
Using *FullProf* to analyze Time of Flight Neutron Powder Diffraction data

Juan Rodríguez-Carvajal, Laboratoire Léon Brillouin (CEA-CNRS), Dec. 2003
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Introduction

A reorganization of the subroutines calculating the peak shape function and derivatives for time of flight neutron powder diffraction has been performed. The result of the new implementation is a better stability for the refinement of instrumental parameters. In this document we provide the detailed mathematical expressions of the peak shape functions used presently in *FullProf*. From the point of view of the input of the PCR file nothing has changed except the values of some parameters. The third function for TOF, convolution of the Ikeda-Carpenter function with a pseudo-Voigt, is now working thanks to the work performed by Laurent Chapon who wrote the corresponding subroutine.

Another important aspect of the modifications performed recently in *FullProf* is the use of external files containing the instrumental resolution function (IRF). Most of the instrumental parameters can be read from an external IRF file and the corresponding values in the PCR file have to be set to zero. The refinable parameters of the PCR file are additive with respect to the instrumental values. After giving the mathematical expressions corresponding to the different functions we provide some examples with and without the use of IRF files.

At present, only the TOF data that have been corrected from the incident spectrum can be safely analyzed with *FullProf*. The correction of the incident spectrum is included but not tested sufficiently. It is not recommended to use raw data, instead use one of the conversion programs existing in the spallation neutron source centers to get the appropriate files. The program can read some of the GSAS input files but not all formats (see manual and `fp2k.inf` for details). If the data of different detector banks are in a single file it suffices to give the same name for the data file of each pattern. This option works with some GSAS input files (`INSTRM=12`) and with X-Y-Sigma files (`INSTRM=14`) as recently adopted at most ISIS instruments.

Peak-shape functions for Neutron Time of Flight in *FullProf*. The cases `NPROF=9, 10`.

The profile function Ω for TOF corresponds to the control variable `NPROF=9, 10, 13`. The peak shape in the first two cases (`NPROF=9, 10`) is the same but the TOF position of the Bragg peaks are calculated in different ways for the two functions. This peak-shape is the same as that corresponding to TOF profile function 4 in GSAS, except that the Gaussian and Lorentzian components of the Voigt functions have different models for anisotropic strain and size broadening. The third case will be treated in the next paragraph. The peak shape for `NPROF=9, 10` is a convolution of a pseudo-Voigt function with a pair of back-to-back exponentials. If we take the origin of time (t) at the Bragg position of a particular peak we have:

Panel 1:

$$\Omega(x) = pV(x) \otimes E(x) = \int_{-\infty}^{+\infty} pV(x-t)E(t)dt$$

With:

Panel 2:

$$\begin{aligned} E(t) &= 2Ne^{\alpha t} & t \leq 0 \\ E(t) &= 2Ne^{-\beta t} & t > 0 \\ N &= \frac{\alpha\beta}{2(\alpha + \beta)} \end{aligned}$$

The parameter α corresponds to the rising time constant and β to the decay constant. Both parameters have a dependency with the d-spacing (total time of flight). We will discuss this point later. The argument x corresponds to the shift in microseconds with respect to the Bragg position: $x=T_i - T_h$. The result of the convolution is:

Panel 3:

$$\Omega(x) = (1 - \eta)N \left\{ e^u \operatorname{erfc}(y) + e^v \operatorname{erfc}(z) \right\} - \frac{2N\eta}{\pi} \left\{ \operatorname{Im}[e^p E_1(p)] + \operatorname{Im}[e^q E_1(q)] \right\}$$

Where erfc is the complementary error function and E_1 is the exponential integral with complex argument. The function Im corresponds to the imaginary component of its argument.

