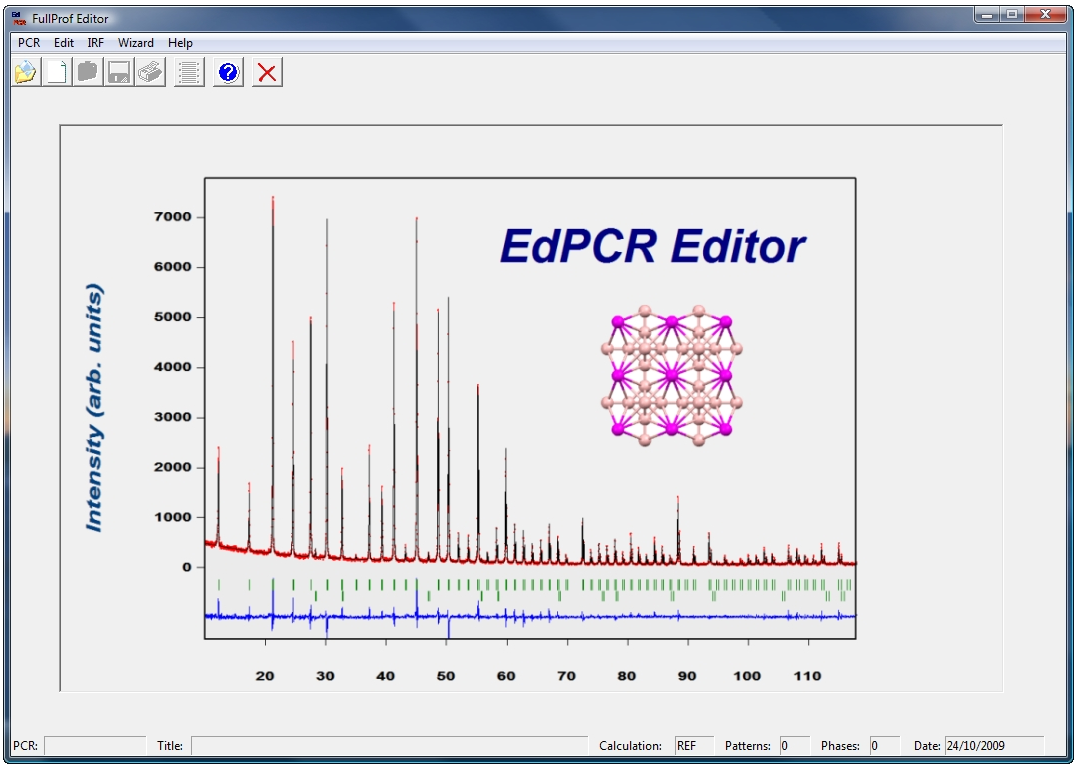
EdPCR

EdPCR

A GUI Editor program for PCR files for FullProf program



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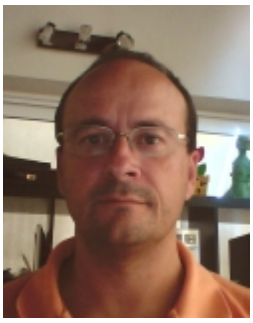

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Introduction

EdPCR is a graphical editor for *PCR files* which are the input file for ***FullProf*** program.

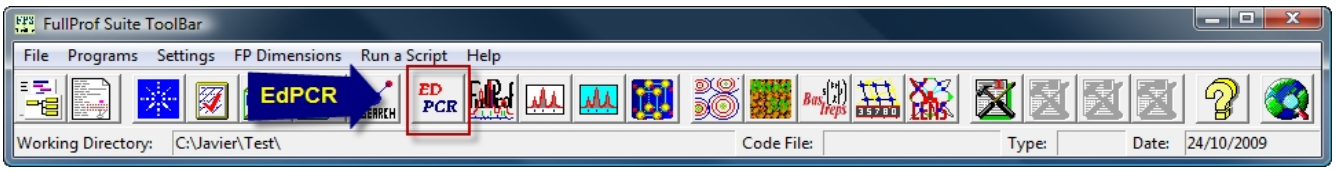
As you probably knows, ***FullProf*** has been mainly developed for *Rietveld analysis* (structure profile refinement) of neutron (nuclear and magnetic scattering) or X-ray powder diffraction data collected at constant or variable step in scattering angle 2θ. The program can be also used as a *profile matching* (or pattern decomposition) tool, without the knowledge of the structure. Single Crystal refinements can also be performed alone or in combination with powder data. Time-of-flight (*TOF*) neutron data analysis is also available. Energy dispersive X-ray data cal also be treated but only in profile matching mode.

The program ***EdPCR*** is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY of being free of internal errors. In no event will the authors be liable to you for damages, including any general, special, incidental or consequential damages arising out of the use or inability to use the program (including but not limited to loss of data or data being rendered inaccurate or losses sustained by you or third parties or a failure of the program to operate with any other programs). The authors are not responsible for erroneous results obtained with ***EdPCR*** program.

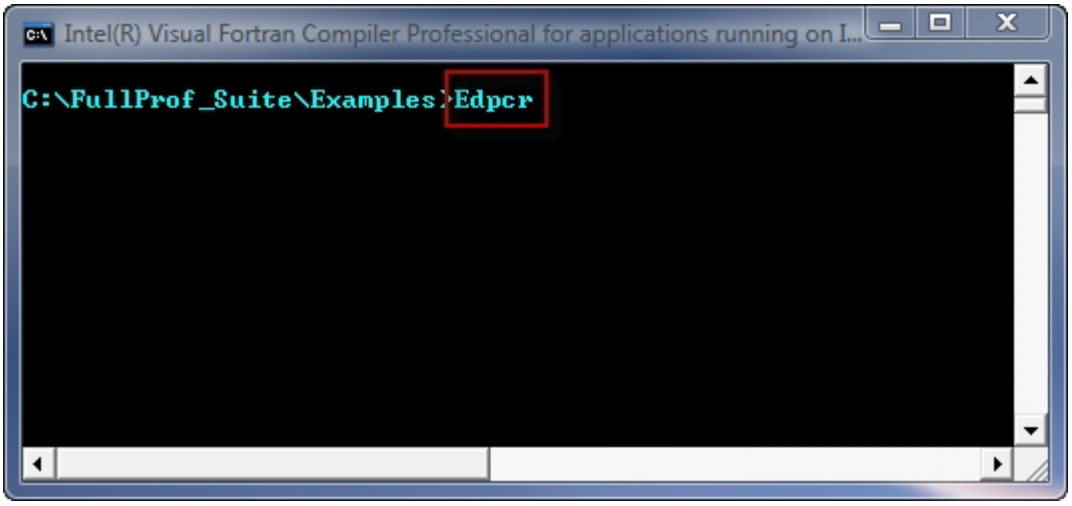
Running the program

For run the ***EdPCR*** program can be done as:

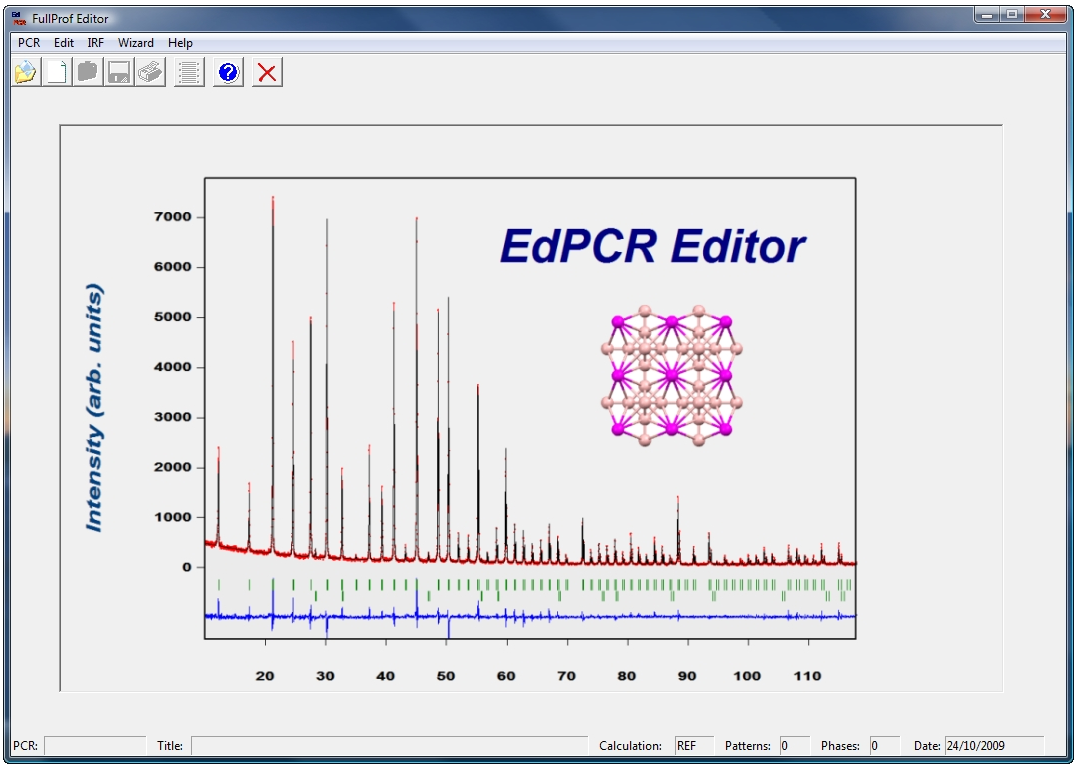
- From Toobar of ***FullProf Suite***



- Terminal window



In a few seconds, you will see the main window of ***EdPCR*** program in your screen.



In the main toolbar of the program you can select the next procedures:

Open an existent ***PCR*** file

Create a new ***PCR*** file

Close the actual ***PCR*** file

Save the actual ***PCR*** file

Print the actual ***PCR*** file loaded in ***EdPCR*** program

View the actual ***PCR*** file using an ASCII editor

Help / Manual of ***EdPCR*** program

Exit of ***EdPCR*** program

Information Dialogs

When a ***PCR*** file is loaded or created using ***EdPCR*** program a new toolbar will be showed on the left side of the main window.

