Introduction to the programs of the FullProf Suite

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Web site for the

FullProf Suite

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

Or go to the ILL web site: http://www.ill.eu

Look for "users and science", "groups and instruments" "diffraction", "software", …

The programs of the *FullProf Suite* are available for the following platforms:

Windows, Linux and MacOS (Intel)

Web site: http://www.ill.eu/sites/fullprof/index.html

FullProf Suite

Crystallographic tools for Rietveld, profile matching & integrated intensity refinements of X-Ray and/or neutron data

Introduction · What's new · Programs · Downloads · Examples & Tutorials · Support · References

Name:	Version date:	Platform:	File size	Link:
FullProf_Suite Windows	Aug - 2008	Windows 9X/NT/2k/XP/Vista	33,234,165	Download
FullProf_Suite Linux	Aug - 2008	Linux - PC	34,623,623	Download
FullProf_Suite Mac	Aug - 2008	Mac OS - Intel	37,758,982	Download

```
INSTALLATION OF THE FULLPROF SUITE FOR WINDOWS
==============================================

Download the package, which is an executable file (installer), in a temporary directory and run it.
Follow the indications of the installer and pay attention not to use, for holding the files, directories
with blanks or non ASCII character in their names

INSTALLATION OF THE FULLPROF SUITE FOR Mac OS AND/OR LINUX
==========================================================

Download the file of the version you wish to install in your system from the WEB page of the FullProf Suite.
The steps to follow are the following:

General Mode (for all the users of the system)
----------------------------------------------
1.- Activate the super-user mode
2.- Create a directory in which you want to hold the programs of the FullProf_Suite.
    For instance: /Applications/FullProf_Suite in Mac OS or
    /usr/local/bin/FullProf_Suite in some Linux systems
3.- Copy the file FullProf_Suite_XXXNN_OP.tgz (XXX=Month NN=year, OP=Lin or Mac) in the
    directory just created in step 2
```

Web site: http://www.ill.eu/sites/fullprof/index.html

FullProf Suite

Crystallographic tools for Rietveld, profile matching & integrated intensity refinements of X-Ray and/or neutron data

Introduction · What's new · Programs · Downloads · Examples & Tutorials · Support · References

Available items in Catalogs section:

Name:	Description:	File size	Link:
FullProf Manual	Users' Guide of FullProf	1,769,341	Download

Available items in Tutorials section:

Name:	Description:	File size	Link:
Atlanta-doc	PDF-docs of a School in Atlanta	2,171,360	Download
ECM-21-Workshop	PDF-docs of ECM-21 Workshop	1,055,669	Download
Exercises-dat	Data files, FullProf exercises	54,250	Download
Exercises-pcr	PCR filese, FullProf exercises	35,608	Download
HoCu_Tutorial	Tutorial magnetic structure	1,130,682	Download
KTb3F12_Tutorial	Tutorial magnetic structure	501,244	Download
Microstructural_effects	Documents about microstructure	544,914	Download
pcr_dat	Data and PCR files	824,597	Download
size-sph	Notes about size effects	14,298	Download
sr_oxalate	Simulated annealing in FullProf	30,958	Download

Available items in Examples section:

Name:	Description:	File size	Link:
FullProf examples	A set of PCR examples files to run on FullProf program	546,446	Download

Programs of the FullProf Suite

FP_Suite_Toolbar: Program for accessing the whole set of the FullProf Suite.

WinPLOTR / WinPLOTR-2006: Programs for visualising powder diffraction patterns. Fitting independent peaks (CW and TOF), interface for FullProf and many of the programs of the FullProf Suite

FullProf : Crystal and magnetic structure refinement, powder/single crystals, polarised neutrons, constant wavelength, TOF, energy dispersive, multiple patterns, simulated annealing for **solving crystal and magnetic** structures (integrated and profile intensities).

EdPCR: Editor of the FullProf input control file

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

SuperCell/K_Search: Program for searching propagation vectors

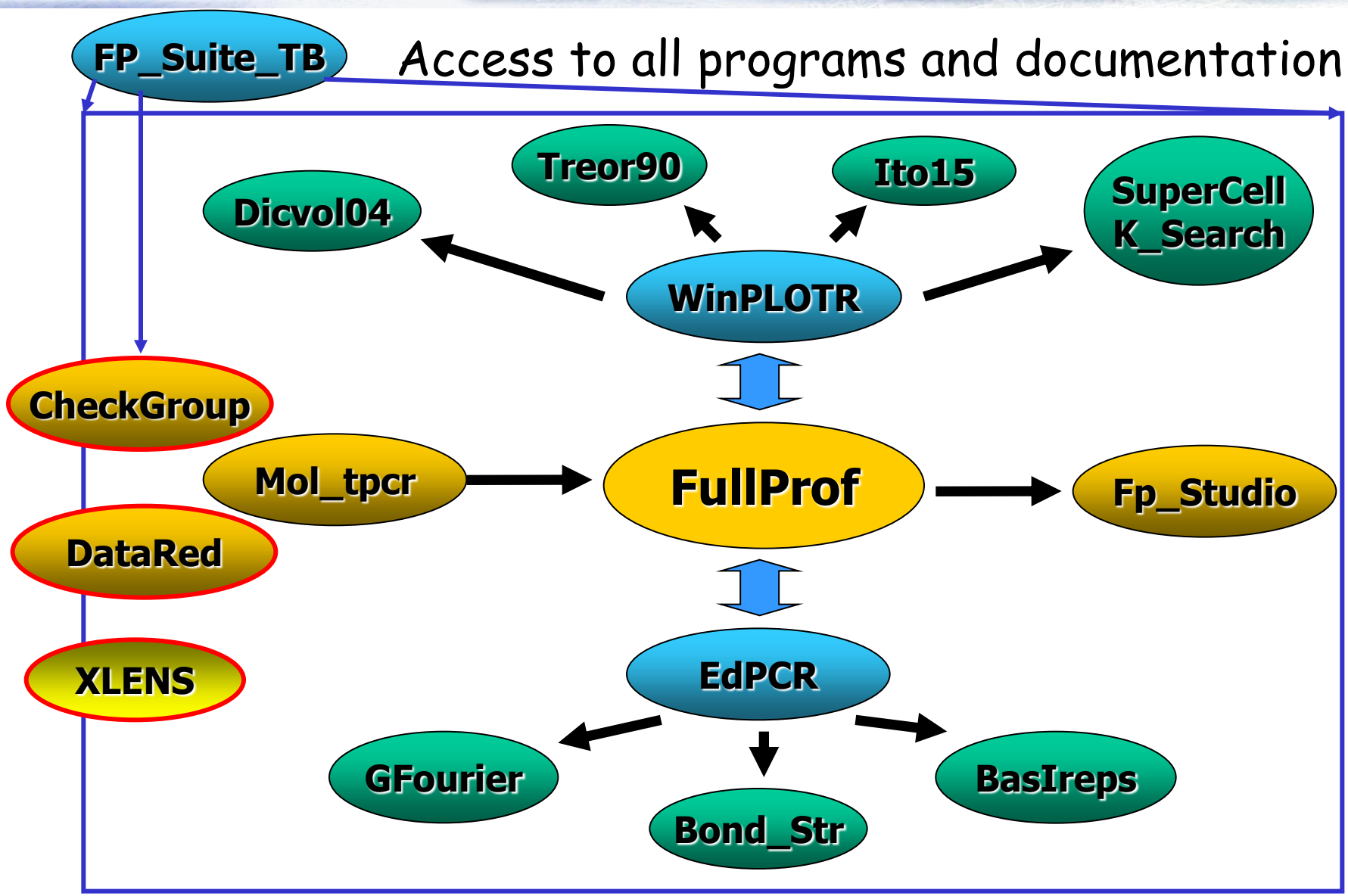
BasIREPS: Program for calculating basis functions of irreducible representations of space groups. Useful for determining magnetic structures .

Fp_Studio: Program for visualising crystal and magnetic structures

Check_Group: Program for getting the space group (powders and single crystals)
Datared/GDatared: Program for single crystal data reduction
Mol_tpcr: console utility for creating Rigid body groups