The complementary error function and the exponential integral are defined, respectively, as:

Panel 4:

$$\operatorname{erfc}(x) = 1 - \operatorname{erf}(x) = 1 - \frac{2}{\sqrt{\pi}} \int_0^x e^{-u^2} du = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-u^2} du$$

$$E_1(z) = \int_z^\infty \frac{e^{-t}}{t} dt; \quad (|\arg z| < \pi)$$

The calculations of these two functions are performed using an approximated formula for the complementary error function (code based on that given in Numerical Recipes,) and an algorithm based in continuous fractions for the exponential integral (based in code provided in *Computation of Special Functions*, by Shanjie Zhang and Jianming Jin, John Wiley and Sons Inc., 1996). The calculation of exponentials in the function of Panel 3 are performed by optimized partitions in multiplicative factors in order to avoid intermediate over-flloats and erroneous final results.

The arguments of the different functions in Panel 3 are:

Panel 5:

$$u = \frac{1}{2} \alpha (\alpha \sigma^2 + 2x) \quad v = \frac{1}{2} \beta (\beta \sigma^2 - 2x)$$

$$y = \frac{\alpha \sigma^2 + x}{\sqrt{2\sigma^2}} \quad z = \frac{\beta \sigma^2 - x}{\sqrt{2\sigma^2}}$$

$$p = \alpha x + \frac{i\alpha H}{2} \quad q = -\beta x + \frac{i\beta H}{2}$$

The pseudo-Voigt function has a Gaussian and a Lorentzian components with the same FWHM, so that σ and H are related here by: $H^2 = \gamma^2 = 8 \ln 2 \sigma^2$. Both η and H are functions of the Gaussian and Lorentzian components of the Voigt function (σ_G and γ_L , see the Thompson-Cox-Hasting relations in the manual) that have the following dependence with d -spacing:

Panel 6:

$$\sigma_G^2 = \sigma_0^2 + \left(\sigma_1^2 + DST2(1 - \zeta)^2 \right) d^2 + \left(\sigma_2^2 + Gsize \right) d^4 = \frac{H_G^2}{8 \ln 2}$$

$$\gamma_L = \gamma_0 + \left(\gamma_1 + \zeta \sqrt{8 \ln 2 DST2} \right) d + \left(\gamma_2 + F(SZ) \right) d^2 = H_L$$

The actual values of η and H (or σ) are calculated from σ_G and γ_L by using the TCH relations. The coefficients of σ_G and γ_L are called sig-0 (σ_0^2), sig-1 (σ_1^2), sig-2 (σ_2^2), gam-0 (γ_0), gam-1 (γ_1), and gam-2 (γ_2), within

FullProf. *Gsize* is a Gaussian size parameter, *DST2* is the contribution of the anisotropic strain, ζ is the

Lorentzian strain fraction and $F(SZ)$ represents a Lorentzian anisotropic size contribution. See the microstructure section of the manual for details.

The difference between the functions NPROF=9 and NPROF=10 are related to the dependence of the decay and rise constants with d -spacing. For the function NPROF=9, the TOF corresponding to a Bragg peak of d -spacing d_h is simply quadratic:

Panel 7:

$$T_h = Z_0 + D_1 d_h + D_2 d_h^2$$

And the function for α and β are:

Panel 8:

$$\alpha = \alpha_0 + \frac{\alpha_1}{d_h} \quad \beta = \beta_0 + \frac{\beta_1}{d_h^4}$$

For the function NPROF=10, the TOF corresponding to a Bragg peak of d -spacing d_h is calculated using a more complex function related to thermal and epithermal components of the neutron spectrum. The expressions below have been developed by Jason Hodges (unpublished) by fitting experimental data obtained in GPPD at Argonne. The Bragg position in microseconds is calculated using the expressions:

Panel 9:

$$\begin{aligned} T_h &= nT_h^e + (1-n)T_h^t \\ T_h^e &= Z_0^e + D_1^e d_h \\ T_h^t &= Z_0^t + D_1^t d_h - \frac{A^t}{d_h} \\ n &= \frac{1}{2} \operatorname{erfc}\left\{w_{cross} \left(T_{cross} - \frac{1}{d_h}\right)\right\} \end{aligned}$$

Where the superscripts e and t correspond to epithermal and thermal components respectively. w_{cross} and T_{cross} are the width and position of the crossover between thermal and epithermal components. The reciprocal of the decay and rise constants are here modeled as a function of d -spacing by the following functions:

Panel 10:

$$\begin{aligned} \frac{1}{\alpha} &= n\alpha^e + (1-n)\alpha^t & \frac{1}{\beta} &= n\beta^e + (1-n)\beta^t \\ \alpha^e &= \alpha_0^e + \alpha_1^e d_h & \beta^e &= \beta_0^e + \beta_1^e d_h \\ \alpha^t &= \alpha_0^t - \frac{\alpha_1^t}{d_h} & \beta^t &= \beta_0^t - \frac{\beta_1^t}{d_h} \end{aligned}$$

Below we give the correspondence of the above instrumental parameters and those written in the PCR file.

For the peak shape function NPROF=9, the global parameters Z_0 , D_1 and D_2 are called, respectively: **zero**, **dt1** and **dt2**.

The parameters governing the variation with d -spacing of the rise/decay constants for NPROF=9 α_0 , β_0 , α_1 , and β_1 are called, respectively, **alph0**, **beta0**, **alph1** and **beta1**.

For the peak shape function NPROF=10, the global parameters Z_0^e , D_1^e , Z_0^t , D_1^t , A^t , w_{cross} and T_{cross} are called, respectively: **Zero**, **Dtt1**, **Zerot**, **Dtt1t**, **Dtt2t**, **Width**, and **x-cross**. The parameters governing the variation with d -spacing of the thermal and epithermal components of the rise and decay constants for

NPROF=10, $\alpha_0^e, \beta_0^e, \alpha_1^e, \beta_1^e, \alpha_0^t, \beta_0^t, \alpha_1^t, \beta_1^t$, are called respectively: **alph0**, **beta0**, **alph1**, **beta1**, **alph0t**, **beta0t**, **alph1t**, and **beta1t**.

It must be remembered that the units of parameters entering in the expressions of the rise, α , and decay, β , time constants for NPROF=10 are reciprocal of those corresponding to the function NPROF=9. The rise and decay time constants, as defined in Panel 2, have units of reciprocal microseconds, so the constants α_0, β_0 have also the same units, however the constants $\alpha_0^e, \beta_0^e, \alpha_0^t, \beta_0^t$, have units of microseconds.

Peak-shape functions for Neutron Time of Flight in *FullProf*. The case NPROF=13.

The third TOF peak shape function, NPROF=13, has been developed, according to the GSAS manual, by W.I.F. David and R.B. Von Dreele (unpublished) and incorporates the moderator pulse shape of S. Ikeda & J.M. Carpenter, Nuc. Inst. and Meth., **A239**, 1985, 536-544. The calculation method in *FullProf* is different of that used in GSAS but the results should in principle be the same. We use similar algorithms to those used for calculating the previous function (NPROF=9, 10).

The Ikeda-Carpenter function is composed of a convolution of two functions; the first represents the slowing down spectrum from the moderator and the second is a mixing of a δ -function and an exponential decay:

Panel 11:

$$S_k(t) = \frac{\alpha^3}{2} t^2 e^{-\alpha t} \quad R_k(t) = (1-R)\delta(t) + R\beta e^{-\beta t}$$

The two parts describe the leakage of fast and slow neutrons from the moderator and have *fast* and *slow* decay constants, α and β , respectively, which are related to the moderator material and dimensions. The mixing coefficient, R, is related to the moderator temperature. Both functions are defined only for $t > 0$; for $t < 0$ both are zero. The result of the convolution is the Ikeda-Carpenter function.

$$I_k(t) = S_k(t) \otimes R_k(t)$$

The direct convolution of the above functions is analytical and gives the result:

$$\begin{aligned} I_k(t) &= S_k(t) \otimes R_k(t) = (1-R)S_k(t) \otimes \delta(t) + R\beta S_k(t) \otimes e^{-\beta t} = \\ &= (1-R)S_k(t) + R\beta \int_{-\infty}^{\infty} S_k(\tau) \left[e^{-\beta(t-\tau)} \right] d\tau = (1-R)S_k(t) + R\beta e^{-\beta t} \int_0^t S_k(\tau) e^{\beta\tau} d\tau \\ I_k(t) &= \frac{\alpha^3}{2} \left[(1-R)t^2 e^{-\alpha t} + \frac{2R\beta}{(\alpha-\beta)^3} \left\{ e^{-\beta t} - e^{-\alpha t} \left((\alpha-\beta)^2 \frac{t^2}{2} + (\alpha-\beta)t + 1 \right) \right\} \right] \end{aligned}$$