The input parameters for ***FullProf*** program are classified according to the next distribution:

 General Information

 Pattern Information

 Phase Information

 Refinement Information

 Simulated Annealing Information

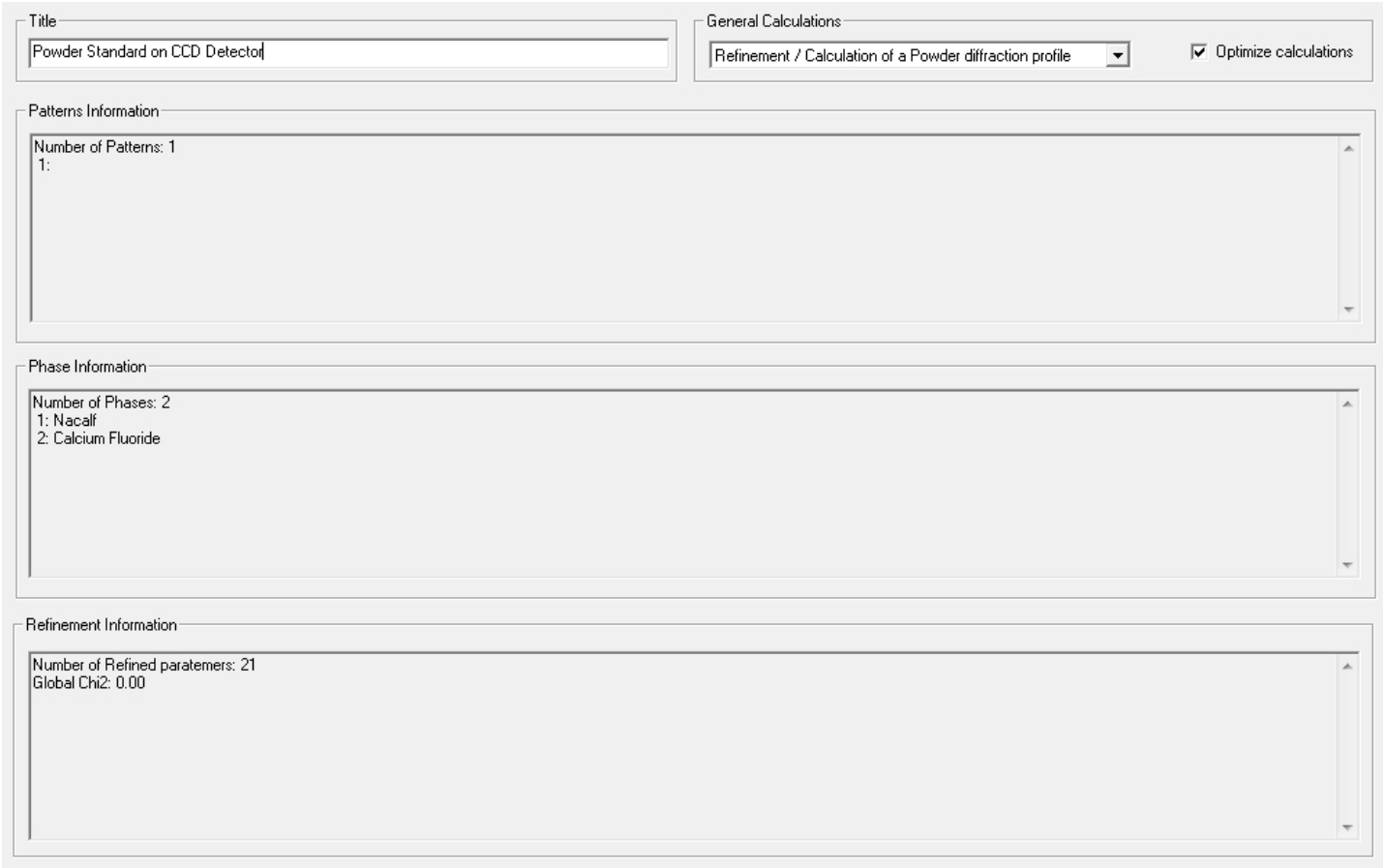
 Constraints Information

 Restraints Information

 Output Information

General Information

User can select this dialog pressing on  button on left Toolbar of ***EdPCR*** program



Options on this dialog are:

Title **[Titl]**
80 characters used to label the printout.

General calculations **[Cry]**
The options are:

- Refinement/Calculation of a Powder diffraction profile
- Refinement on single crystal data / Integrated intensity
- Simulated Annealing optimization (Integrated intensities)
- Simulated Annealing optimization (Powder profile)

Optimize calculations **[Opt]**
The program tries to optimise the calculations looking for the particular options used in the job. In some cases the calculation proceeds up to a 30% faster.

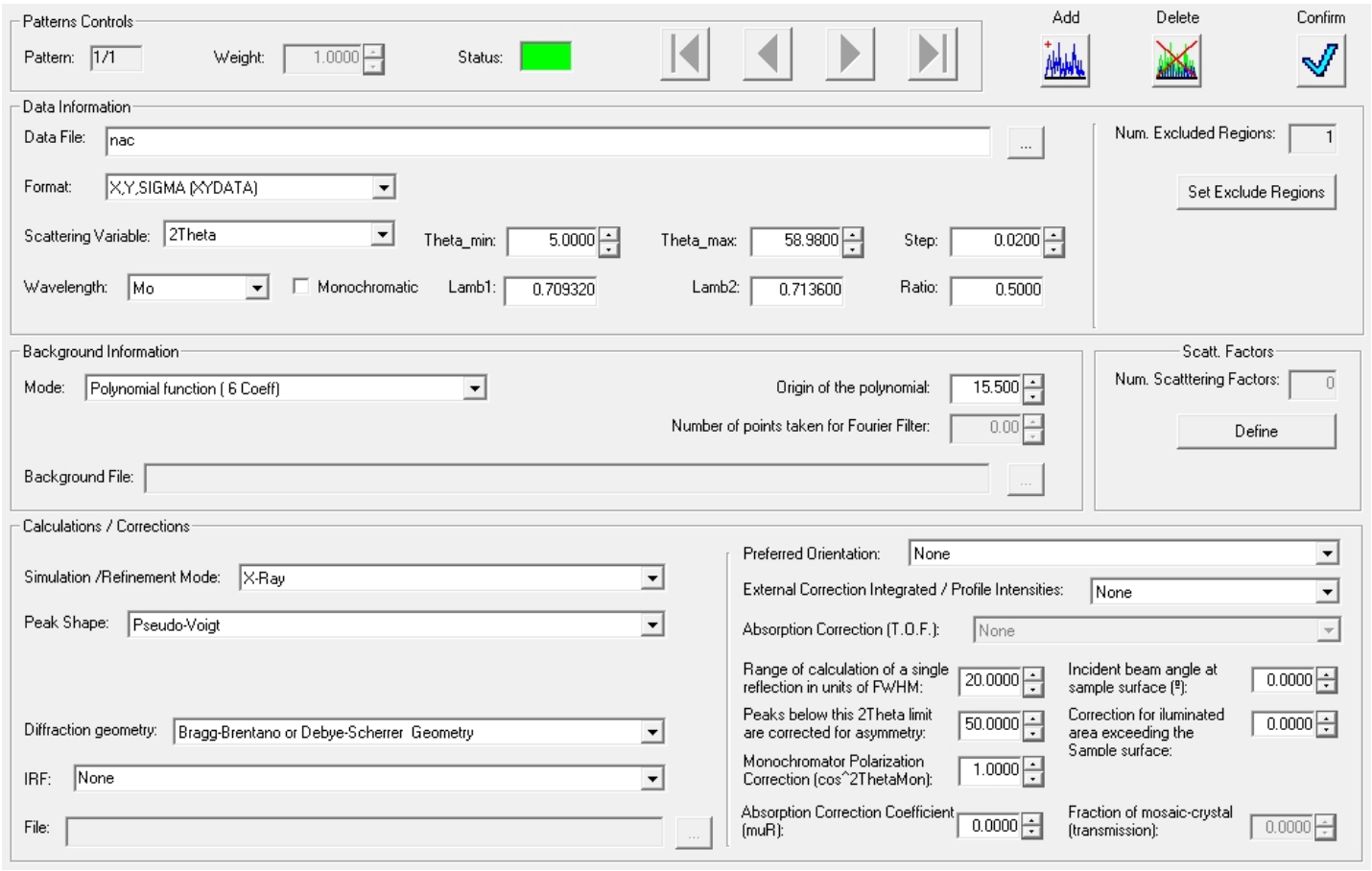
The rest of Dialog contains information included on ***PCR*** file about *Patterns*, *Phases* and *Refinement* information

Equivalence on PCR file

```
COMM Title
! Files => DAT-file: ,  PCR-file: nac
!Job Npr Nph Nba Nex Nsc Nor Dum Iwg Ilo Ias Res Ste Nre Cry Uni Cor Opt Aut
   0   7   2   0   0   0   0   0   0   0   0   0   0   0   0   0   1   1
```

Pattern Information

User can select this dialog pressing on  button on left Toolbar of ***EdPCR*** program.

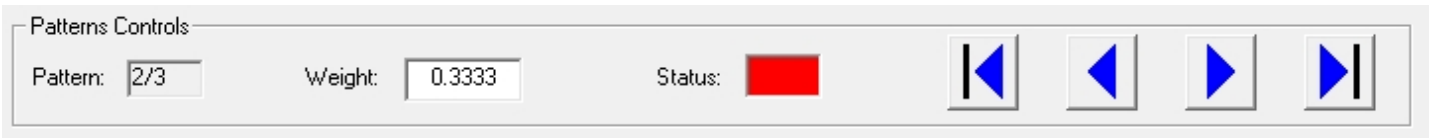


All Patterns information is controlled by this dialog ***except*** refinement parameters.

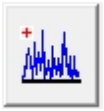
Pattern Parts:

- Patterns controls
- Data Information
- Background Information
- Scattering Factors
- Calculations/Corrections

Patterns Control



Buttons



Add a new pattern

Delete the current pattern

Confirm all information about the current dialog.

Controls

Go to first pattern

Go previous pattern

Go to next pattern

Go to last pattern

Status

Unsaved information

Saved information

Options on this dialog are:

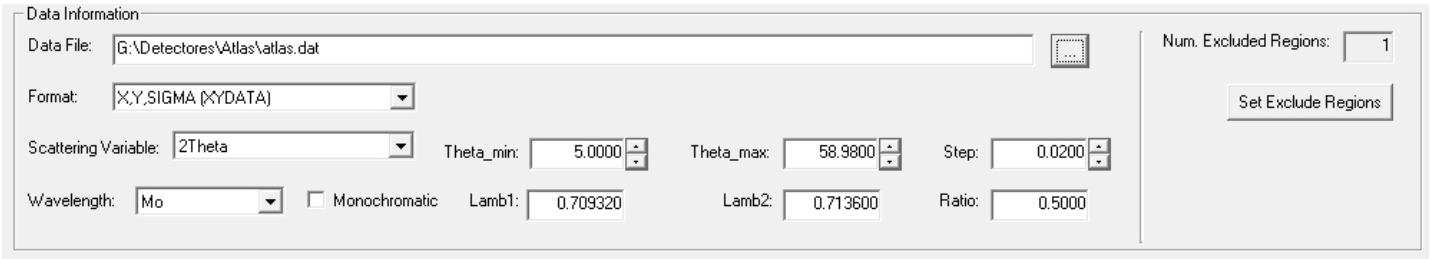
Weight
Useful for *multipattern* option. Is the weight for actual pattern.

Equivalence on PCR file

```
COMM MultiPattern Test
NPATT      2        0 0 <- Flags for patterns (1:refined, 0: excluded)
W_PAT    1.000 0.000
```

Data Information

Data file information is concentrate in this zone



Data file
Name of the pattern file. If necessary the user can select it using the button 

Format **[Ins]**
Select the format of the pattern file.
For some formats, ***EdPCR*** program is able to read the information directly and fill them on the rest of fields. If not, the user
will have to introduce them writing himself.