External programs: **DICVOL04, TREOR90, ITO, XLENS**

FullProf Suite



Toolbar of the FullProf Suite

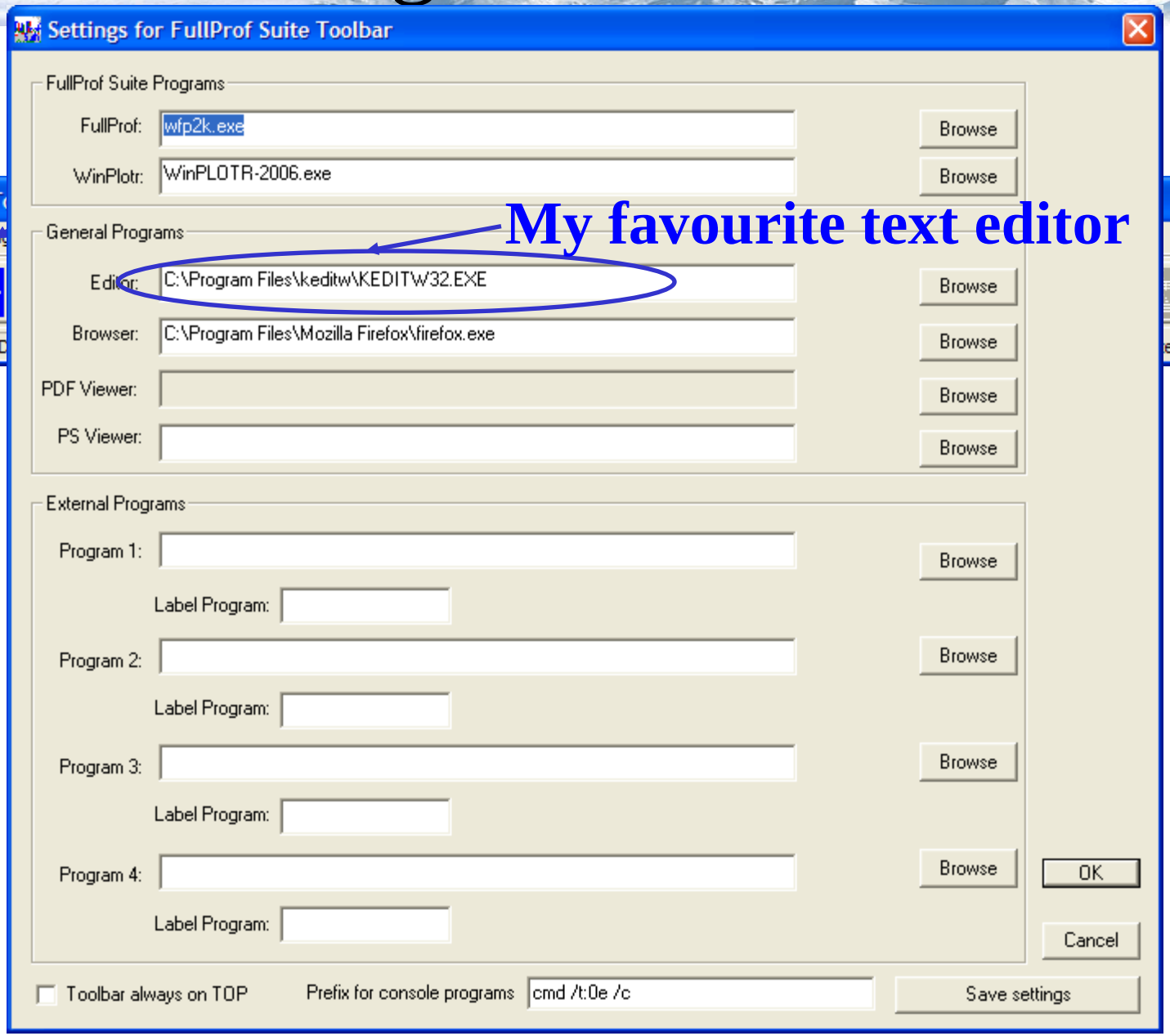
File: Select working directory

Run Programs

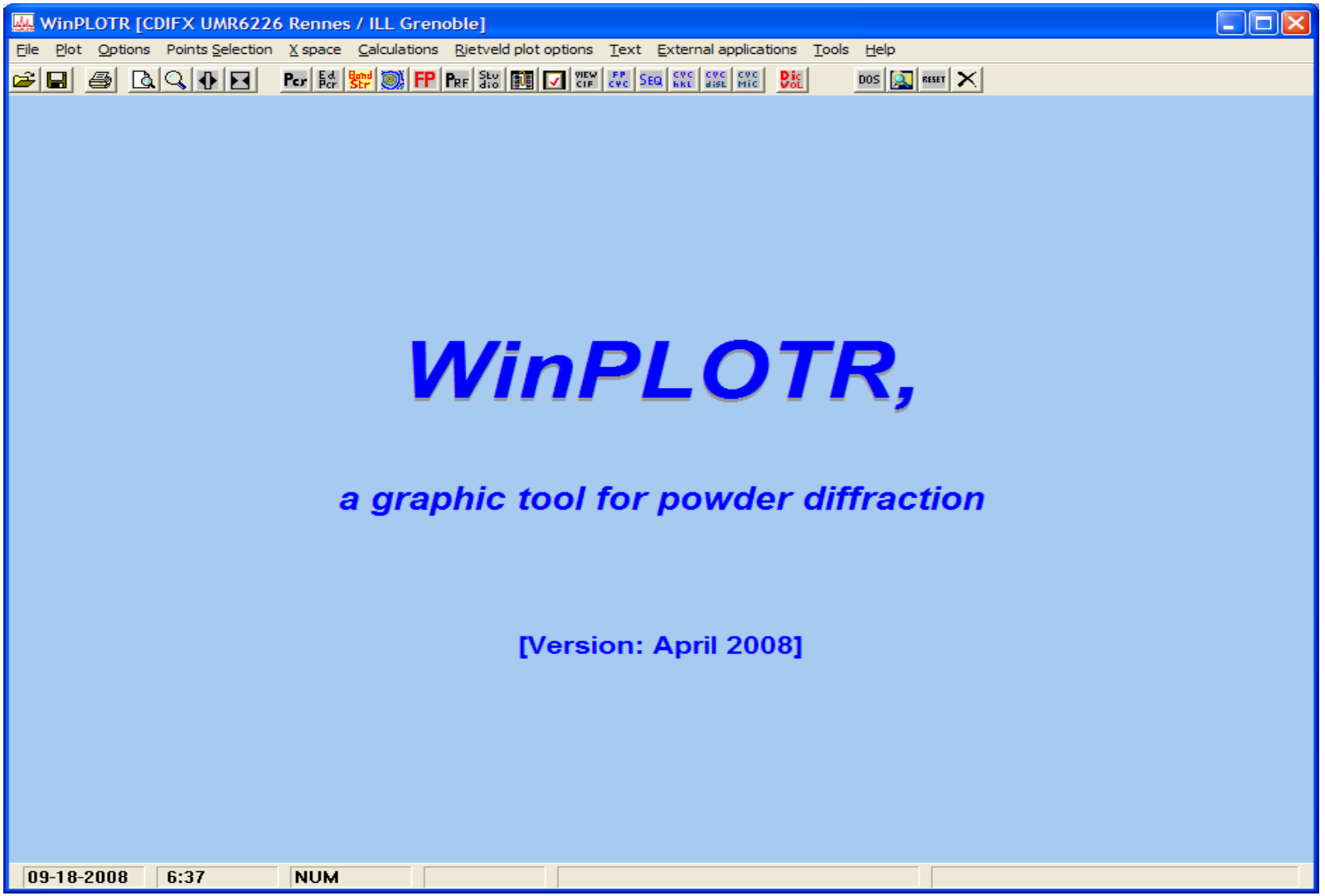
Edit current file

Charge PCR or recognised files

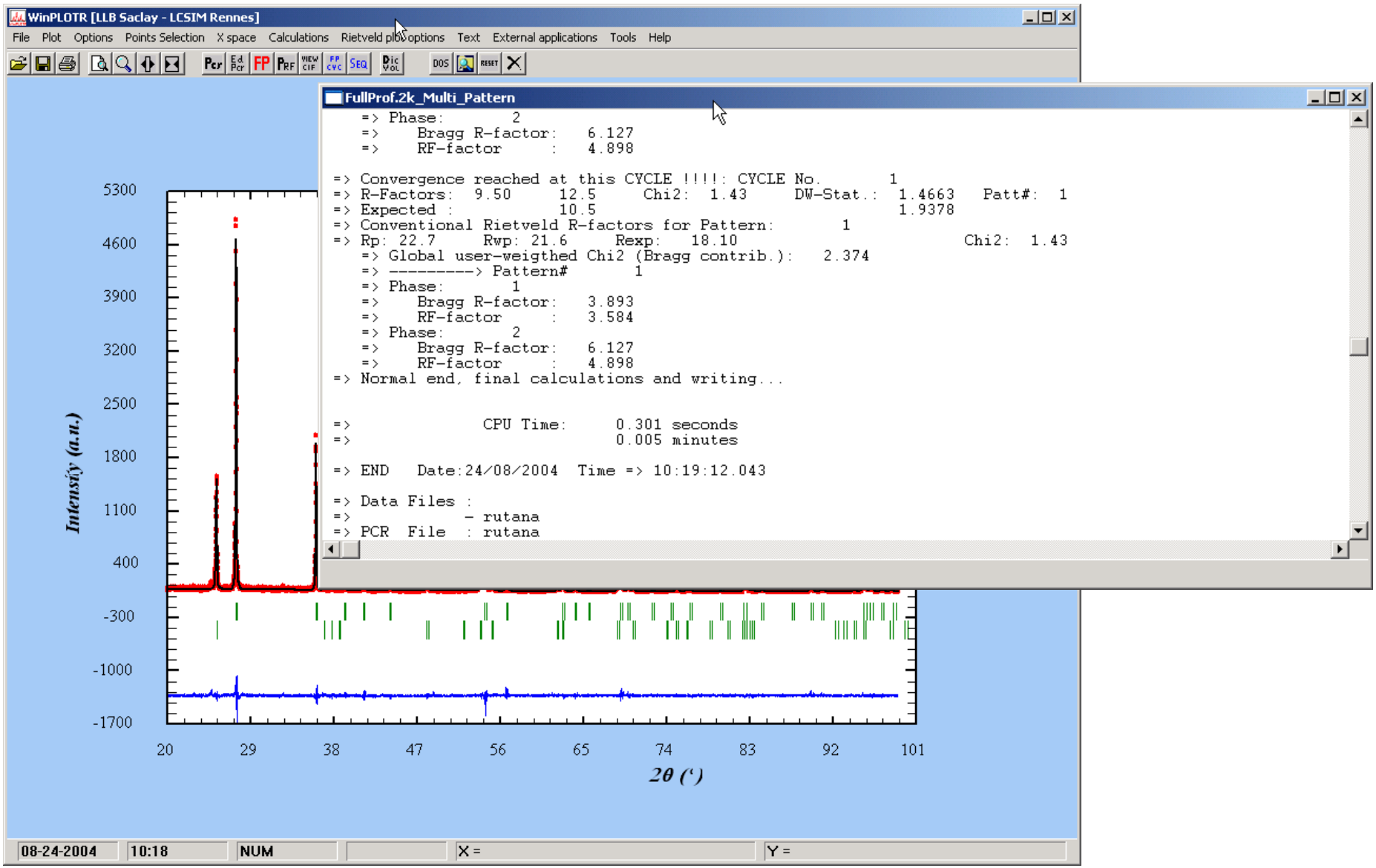
Setting of the Toolbar



WinPLOTR: program to access the whole FullProf Suite



Running FullProf from WinPLOTR



WinPLOTR: reading the X-ray and neutron diffraction patterns, running indexing programs, fitting peaks, etc

Basics operations for configuring WinPLOTR

The file WinPLOTR.set

Accessing general applications, Explorer, Acrobat reader, …

1: Automatic peak search for indexing

2: Saving peaks as DICVOL04, Treor90, etc

3: Running indexing programs

4: Automatic generation of PCR file for cell refinement and integrated intensity extraction