Where the symbol [] around the exponential function within the integral symbol means that we are taking an exponential function $e^{\beta(\tau-t)}$ for $\tau < t$, and zero for $\tau > t$ and for $\tau < 0$. This explains the change of integration limits.

The profile function NPROF=13 corresponds to the convolution of the above function with a pseudo-Voigt using the TCH approximation to the Voigt function. Using the same simplification for the Ikeda-Carpenter function as that used in GSAS, we have:

Panel 12:

$$\begin{aligned} I_k(t) &= (1-R) \frac{\alpha(1-k^2)}{2k^2} \left[e^{-\alpha t(1-k)} + e^{-\alpha t(1+k)} - 2e^{-\alpha t} \right] + \\ &= \frac{R\alpha\beta(1-k^2)}{2k^2} \left[\frac{2\alpha^2 k^2}{xyz} e^{-\beta t} - \frac{1}{z} e^{-\alpha t(1-k)} - \frac{1}{x} e^{-\alpha t(1+k)} + \frac{2}{y} e^{-\alpha t} \right] \end{aligned}$$

The meaning of each parameter is given below.

The convolution of the I_k function with the pseudo-Voigt function is slightly more complicated than the functions considered in previous section. However, there are no major changes in the mathematics and the same special functions (complementary error function and exponential integral function) are used in the program.

Definition of the parameters used in the function (Laurent Chapon): Here the variable called x in previous functions has been replaced by $dt = T_i - T_h$. In the present paragraph the variable x has another meaning as summarized in the following panels:

Panels 13:

| | | | | |
|--|---|---|---|--|
| $R = e^{\left(-\frac{81.799}{\kappa\lambda^2}\right)}$ $k = 0.05$ $\alpha^- = \alpha(1 - k)$ $\alpha^+ = \alpha(1 + k)$ $x = \alpha^- - \beta$ $y = \alpha - \beta$ $z = \alpha^+ - \beta$ | $z_s = -\alpha dt + i\frac{1}{2}\alpha\gamma$ $z_u = -\alpha^- dt + i\frac{1}{2}\alpha^- \gamma = (1-k)z_s$ $z_v = -\alpha^+ dt + i\frac{1}{2}\alpha^+ \gamma = (1+k)z_s$ $z_r = -\beta dt + i\frac{1}{2}\beta\gamma$ | $u = \frac{1}{2}\alpha^- (\alpha^- \sigma^2 - 2dt)$ $v = \frac{1}{2}\alpha^+ (\alpha^+ \sigma^2 - 2dt)$ $s = \frac{1}{2}\alpha (\alpha \sigma^2 - 2dt)$ $r = \frac{1}{2}\beta (\beta \sigma^2 - 2dt)$ | $N = \frac{1}{4}\alpha \frac{(1-k^2)}{k^2}$ $N_u = 1 - R \frac{\alpha^-}{x}$ $N_v = 1 - R \frac{\alpha^+}{z}$ $N_s = -2(1 - R \frac{\alpha}{y})$ $N_r = 2R\alpha^2 \beta \frac{k^2}{xyz}$ | $y_u = \frac{(\alpha^- \sigma^2 - dt)}{\sqrt{2\sigma^2}}$ $y_v = \frac{(\alpha^+ \sigma^2 - dt)}{\sqrt{2\sigma^2}}$ $y_s = \frac{(\alpha \sigma^2 - dt)}{\sqrt{2\sigma^2}}$ $y_r = \frac{(\beta \sigma^2 - dt)}{\sqrt{2\sigma^2}}$ |
|--|---|---|---|--|