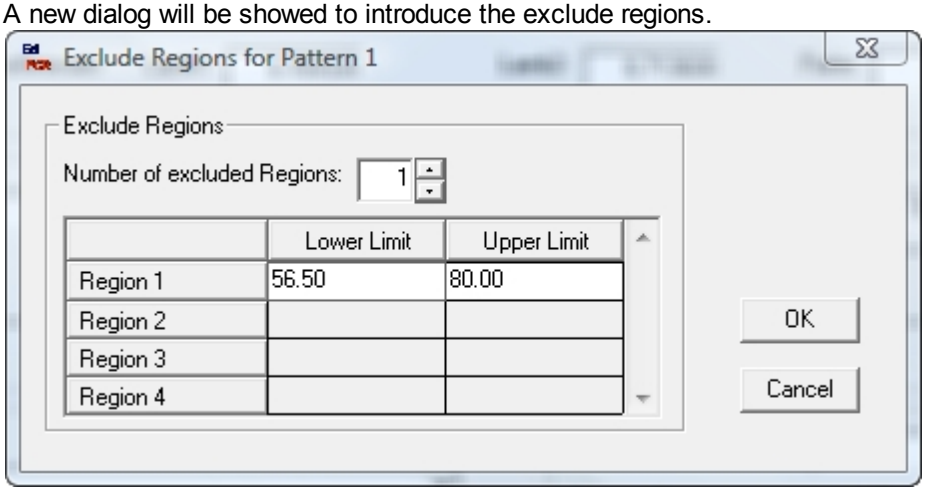
Scattering variable **[Uni, Thmin, Step, Thmax]**
The options are: 2Theta, μsecs for TOF and Energy (KeV). Minimum, maximum and step values are also necessary.

Wavelength **[lambda1, lambda2, ratio]**
Define the current wavelengths for actual pattern.
The user can select some of them in a list or directly by hand is ***user defined*** is selected. ***Ratio*** is the relation (I_2/I_1).

Excluded regions

If the user need define different exclude regions, then click on [Set Exclude Regions] button.

A new dialog will be showed to introduce the exclude regions.

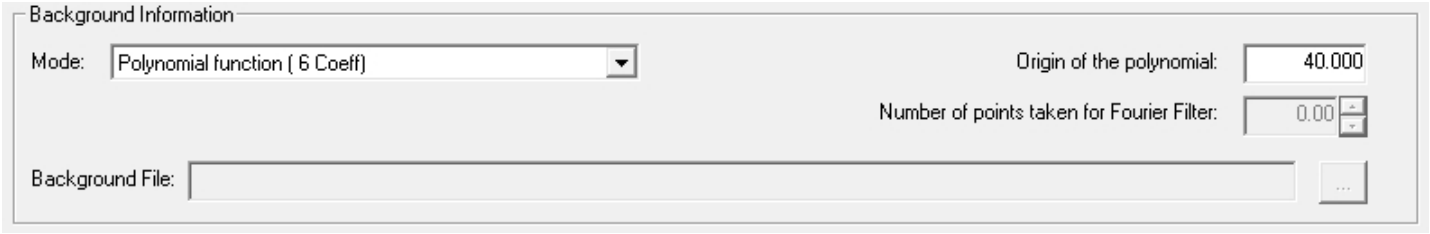


Equivalence on PCR file

```
! Files => DAT-file: NAC,  PCR-file: nac
!Job Npr Nph Nba Nex Nsc Nor Dum Iwg Ilo Ias Res Ste Nre Cry Uni Cor Opt Aut
   0   7   2   0   2   0   0   0   0   0   0   0   0   0   0   0   1   1
!
!Ipr Ppl Ioc Mat Pcr Ls1 Ls2 Ls3 NLI Prf Ins Rpa Sym Hkl Fou Sho Ana
   0   0   1   0   1   0   4   0   0   1  13   0   0   0   0   0   0
!
! lambda1 Lambda2    Ratio     Bkpos     Wdt     Cthm      muR   AsyLim   Rpolarz ->Patt# 1
 1.540560 1.544390  0.5000   40.000 50.0000  1.0000   0.0000   60.00    0.0000
!
!NCY  Eps  R_at  R_an  R_pr  R_gl      Thmin       Step       Thmax     PSD    Sent0
 20  0.10  1.00  1.00  1.00  1.00     10.0100   0.020054   119.9835   0.000   0.000
!
! Excluded regions (LowT  HighT) for Pattern#  1
       0.00       10.00
     100.00      150.00
```

Background Information

Background information is located in this zone



Mode **[Nba]**
Define the type of model for background calculations.

Origin of the polynomial **[Bkpos]**
This option is enabled when the user selected a polynomial function to modeled the background. It represents the origin of polynomial
for background (in 2θ degrees or μseconds for TOF).

Number of points taken for Fourier Filter **[FWindow]**
Window for Fourier filtering.
This option is enabled if the Fourier Filtering is selected as model for background calculations. The value of ***FWINDOW*** must be much
greater than the number of points subtended by the base of a single Bragg reflections in the widest region (a factor greater than five,
at least!).

Background File
This option is enabled depending of the model selected for background calculations.

Equivalence on PCR file

```
!Job  Npr  Nph  Nba  Nex  Nsc  Nor  Dum  Iwg  Ilo  Ias  Res  Ste  Nre  Cry  Uni  Cor  Opt  Aut
   0    7    2    0    2    0    0    0    0    0    0    0    0    0    0    0    1    1
. . .
. . .

! lambda1 Lambda2    Ratio    Bkpos    Wdt     Cthm      muR    AsyLim   Rpolarz ->Patt# 1
 1.540560 1.544390  0.5000   40.000 50.0000  1.0000   0.0000    60.00    0.0000
'
```

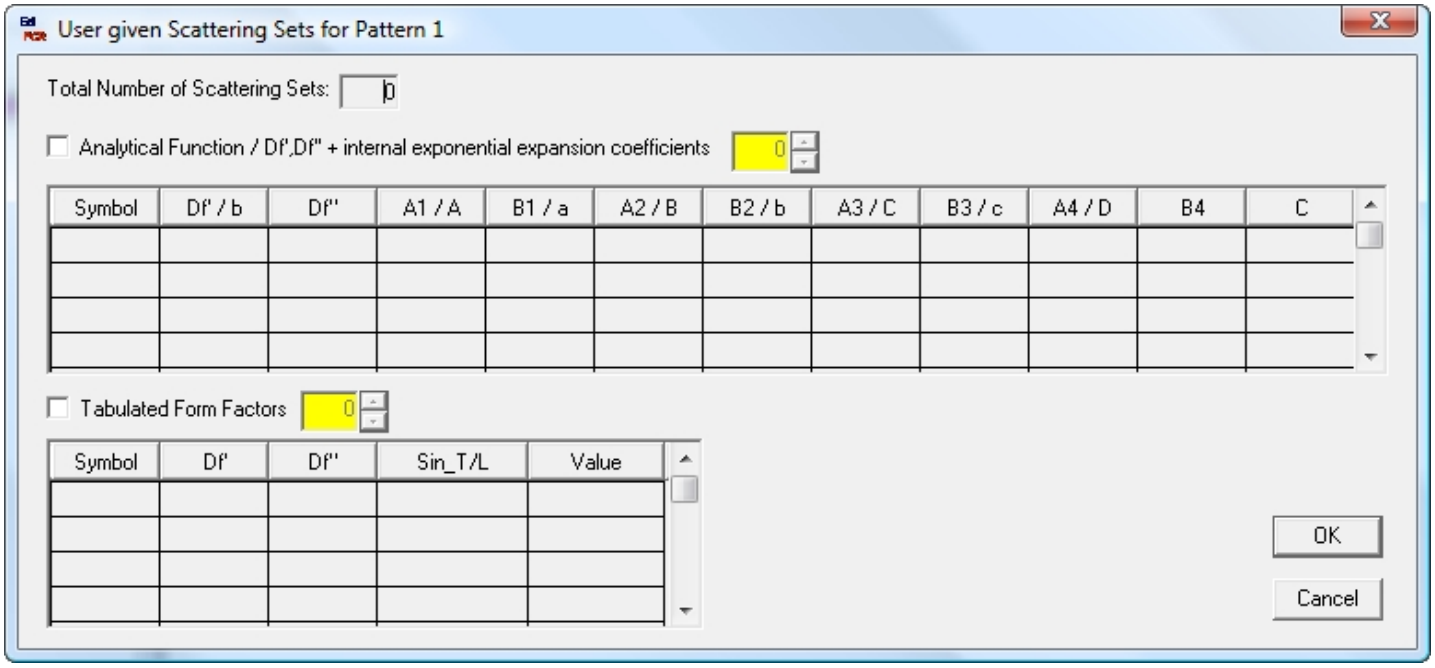
Scattering Factors

The user can define special scattering factors. To do this, click on 

button.

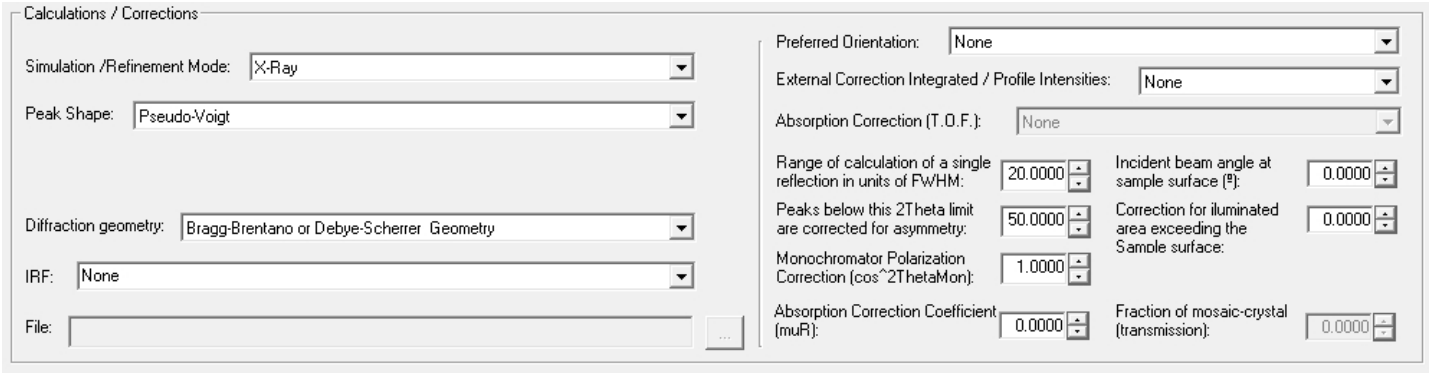
There are two options to define the scattering factors:

- Analytical function
- Tabulated form factors



Calculations / Corrections

Main parameters used on profile calculations are presented here.



Simulation / Refinement mode **[Job]**
Define the type of job for this pattern

Peak shape **[Npr]**
Default value for selection of a normalized peak shape function.

