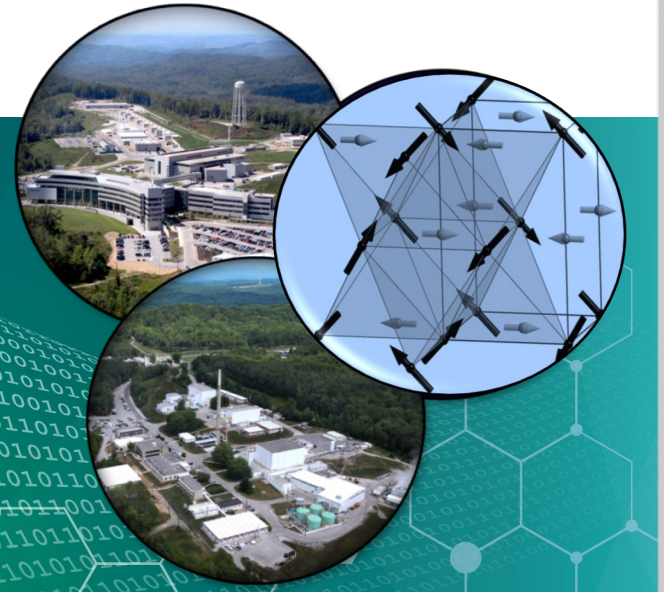
OAK RIDGE National Laboratory

Introduction to Fullprof Suite and Sarah Representational Analysis



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Oak Ridge National Laboratory

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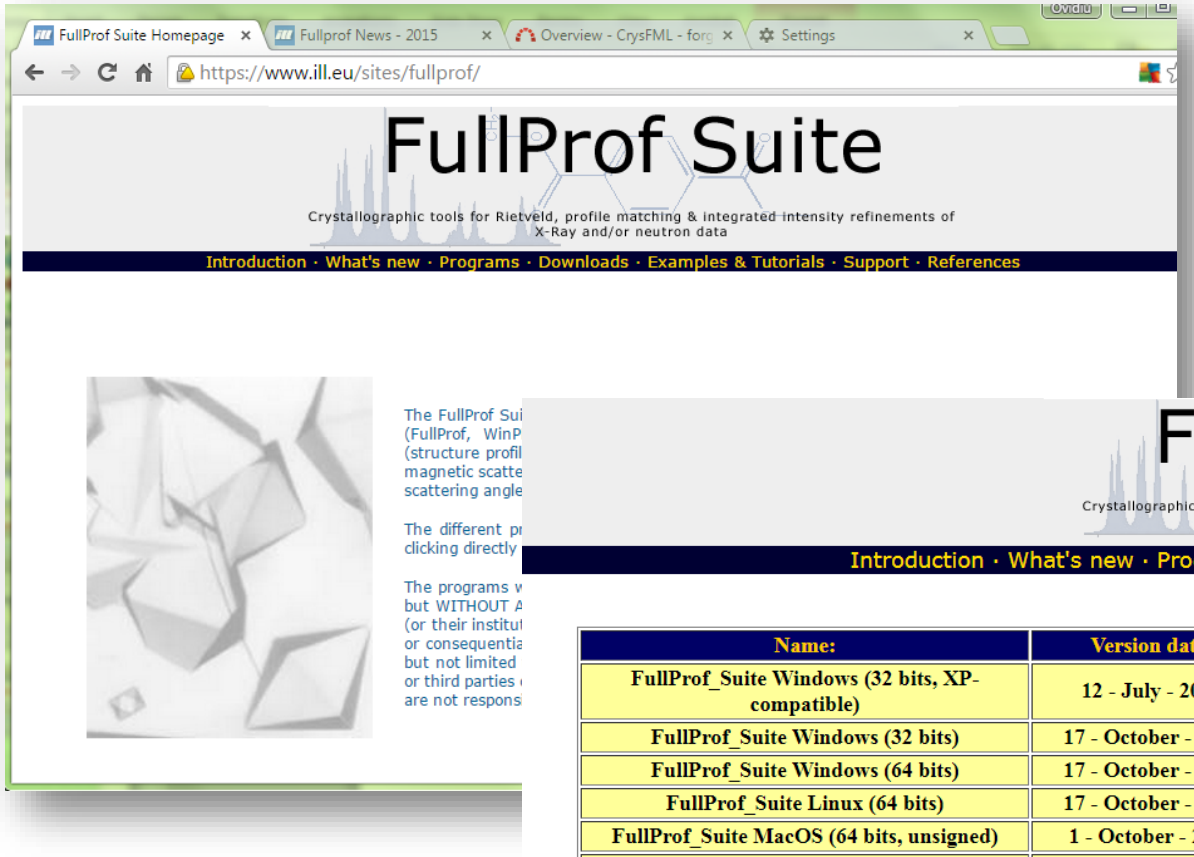
U.S. DEPARTMENT OF ENERGY

Where to download FullProf Suite

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

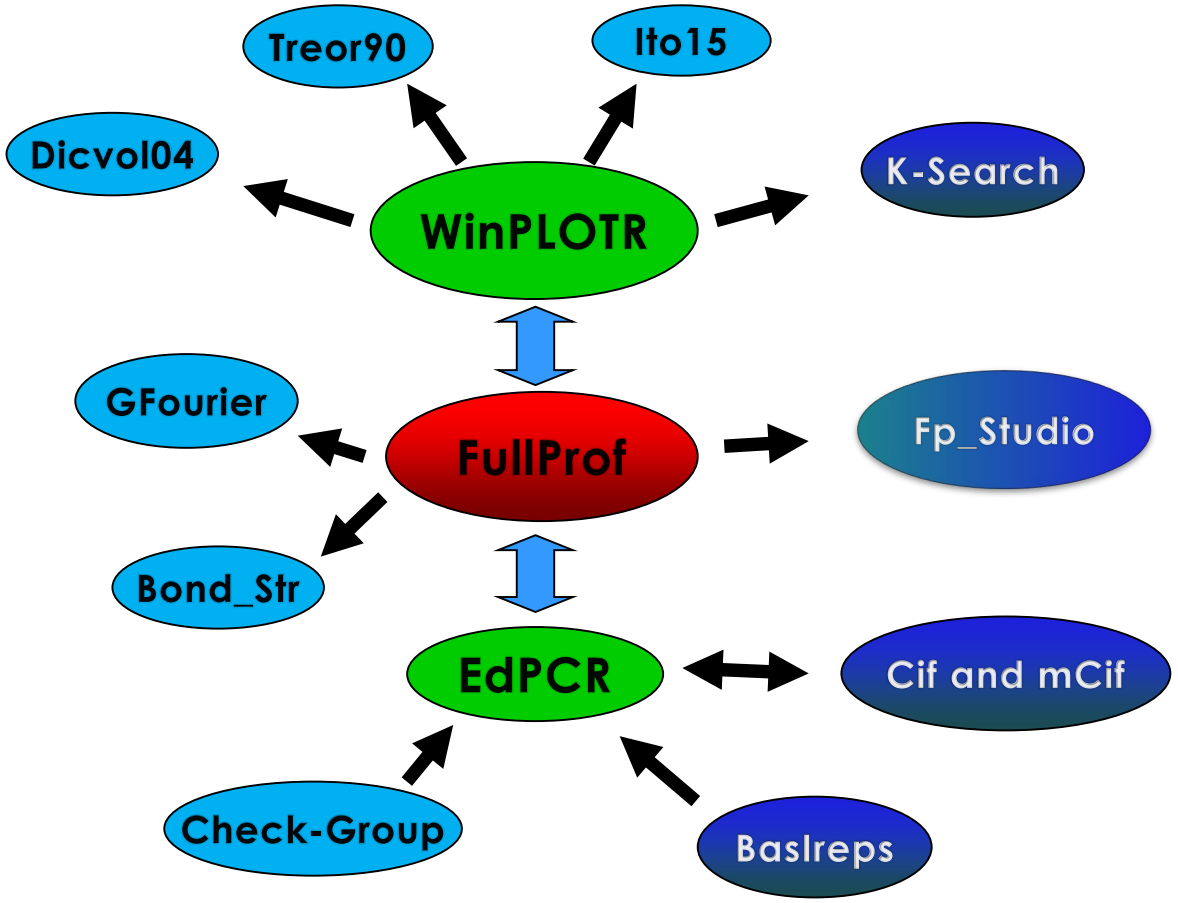


Name:	Version date:	Platform:	File size	Link:
FullProf_Suite Windows (32 bits, XP-compatible)	12 - July - 2019	Windows XP-7-10 (Last Supported Version)	91,601,889 bytes	Download
FullProf_Suite Windows (32 bits)	17 - October - 2019	Windows 7-10	96,205,541 bytes	Download
FullProf_Suite Windows (64 bits)	17 - October - 2019	Windows 7-10	106,717,268 bytes	Download
FullProf_Suite Linux (64 bits)	17 - October - 2019	Linux - Intel	113,800,467 bytes	Download
FullProf_Suite MacOS (64 bits, unsigned)	1 - October - 2018	macOS - Intel (.tgz)	116,326,479 bytes	Download
FullProf4Mac.app (64 bits, signed) - v2.5.4	18 - May - 2018	macOS - Intel (.dmg)	116,707,285 bytes	Download