Gaussian part of the function Ω_G (Panel 14):

$$\Omega_G = \left\{ N_u e^u \operatorname{erfc}(y_u) + N_v e^v \operatorname{erfc}(y_v) + N_s e^s \operatorname{erfc}(y_s) + N_r e^r \operatorname{erfc}(y_r) \right\}$$

$$\Omega_G = (N_u \Omega_G^u + N_v \Omega_G^v + N_s \Omega_G^s + N_r \Omega_G^r)$$

Lorentzian part of the function Ω_L (Panel 15):

$$\Omega_L = -\frac{2}{\pi} \left\{ N_u \operatorname{Im}[e^{z_u} E_1(z_u)] + N_v \operatorname{Im}[e^{z_v} E_1(z_v)] + N_s \operatorname{Im}[e^{z_s} E_1(z_s)] + N_r \operatorname{Im}[e^{z_r} E_1(z_r)] \right\}$$

$$\Omega_L = (N_u \Omega_L^u + N_v \Omega_L^v + N_s \Omega_L^s + N_r \Omega_L^r)$$

The complete function is then obtained as (Panel 16):

$$\Omega = N \left\{ (1 - \eta) \Omega_G + \eta \Omega_L \right\}$$

The profile parameters concerning the Lorentzian and Gaussian broadening are the same as those in the previous functions. The dependence of the fast and slow decay constants and the mixing coefficient R with wavelength is given by:

Panel 17

$$\alpha = \frac{1}{\alpha_0 + \lambda \alpha_1} \quad \beta = \frac{1}{\beta_0}$$

$$R = e^{\left(-\frac{81.799}{\kappa\lambda^2}\right)}$$

The refinable peak-shape parameters are: α_0 , α_1 , β_0 and κ . are called, respectively, **alph0**, **alph1**, **beta0**, and **kappa**. The dependence of TOF versus d-spacing is the same as that used for NPROF=9. But remember that the values of the global parameters Z_0 , D_1 and D_2 (**zero**, **dt1** and **dt2**) do not coincide with those of NPROF=9 because the peak position in NPROF=9 coincides with the rising of the peak on the low TOF side.

External instrumental resolution function files for Neutron Time of Flight

If an IRF file is provided to treat TOF data (**Res** = 5, 6) the values of the major part of parameters are added to those given in the PCR file. Only fixed parameters, like the 2θ angle of a detector bank (called **2ThetaBank**), will substitute the value provided in the PCR file. An example of IRF file that is valid for NPROF=9 (for NPROF=13 the place of **kappa** is that of **beta1**) is given below:

```

IRF of TOF of GPPD at IPNS (Argonne) (from NBS-Si) ireso: 5
! Test of the IRF for TOF in FullProf. RES=5
! This is a comment
# This is also a comment
# IRF valid for profile function number 9 in FullProf
!      Tof-min(us)      step      Tof-max(us)
TOFRG  2500.0000      5.0000      29995.0000
!      Dtt1_i      Dtt2_i
D2TOF  7476.910      -1.040
!      TOF-TWOTH of the bank in degrees
TWOTH  144.845
!      Sig-2_i      Sig-1_i      Sig-0_i
SIGMA  0.000      31.973      0.000
!      Gam-2_i      Gam-1_i      Gam-0_i
GAMMA  0.000      2.513      0.000
!      alph0_i      beta0_i      alph1_i      beta1_i
ALFBE  0.00000      0.040675      0.584103      0.011220

```

The first line of this file is always considered as a title. The keyword **TOFRG** is only for informative or for simulation purposes. The TOF at each channel is read with the input data and it is not needed to have a fixed step. The keyword **TWOTH** fixes the value of **2ThetaBank** to the given numerical value (**twoth-given**). The corresponding value in the PCR file is replaced with **twoth-given**.