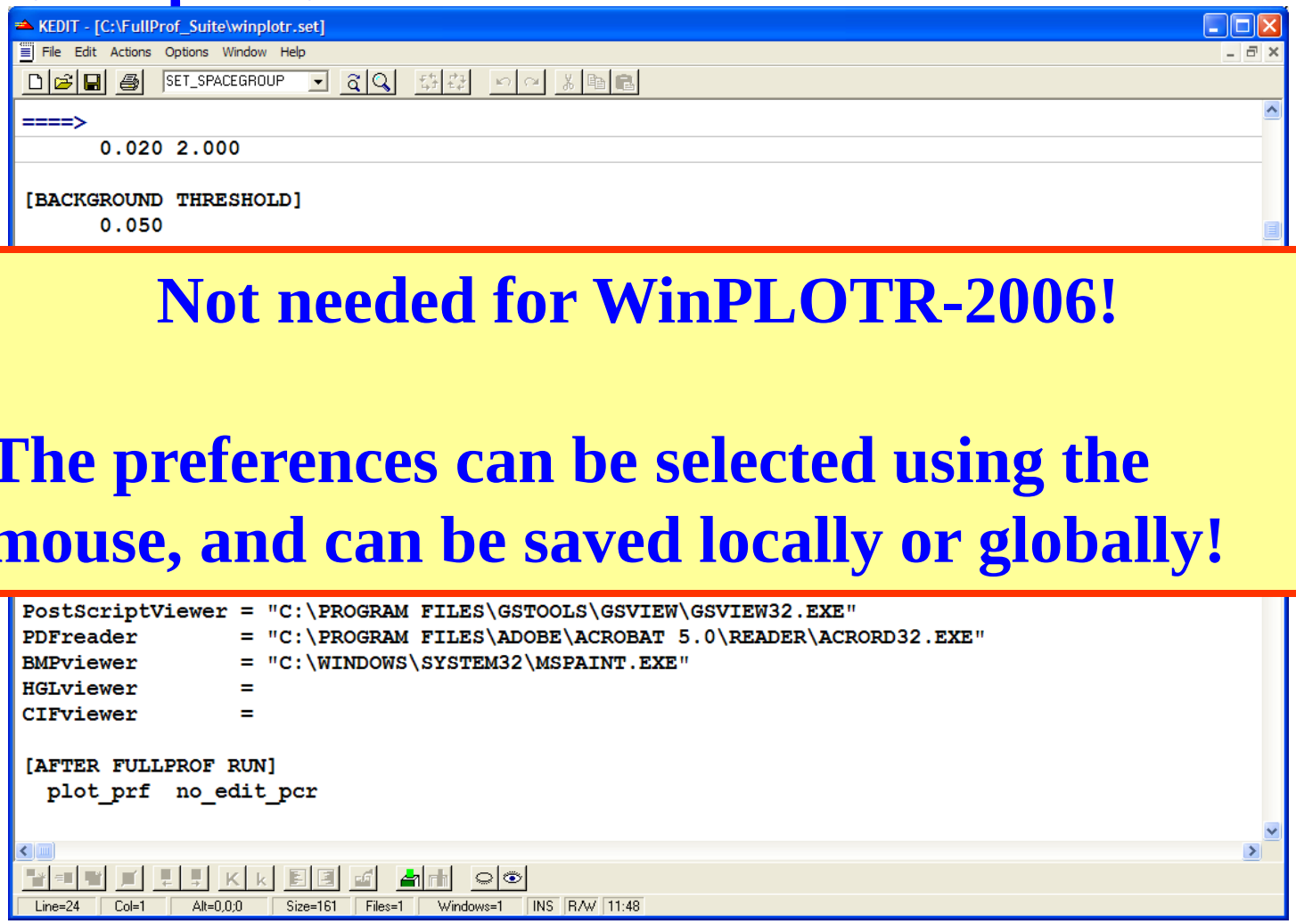
5: Making individual peak fits

6: Exporting a background file

7: Invoking other programs

Configuration of WinPLOTR

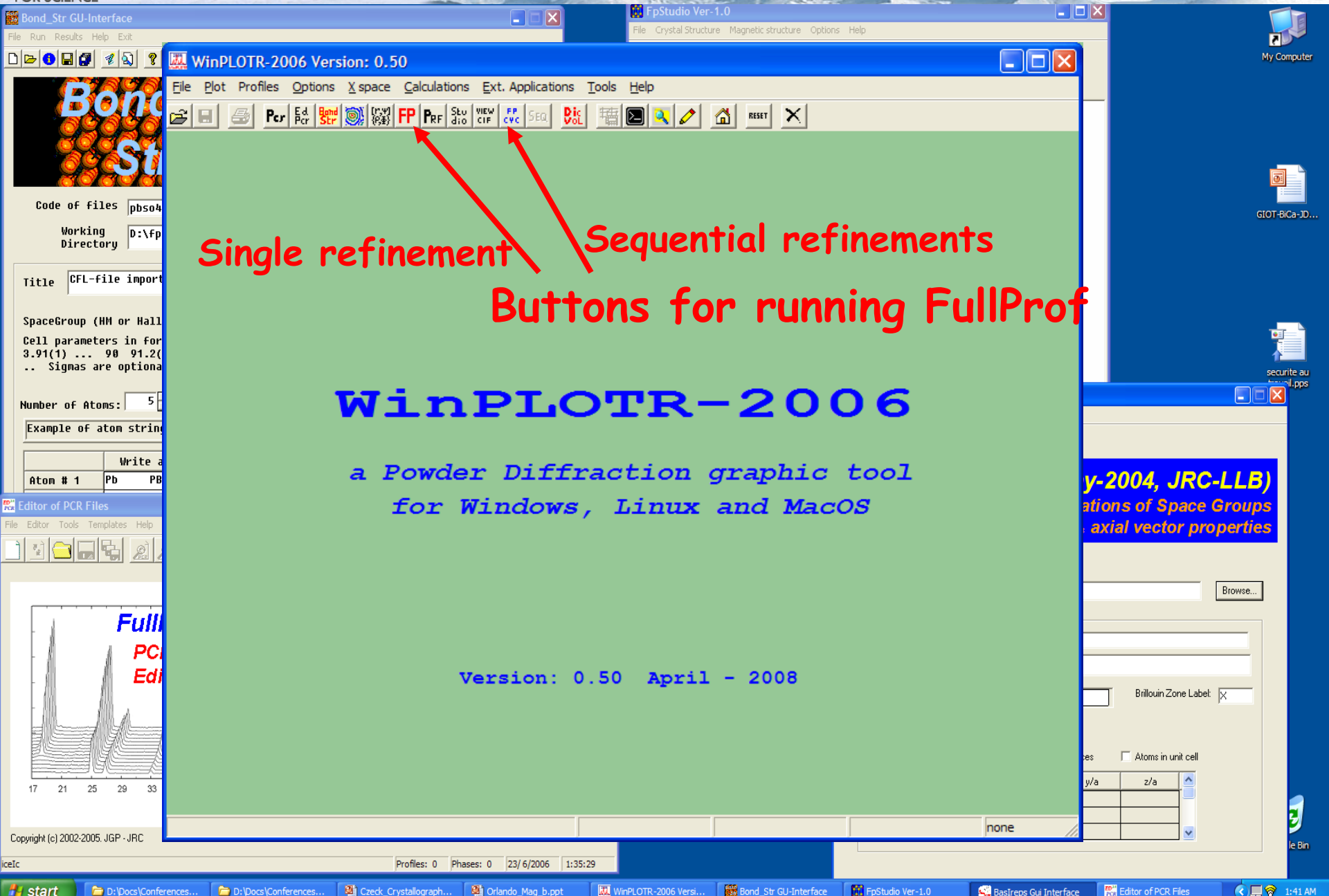
File: winplotr.set

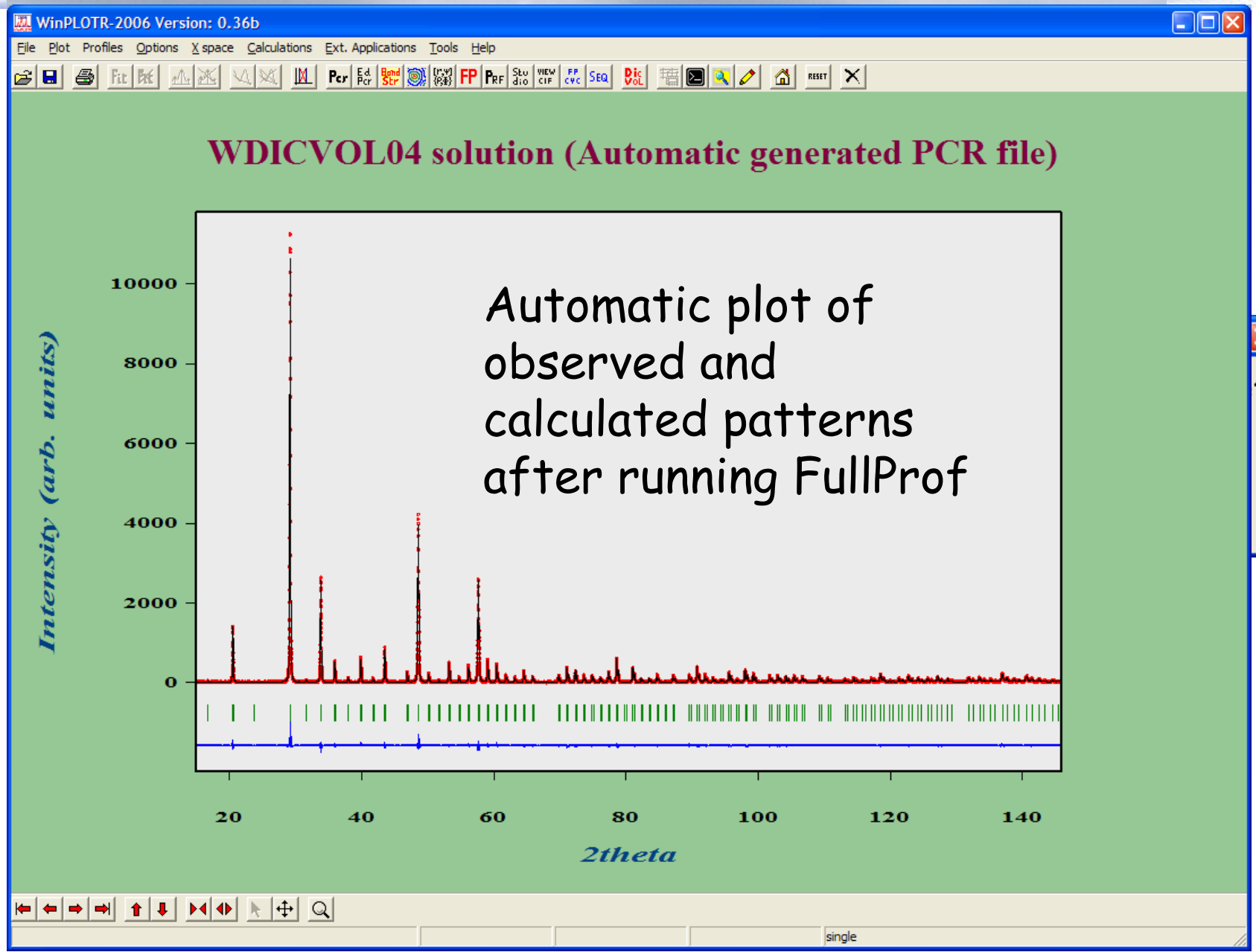


Not needed for WinPLOTR-2006!

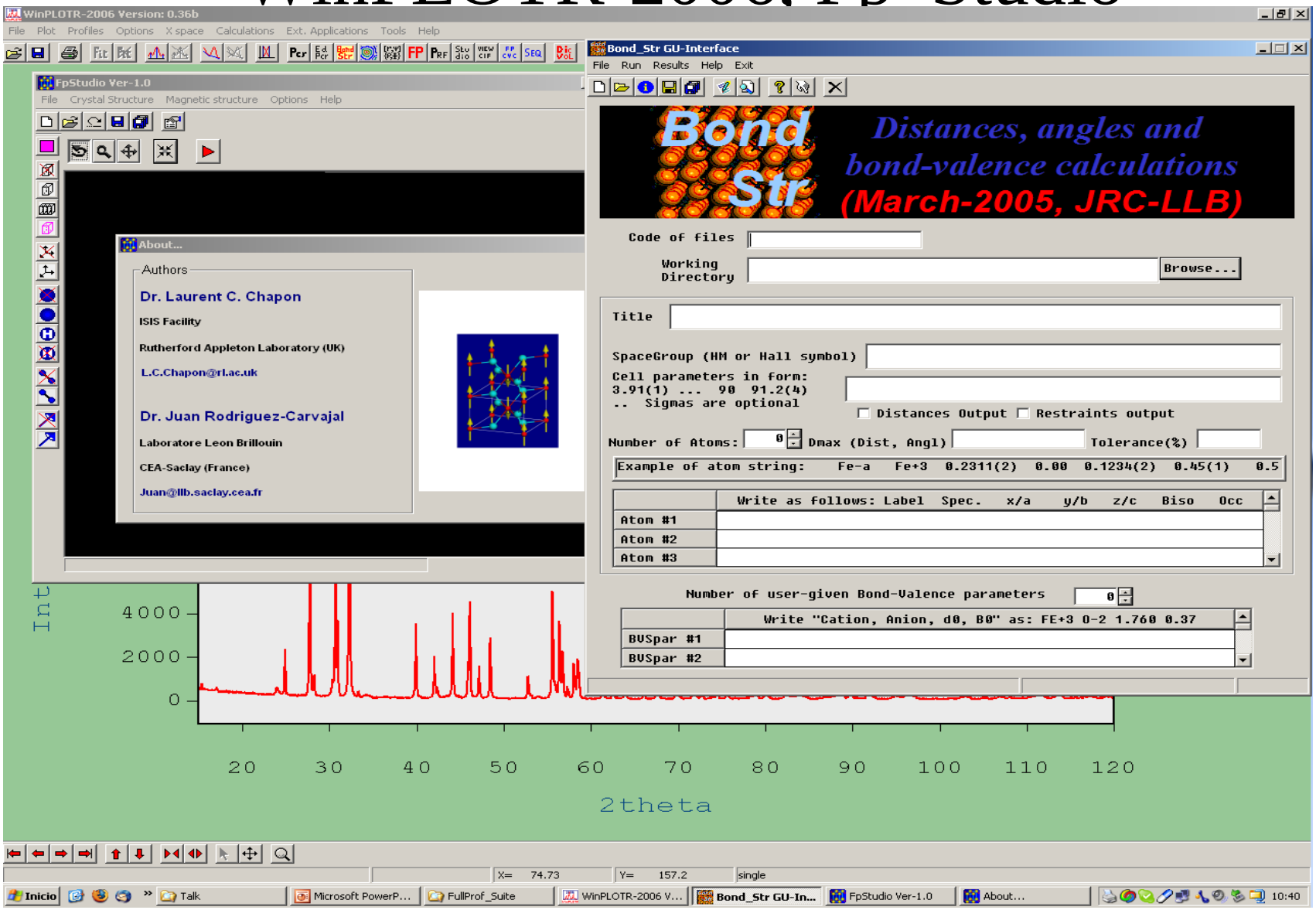
The preferences can be selected using the mouse, and can be saved locally or globally!