- Gaussian
- Lorentzian
- Modified Lorentzian
- Intermediate Lorentzian
- Tripled Pseudo Voigt
- Pseudo Voigt
- Thompson-Cox-Hastings Pseudo Voigt convoluted with axial divergence asymmetry function
- Numerical profile
- T.O.F. Pseudo Voigt convoluted with back-to-back exponential functions
- T.O.F. Pseudo Voigt convoluted d-spacing
- Split Pseudo Voigt
- Pseudo Voigt convoluted with axial divergence asymmetry function

The rest of parameters are related about corrections on the calculated profiles

***Diffraction geometry* [Ilo]**
Lorentz and polarization corrections depending of geometry of the diffractometer.

***IRF* [Res]**
Instrumental resolution file is used or not and define the model to use

***Preferred orientation* [Nor]**
Define the model for preferred orientation

***External correction integrated / Profile intensities* [Cor]**
Apply external intensity correction with external file

***Absorption correction (T.O.F)* [Iabscor]**
Type of absorption correction for T.O.F. data

***Range of calculation of a single reflection in units of FWHM* [Wdt]**
Represent the width of calculated profile of a single Bragg reflection in units of FWFH.
Typical values are:

- For Gaussian profiles: 4
- For Lorentzian profiles: 20-30
- For T.O.F. profiles: 4-5

***Peaks below this 2Theta limit are corrected for asymmetry* [AsyLim]**
Peaks below this 2θ limit are corrected for asymmetry

***Monochromator polarization correction* [Cthm]**
Coefficient for monochromator polarization correction

***Absorption correction coefficient (μR)* [muR]**
Absorption correction coefficient μR (μ is the effective absorption coefficient; R the radius or thickness of the sample), used only
for refinement on cylindrical samples and flat samples with symmetrical θ-2θ scanning (the scattering vector lying within the sample plane).

***Incident beam angle at sample surface* [PSD]**
Incident beam angle at sample surface in degrees

***Correction for illuminated area exceeding the sample surface* [Sent0]**
Theta angle at which the sample intercepts completely the x-ray beam.
Below ***SENT0*** part of the beam doesn't touch the sample and the intensity of reflections below ***SENT0*** have to be multiplied by the factor:

$$sclow = \sin\theta / \sin(SENT0)$$

***Fraction of mosaic crystal (Transmission) / Polarization factor* [Rpolarz]**
The value is the Polarization factor in a synchrotron experiment (Ilo=2) or the Fraction mosaic-crystal for transmission geometry.

Equivalence on PCR file

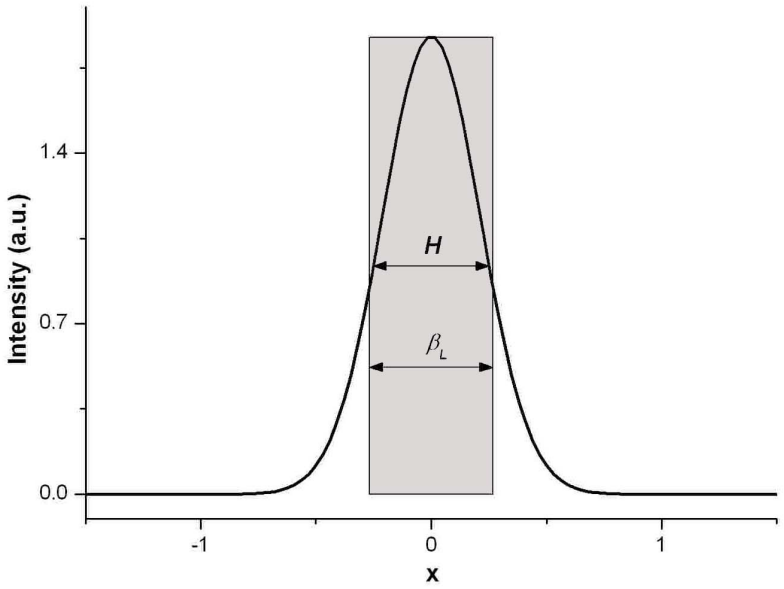
```
!Job  Npr  Nph  Nba  Nex  Nsc  Nor  Dum  Iwg  Ilo  Ias  Res  Ste  Nre  Cry  Uni  Cor  Opt  Aut
  0    7    2    0    2    0    0    0    0    0    0    0    0    0    0    0    1    1
!
!Ipr  Ppl  Ioc  Mat  Pcr  Ls1  Ls2  Ls3  NLI  Prf  Ins  Rpa  Sym  Hkl  Fou  Sho  Ana
  0    0    1    0    1    0    4    0    0    1   13    0    0    0    0    0    0
!
! lambda1  Lambda2     Ratio     Bkpos     Wdt     Cthm     muR     AsyLim   Rpolarz  ->Patt# 1
 1.540560 1.544390   0.5000    40.000  50.0000  1.0000   0.0000   60.00    0.0000
!
!NCY  Eps   R_at  R_an  R_pr  R_gl      Thmin        Step        Thmax     PSD     Sent0
 20  0.10   1.00  1.00  1.00  1.00      10.0100    0.020054    119.9835   0.000    0.000
```

Peak Shape Functions

The peak shape functions define on ***FullProf*** program are:

- Gaussian
- Lorentzian
- Modified Lorentzian
- Intermediate Lorentzian
- Tripled PseudoVoigt
- PseudoVoigt
- Pearson VII
- Thompson-Cox-Hastings pseudo-Voigt convoluted with axial divergence asymmetry function
- Numerical profile(CODFIL.shp, GLOBAL.shp)
- T.O.F. Convolution pseudo-Voigt with back-to-back exponential functions
- T.O.F. Convolution pseudo-Voigt versus d-spacing
- Split pseudo-Voigt function
- Pseudo-Voigt function convoluted with axial divergence asymmetry function
- T.O.F. Pseudo-Voigt function convoluted with Ikeda-Carpenter function

Gaussian



$$\Omega_0(x) = G(x) = a_G \exp\left(-b_G x^2\right)$$

where:

$$a_G = \frac{2}{H}\sqrt{\frac{\ln 2}{\pi}} \qquad b_G = \frac{4\ln 2}{H^2}$$

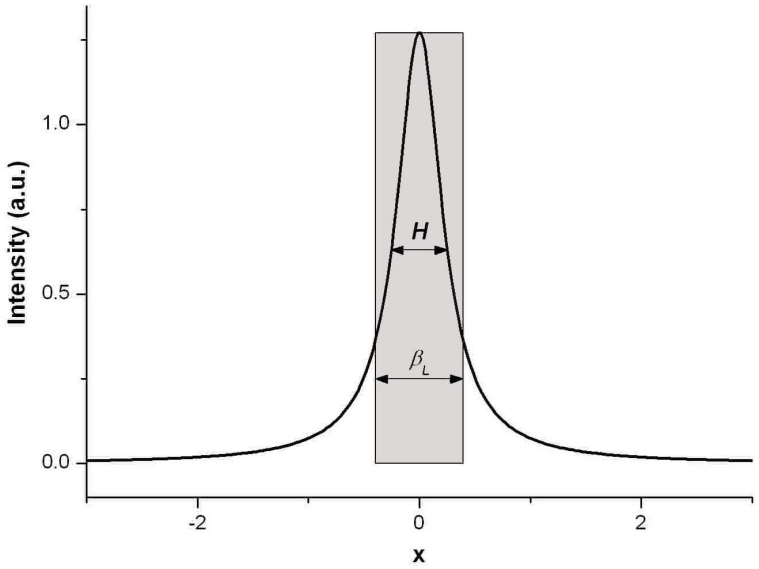
and *H* is the *FWHM*.

$$H^2 = \left(U + D_{ST}^2\right)\tan^2\theta + V\tan\theta + W + \frac{I_G}{\cos^2\theta}$$

The integral breadth of the Gaussian functions is:

$$\beta_G = \frac{1}{a_G} = \frac{H}{2}\sqrt{\frac{\pi}{\ln 2}}$$

Lorentzian



$$\Omega_1(x) = L(x) = \frac{a_L}{1 + b_L x^2}$$

where

$$a_L = \frac{2}{\pi H} \qquad b_L = \frac{4}{H^2}$$

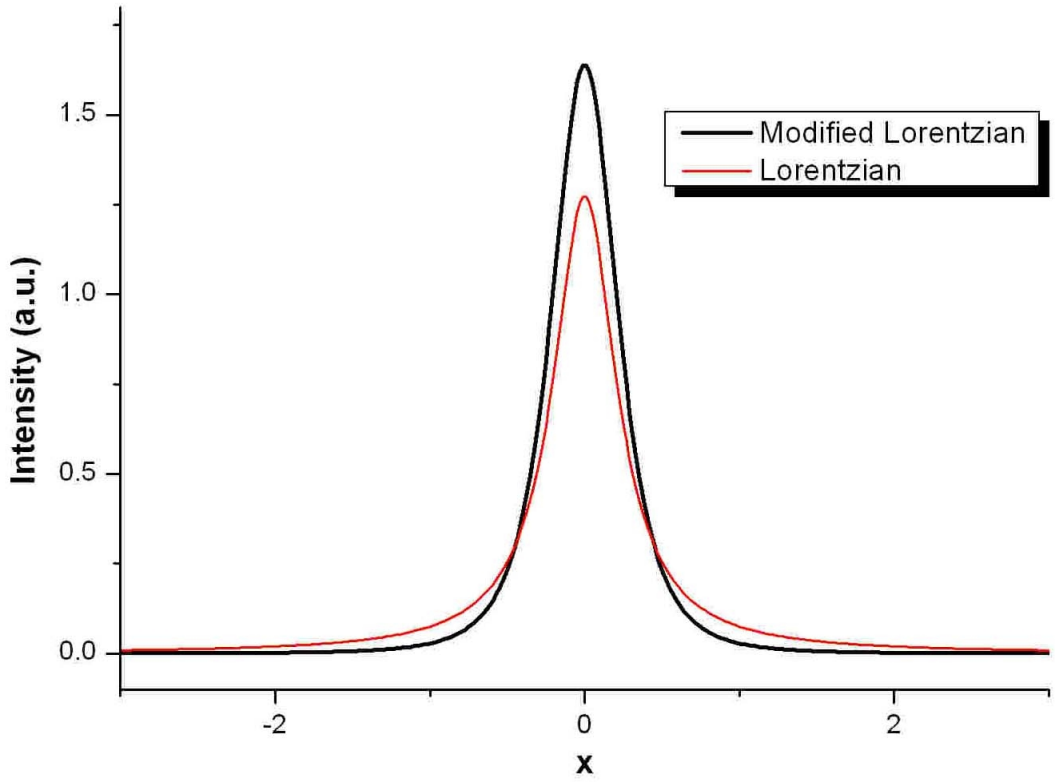
and H is the FWHM

$$H^2 = \left(U + D_{ST}^2\right)\tan^2\theta + V\tan\theta + W + \frac{I_G}{\cos^2\theta}$$