The keyword **D2TOF** introduces two instrumental parameters that do not substitute those given in the PCR file. Instead the effective parameter used within **FullProf** to calculate the TOF for a particular d-spacing is:

$$\text{TOF} = \text{ZERO} + (\text{dtt1} + \text{dtt1}_i) d + (\text{dtt2} + \text{dtt2}_i) d^2$$

Where **dtt1** and **dtt2** are refinable parameters given within the PCR file. So, if the IRF parameters are good enough the values to be put in the PCR file are 0! Notice that the global zero-shift is not accepted as an instrumental parameter. The user may refine it directly.

The same procedure is used for the rest of instrumental parameters. For instance the Gaussian variance is calculated as

$$\text{variance} = (\text{Sig-2}_i + \text{sig-2} + \text{Gsize}) d^4 + (\text{Sig-1}_i + \text{sig-1} + \text{XST2}) d^2 + (\text{Sig-0}_i + \text{sig-0})$$

where **XST2** represents the anisotropic strain contribution (see Panel 6). The rest of profile parameters follow the same pattern as that of **sigma** and **dtt**-values.

Another example of IRF, appropriate for NPROF=10, is the following:

```

IRF of GPPD at IPNS (Argonne) Res: 6
! Test of the IRF for TOF in FullProf. RES=6 Jason Hodges' TOF vs d
! This is a comment
# This is also a comment
# IRF valid for profile function number 10 in Fullprof
!      Tof-min(us)      step      Tof-max(us)
TOFRG  2500.0000      10.0000      30000.0000
!      Dtt1_i      Unused
D2TOF  7478.332      0.0
!      Dtt1t_i      Dtt2t_i      x-cross_i      Width_i
D2TOT  7459.7754      19.9522      1.2640      2.3630
!      TOF-TWOTH of the bank
TWOTH  144.845
!      Sig-2_i      Sig-1_i      Sig-0_i
SIGMA  0.000      32.000      0.000
!      Gam-2_i      Gam-1_i      Gam-0_i
GAMMA  0.000      0.000      0.000
!      alph0_i      beta0_i      alph1_i      beta1_i
ALFBE  1.470500      2.483000      -0.853300      9.298000
!      alph0t_i      beta0t_i      alph1t_i      beta1t_i
ALFBT  7.387000      27.180000      4.012400      4.733000

```

The first line of this file is always considered as a title and the rest of keywords provide parameters that are additive with respect to those given in the PCR file.

In the near future, new values of the variable RES will be introduced in order to manage complicated dependence of the peak shape instrumental parameters. In principle a look-up table for interpolating the peak shape parameters close to a particular TOF value will be introduced in order to handle the most complex situations.

Examples of simple Neutron Time of Flight refinements using *FullProf*

In the *examples* subdirectory of the *FullProf* suite directory there are several cases using refinement of TOF data coming from different sources.

The best way to start the data treatment of a TOF neutron powder pattern is by modifying a previous PCR file that works with a standard sample passed in the same instrument. It is still better to get an IRF file appropriate to the instrument on which the measurements has been performed. If this is the case, the user may take advantage of the GUI *EdPCR* that allows importing an external CIF/Shellx/Ascii file containing the structural parameters