FullProf Suite for Windows, Linux and MacOS

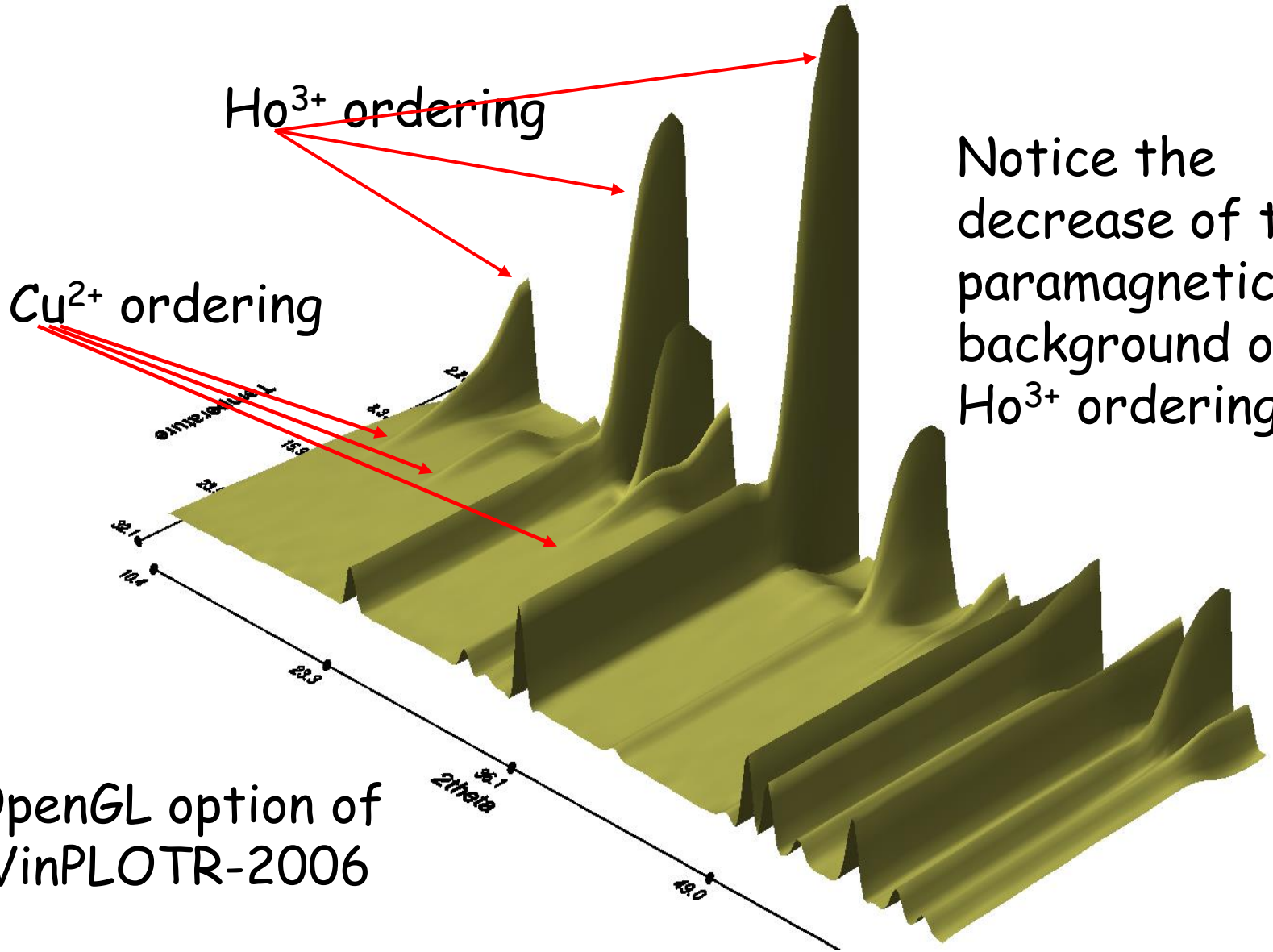



WinPLOTR-2006 Version: 0.36b
File Plot Profiles Options X space Calculations Ext. Applications Tools Help
WDICVOL04 solution (Automatic generated PCR file)
Intensity (arb. units)
10000
8000
6000
4000
2000
0
20
40
60
80
100
120
140
2theta
Automatic plot of observed and calculated patterns after running FullProf
single

FullProf Suite: Bond_Str, WinPLOTR-2006, Fp_Studio



Magnetic ordering of Ho and Cu ions in Ho_2BaCuO_5 (D1B)



How to use the FullProf Suite: Old way

➔ **Open WinPLOTR**

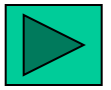
➔ **A button on WinPLOTR gives access to EdPCR**

➔ **Within EdPCR you have access to a series of programs of the FullProf_Suite**

➔ **BasIreps: Irreducible representations of space groups**

➔ **GFourier: Fourier maps**

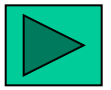
➔ **FullProf_Studio: visualization Xtal & Magnetic Structures**



Execute WinPLOTR

How to use the FullProf Suite: New way

- ➔ **Open the ToolBar and select Working Directory**
- ➔ **Select the working file (normally a PCR file)**
- ➔ **When running a program it tries to use the code of the charged file for obtaining the input file**
- ➔ **Access to WinPLOTR, EdPCR, Bond_Str, DicVOL, DataRed, CheckGroup, XLENS, etc**
- ➔ **BasIreps: Irreducible representations of space groups**
- ➔ **GFourier: Fourier maps**
- ➔ **FullProf_Studio: visualization Xtal & Magnetic Structures**



Execute ToolBar

A program for analysis of diffraction patterns: *FullProf*

- **A program for :**
  - **Simulation of powder diffraction patterns**
  - **Pattern decomposition⇨ integrated intensities**
  - **Structure refinement**
  - **Powder and single crystal data**
- **Crystal and magnetic structures: special form factors, rigid bodies, symmetry adapted modes, incommensurate magnetic structures, restraints, microstructure effects, etc.**
- **Multiple data sets: simultaneous treatment of several powder diffraction patterns (CW X-rays & neutrons, Energy dispersive X-rays, TOF neutron diffraction)**
- **Combined treatment of single crystal and powder data**
- **Crystal and magnetic Structure determination capabilities: simulated annealing on integrated intensity and profile data**

Inside the programs of the FullProf Suite

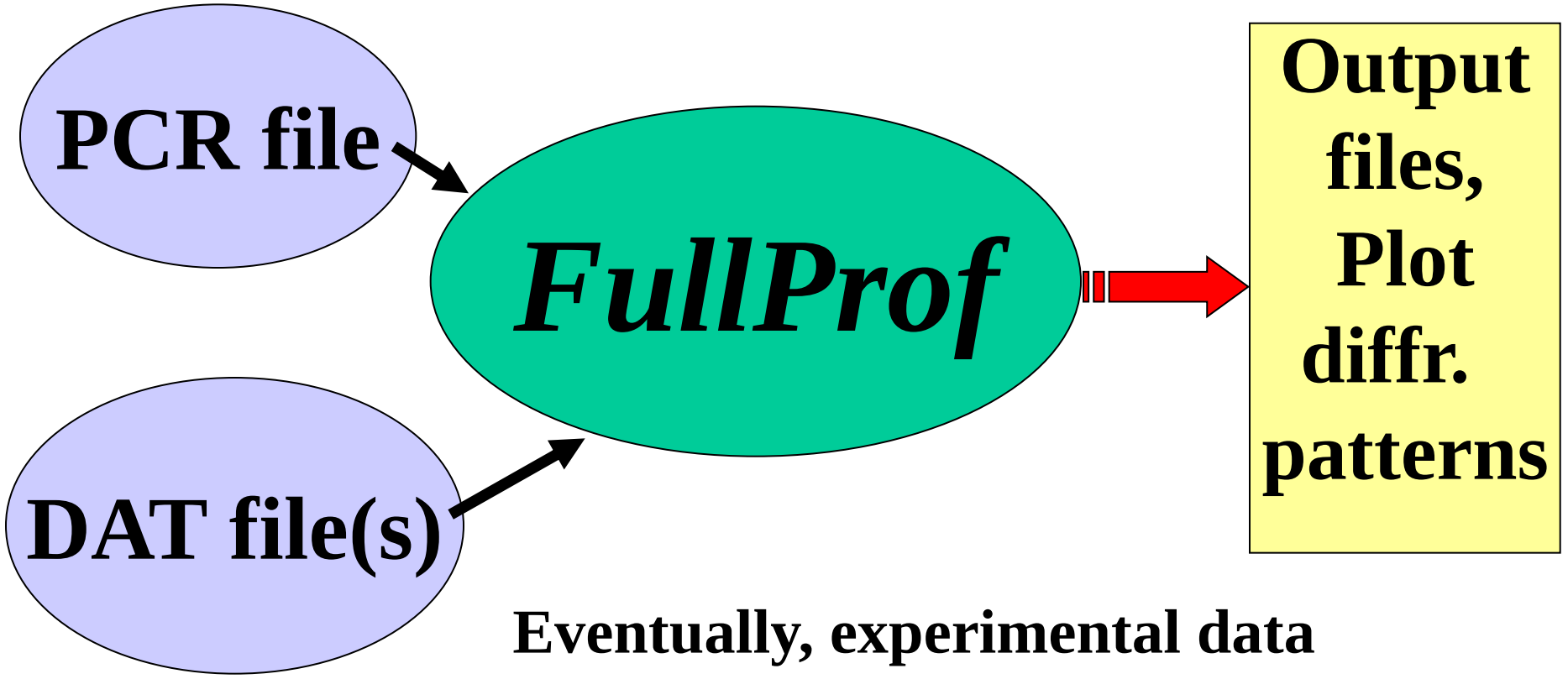
- **The programs are written in Fortran 95**
- **All of them are based in CrysFML: a series of Fortran 95 modules constituting a mathematical and crystallographic library.**
- **GUIs completely separated from the calculation kernels.**

How works *FullProf*

Minimal input:

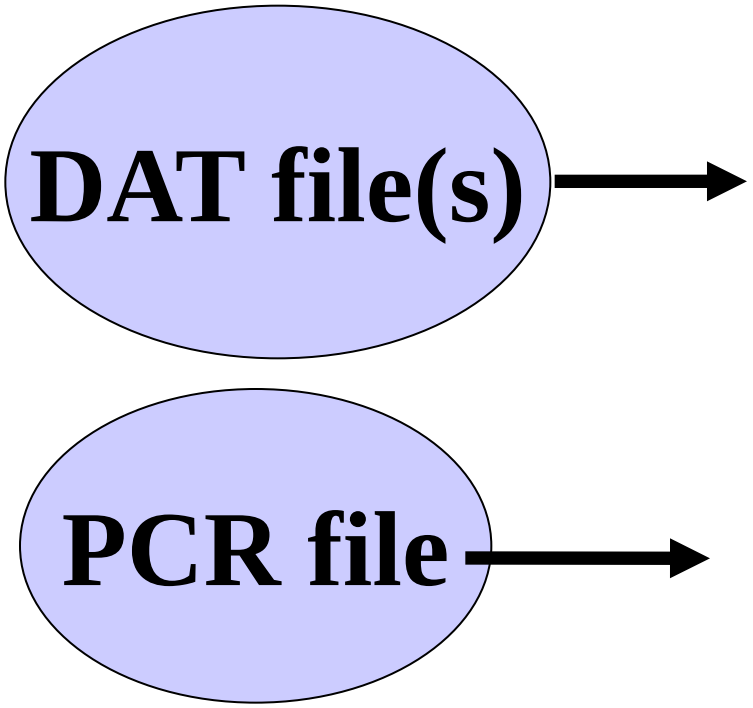
Input control file (extension ‘ *.pcr* ’): PCR-file

Model, crystallographic/magnetic information



Eventually, experimental data

The PCR file: steep learning curve



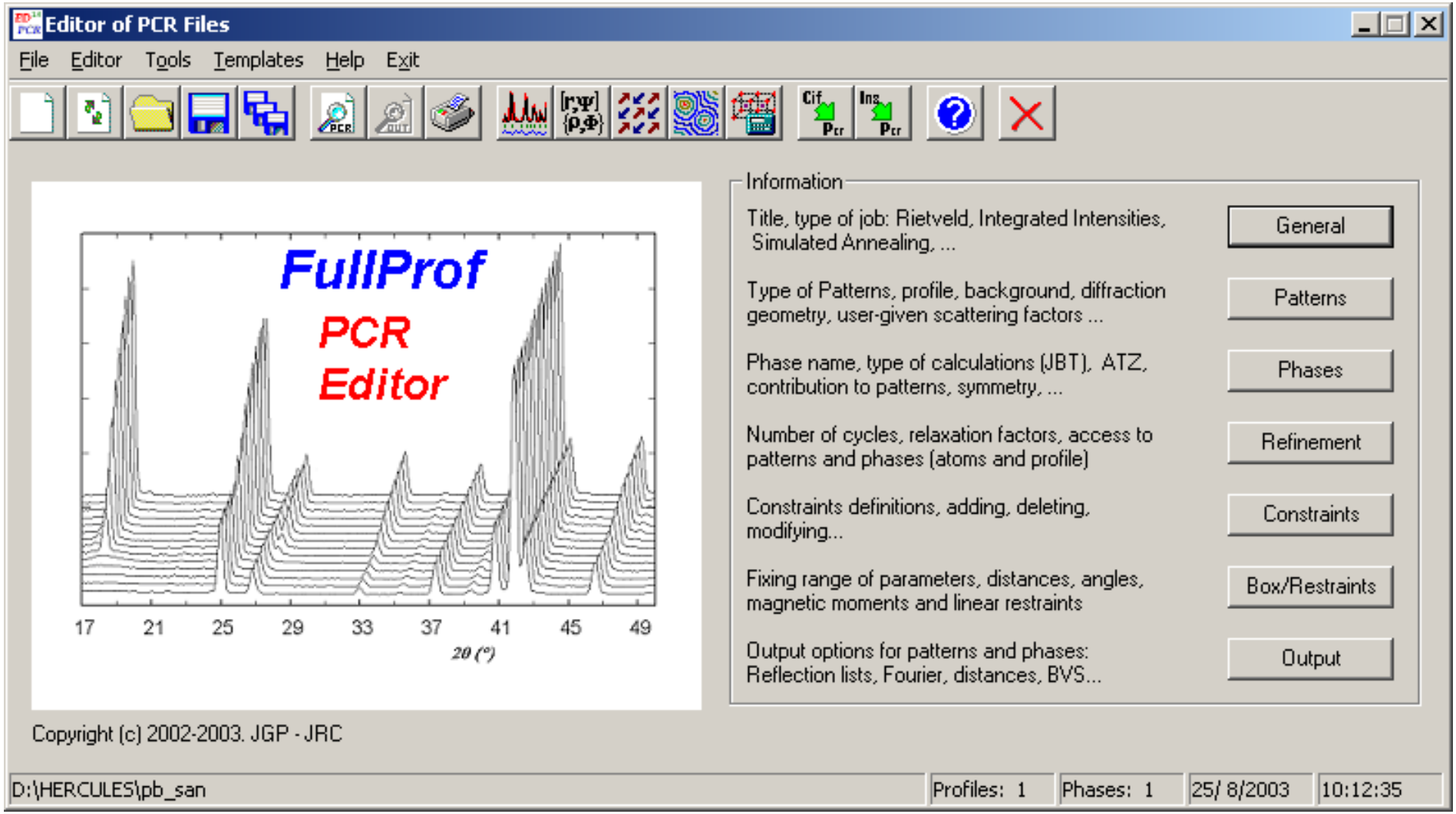
Format depending on the instrument, usually simple

- ➔ **Many variables and options**
- ➔ **Complex to handle**

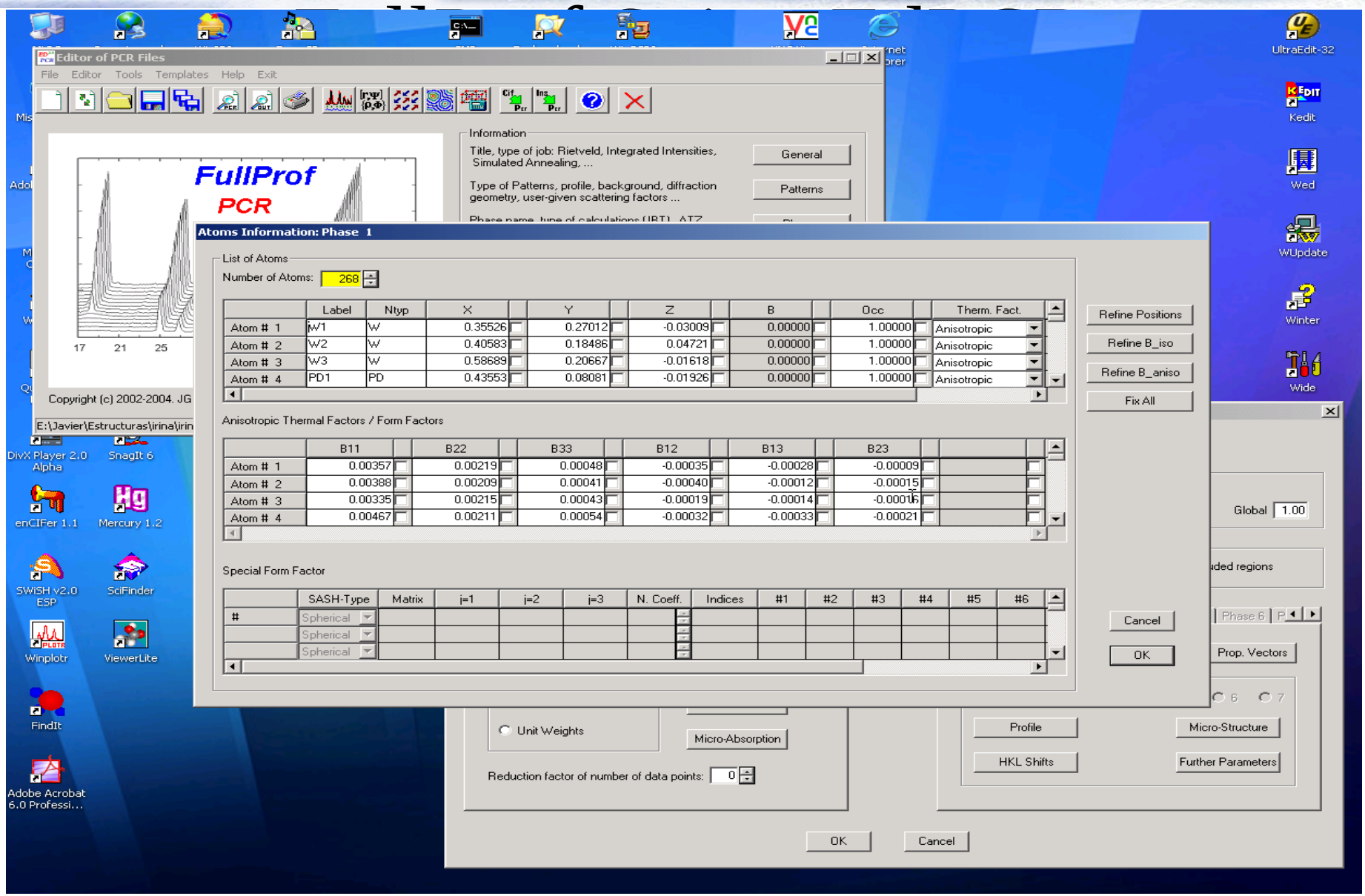
➔ **Hint: copy an existing (working) PCR-file and modify it for the user case, or...**

