm'm' number: 123.345 <-- Magnetic Space Group Symbol (BNS symbol and number) Transform to standard: a,b,c;0,0,0 <--Basis transformation from alt setting to standard BNS Parent space group: Pm-3m IT number: 221 <--Nonmagnetic Parent Group Transform from Parent: b,c,a;0,0,0 <--Basis transformation from parent to current setting ! Atom Typ Mag Vec Occ N type Spc/Fftype Х Y Z Biso Rx Ry Rz Ιx Iy Ιz MagPh 0.50000 0.50000 La 1 0.06250 LA 0 0 0.50000 0.50000 0 1 0.00 0.00 0.00 0.00 0.00 Mn 1 MN 0.00000 0.00000 0.00000 0.50000 0.06250 1 2 1 0 0.00 0.00 0.00 0.00 0.00 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00 0.00 0.00 0.00 0.00 0.00000 0.00000 0.50000 01 0 0 0.50000 0.06250 0 3 0 0.00 0.00 0.00 0.00 0.00 O 2 0 0 0.00000 0.50000 0.00000 0.50000 0.12500 0 3 0 0.00 0.00 0.00 0.00 0.00 ! Basis vectors of magnetic symmetry modes for each atom M MODES 1 ! Nm Atom Irrep Coeff Mx My Mz mGM4+ 0.0000 0.0000 0.2538 1.00 1 Mn 1 ! Amplitudes of Magnetic Symmetry Modes MA MODES 1 2 A1 mGM4+ 0.00000 1.00 Str3 Strain-Model Scale Shape1 Bov Strl Str2 2.00 0.00000 0.00000 0.00000 0.00000 0.00000 0 0.000 0.00000 0.000 0.000 0.000 0.000

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FullProf : IC using Superspace description (mcif to pcr)

DyMn6Ge6 magnetic VARY mxmymz McosMsin

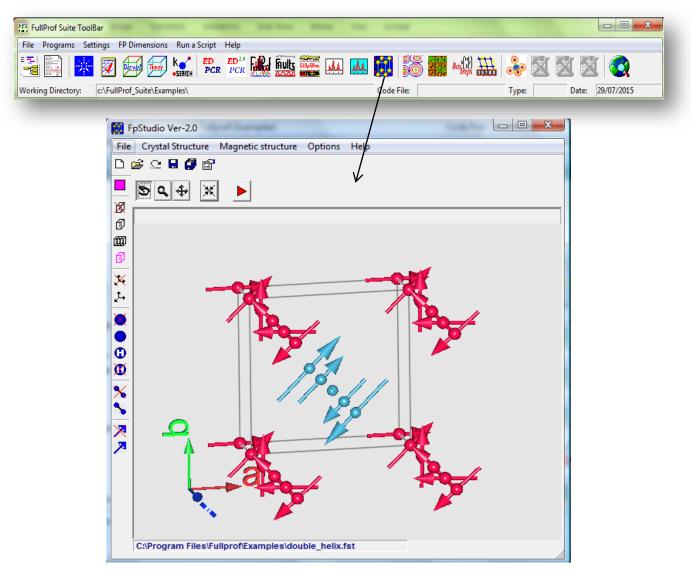
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt of Isy Str Furth ATZ Nvk Npr More 5 0 0 0. 0 0.0 1. 7 🛝 2 🖉 133584,188 1 7 0 0 <-- Magnetic SuperSpace group symbol P62'2'(0,0,q)h00 generators x-y,x,z,t+1/6,+1; x-y,-y,-z,-t+1/3,-1 N_{qc} 1 Q_coeff Atom Typ Max_Qcoeff Y Ζ Biso Occ N_type Spc / Line below:Codes Х Mcosx Msinx Msinz / Line below:Codes Mcosy Mcosz Msiny beta13 beta23 beta11 beta22 beta33 beta12 / Line below:Codes 0.00000 0.00000 1.00000 Dy JDY3 0.00000 0.00000 1 0 0.00000 0.00000 0.00000 0.00000 0.00000 MagM0-Moment: 0.00000 0.00000 3.80587 <- Homogeneous magnetic moment 0.00000 0.00000 101.00000 0.00000 Mcos-Msin-1: 7.12688 3.56344 0.00000 6.17206 0.00000 <-Amplitudes of Modulated moments 92.00000 91.00000 0.00000 0.00000 91.73205 0.00000 0.00000 6.00000 1 0 Mn1 MMN2 0.00000 0.50000 0.25030 0.00000 0.00000 0.00000 0.00000 0.00000 MagM0-Moment: 0.00000 0.00000 -1.08612 <- Homogeneous magnetic moment 0.00000 0.00000 81.00000 Mcos-Msin-1: -2.28216 -1.22194 0.00000 0.33498 -1.23195 0.00000 <-Amplitudes of Modulated moments 71.00000 61.00000 0.00000 51.00000 41.00000 0.00000 0.50000 0.00000 Gel GE 0.66667 0.33333 2.00000 0 0 0 0.00000 0.00000 0.00000 0.00000 0.00000 Ge2 GE 0.66667 0.00000 0.00000 2.00000 0 0.33333 0 0 0.00000 0.00000 0.00000 0.00000 0.00000 Ge3 GE 0.00000 0.00000 0.34450 0.00000 2.00000 0 0 0.00000 0.00000 0.00000 0.00000 0.00000 » Drofile Decemptors for Dettern # 1