The integral breadth of the Lorentzian function is

$$\beta_L = \frac{1}{a_L} = \frac{\pi H}{2}$$

Modified Lorentzian



$$\Omega_2(x) = ML(x) = \frac{a_{ML}}{\left(1 + b_{ML} x^2\right)^2}$$

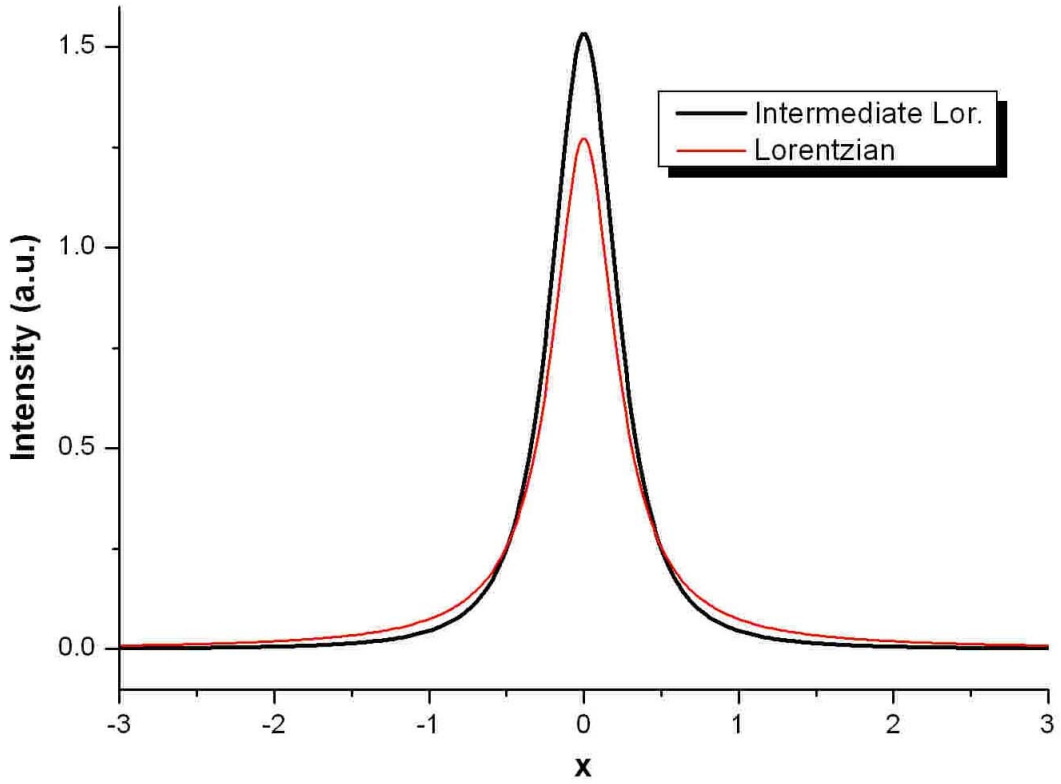
where

$$a_{ML} = \frac{4\sqrt{\sqrt{2}-1}}{\pi H} \qquad b_{ML} = \frac{4\left(\sqrt{2}-1\right)}{H^2}$$

and H is the FHWH

$$H^2 = \left(U + D_{ST}^2\right)\tan^2\theta + V\tan\theta + W + {}^{I_G}\!/_{\cos^2\theta}$$

Intermediate Lorentzian



$$\Omega_3(x) = IL(x) = \frac{a_{IL}}{\left(1 + b_{IL}x^2\right)^{3/2}}$$

where

$$a_{IL} = \frac{\sqrt{2^{2/3} - 1}}{H} \qquad b_{IL} = \frac{4\left(2^{2/3} - 1\right)}{H^2}$$

and H is the FHWH

$$H^2 = \left(U + D_{ST}^2\right)\tan^2\theta + V\tan\theta + W + {}^{I_G}\!/_{\cos^2\theta}$$

Tripled PseudoVoigt

$$\Omega_4(x) = X \cdot pV(x - D) + (1 - X - Y) \cdot pV(x) + Y \cdot pV(x + D)$$

where

$D = \frac{S_{hl}}{d\cos\theta}$ and S_{hl} is addtitional shape parameter.

The pseudovoigt function is defined as follow:

$$pV(x) = \eta L(x) + (1-\eta)G(x)$$

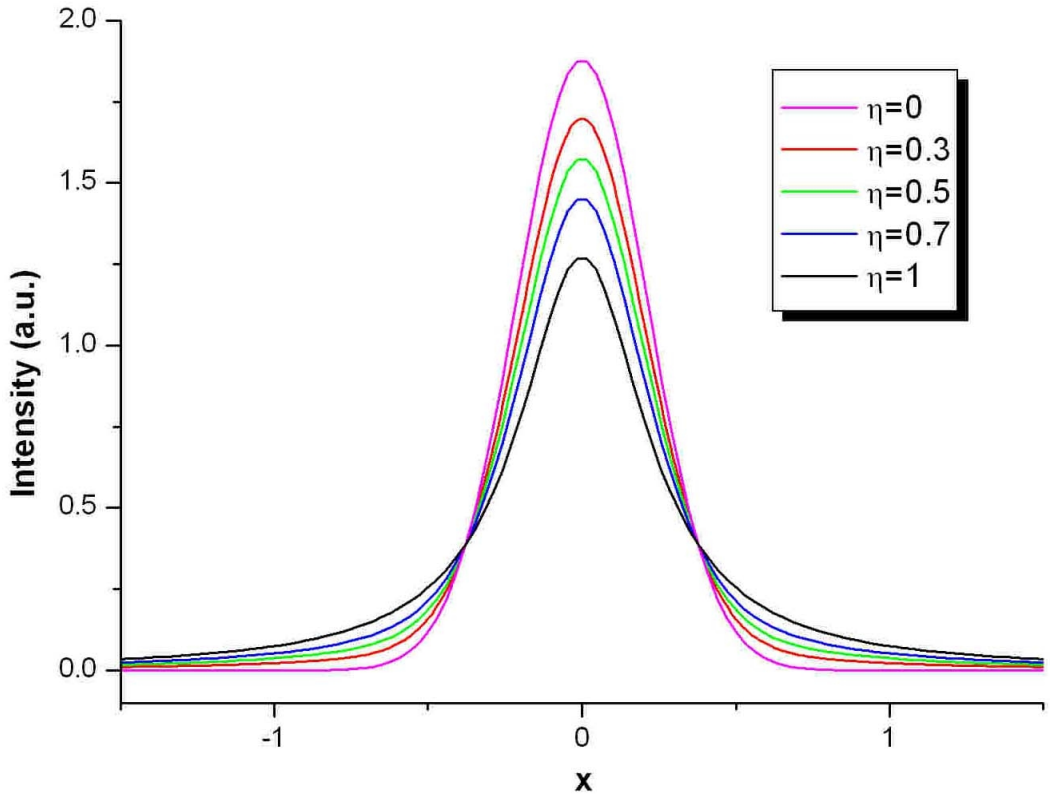
where

$$\eta = \eta_0 + X \cdot 2\theta$$

and the FHWM as

$$H^2 = \left(U + D_{ST}^2\right)\tan^2\theta + V\tan\theta + W + \frac{I_G}{\cos^2\theta}$$

PseudoVoigt



$$\Omega_5(x) = pV(x) = \eta L(x) + (1-\eta)G(x)$$

$$\eta = \eta_0 + X \cdot 2\theta$$

where $0 \le \eta \le 1$.

The ***pV(x)*** function is a linear combination of a ***Lorentzian*** (*L*) and a ***Gaussian*** (*G*) of the same FWHM (*H*), so there two parameters
characterizing the peak shape:

$$pV(x) = pV(x, \eta, H)$$

If *L(x)* and *G(x)* are normalized, *pV(x)* is also normalized. The integral breadth of a normalized pseudoVoigt function is just the inverse of the maximum value. The FWHM is the same for *L(x)*, *G(x)* and *pV(x)*.

Pearson VII

$$\Omega_6(x) = PVII(x) = \frac{a_{VII}}{\left(1+b_{VII}x^2\right)^m}$$

where

$$a_{VII} = \frac{\Gamma(m)}{\Gamma(m)-1/2}\frac{2\sqrt{2^{1/m}-1}}{\sqrt{\pi}H} \qquad b_{VII} = \frac{4\left(2^{1/m}-1\right)}{H^2}$$

$$m = m_0 + 100\frac{X}{2\theta} + 10000\frac{Y}{(2\theta)^2}$$

and the FWHM is

$$H^2 = \left(U + D_{ST}^2\right)\tan^2\theta + V\tan\theta + W + {I_G}/{\cos^2\theta}$$

Thopson-Cox-Hastings pseudoVoigt

$$\Omega_7(x) = pV(x)$$

The pseudoVoigt function is an approximation to the Voigt function defined as the convolution of a Lorentzian and a Gaussian:

$$pV(x) = L(x) \otimes G(x) = \int_{-\infty}^{+\infty} L(x-u)G(u)du$$

where *L(x)* and *G(x)* have different FWHM (H_L and H_G respectively). The *pV(x)* function is an approximation that substitutes the two shape parameters H_L and H_G by the pair (η, *H*):

$$H^5 = H_G^5 + 2.69269H_G^4H_L + 2.42843H_G^3H_L^2 + 4.47163H_G^2H_L^3 + 0.07842H_GH_L^4 + H_L^5$$

$$\eta = 1.36603\frac{H_L}{H} - 0.47719\left(\frac{H_L}{H}\right)^2 + 0.11116\left(\frac{H_L}{H}\right)^3$$

The inversion of the above two expressions leads to the relations:

$$\frac{H_L}{H} = 0.72928\eta + 0.19289\eta^2 + 0.07783\eta^3$$

$$\frac{H_G}{H} = \left(1 - 0.74417\eta - 0.24781\eta^2 - 0.00810\eta^3\right)^{1/2}$$

The FWHM of the Gaussian (H_G) and Lorentzian (H_L) components is calculated as:

$$H_G^2 = (U + D_{ST}^2)\tan^2\theta + V\tan\theta + W + {I_G}/{\cos^2\theta}$$

$$H_L = X\tan\theta + \frac{\left[Y + F(S_Z)\right]}{\cos\theta}$$

Numerical

PseudoVoigt x BB exponential functions (TOF)

PseudoVoigt x d spacing (TOF)

Split PseudoVoigt

$$\Omega_{11}(x) = pV(x) = \eta L(x) + (1-\eta)G(x)$$

Split left and right parts of the profile function as:

Left part

$$H_l^2 = (U_l + D_{ST}^2)\tan^2\theta + V_l\tan\theta + W_l + \frac{I_G}{\cos^2\theta} + \frac{Shape1}{\tan^2 2\theta}$$

Shape1 is applied only for ***2***θ ***< 90º***

$$\eta_l = \eta_0 + X_l \cdot 2\theta$$

Right part

$$H_r^2 = (U_r + D_{ST}^2)\tan^2\theta + V_r\tan\theta + W_r + \frac{I_G}{\cos^2\theta} + \frac{Shape2}{\tan^2 2\theta}$$