➔ **USE the new GUI: EdPCR**

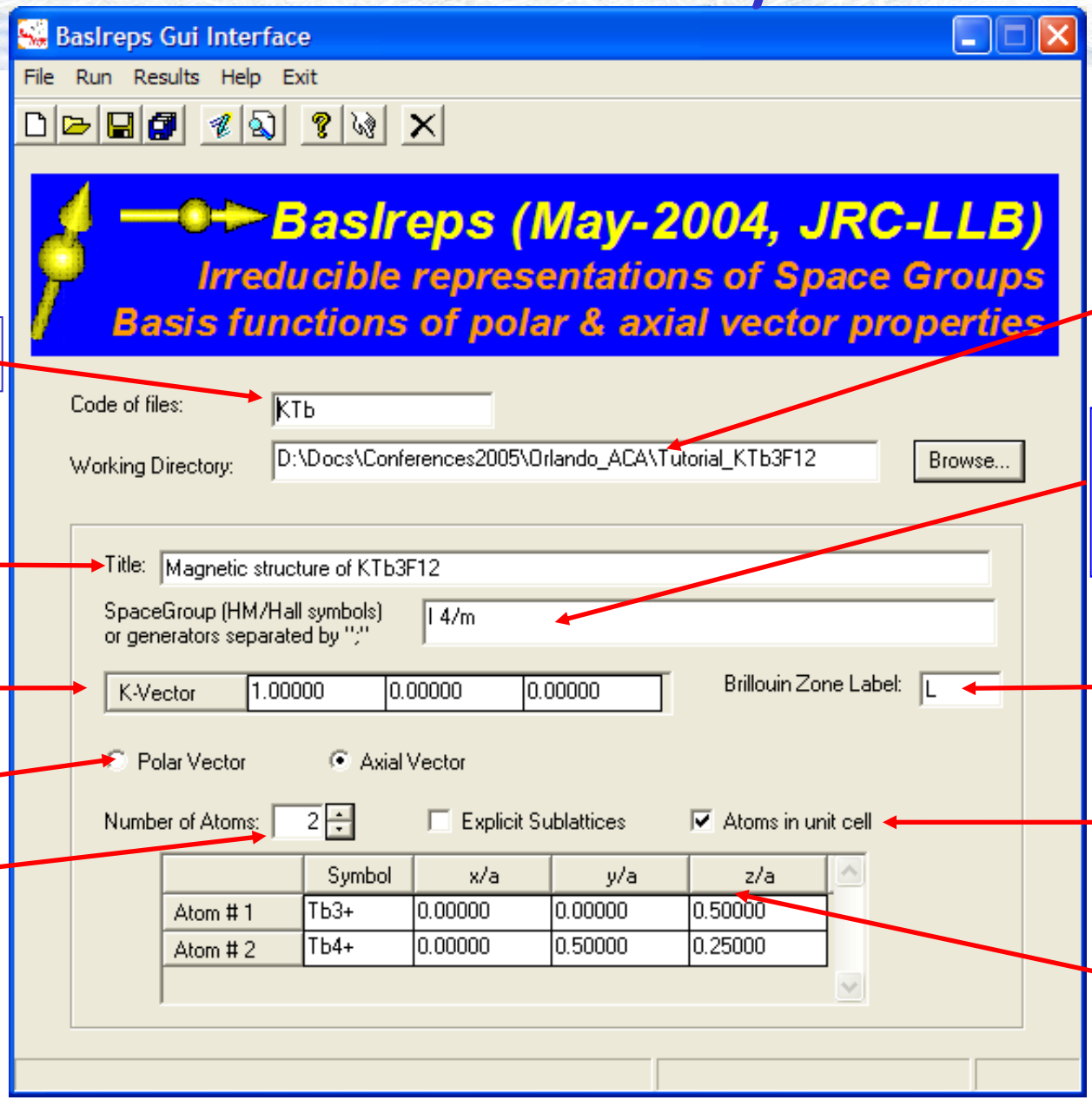
A GUI for *FullProf*: EdPCR



GUI using Winteracter: http://www.winteracter.com


Editor of PCR Files
File Editor Tools Templates Help Exit
FullProf
PCR
Information
Title, type of job: Rietveld, Integrated Intensities, Simulated Annealing, ...
General
Type of Patterns, profile, background, diffraction geometry, user-given scattering factors ...
Patterns
Copyright (c) 2002-2004. JG
E:\Javier\Estructuras\irina\irin
Atoms Information: Phase 1
List of Atoms
Number of Atoms: 268
Label Ntyp X Y Z B Occ Therm. Fact.
Atom # 1 W1 W 0.35526 0.27012 -0.03009 0.00000 1.00000 Anisotropic
Atom # 2 W2 W 0.40583 0.18486 0.04721 0.00000 1.00000 Anisotropic
Atom # 3 W3 W 0.58689 0.20667 -0.01618 0.00000 1.00000 Anisotropic
Atom # 4 PD1 PD 0.43553 0.08081 -0.01926 0.00000 1.00000 Anisotropic
Refine Positions
Refine B_iso
Refine B_aniso
Fix All
Anisotropic Thermal Factors / Form Factors
B11 B22 B33 B12 B13 B23
Atom # 1 0.00357 0.00219 0.00048 -0.00035 -0.00028 -0.00009
Atom # 2 0.00388 0.00209 0.00041 -0.00040 -0.00012 -0.00015
Atom # 3 0.00335 0.00215 0.00043 -0.00019 -0.00014 -0.00016
Atom # 4 0.00467 0.00211 0.00054 -0.00032 -0.00033 -0.00021
Special Form Factor
SASH-Type Matrix j=1 j=2 j=3 N. Coeff. Indices #1 #2 #3 #4 #5 #6
Spherical
Cancel
OK
Global 1.00
Prop. Vectors
Unit Weights
Micro-Absorption
Reduction factor of number of data points: 0
Profile
Micro-Structure
HKL Shifts
Further Parameters
OK
Cancel
UltraEdit-32
Kedit
Wed
WUpdate
Winter
Wide
DivX Player 2.0 Alpha
SnagIt 6
enCIFer 1.1
Mercury 1.2
SWiSH v2.0 ESP
SciFinder
Winplotr
ViewerLite
FindIt
Adobe Acrobat 6.0 Professi...

GUI for *BasIreps*



Code of files

Working directory

Title

Space group symbol or generators

k-vector

Brillouin Zone label

Axial/polar

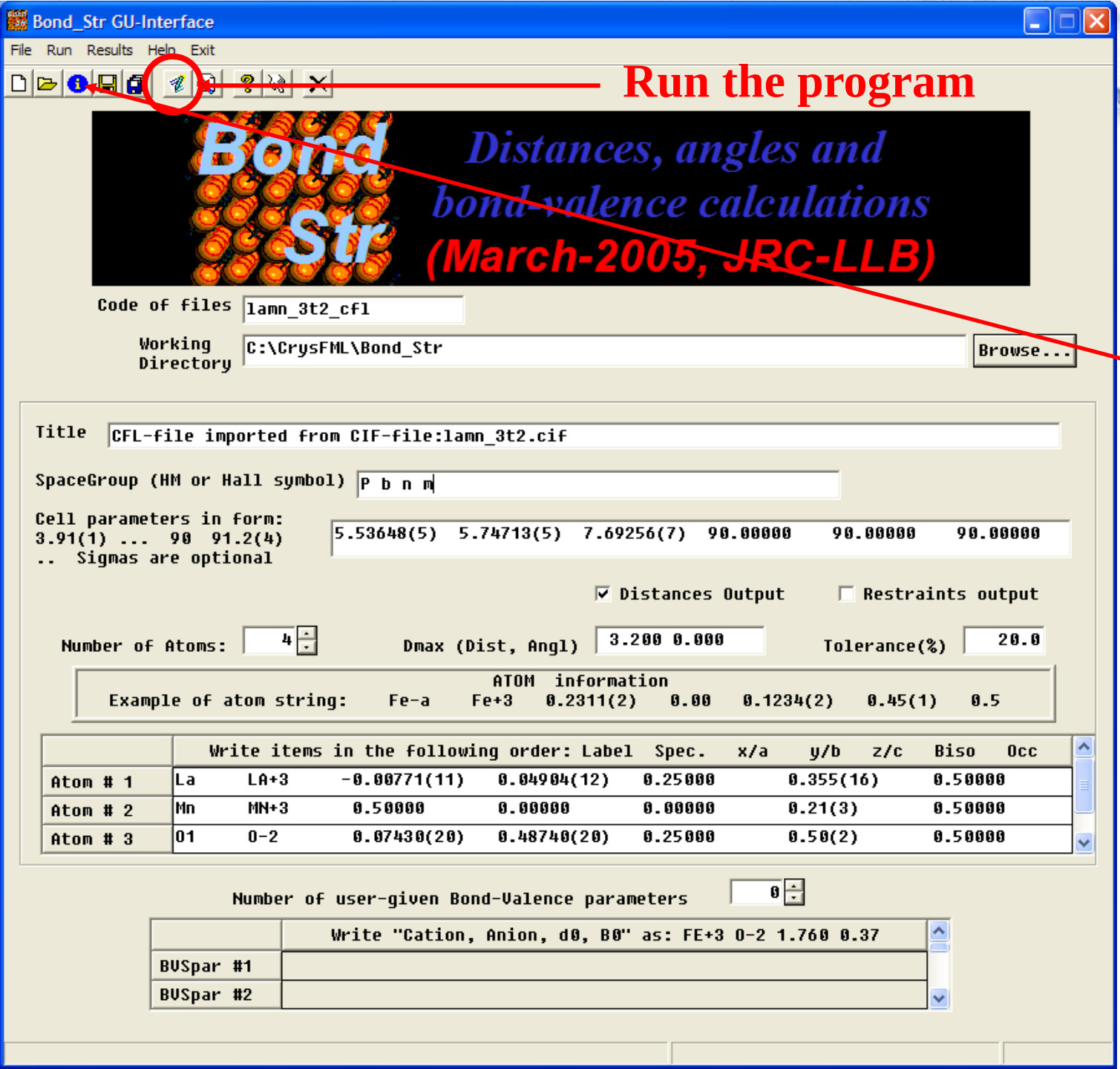
Atoms in Unit Cell

Number of atoms

Atoms positions

Example of *BasIreps* output: *.bsr

```
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
=> Basis functions of Representation IRrep( 1) of dimension  2 contained 3 times in GAMMA
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

SYMM  x,y,z    -x+1/2,-y,z-1/2    y+3/4,-x+1/4,-z+3/4    -y+1/4,x+1/4,-z+3/4
Atoms:      Cu_1                Cu_2                Cu_3                Cu_4
 1:Re (    1    0    0) (    0    0    0) (    0   -1    0) (    0   -1    0)
   Im (    0    0    0) (   -1    0    0) (    0    0    0) (    0    0    0)
 2:Re (    0    1    0) (    0    0    0) (    1    0    0) (    1    0    0)
   Im (    0    0    0) (    0   -1    0) (    0    0    0) (    0    0    0)
 3:Re (    0    0    1) (    0    0    0) (    0    0   -1) (    0    0    1)
   Im (    0    0    0) (    0    0    1) (    0    0    0) (    0    0    0)
 4:Re (   -1    0    0) (    0    0    0) (    0    0    0) (    0    0    0)
   Im (    0    0    0) (   -1    0    0) (    0    1    0) (    0   -1    0)
 5:Re (    0    1    0) (    0    0    0) (    0    0    0) (    0    0    0)
   Im (    0    0    0) (    0    1    0) (    1    0    0) (   -1    0    0)
 6:Re (    0    0    1) (    0    0    0) (    0    0    0) (    0    0    0)
   Im (    0    0    0) (    0    0   -1) (    0    0   -1) (    0    0   -1)


----- LINEAR COMBINATIONS of Basis Functions: coefficients u,v,w,p,q ....
      General expressions of the Fourier coefficients Sk(i) i=1,2,...nat

      SYMM x,y,z                                        Atom: Cu_1      0.0000  0.0000  0.5000
      Sk(1): (u-p,v+q,w+r)

      SYMM -x+1/2,-y,z-1/2                              Atom: Cu_2      0.5000  0.0000  0.0000
      Sk(2): i.(-u-p,-v+q,w-r)

      SYMM y+3/4,-x+1/4,-z+3/4                          Atom: Cu_3      0.7500  0.2500  0.2500
      Sk(3): (v,-u,-w)+i.(q,p,-r)

      SYMM -y+1/4,x+1/4,-z+3/4                          Atom: Cu_4      0.2500  0.2500  0.2500
      Sk(4): (v,-u,w)+i.(-q,-p,-r)
```



GUI for Bond_Str

Can read CIF files

Bond_Str Text Editor - [C:\CrysFML\Bond_Str\lamn_3t2_cfl.bvs]