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



Developers of FullProf Suite

Juan Rodríguez-Carvajal (ILL, France)

FullProf, CrysFML, BasIreps, …

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

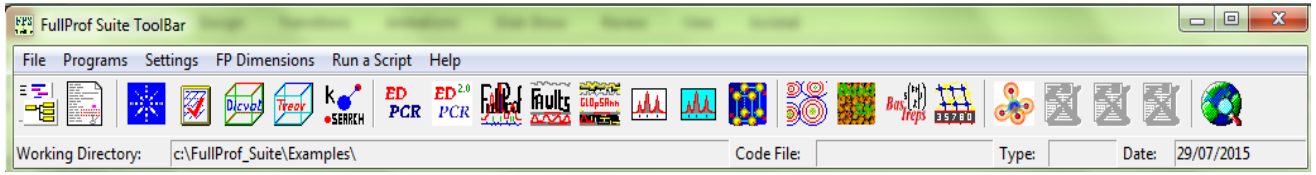
Oscar Baltuano (IPEN, Peru): WinPLOTR-2006

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

FullProf Suite

Toolbar:



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

```
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>> 9    October 2019 :  Extensive changes in the new version of FullProf concerning Simulated Annealing and Superspace.
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   - 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 FP_Studio yet.
```
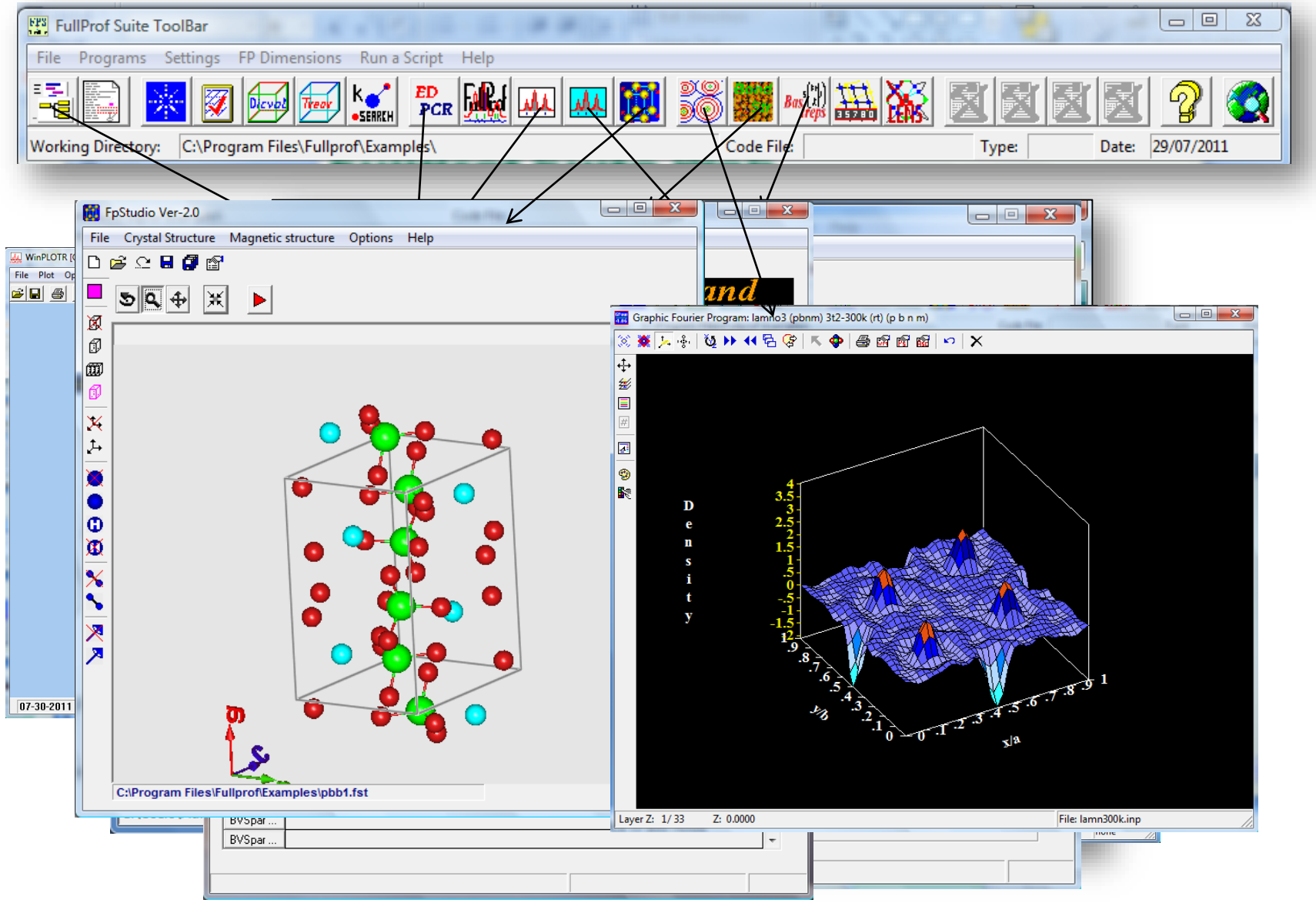
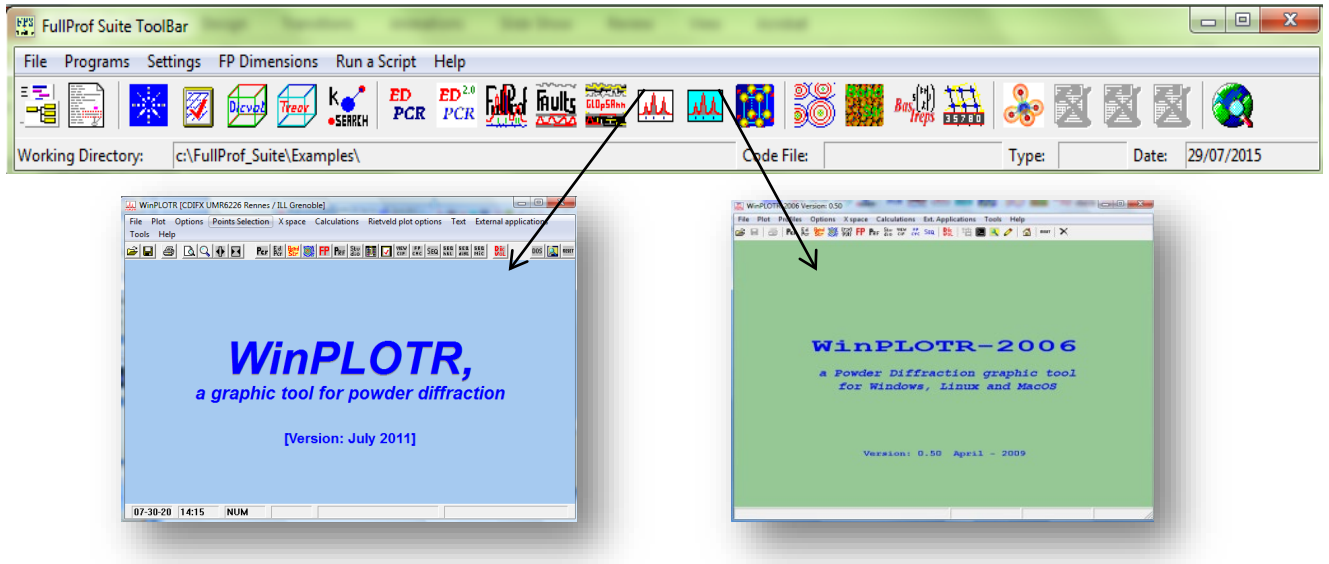