Shape2 is applied only for ***2***θ ***> 90º***

$$\eta_r = \eta_0 + X_r \cdot 2\theta$$

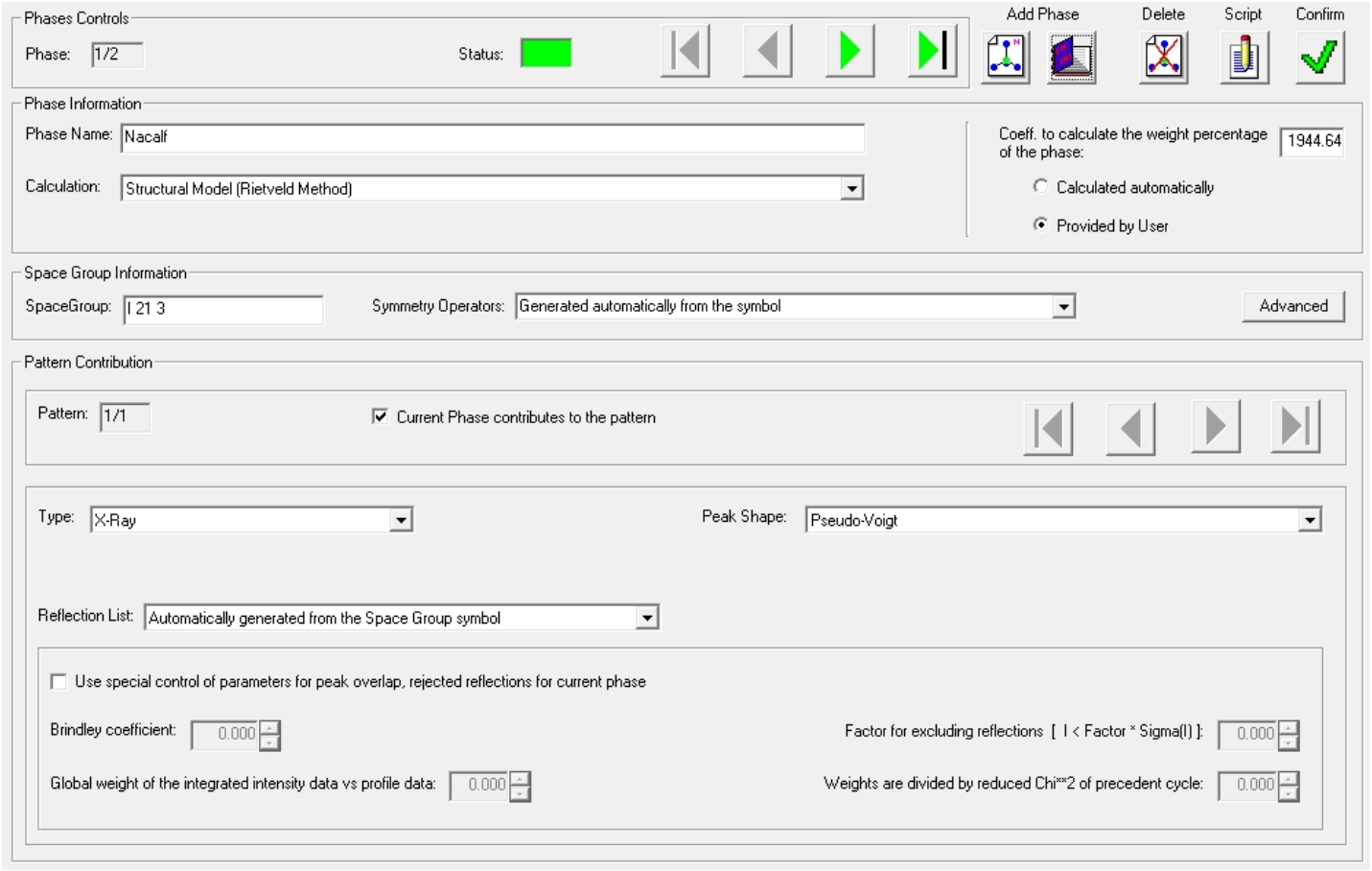
PseudoVoigt x Axial divergence assymetry

PseudoVoigt x Ikeda-Carpenter (TOF)

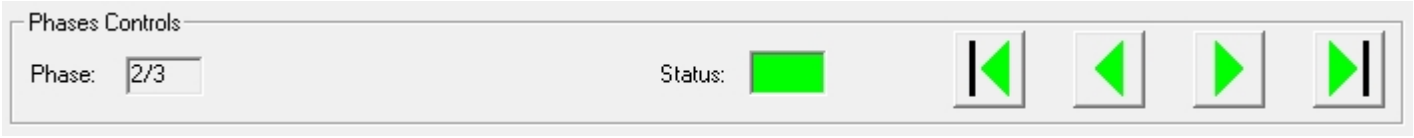
Phase Information

User can select this dialog pressing on  button on left Toolbar of ***EdPCR*** program.

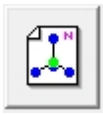
All Phases information is controlled by this dialog ***except*** refinement parameters.



Phases Control



Buttons



Add a new phase

Add a new phase from CIF or SHELX files

Delete the current phase information

Macro information for current phase

Confirm all information about the current dialog.

Controls

Go to first phase

Go previous phase

Go to next phase

Go to last phase

Status

Unsaved information

Saved information

Equivalence on PCR file

```
!Job  Npr  Nph  Nba  Nex  Nsc  Nor  Dum  Iwg  Ilo  Ias  Res  Ste  Nre  Cry  Uni  Cor  Opt  Aut
   0    7    2    0    2    0    0    0    0    0    0    0    0    0    0    0    1    1
'
```

Phase Information

Phase name
Name of current phase

***Calculation* [Jbt]**
Select the type of calculation for current phase

***Coefficient to calculate the weight percentage of the phase* [ATZ]**
Calculation for the coefficient according to

$$ATZ = Z\, M_w\, f^2 / t$$

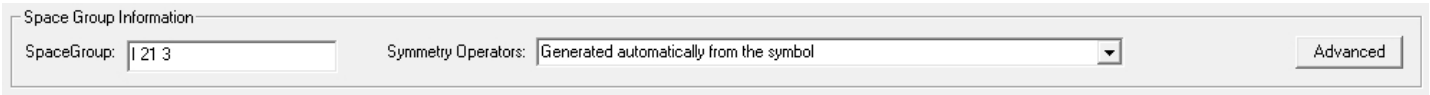
where

Z	Number of formula units per cell
M_W	Molecular weight
f	Used to transform the site multiplicities. For a stoichiometric phase *f*=1 if these multiplicities are calculated by dividing the Wyckoff multiplicity *m* of the site by general multiplicity *M*. Otherwise *f*=*Occ M*/*m* , where *Occ* is the occupation factor.
t	Brindley coefficient that accounts for microabsorption effects It is required for quantitative phase analysis only. When different phases have similar absorption (in most neutron uses), *t*≈1.0

Equivalence on PCR file

```
!-------------------------------------------------------------------------------
!  Data for PHASE number:   1  ==> Current R_Bragg for Pattern#  1:     0.00
!-------------------------------------------------------------------------------
NaCaAlF
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth      ATZ     Nvk Npr More
   6   0   0 0.0 0.0 1.0   0   0   0   0   0     1944.635   0   7   0
```

SpaceGroup Information



Spacegroup
Define the space group for current phase using Hermann-Mauguin representation

***Symmetry Operators* [Sym]**
Selecting in which mode are used the symmetry operators.

If the user wants a more interactive process or introduce magnetic operators then need do click on Advanced button.

A new dialog will be showed with 3 subdialogs:

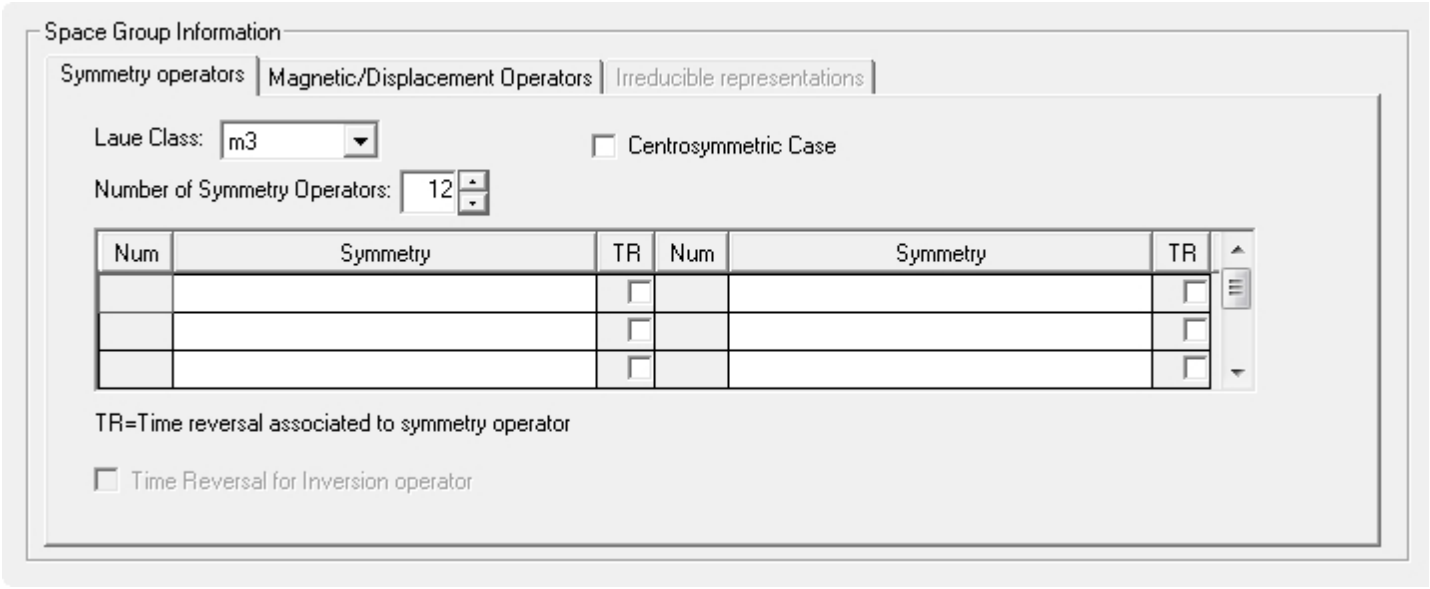
- Symmetry operators
- Magnetic / Displacement operators
- Irreducible operators

Equivalence on PCR file

```
!
!Ipr  Ppl  Ioc  Mat  Pcr  Ls1  Ls2  Ls3  NLI  Prf  Ins  Rpa  Sym  Hkl  Fou  Sho  Ana
   0    0    1    0    1    0    4    0    0    1   13    0    0    0    0    0    0
...
...

!
I 21 3                    <--Space group symbol
```