File Edit Search

```
(O1  )-(Mn  ) :  1.9680(   2)   0.570(  0)

Coordination number:     4      Eff.Coor. number:  4.00  for atom: O1
Average distance  :  2.2304(   5)  Distortion:   142.929 xE-04
Predicted distance:  2.0165        Single bond-valence S= 0.500
                                     Valence:   -2.000
                                        Sums:    1.994(  2)
Deviation from the Valence Sum Rule (r1,%dev):  -0.006   0.277
{r1=Sumj(sij)-Vi, %dev=100abs(r1)/Vi}
Deviation from the Equal Valence Rule    (r2):   0.090
{r2=<sij-<sij>>rms}


   ---------------------------------------------------------------
=> Bond-valence and coordination of atom: O2   occupancy: 1.000(  0)
   ---------------------------------------------------------------

(O2  )-(La  ) :  2.6496(  11)   0.275(  1)
(O2  )-(La  ) :  2.6975(  10)   0.242(  1)
(O2  )-(La  ) :  2.4599(  11)   0.459(  1)
(O2  )-(Mn  ) :  2.1787(  10)   0.323(  1)
(O2  )-(Mn  ) :  1.9063(  10)   0.673(  2)

Coordination number:     5      Eff.Coor. number:  5.00  for atom: O2
Average distance  :  2.3784(   5)  Distortion:   157.256 xE-04
Predicted distance:  2.0990        Single bond-valence S= 0.400
                                     Valence:   -2.000
                                        Sums:    1.972(  3)
Deviation from the Valence Sum Rule (r1,%dev):  -0.028   1.408
{r1=Sumj(sij)-Vi, %dev=100abs(r1)/Vi}
Deviation from the Equal Valence Rule    (r2):   0.158
{r2=<sij-<sij>>rms}

=> Lines concerning predicted average distances and single
   bond-valence values, as well as the deviations from the
   Equal Valence Rule,  apply only to those central atoms
   having N coordination-atoms of the same chemical species.
   (The term 'single bond-valence' refers to the valence value
   of a single bond for a regular polyhedron, so S=Valence/N)


=> The Old Global Instability Index (GII) is calculated with the atoms of the asymetric unit (Num_Atoms).
   The normalized GII(a,b,c) below are calculated using the sum over asymmetric unit but multiplying
   differences by the multiplicity of the site. N_Atoms_UCell is the total number of atoms in the
   conventional unit cell. In all cases the result of the different expressions is multiplied by 100.0

=>  Old Global Instability Index (  GII=SQRT{SUM{|BVS-abs(q)|^2}/Num_Atoms} ) =  11.80 /100
=>  Normalized   GII(a)=       SUM {|BVS-abs(q)|  *mult}       /N_Atoms_UCell =   7.74 /100
=>  Normalized   GII(b)=       SUM {|BVS-abs(q)|  *mult/abs(q)}/N_Atoms_UCell =   2.79 %
=>  Normalized   GII(c)= SQRT{ SUM {|BVS-abs(q)|^2*mult}       /N_Atoms_UCell}=  10.63 /100
```

Line:1 Col:1 INS

Last minute changes in *FullProf*

Documented in "fp2k.inf"

```
 ------------------------------------------------------------------------
  In this file new features, as well as discovered bugs, of FullProf.2k
  are periodically documented. For details consult the manual of FullProf.
  From 10 May 2003, comments on the programs constituting the FullProf suite
  are also provided.
       Juan Rodriguez-Carvajal (Institut Laue-Langevin, Grenoble, France)
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>>  29  August   2008:  New version of FullProf. Symmetry modes with AMPLIMODES.
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   - A new version of FullProf has been produced incorporating the possibility
     for refinement (powder, single crystals, simulated annealing) of amplitudes
     of symmetry modes. The present version is:

        ***********************************************************'
        ** PROGRAM FullProf.2k (Version 4.40 - Aug2008-ILL JRC) **'
        ***********************************************************'

   - In the present version of FullProf the refinement of a crystal structure can be done
     in terms of symmetry adapted modes. FullProf uses the output of the program AMPLIMODES
     from the Bilbao Crystallographic Server (http://www.cryst.ehu.es/cryst/amplimodes.html)
     The free parameters, instead of atom positions, are the amplitudes of symmetry modes.
     The provided atom positions should not be refined. They are given as a reference of the
     high symmetry (HS) phase described in the low symmetry (LS) frame.

     This option is accessible by putting the variable JBT=6.
     The input is exactly the same as for JBT=0, except that no refinement codes are allowed for
     atom positions. This is taken into account by the program when Aut=1 (automatic mode).
```

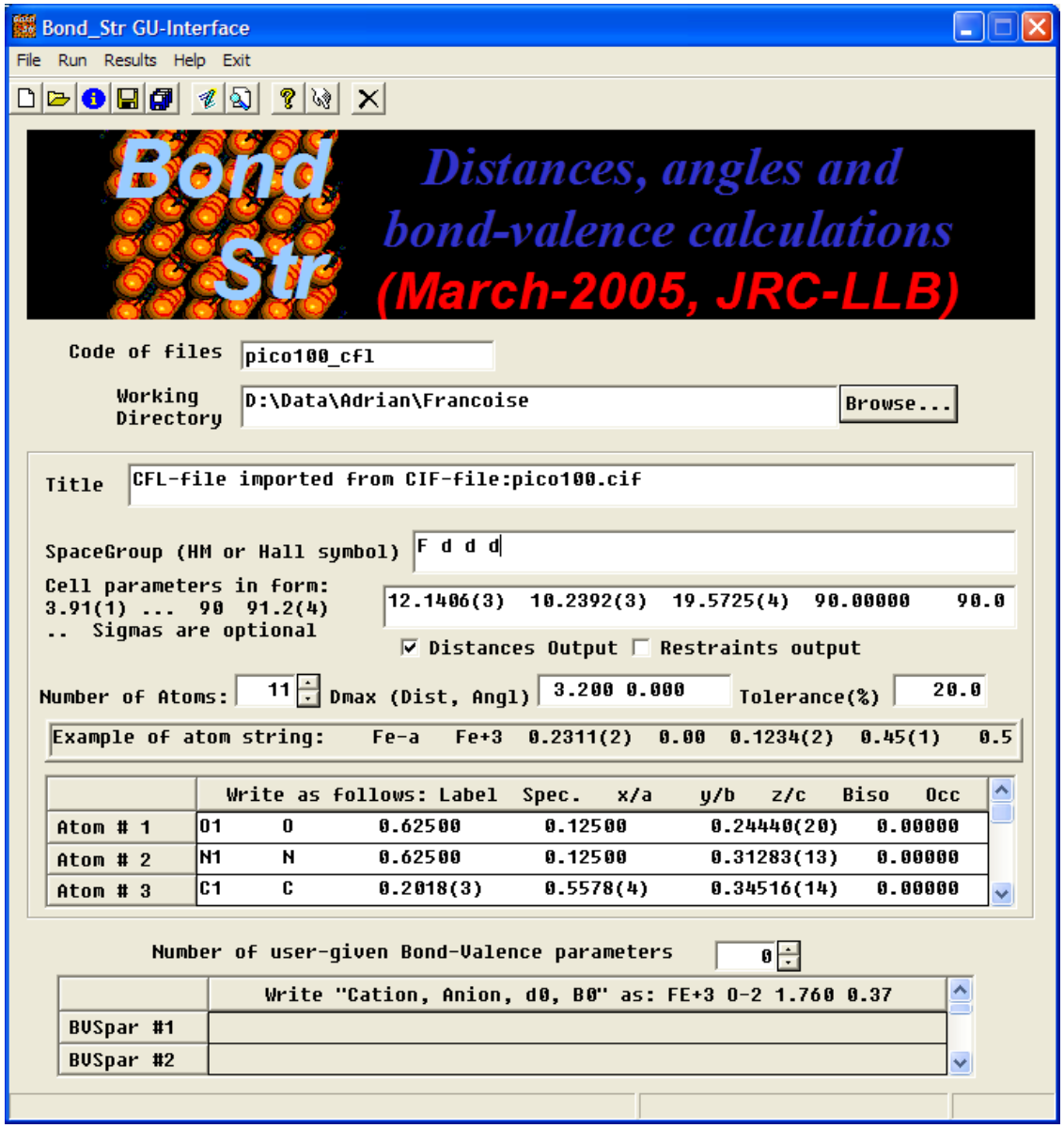
Some useful features in *FullProf*

- ➔ **Facilities concerning symmetry, symmetry modes**
- ➔ **Automatic mode for handling refinement codes and symmetry constraints**
- ➔ **Rigid body refinements + distances and angles restraints**
- ➔ **Special form factors, sym. adapted spherical harmonics**
- ➔ **Simulated Annealing on integrated intensities or profile**
- ➔ **The treatment of micro-structural effects**
- ➔ **Different formats of the file containing the Instrumental Resolution Function (FPA)**

Constraints: reduce the number of free parameters (rigid body refinements)

Restraints: same number of free parameters + additional observations

How to generate restraints for *FullProf*?



1: Calculating distances from FullProf

2: Using Bond_Str importing a CIF file

Both programs generate a file called CFML_Restraints.tpcr

How to generate restraints for *FullProf*?

```
List of possible restraints:

 At1    At2   ITnum      T1          T2          T3          DIST    SIGMA
  O1     N1       1   0.00000     0.00000     0.00000       1.3393  0.0047
  O1     C1       1   0.50000    -0.50000     0.00000       2.2874  0.0045
  O1     C1      -2   0.25000    -0.25000     0.50000       3.3163  0.0041
  O1     C2      -4   1.00000    -0.25000    -0.25000       3.1481  0.0046
  O1     H1       1   0.50000    -0.50000     0.00000       2.5023  0.0051
. . . .
```

Lines to be pasted into the PCR file

```
DFIX    1.33935   0.00467   O1   N1
DFIX    2.28738   0.00455   O1   C1_9.545
DFIX    3.31627   0.00413   O1   C1_24.545
DFIX    3.14808   0.00457   O1   C2_6.644
DFIX    2.50228   0.00510   O1   H1_9.545
```

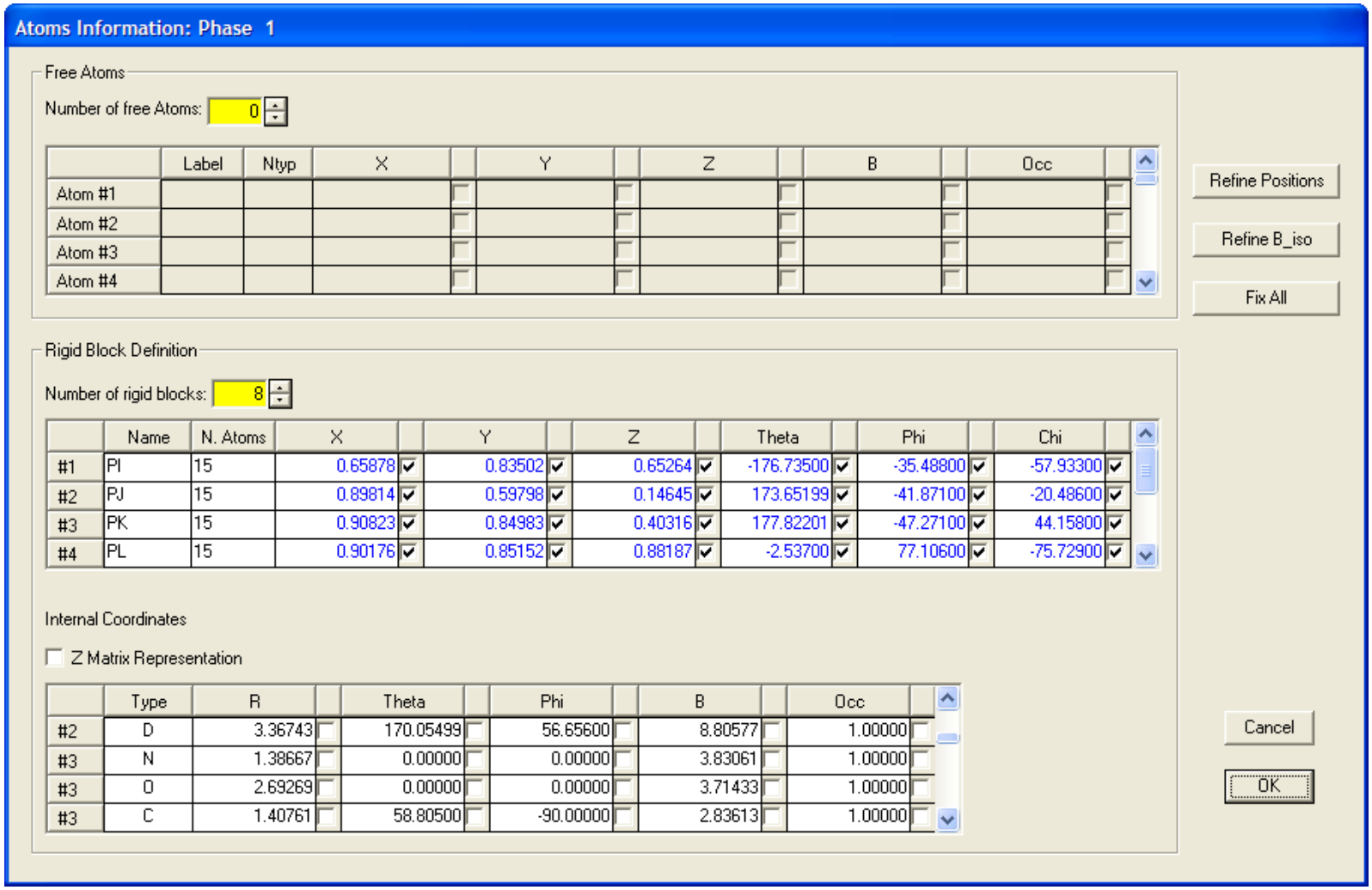
In CFL format

Rigid body constraints

A utility called ***mol_tpcr.exe*** can be used to generate a piece of PCR file containing information about a rigid body.