FullProf Suite ToolBar

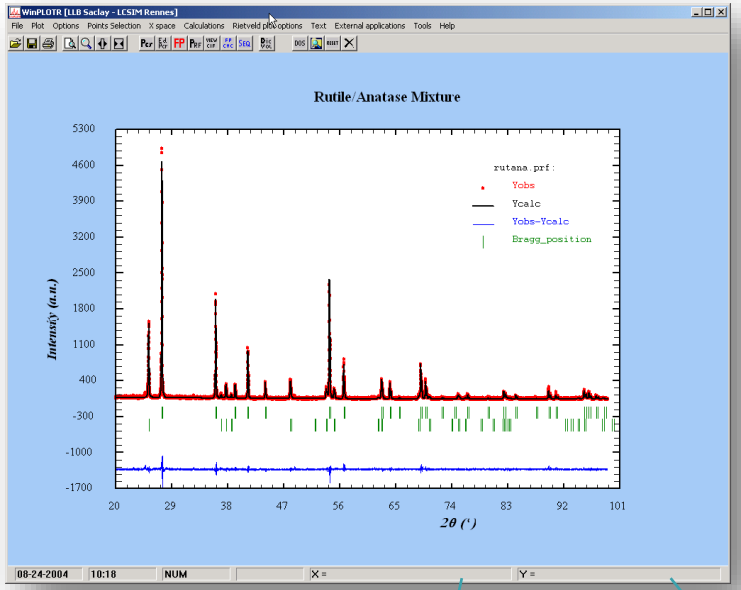


FullProf Suite: WinPLOTR

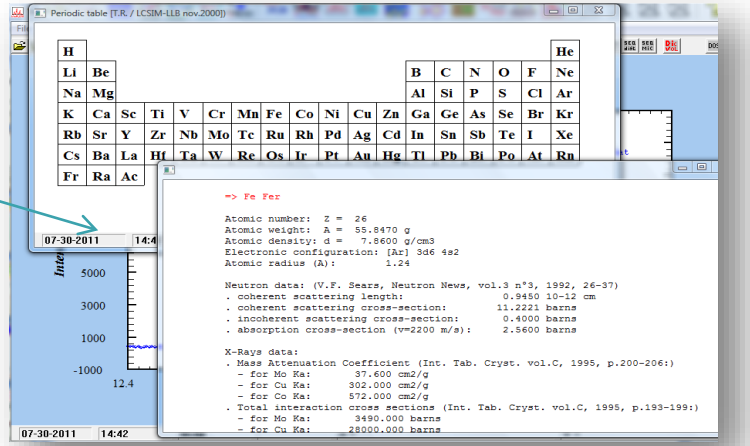


- ✓ Reading the X-ray and neutron diffraction patterns
- ✓ Automatic peak search for indexing
- ✓ Saving peaks as input for DICVOL04, Treor90, K-Search ...
- ✓ Making individual peak fit
- ✓ Exporting a background file
- ✓ Invoking other programs of FullProf Suite

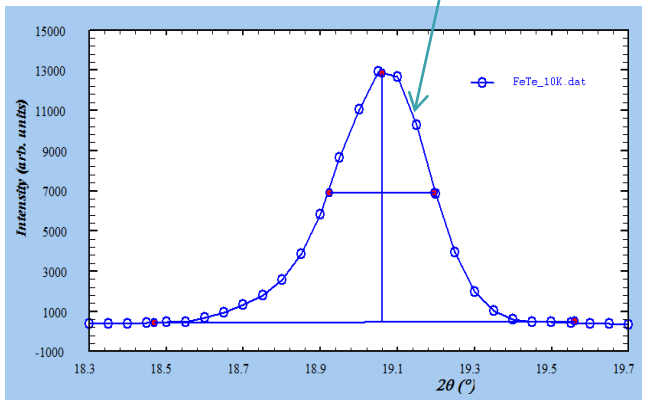
FullProf Suite: WinPLOTR



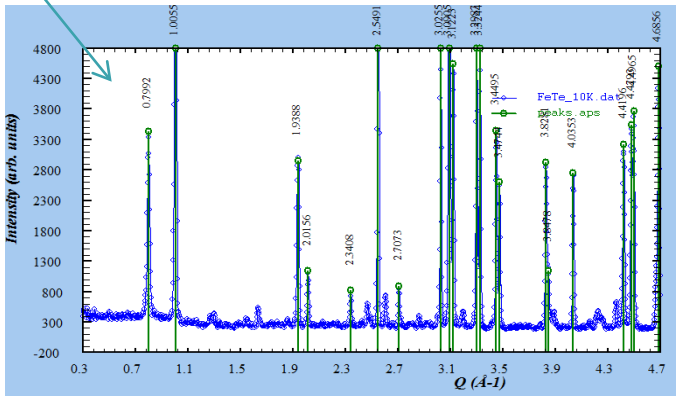
Access to other programs:
(e.g., periodic table of elements, space groups info, molecular weight and unit cell volume calculation …)



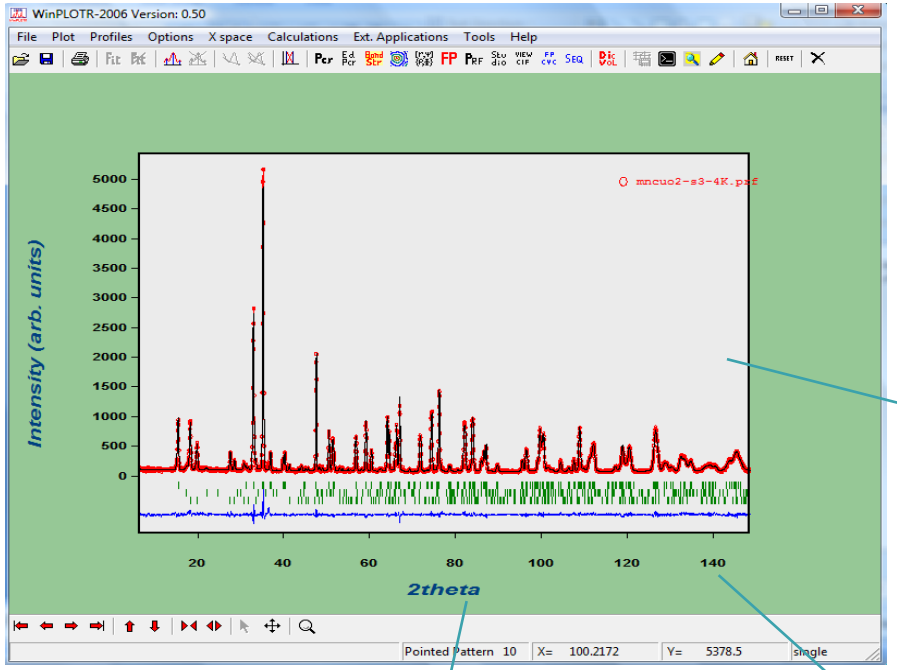
Individual peak fit



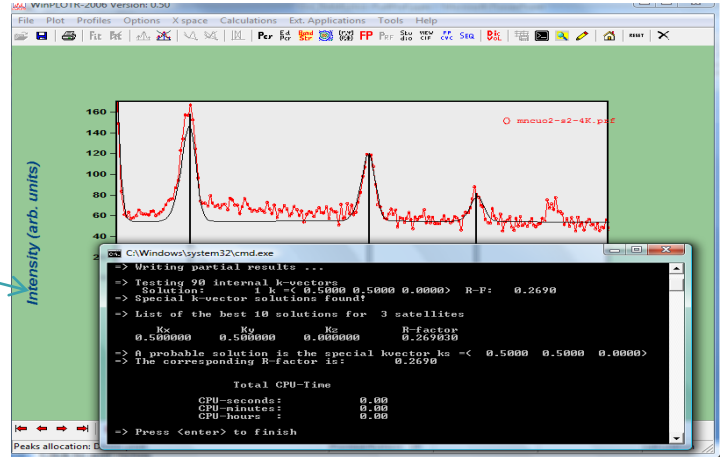
Automatic peak & background search



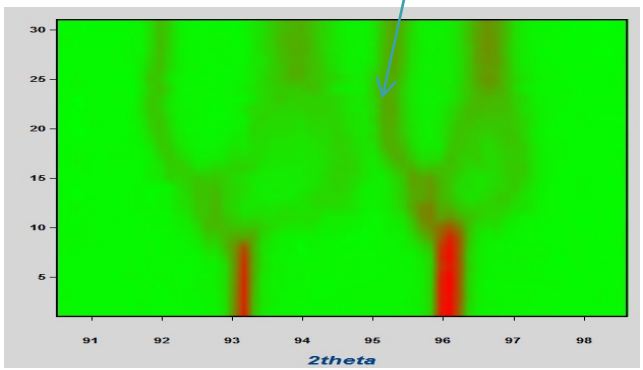
FullProf Suite: WinPLOTR-2006



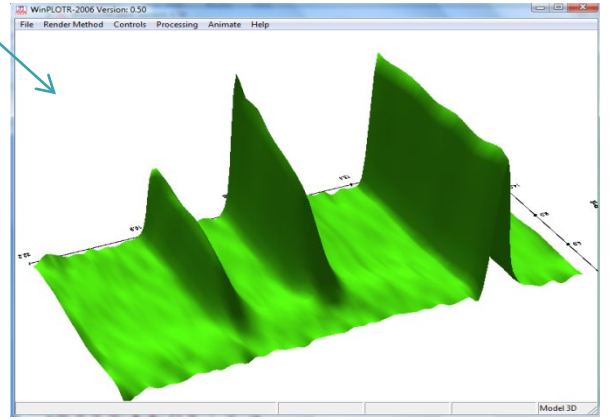
Search for the magnetic propagation vector (k-search)