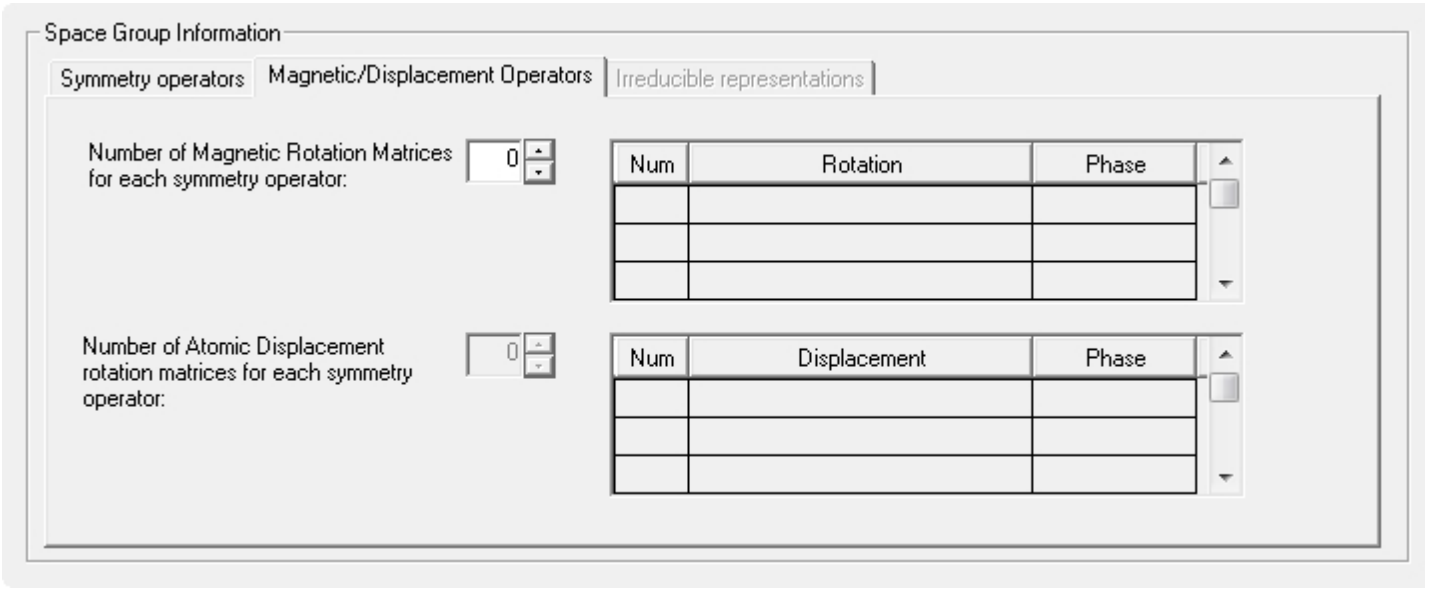
Symmetry operators



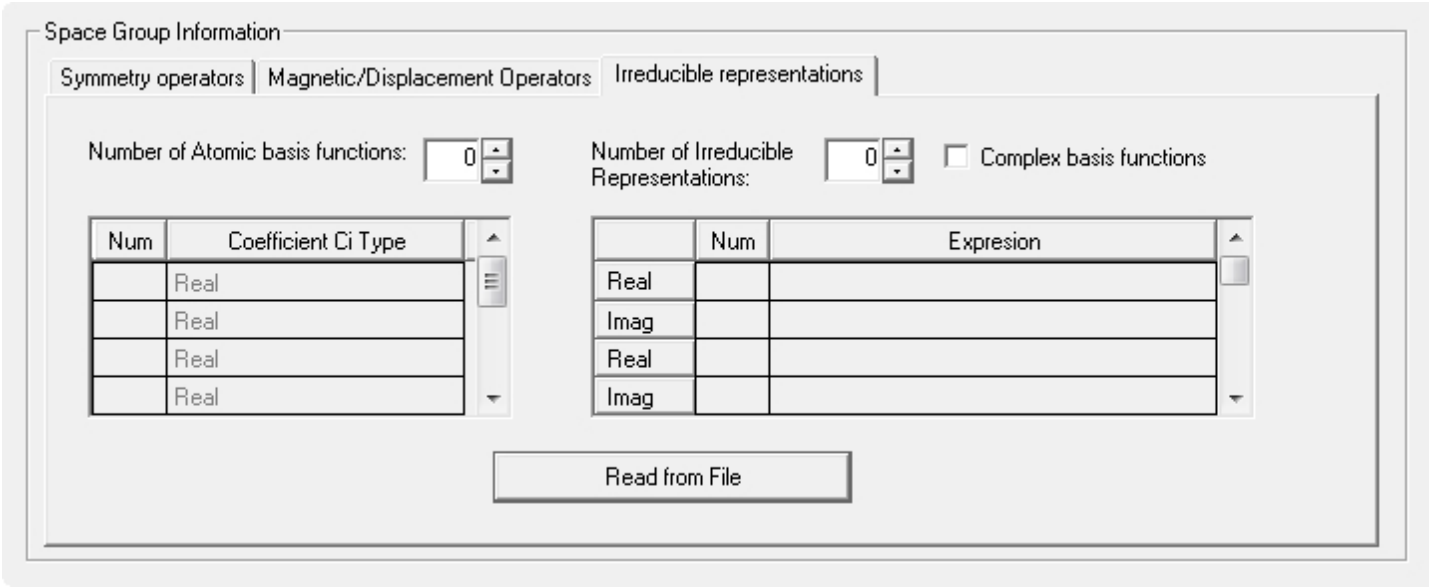
When Space group information is generated automatically all fields are filled with respectively information.

Only when the user define it, these fields can be modified.

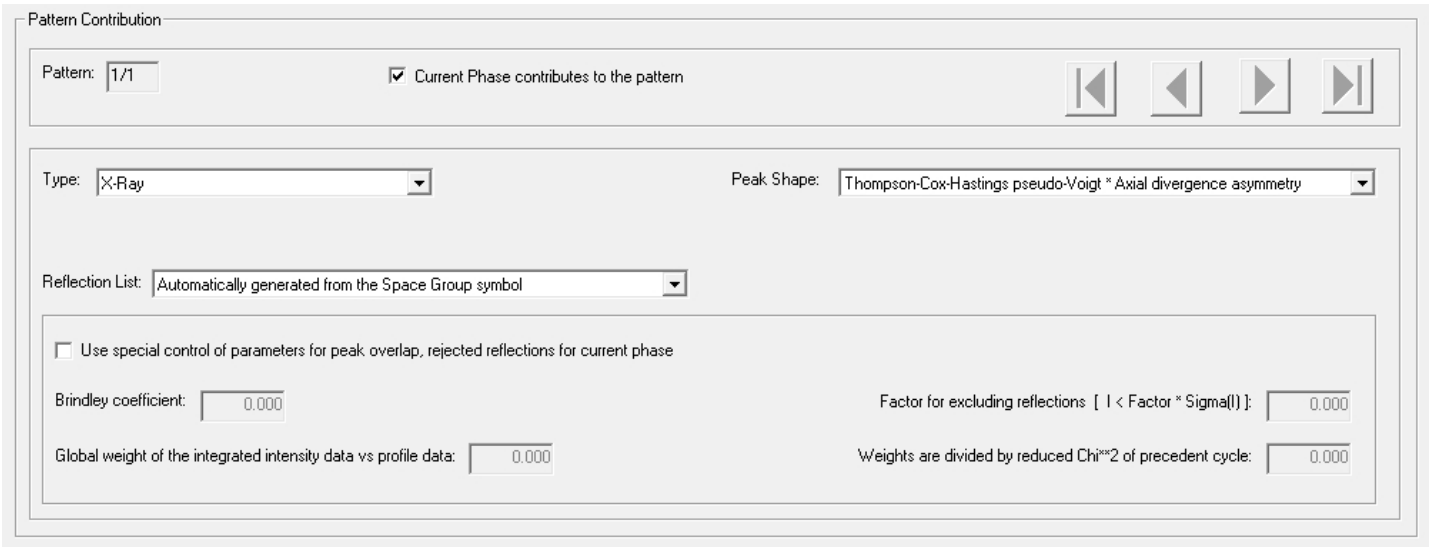
Magnetic/Displacement operators



Irreducible operators



Pattern Contributions



This is the part for pattern contribution of the current phase.

Current phase contributes to the pattern **[JCONTR]**
Checkbox to active if the current phase contributes in this pattern.

Controls


Go to first pattern


Go previous pattern


Go to next pattern


Go to last pattern

***Type of Pattern* [Jbt]**
Select the job type for current phase.

***Peak shape* [Npr]**
Specific profile function for the current phase

***Reflection list* [Irf]**
Control for reflections generation or use of a reflections file

Equivalence on PCR file

```
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth        ATZ     Nvk Npr More
   6   0   0 0.0 0.0 1.0   0   0   0   0   0       1944.635   0   7   0
```

The user can activate control parameters for peak overlap or rejected reflections for current phase. Then the next fields are activated.

***Brindley coefficient* [Brind]**
Brindley coefficient

***Global weight of the integrated intensity respect global profile* [Rmua]**
Used when a list of integrated intensities is given as observations for the current phase (see ***Irf*** parameter).

If ***Rmua*** is equal to zero then ***FullProf*** program puts it to 1.0. The value of this variable corresponds to the global weight of the integrated intensity
observations with respect to the global profile. The contribution to the normal equations of the integrated intensity part is multiplied by ***Rmua***.

***Factor for excluding reflections* [Rmub]**
Used when a list of integrated intensities is given as observations for the current phase (see ***Irf*** parameter).

Rmub is a factor for excluding reflections: only the reflections verifying the constraint

$$G_{obs} \geq Rmub \cdot \sigma(G_{obs})$$

are considered in the refinement. G_{obs} is the integrated intensity, structure factor or structure factor squared of the current reflection.

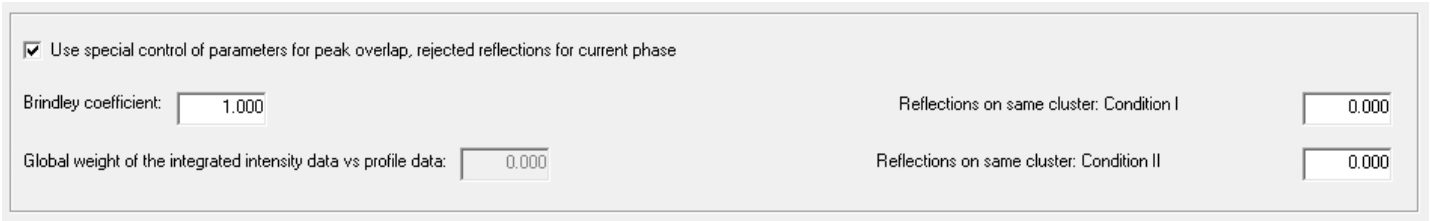
***Weights are divide by reduced χ^2 of precedent cycle* [Rmuc]**
Used when a list of integrated intensities is given as observations for the current phase (see ***Irf*** parameter).

If ***Rmuc*** is greater than 0.9 the weights are divided by the reduced χ^2 of the precedent cycle.

Equivalence on PCR file

```
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth        ATZ     Nvk Npr More
   6   0   0 0.0 0.0 1.0   0   0   0   0   0       1944.635   0   7   1
!
!Jvi Jdi Hel Sol Mom Ter  Brind   RMua     RMub     RMuc    Jtyp  Nsp_Ref Ph_Shift N_Domains
   0   0   0   0   0   0  0.0000  0.0000   0.0000   0.0000    0       0       0       0
```

When the current job is a Profile matching with constant scale factor and using a list of overlapped peak cluster then a control for two consecutive
reflections belongs to a same cluster will be used.