It is possible to generate a CFL file from a CIF, using Bond_Str, and then, doing a minimal editing work, create an appropriate file for ***mol_tpcr***

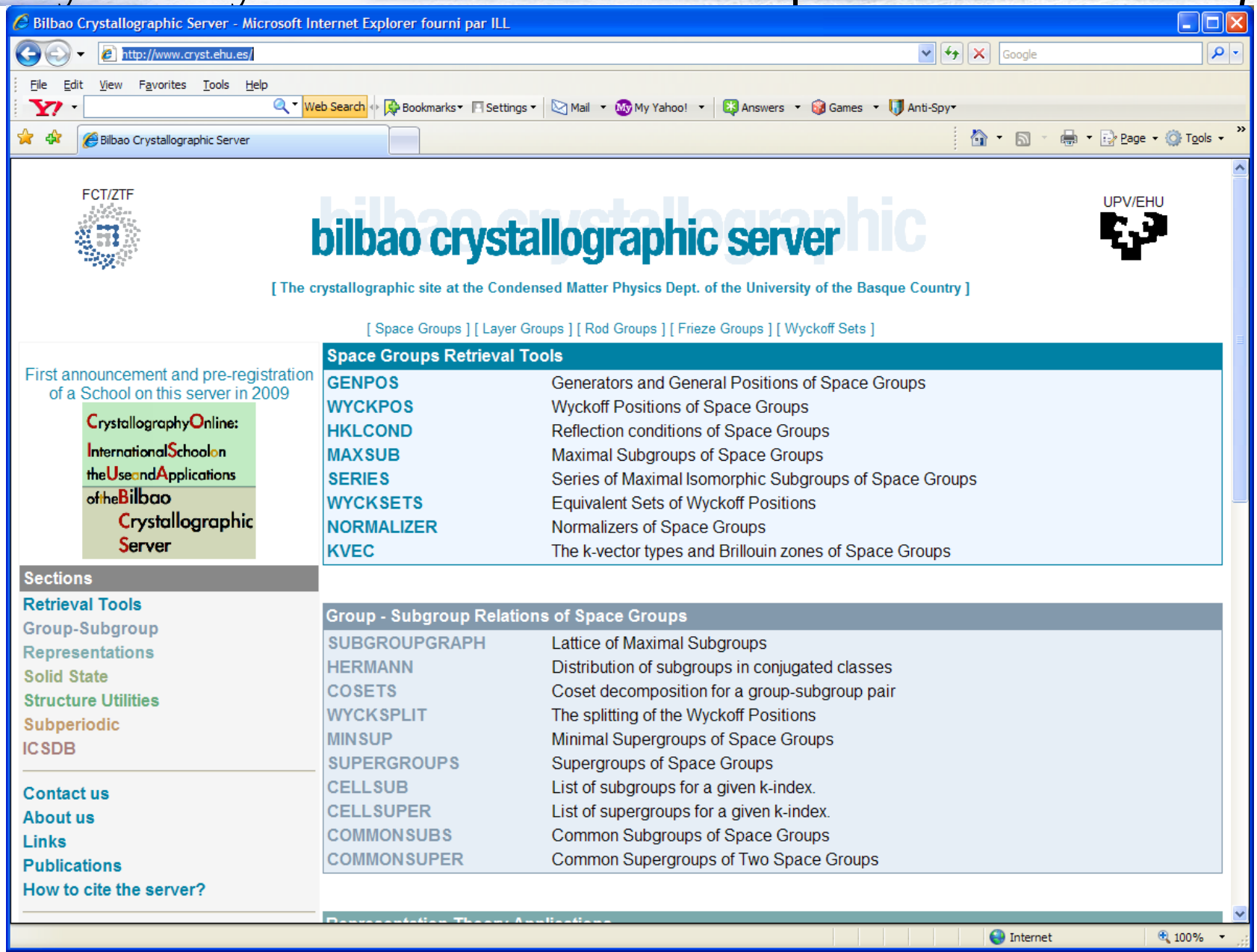
EdPCR allows an easy edition of Rigid Bodies (problem with free atoms!)



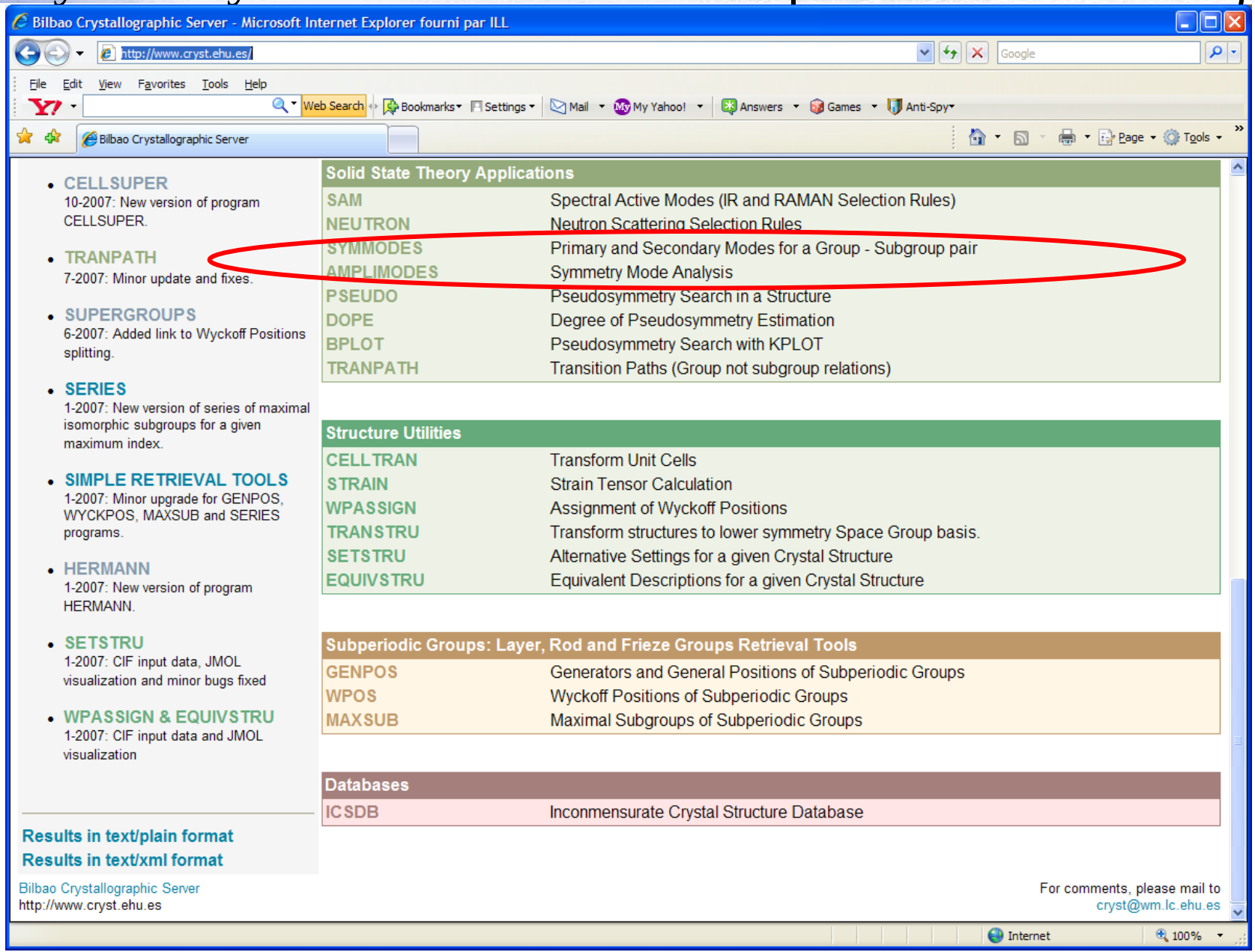
PCR file generated by EdPCR

```
!-------------------------------------------------------------------------------
!  Data for PHASE number:   1  ==> Current R_Bragg for Pattern#  1:     4.95
!-------------------------------------------------------------------------------
C5H4NO(CH3) ,ESRF 10K
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth        ATZ     Nvk Npr More
 120   0   0 0.0 0.0 1.0   4   0   0   1   0        929.020    0   7   0
!
P 41                      <--Space group symbol
!Atom Typ       x         y         z         B       Occ       P6      THETA      PHI   Spc
!  r/xc/rho the/yc/phi phi/zc/z    X0        Y0        Z0       CHI     P16:SAT    DEG  KIND
PI1  N       0.65457   0.83848   0.58247   3.83061   1.00000   1.00000 -176.735  -35.488   0  #CONN C C 0 1.8
               0.00      0.00      0.00      0.00      0.00      0.00   111.00    121.00
    1.38667    0.000     0.000   0.65878   0.83502   0.65264  -57.933     0.000      1      0
       0.00      0.00      0.00    351.00    361.00    371.00    131.00
PI2  O       0.65070   0.84127   0.51616   3.71433   1.00000           0   0   0          0  #CONN C N 0 1.8
               0.00      0.00      0.00      0.00      0.00
    2.69269    0.000     0.000
       0.00      0.00      0.00
PI3  C       0.68712   0.76540   0.61290   2.83613   1.00000           0   0   0          0  #CONN O N 0 1.8
               0.00      0.00      0.00      0.00      0.00
    1.40761   58.805   -90.000
       0.00      0.00      0.00
PI4  C       0.62593   0.90874   0.61882   2.83613   1.00000           0   0   0          0  #CONN D C 0 1.2
               0.00      0.00      0.00      0.00      0.00
    1.40761   58.805    90.000
       0.00      0.00      0.00
. . . . .
```

Refinement of crystal structures using amplitudes of symmetry modes instead of atom positions in *FullProf*



Refinement of crystal structures using amplitudes of symmetry modes instead of atom positions in *FullProf*



Tutorials on the FullProf Suite

Tutorial 1

How to extract structure factors from X-ray powder diffraction and solve the structure using direct space methods. A *trivial* example: Y_2O_3

Data: powder diffraction pattern or Y_2O_3

Tutorial 2

Tutorial on Magnetic Structure Determination and Refinement using Neutron Powder Diffraction and FULLPROF

Data: LaMnO3 at 150K and 50K

PCR file with the crystal structure at 150K

Tutorials on the FullProf Suite

Tutorial 3

How to work with symmetry modes using FullProf and AMPLIMODES.

Two simple examples: $CaTiO_3$ and $LaMnO_3$

Data: powder diffraction patterns of $CaTiO_3$ and $LaMnO_3$.

Tutorial 4

How to use restraints and the rigid body description of molecular fragments in the program FullProf.

Data: Sr-oxalate, naphtalene, urea

PCR files