2D contour plot



3D surface plot



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

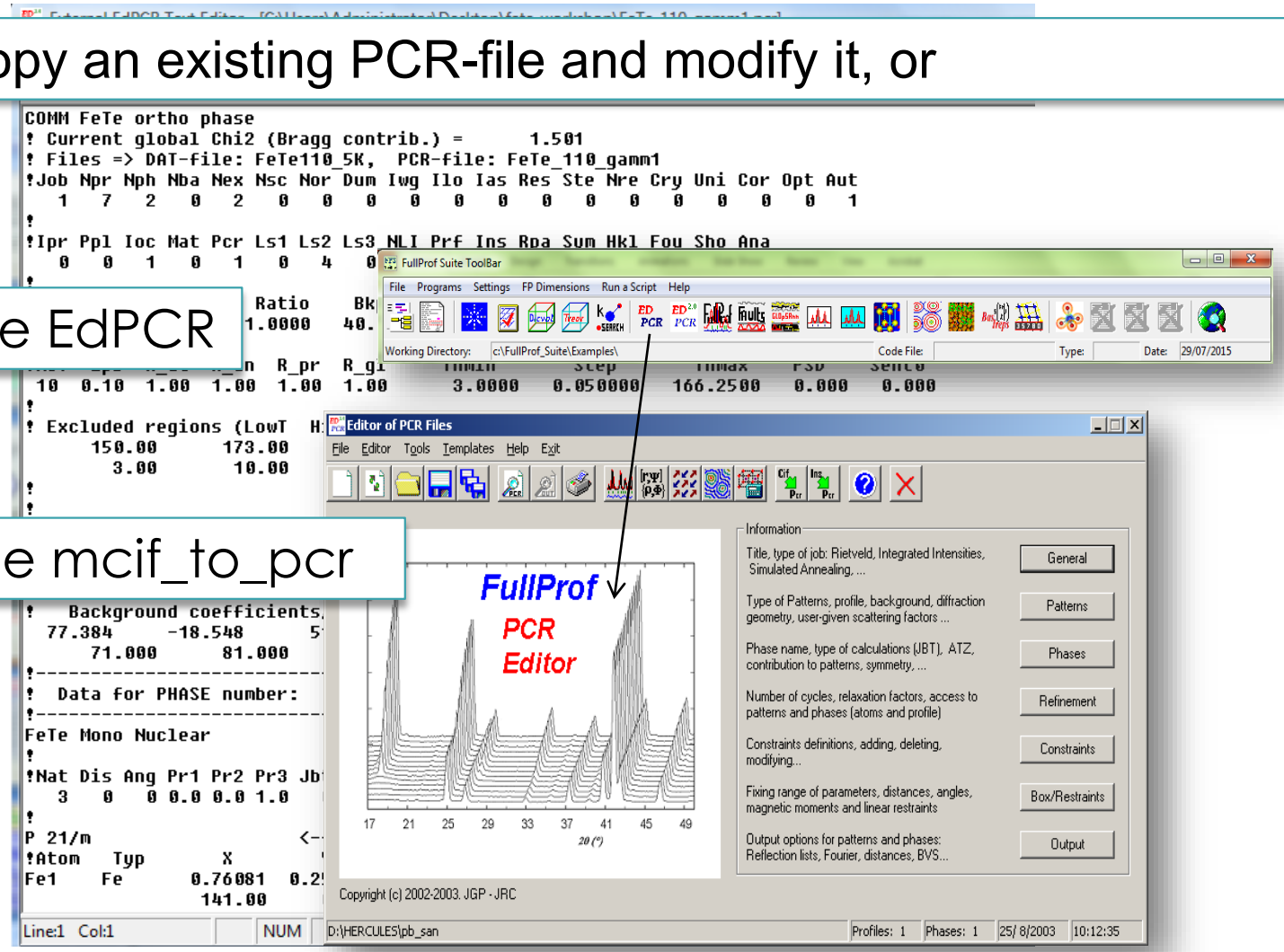
PCR file

- Many variables and options
- Complex to handle

→ Copy an existing PCR-file and modify it, or

→ use EdPCR

→ use mcif_to_pcr



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

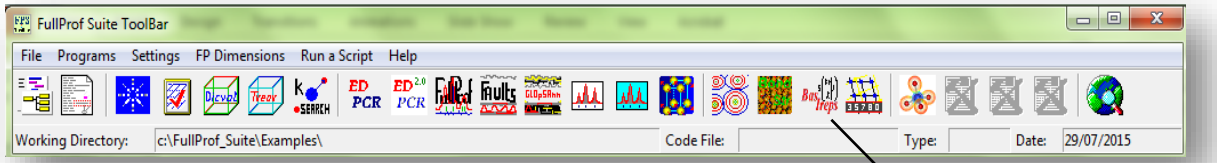
III. Perform Symmetry Analysis
FP_Suite -BasIreps, SARAh
Bilbao Cryst. Server, Isodistort

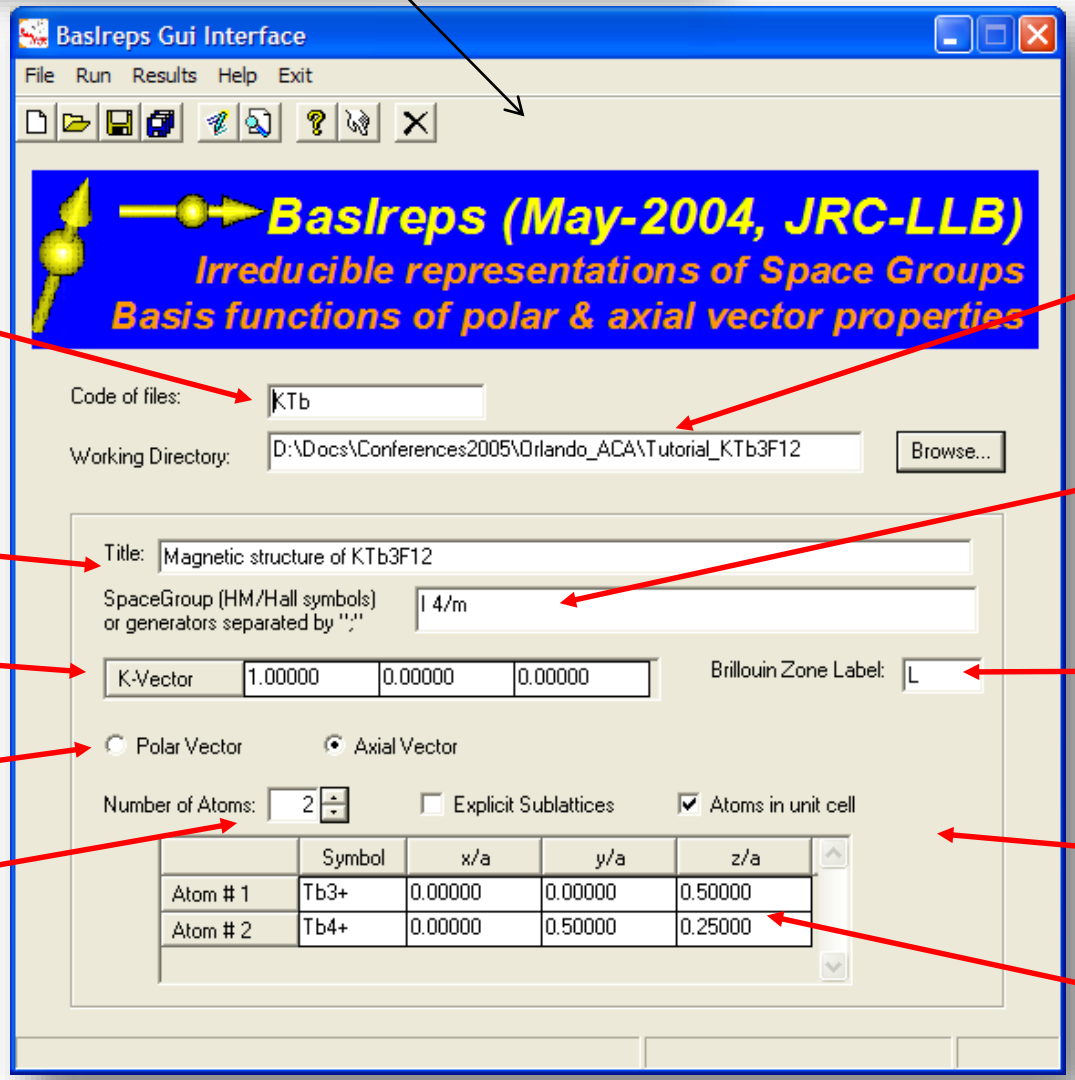
Propagation vector
⇐ *Space Group*
Atom positions