The reflections *i* and *i+1* belong to the same cluster if

Condition I:

$$T_{i+1} - T_i < 0.5\, Rmub \left(H_i + H_{i+1} \right)$$

Condition II:

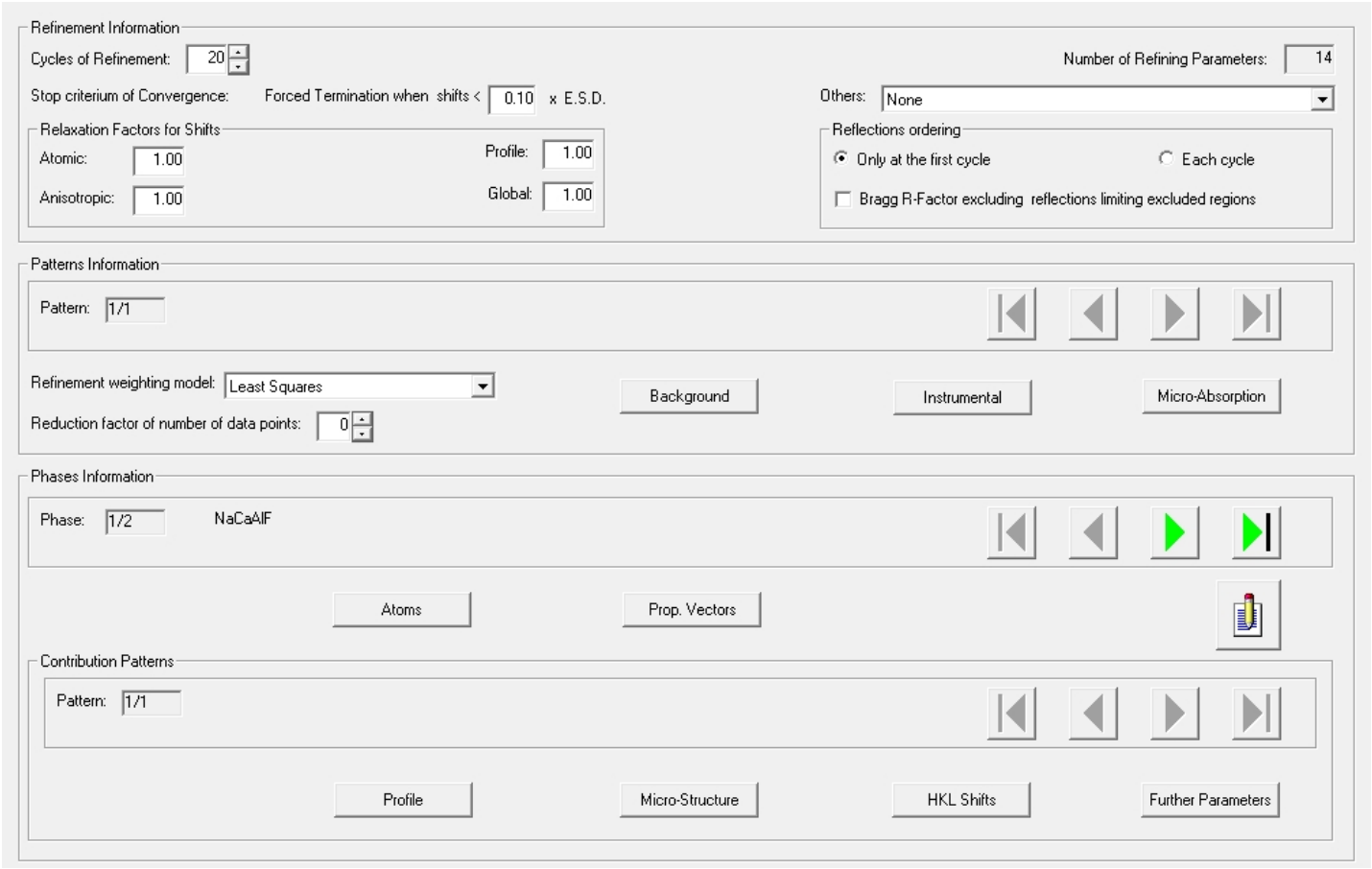
$$T_{i+1} - T_i < 0.5 \left(H_i + H_{i+1} \right)$$
$$and$$
$$G_{i+1} < G_{sum} \cdot Rmuc$$

where G_i is the integrated intensity, T_i is the Bragg position, H_i is the FWHM of reflection *i*, G_{sum} is the cumulated integrated intensity of the current cluster. If ***Rmub*** and ***Rmuc*** are given as zeroes, ***FullProf*** program put ***Rmub*** equal to 1.0 and ***Rmuc*** as 0.2

Refinement Information

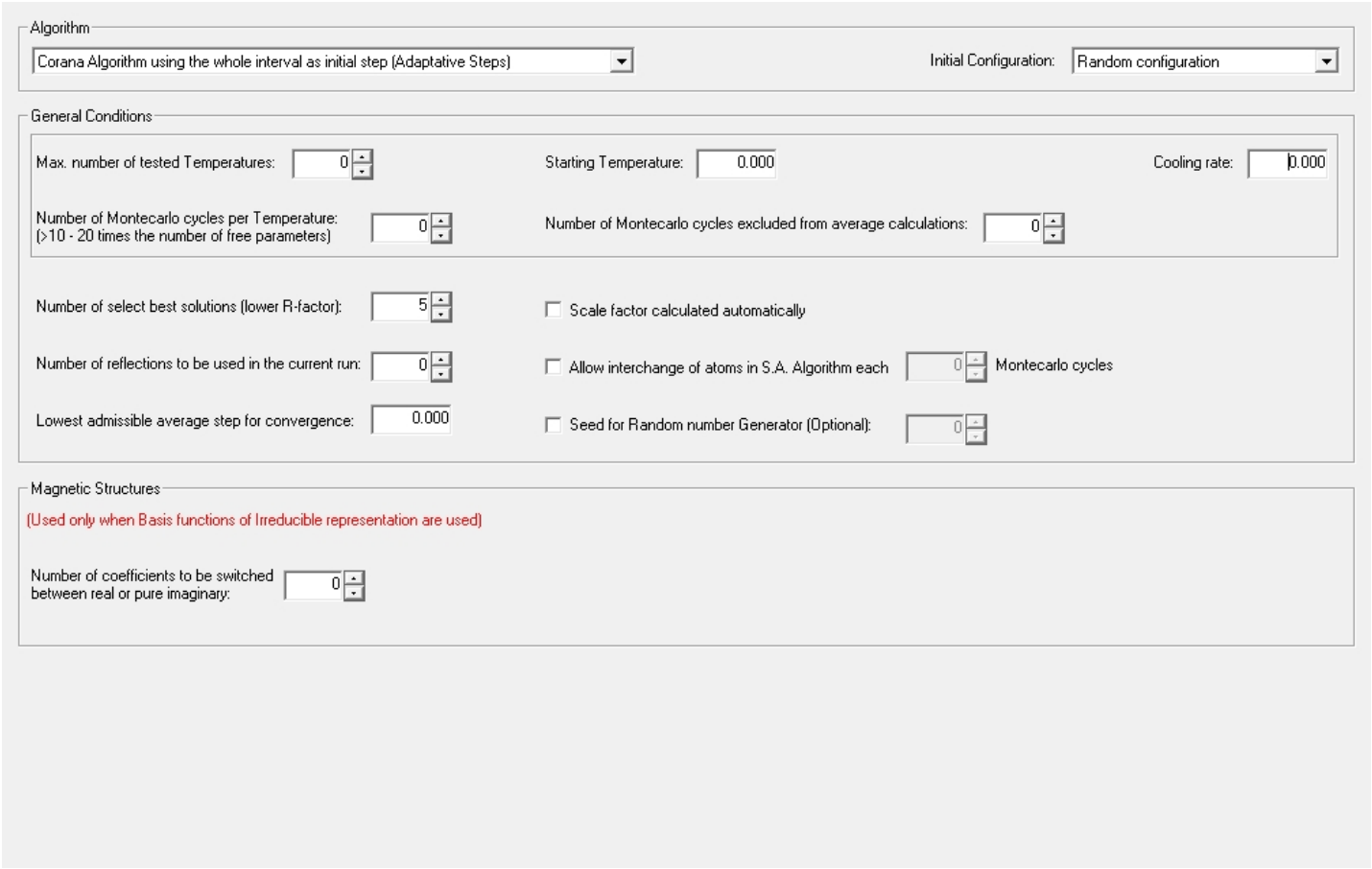
User can select this dialog pressing on  button on left Toolbar of ***EdPCR*** program

All refinement parameters are located in this main dialog.



Simulated Annealing Dialog

User can select this dialog pressing on  button on left Toolbar of ***EdPCR*** program



Constraints Information

User can select this dialog pressing on  button on left Toolbar of ***EdPCR*** program

Restraints Dialog

User can select this dialog pressing on  button on left Toolbar of ***EdPCR*** program

Output Information

User can select this dialog pressing on  button on left Toolbar of ***EdPCR*** program

General Output Files

- [x] Classical Output Format for a Single Pattern in PCR
- [ ] Debug Mode for PCR File
- [ ] Summary of Refined Parameters (RPA)
- (•) Overwrite PCR File
- [ ] Symmetry Operator List (SYM)
- [ ] Crystallographic Information File (CIF)
- ( ) NEW PCR File

Patterns Information

Pattern: 1/1 — Equal Settings for all Patterns

Files

- Output Information (OUT)
- Profile Refinement (PRF)
- Calculated Profile (SUB)
- Background File (BAC)
- Reflections File (HKL)
- List Reflections (SAV)
- Structure Factors (FOU)
- Simulated Diffraction (SIM)
- Summary Pattern (SUM)
- Refinement Plots

- [ ] Only Information from the last cycle is printed

Correlation Matrix Output: None

- [ ] Reflection list is written before starting cycle
- [ ] Cal. and Obs. profile intensities are written
- [ ] Corrected profile intensities are written
- [x] Cal. and Obs. integrated intensities are written
- [ ] Merged reflections list is written
- [ ] List reflec. from second wavelength is written

Phases Information

Phase: 1/1 — Equal Settings for all Phases

Atoms Information (ATM)

- [ ] Atoms inside a conventional cell
- [ ] Atoms within a primitive cell for magnetic phase
- [ ] Magnetic phase information for MOMENT program

Overlapped Peaks (INT)

- [ ] Overlapped peaks

Graphics Formats (SCH)

- [ ] SCHAKAL
- [ ] STRUPLO

Geometric Calculations

- [ ] Active

Distance Max: 0.0000 — Distance Max. (Angle Calc.): 0.0000

Bond Valence Sum Calculations

- [ ] Active

Num. Cations: 0

Num. Anions: 0

Tolerance (%): 0.000

	Cation
1	
2	
3	
4	

	Anion
1	
2	
3	
4	