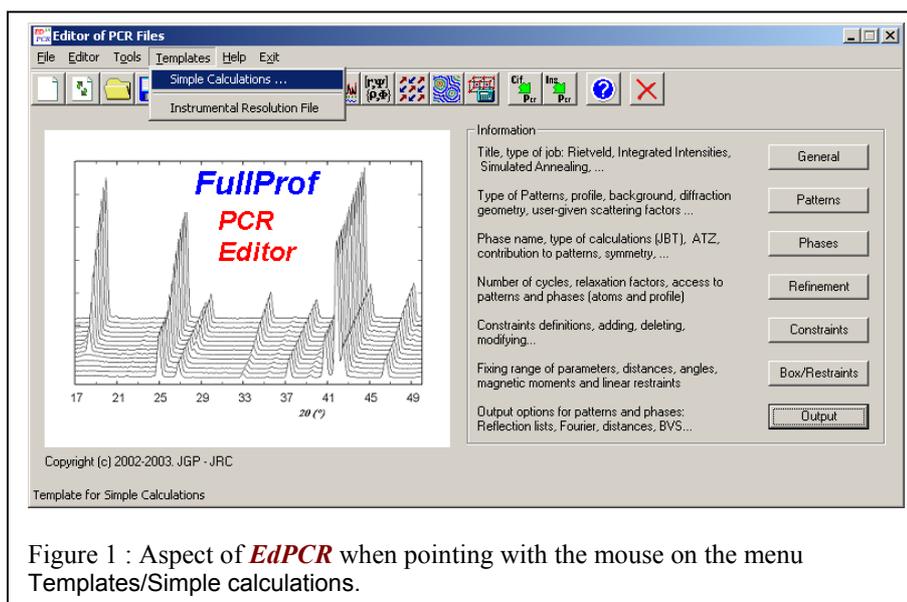


Figure 1 : Aspect of *EdPCR* when pointing with the mouse on the menu Templates/Simple calculations.

and an IRF file for profile parameters. The number of clicks for doing this task is only 4. First start *EdPCR* from *WinPLOTR* or from a DOS console, the aspect is that of the figure 1. After selecting **Simple Calculations** from the **Templates** menu, the following windows is opened:

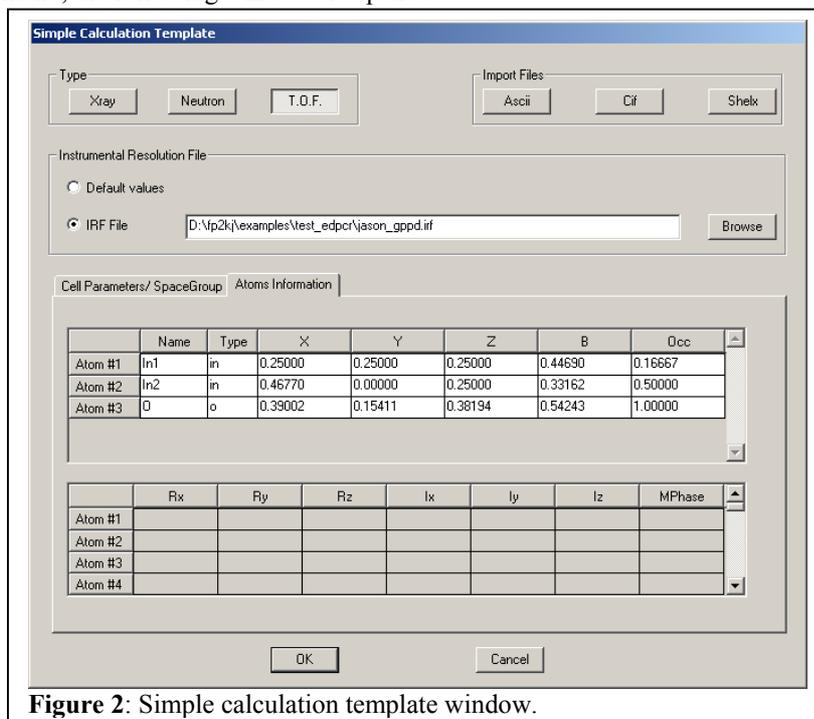


Figure 2: Simple calculation template window.

After selecting the type of job (T.O.F.) and importing a CIF file (for instance), the user should select an IRF file by browsing his(her) directory tree. Clicking the OK button terminates the procedure and one comes back to the window in Figure 1. Clicking on the save button a PCR file is automatically created. *FullProf* can now be run to

calculate the diffraction pattern according to the values for instrumental parameters given in the IRF file and the crystal structure imported from the CIF file.