IV. Introduce and refine the magnetic phase
FP_Suite: FullProf

⇐ *Atomic components of Fourier basis functions*

Symmetry Analysis using *BasIreps*





Code of files

Working director y

Space group symbol or generators

Title

k-vector

Brillouin Zone label

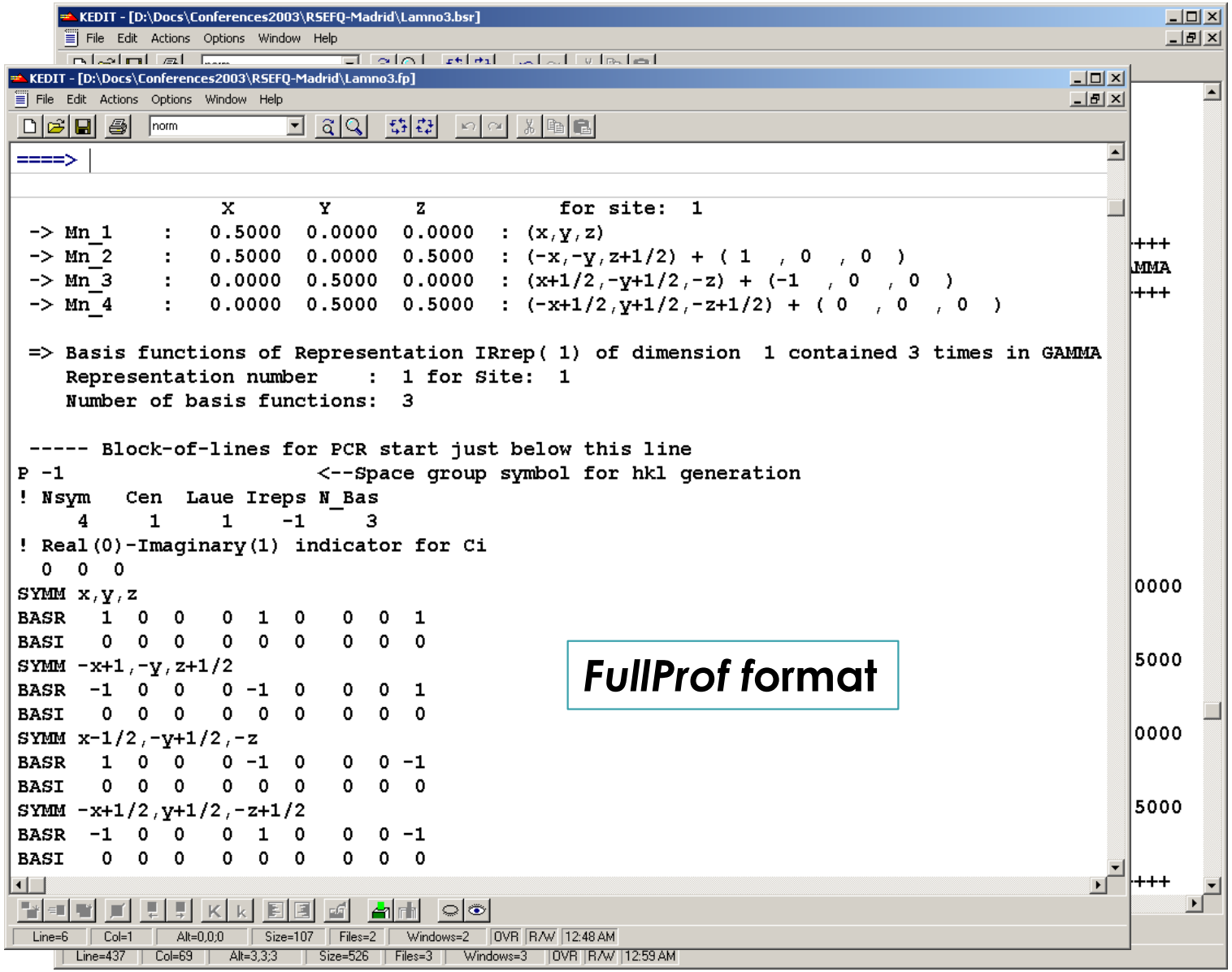
Axial/polar

Number of atoms

Atoms in Unit Cell

Atoms positions

Symmetry Analysis using *BasIreps*



FullProf format

FullProf : Magnetic Structure Factor

magnetic moment

expanded as Fourier series

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

S_{kjs} : Fourier coefficients are complex vectors

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

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

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

The magnetic structure factor:

$$\mathbf{M}(\mathbf{h}) = p\sum_{j=1}^{n} O_j f_j(\mathbf{h}) T_j \sum_s \mathbf{S}_{\mathbf{k}js}\ exp\left\{2\pi i\left[(\mathbf{H}+\mathbf{k})\left\{S|\mathbf{t}\right\}_s \mathbf{r}_j\right]\right\}$$

$\left\{S|\mathbf{t}\right\}_s$ Symmetry operators

FullProf: Magnetic Structure Refinement

many different ways of treating magnetic structures

➢ Fourier coefficients refinement:

- The magnetic symmetry is introduced together with explicit symmetry operators of the crystal structure.
- The refined variables are directly the components of the S_{kjs} vectors.
- A relation exist between S_{kj1} and S_{kjs} $\quad \mathbf{S}_{\mathbf{k}js} = M_{js}\,\mathbf{S}_{\mathbf{k}j1} exp\left\{-2\pi i \phi_{\mathbf{k}j}\right\}$

➢ 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

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

- 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, ….

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

```
Magnetic phase
!
!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  -1   0   0          0.000    0   7   0
!
P m m m                      <--Space group symbol
!Nsym Cen Laue MagMat
   4   1   3   1
!
SYMM   x,y,z
MSYM   u,v,w,0.0
SYMM   -x,-y,z+1/2
MSYM   -u,-v,w,0.0
SYMM   -x+1/2,y+1/2,-z+1/2
MSYM    u,-v,w,0.0
SYMM   x+1/2,-y+1/2,-z
MSYM   -u, v,w,0.0
!
!Atom Typ  Mag Vek     X        Y        Z        Biso    Occ       Rx       Ry       Rz
!     Ix      Iy      Iz     beta11   beta22   beta33   MagPh
Mn1  MMN3  1   0   0.50000 0.00000 0.00000 0.04338 1.00000   0.000    3.847    0.000
                       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
```

FullProf : Symmetry operators between Fourier components (Polar coordinates)

```
!-------------------------------------------------------------------------------
NiO |Magnetic Phase
!
!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   -1   -1    0    0        0.000    1   7     0
!
R -1                  <--Space group symbol for hkl generation
!
!Nsym Cen Laue MagMat
  1   1   1   1
!
SYMM X, Y, Z
MSYM u,v,w, 0.000
!
!Atom   Typ   Mag  Vek    X         Y         Z          Biso    Occ       Rm     Rphi  Rtheta
!    Im   Iphi   Itheta  beta11  beta22  beta33    MagPh
 Ni1    MNI3  1      0  0.00000 0.00000 0.00000 0.30000  1.00000   1.651   0.000  90.000
                        0.00      0.00      0.00       0.00       0.00      171.00   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
```