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3D visualization program: FpStudio

➤ reads ".fst" files - automatically generated by FullProf

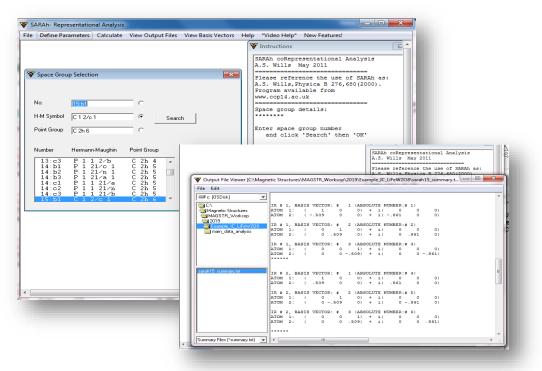


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SARAh <u>http://fermat.chem.ucl.ac.uk/spaces/willsgroup/software/</u>

Sarah-Representational Analysis



Sarah-Refine

GSAS Controls FullProf Controls Topas Controls View bas	s vectors Tools Help "Video Help" Ne	w Features!
		W Instructions
		SARAh-Refine for FullProf A.S. Wills (Version: 9.0.16 July 20
V SARAh- Generate/Edit FullProf 2K *.PCR File		Diesse reference the use of SiDih
		Shubnikov and Normal Point Group Information
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\square A(1) $\Gamma(9) \Psi(6)$		6) 2/m m'm'm Pnn'm' 58.398
$\square A(1) \Gamma(9) \Psi(7)$	2) Edit PCR/Replace Basis Vectors	7) N/A N/A C/B C/B
A(1) Γ(9) Ψ(8)	PCR undefined	8) N/A N/A C/B C/B
A(1) Γ(10) Ψ(9)		9) mm2 mmm' Pn'nm 58.395
A(1) Γ(10) Ψ(10)		10) mm2 mmm' Pn'nm 58.395
1	Select PCR Edit File	< □ →
Select Basis Vectors Select All Unselect All	Make FST file	Click on the basis vector label in the main window to move to its Point Group and Shubnikov Group in this list.
	Options:	The symmetry of a basis vector will be highlighted
Common Irreducible Representations	Use Complex	when it is selected.
$\Box \Gamma(2)$ $\Box \Gamma(8)$	Coefficients C_i	N/A indicates that the basis vector does not
□ Γ(3) □ Γ(9) Select □ Γ(5) □ Γ(10) Unselect All	Close	have a valid Point or Shubnikov Group. C/B indicates a change of is required. See tst2 file for explanation.

calculates the Irreducible representations and basis vectors associated with a space grou, propagation vector and atomic positions Output files includes a tailored summary with cut-and-paste tables written in LaTeX

adds functionalities to GSAS, FullProf and TOPAS, to allow them to refine magnetic structures in terms of the basis vectors. It sets up the pcr file for the magnetic refinement, and enables the searching of magnetic propagation vectors with reverse-Monte Carlo routines

SARAh creates a Magnetic phase to use in Fullprof

26

Edit Format View Help		File Edit Search
Note for DUACE number 1 - > Current D. Drogg for Dattern # 1: - 1.00	<u>^</u>	🕒 🖻 🖶 🖶 🔍 💃 🛍 🛱 🗂 🖱
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it Dis Mom Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nvk Npr More		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 0.00
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2 1 1 -1 6 eal(0)-Imaginary(1) indicator for Ci		Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nvk Npr More
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SI 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		W1 W 0.24831 0.09192 0.24478 0.42000 1.00000 0 0 0 0 0.00 0.00 0.00 0.00
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SARAh – web Representational Analysis

http://fermat.chem.ucl.ac.uk/spaces/willsgroup/web-software/sarah-webrepresentational-analysis/

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 pr has been entirely rewritten. It is still in a development phase and please contact me if you find problems or have suggestions 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 seconds.