The user can create (modify) his(her) own IRF file by selecting, from the **Templates** menu, the **Instrumental resolution file** item. This opens a window like that of Figure 3:

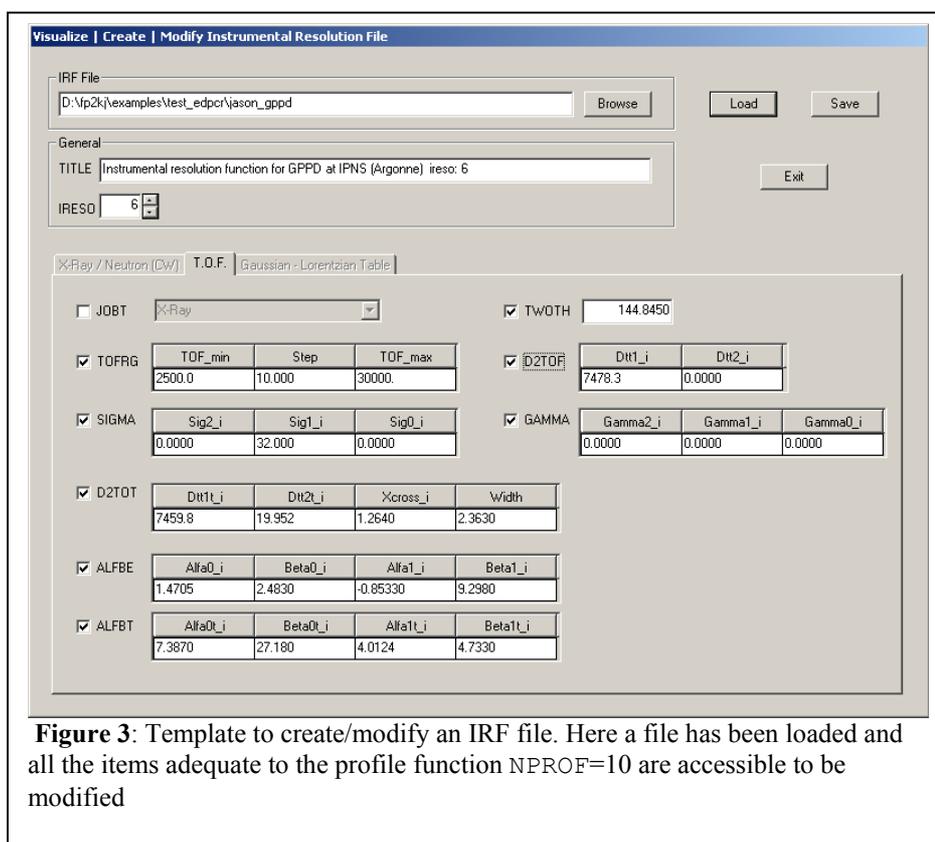


Figure 3: Template to create/modify an IRF file. Here a file has been loaded and all the items adequate to the profile function $N_{PROF}=10$ are accessible to be modified

An example that illustrates another interesting feature recently introduced in **FullProf** (the treatment of special reflections. See **fp2k.inf**) is the case of data collected in OSIRIS on the compound $Na_2Ca_3Al_2F_{14}$ (NAC for short: **nac-osiris.dat**). The files **nac-osiris.pcr** and **nac-osirisn.pcr** refine the structure of NAC considering the profile function $N_{PROF}=9$. In the second case shifts of individual reflections are allowed improving considerably the fit (see figure 4).

The second phase is the impurity CaF_2 that was present in the sample. The third phase is Cd coming from the sample holder. This phase is treated using $J_{BT}=3$, the relative intensities are fixed and read from the input files **nac-osiris3.hkl** and **nac-osirisn3.hkl** because the texture prevents a normal Rietveld treatment by calculating the structure factors.

Other cases, treating TOF data, exist in the "examples" subdirectory of the **FullProf** suite directory. A provisional list is the following (the data file name is the same as that of the PCR file):

- arg_si.pcr** : Corrected TOF data of Si from SEPD at Argonne
- cecoal.pcr** and **cecual.pcr** : TOF data from POLARIS at ISIS – Intermetallic compounds (O. Moze)
- CeO2-PEARL.pcr** : CeO_2 data collected at PEARL (ISIS) (Bill Marshall)
- lamn_pol.pcr** : $LaMnO_3$ data collected at RT on POLARIS
- nac-osiris.pcr** and **nac-osirisn.pcr**: NAC data collected on OSIRIS.
- hrpd.pcr** : CeO_2 (Round Robin) data collected on HRPD (ISIS).

This list will be updated progressively.