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

```
!-------------------------------------------------------------------------------
Nuclear and Magnetic Structure of: /srv/www/bcs_branch_www//bcs/www/tmp//subgrou   VARY mxmymz
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth        ATZ     Nvk Npr More
   4   0   0 0.0 0.0 1.0  10   0   2   0   0          0.000    0   7   0
!
P4/mm'm'  number:123.345      <--Magnetic Space group symbol (BNS symbol & number)
Transform to standard: a,b,c;0,0,0
Parent Space Group:       IT_number:    0
Transform from Parent:
! Nsym   Cen  N_Clat N_Ant
     8     2     0     0
!
! Symmetry operators
  1 x,y,z,+1
  2 -y,x,-z,+1
  3 y,x,z,-1
  4 x,-y,z,-1
  5 -x,y,z,-1
  6 y,x,-z,-1
  7 -x,-y,z,+1
  8 y,-x,-z,+1
!
!Atom   Typ     Mag Vek       X          Y          Z        Biso       Occ     N_type     Spc  /Line b
!       Rx         Ry         Rz         Ix         Iy         Iz       MagPh   / Line below:Codes
!      beta11    beta22    beta33    beta12    beta13    beta23   / Line below:Codes
La_1   La          1  0    0.50000    0.50000    0.50000    0.00000    0.06250     0     0     #
                              0.00       0.00       0.00       0.00       0.00
Mn_1   MMN2        1  0    0.00000    0.00000    0.00000    0.00000    0.06250     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 <-MagPar
       0.00       0.00       0.00       0.00       0.00       0.00       0.00
```

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

```
!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          0.000   0   7   0
!
P m m m                    <--Space group symbol
! Nsym   Cen  Laue Ireps N_Bas
     4     1     1    -1     3
! Real(0)-Imaginary(1) indicator for Ci
  0  0  0
!
SYMM x,y,z
BASR   1  0  0   0  1  0   0  0  1
BASI   0  0  0   0  0  0   0  0  0
SYMM -x+1,-y,z+1/2
BASR  -1  0  0   0 -1  0   0  0  1
BASI   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
SYMM x-1/2,-y+1/2,-z
BASR  -1  0  0   0  1  0   0  0  1
BASI   0  0  0   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
Mn1   MMN3  1   0   0.50000 0.00000 0.00000 0.04338 1.00000   0.000    3.847    0.000
                      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
```

FullProf : using Amplimodes (mcif to pcr – Isotropy)

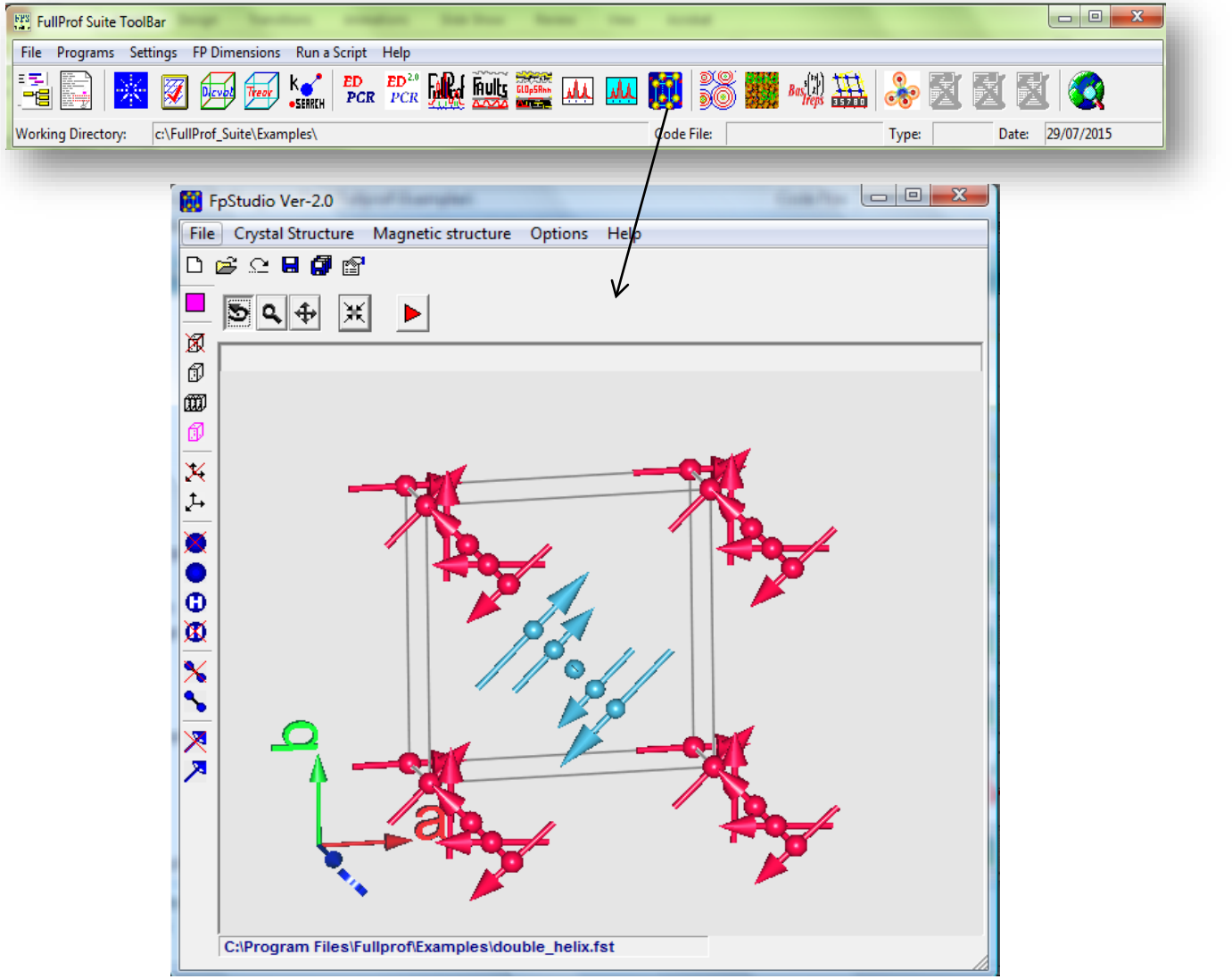
```
!-------------------------------------------------------------------------------
!  Data for PHASE number:   1  ==> Current R_Bragg for Pattern#  1:     0
!-------------------------------------------------------------------------------
AMPLIMODES for FullProf           FIX xyz
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth       ATZ    Nvk Npr More
  4   0   0   0.0 0.0 1.0  -6   0   2   0    1        1000.0  0   7   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      X         Y         Z        Biso      Occ  N_type  Spc/Fftype
!       Rx        Ry        Rz        Ix        Iy        Iz      MagPh
La_1   LA       0    0   0.50000   0.50000   0.50000   0.50000   0.06250      0    1
                             0.00      0.00      0.00      0.00      0.00
Mn_1   MN       1    0   0.00000   0.00000   0.00000   0.50000   0.06250      1    2
                             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
O_1    O        0    0   0.00000   0.00000   0.50000   0.50000   0.06250      0    3
                             0.00      0.00      0.00      0.00      0.00
O_2    O        0    0   0.00000   0.50000   0.00000   0.50000   0.12500      0    3
                             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      Mx       My       Mz       Coeff
  1 Mn_1   mGM4+      0.0000   0.0000   0.2538   1.00
! Amplitudes of Magnetic Symmetry Modes
MA_MODES    1    2
    A1_mGM4+         0.00000    1.00
!
!  Scale        Shape1      Bov       Str1       Str2       Str3    Strain-Model
  2.00         0.00000   0.00000   0.00000   0.00000   0.00000        0
    0.00000      0.000     0.000     0.000     0.000     0.000
```

FullProf : IC using Superspace description (mcif to pcr)

```
!-------------------------------------------------------------------------------------------
DyMn6Ge6 magnetic VARY   mxmymz McosMsin
!
!Nat Dis Ang Pr1 Pr2 Pr3  Jbt  Irf Isy Str Furth      ATZ    Nvk Npr More
  5   0  0 0.   0   0.0  1.0   7   0   2   0    0    133584.188   1   7   0
!
P62'2'(0,0,g)h00            <-- Magnetic  SuperSpace group symbol
generators x-y,x,z,t+1/6,+1;  x-y,-y,-z,-t+1/3,-1
N_qc  1
Q_coeff
  1
!
!Atom   Typ  Max_Qcoeff      X        Y        Z       Biso       Occ   N_type Spc / Line below:Codes
!              Mcosx       Mcosy      Mcosz      Msinx      Msiny      Msinz       / Line below:Codes
!             beta11      beta22     beta33     beta12     beta13     beta23       / Line below:Codes
Dy    JDY3     1        0.00000    0.00000    0.00000    0.00000    1.00000    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
  Mcos-Msin-1:    7.12688    3.56344    0.00000    0.00000    6.17206    0.00000  <-Amplitudes of Modulated moments
               92.00000   91.00000    0.00000    0.00000   91.73205    0.00000
Mn1   MMN2     1        0.00000    0.50000    0.25030    0.00000    6.00000    1    0
                      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
Ge1   GE       0        0.66667    0.33333    0.50000    0.00000    2.00000    0    0
                      0.00000    0.00000    0.00000    0.00000    0.00000
Ge2   GE       0        0.66667    0.33333    0.00000    0.00000    2.00000    0    0
                      0.00000    0.00000    0.00000    0.00000    0.00000
Ge3   GE       0        0.00000    0.00000    0.34450    0.00000    2.00000    0    0
                      0.00000    0.00000    0.00000    0.00000    0.00000
! --> Profile Parameters for Pattern #  1
```