-Andrew (June 2018)

Wolfram

```
Space group : {69, Fmmm} 

Propagation vector :

000

Crystallographic coordinates in the form

or Cu2 1/2 1/2 -1/2

Cu1 1/2 1/2 -1/2
```

{ {	Γ_1 , Cu	¢1 1) 1 2) 1	I. 0. I. 1.	0. 0.	, [Гı Cu	ψ ₂ 1) 2)	0. 0.	1. -1.	. 0.	.,	Г С	ı ∳ u 1 2	³ 3 1) (2) (). ()). ()). 1). 1	. }		
{	Γ ₂ Cu	ψ ₁ 1) 2)	1. -1.	0. -1.	0. 0.	,	Γ ₂ Cu	ψ ₂ 1) 2)	0. 0.	1. 1.	0. 0.	,	Γ ₂ Cu	ψ ₃ 1) 2)	0. 0.	0. 0.	1. -1.	} }	

Table 12. The basis vectors projected from the different IRs

$\left\{ \begin{array}{c cccc} \Gamma_{1} & \psi_{1} \\ Cu_{2} & 1 & 0. & -1. & 0. \end{array} \right\}$,	$ \{ \begin{array}{cccc} \Gamma_2 & \psi_1 \\ Cu_2 & 1 \end{pmatrix} \begin{array}{c} 2 & 1 \\ 2 & 1 \end{array} , \begin{array}{c} 0 \\ 0 \end{array} \} $	_{D.} ,	$\begin{matrix} \Gamma_2 \\ Cu_2 \end{matrix}$	ψ ₂ 1) 0.	0. 2.	}
----------------------------------------------------------------------------------------------------------	---	-------------------------------------------------------------------------------------------------------------------------------------------------------------	-----------------	-------------------------------------------------	-------------------------	-------	---

View - Basis vectors in FullProf pcr format (Copy and paste text

Below are model sections for a FullProf pcr file. Note that the phase of any imaginary basis vector component is reversed to match FullProf's format :

```
***Basis vectors for Atom=1 , \ \mbox{\sc r}=1 , \eta(1)=\{a\}
Magnetic phase by SARAh - web Representational Analysis
!Nat Dis Mom Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth
                                               ATZ Nvk Npr More
     0 0 0.0 0.0 1.0 1 0 -2 0 0
  1
                                               0.00 1 0 0
P -1
                       <--Space group symbol
! Nsym Cen Laue Ireps N Bas
    2 1 1 -1 3
! Real(0)-Imaginary(1) indicator for Ci
000
SYMM X, Y, Z
BASR 1. 0 0 0 1. 0 0 0 1.
BASI 0 0 0 0 0 0 0 0 0
```

Table 13. The basis vectors combined according to the unique 'isotropy groups' of the IR space vector $\boldsymbol{\eta}$:

$\Big\{ \begin{array}{c} \Gamma_1 \\ Cu \end{array} \Big $	$\psi_1^{\eta_1}$ 1) 2)	1. 1.	0 1.	0 0	,	Γ_1 Cu	$\psi_2^{\eta_1}$ 1) 2)	0 0	1. -1.	0 0	,	Γ ₁ Cu	ψ ₃ ^{η1} 1) 2)	0 0	0 0	1. 1.	}

	Γ_2	$\psi_1^{\eta_1}$ 1)				Γ_2	$\psi_{2}^{\eta_{1}}$					Γ_2	$\psi_{3}^{\eta_{1}}$				
{	Cu	1)	1.	0	0,	Cu	1)	0	1.	0	,	Cu	1)	0	0	1.	}
		2	1	1	<u>n </u>		n,	n	1	n			2	n	n	1	

Actional Laboratory REACTOR SOURCE

Thank you !