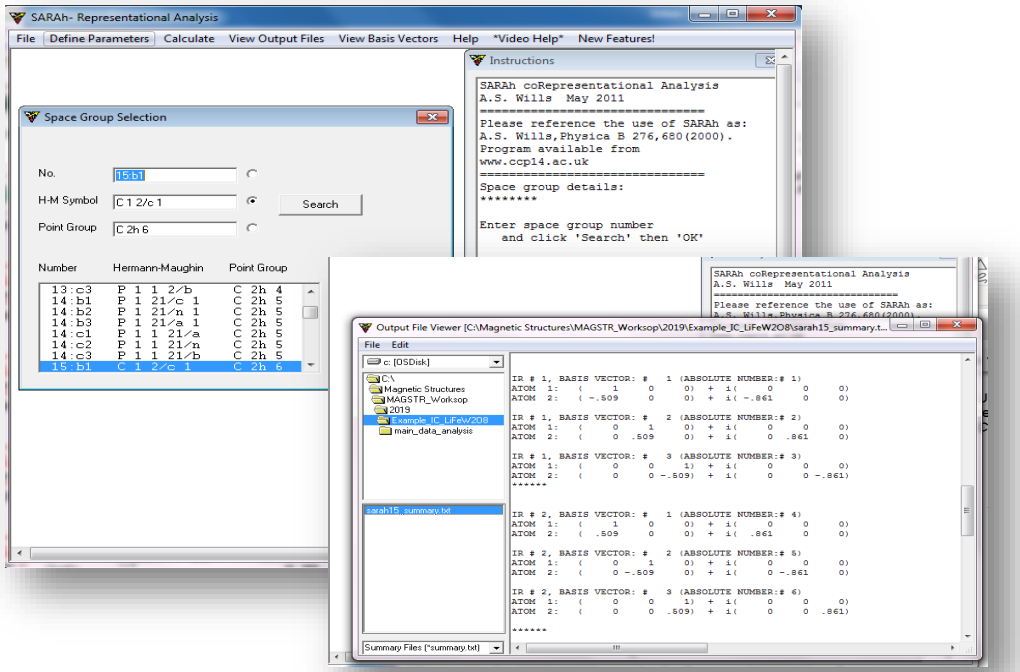
3D visualization program: *FpStudio*

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



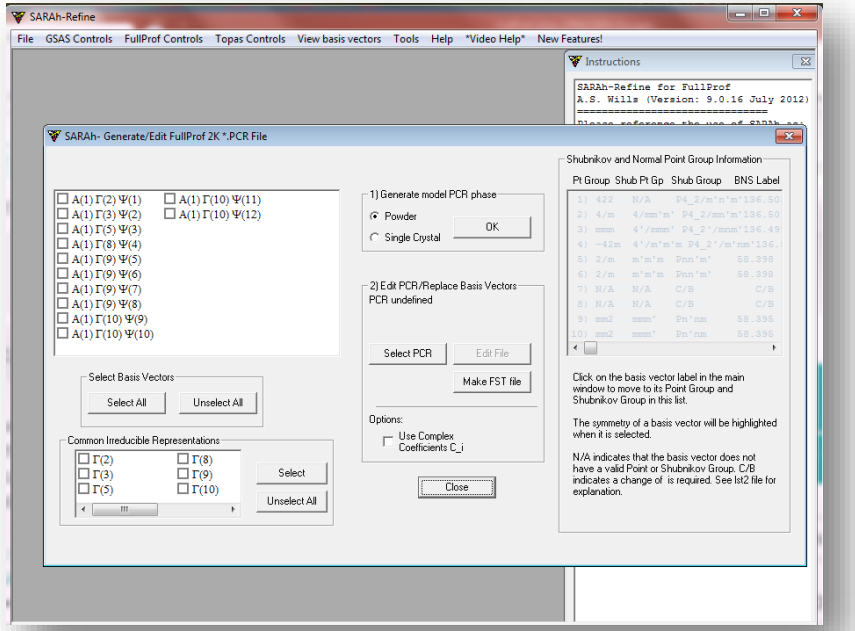
SARAh http://fermat.chem.ucl.ac.uk/spaces/willsgroup/software/

Sarah-Representational Analysis



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

Sarah-Refine



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

sarah15.pcr - Notepad

File Edit Format View Help

```
!-------------------------------------------------------------------------------
! Data for PHASE number:   1  ==> Current R_Bragg for Pattern#  1:    1.00
!
Magnetic Phase
!
!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
!
C -1                    <--Space group symbol
! Nsym   Cen  Laue Ireps N_Bas
    2     1     1    -1     6
! Real(0)-Imaginary(1) indicator for Ci
  0 0 0 0 0 0
!
SYMM X, Y, Z
BASR  1  0  0  0  1  0  0  0  1  1  0  0  0  1  0  0  0  1
BASI  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
SYMM X, -Y+1, Z+1/2
BASR -.5  0  0  0 .51  0  0  0 -.5 .51  0  0  0 -.5  0  0  0 .51
BASI .86  0  0  0 -.9  0  0  0 .86 -.9  0  0  0 .86  0  0  0 -.9
!
!Atom Typ  Mag Vek    X      Y      Z      Biso   Occ      C1      C2      C3
!    C4     C5     C6     C7     C8     C9     MagPh
FE1  MFE3  1   0    .00000 .33532 .25000 .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
   0.000  0.000  0.000  0.000  0.000  0.000  0.000  .00000
    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
   1.08239  -0.23233   0.25618   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
273
    0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
! Pref1    Pref2     Asy1      Asy2      Asy3      Asy4
  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
     0.00     0.00     0.00     0.00     0.00     0.00
! Propagation vectors:
   .8900000   .0000000   .3300000        Propagation Vector  1
```

External EdPCR Text Editor - [C:\Magnetic Structures\MAGSTR_Worksop\2019\Example_IC_LiFeW2O8\LiFeW2O8.pcr]

File Edit Search

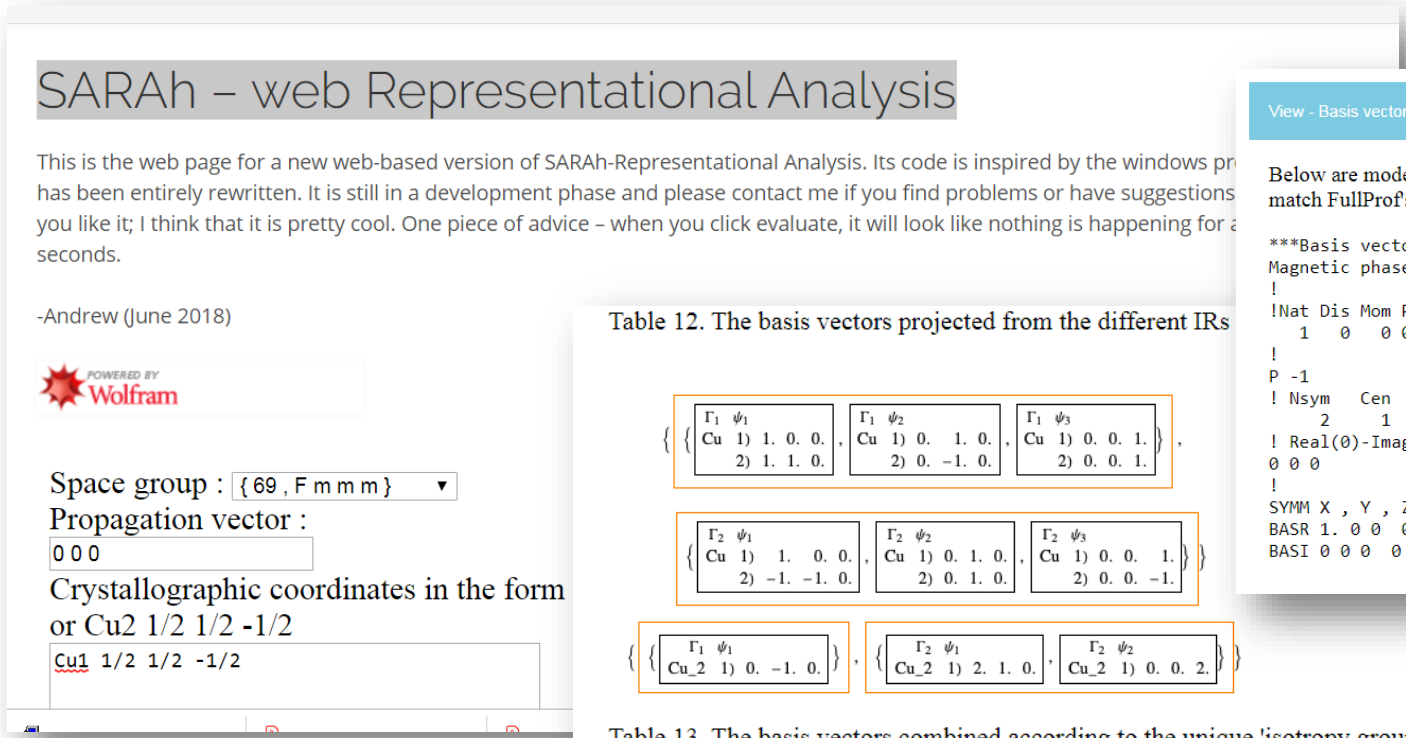
```
     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000
!  Pref1     Pref2      Asy1      Asy2      Asy3      Asy4      S_L       D_L
   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
      0.00      0.00      0.00      0.00      0.00      0.00      0.00      0.00
!-------------------------------------------------------------------------------
!-------------------------------------------------------------------------------
Crystallographic investigation of a double tungstate, Li Fe (W 04)2
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth       ATZ     Nvk Npr More
   7   0   0 0.0 0.0 1.0   0  -1   0   0   0       2233.933  -1   7   0
!
!
C 1 2/c 1                 <--Space group symbol
!Atom   Typ       X         Y         Z        Biso       Occ      In Fin N_t Spc /Codes
W1     W       0.24831   0.09192   0.24478   0.42000   1.00000   0   0   0   0
                  0.00      0.00      0.00      0.00      0.00
Fe1    Fe      0.00000   0.33421   0.25000   0.74000   0.50000   0   0   0   0
                  0.00      0.00      0.00      0.00      0.00
Li1    Li      0.50000   0.34345   0.25000   2.00000   0.50000   0   0   0   0
                  0.00      0.00      0.00      0.00      0.00
O1     O       0.36480   0.05924   0.92493   1.00000   1.00000   0   0   0   0
                  0.00      0.00      0.00      0.00      0.00
O2     O       0.37971   0.18197   0.41116   1.00000   1.00000   0   0   0   0
                  0.00      0.00      0.00      0.00      0.00
O3     O       0.35709   0.54854   0.94233   1.00000   1.00000   0   0   0   0
                  0.00      0.00      0.00      0.00      0.00
O4     O       0.37763   0.69357   0.39354   1.00000   1.00000   0   0   0   0
                  0.00      0.00      0.00      0.00      0.00
!-------> Profile Parameters for Pattern #  1
!  Scale      Shape1      Bov      Str1      Str2      Str3     Strain-Model
 0.25794      0.00000    0.00000   0.00000   0.00000   0.00000       0
     0.00000     0.000     0.000     0.000     0.000     0.000
!       U         V         W         X         Y       GauSiz    LorSiz Size-Model
    0.000000  0.000000  0.012757  0.000000  0.000000  0.000000  0.000000    0
      0.000     0.000     0.000     0.000     0.000     0.000     0.000
!      a         b         c       alpha      beta       gamma      #Cell Info
   9.267413  11.394221   4.893332  90.000000  90.567055  90.000000
    0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
!  Pref1     Pref2      Asy1      Asy2      Asy3      Asy4      S_L       D_L
  0.00000   0.00000   0.00000   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
! Propagation vectors:
```

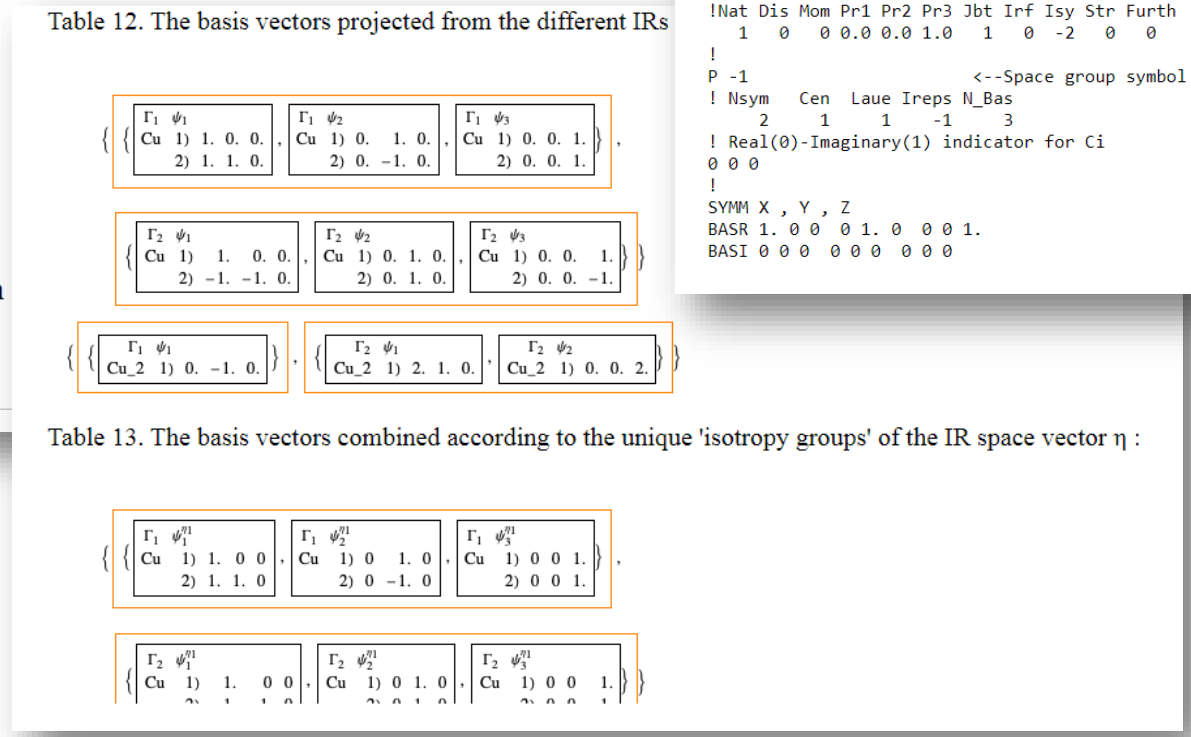
Line:93 Col:1 INS

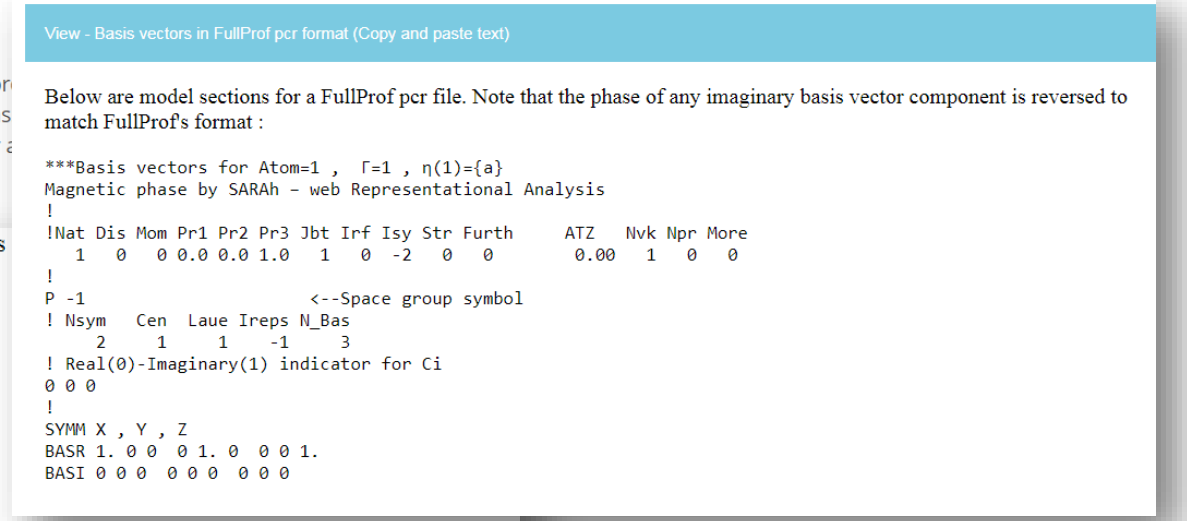
OAK RIDGE National Laboratory | HIGH FLUX ISOTOPE REACTOR | SPALLATION NEUTRON SOURCE

SARAh – web Representational Analysis

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







Thank you !