APPENDIX

DETAILED DESCRIPTION OF INPUT FILES FOR FullProf

In this appendix we describe the following input files:

- Input control file: **CODFIL.pcr**
- Input data files: **FILE.dat**
- Background file: **CODFIL.bac** or **FILE.bac**
- Reflection files: **CODFILn.hkl**, **hkln.hkl**, **CODFIL.int**
- Instrument Resolution File: **MYRESOL.irf**
- Numerical profile file: **CODFIL.shp** or **global.shp**
- Intensity correction file: **CODFIL.cor**

CODFIL.PCR

This file is free format. This does not mean free format in Fortran (*)-sense: a procedure interprets the items given by the user that must obey the order given below. A space is needed between each item (except when the second is a negative number). When the program is run, messages of error reading a line of this file are normally due to a previous error. For example, the number of atoms you really wrote does not correspond to the number you put in the line following the name of the phase. Empty lines as well as lines starting with the symbol "!" in the first column are considered as comments and are ignored by the program. This file is re-written by ***FullProf*** at the end of a job. The original file may be suppressed or conserved depending on the value of a flag. The program generated PCR-file contains comments (mnemonics for each variable) to facilitate the recognition of the different variables.

If the user starts his(her) CODFIL.PCR file with the left-adjusted capital "COMM", the new CODFIL.PCR file conserves the initial format; that is the usual single pattern format, otherwise the program generates a PCR-file with a format adapted to the multiple pattern refinement. If the user introduce his(her) own comments, they are not saved in the new version of the file. The best to start working with ***FullProf*** is to edit a previously existent PCR-file and modify it as wished. The inexperienced user can use some of the programs that are specially developed to edit a PCR-file (see for instance the program AXES by Hugo Mndar [ ]). A dedicated tool will be soon available for the operating systems Windows and Linux.

In the following we use the term LINE as a label for reference purposes in the document. The line number does not correspond to the effective ordinal number of the line appearing in an actual PCR-file. When a block of similar lines have to be repeated for each pattern (it is supposed that we are dealing with NPATT patterns simultaneously) the keyword *NPATT_Lines* starts the block and the block is finished by the keyword *End_NPATT_Lines*, this corresponds to a loop on the index of the pattern. Sometimes the number of lines is less than NPATT. This occurs when the line is optional and depends on the value of a pattern-dependent variable.

In this document we shall describe the format of the PCR-file adapted to multipattern refinements. This format derives from the single pattern one by just splitting some lines where flags depending on the pattern number were written in a single line. The program is, and will continue to be, totally compatible with the old single pattern format even if new items corresponding to new options are concerned. When there are differences between the two formats we will give the lines of the single pattern format in **black**

font preceded with the word ***LINE n*** together with the new ones in **blue font** starting with **LINE n**. In fact the places where differences, apart from the fact that the loops on the number of patterns reduce to 1, are the LINES 2, 3, 4, 5, 7, 9, 19, 19-1, 19-3, and 19-4.

Sometimes we shall use mathematical formulas to clarify the meaning of a variable, the complete explanation is given in the Mathematical section of the ***FullProf*** manual. The scattering variable is represented, in general, by the symbol *T*. When the context requires an explicit reference we use *2θ*, *TOF* or *E*. For multiple patterns refinement we shall use the variable *n_pat* to index a diffraction pattern. We will write **XXX**(*n_pat*) for the name of a variable **XXX** that depends of the diffraction pattern *n_pat*. When the context is clear the variable will be referenced simply as **XXX**.

The content of the file CODFIL.pcr is described in the following.

LINE 1: TITLE (any 80 characters used to label the printout)

If the first four character of TITLE correspond to the word TITL the file is given in "command mode" (not available yet). If the first four characters of TITLE correspond to **COMM**, the new CODFIL.PCR file conserves the initial format; that is the usual single pattern format, otherwise the program generates a PCR-file with a format adapted to the multiple pattern refinement.

The generated PCR-file include comment lines give a keyword for each variable in order to be easily recognised by the user. This comment line has been included below to facilitate the recognition of the different lines.

The next two lines should not be given if one wishes to use the conventional single pattern format of the PCR-file. However the new mutipattern format works properly also for a single pattern.

LINE 2: keyword NPATT (5 characters +1 integer) (OPTIONAL)

Keyword **NPATT** followed by an integer, **npatt**, corresponding to the number of patterns to be treated simultaneously.

This line may be suppressed for a single pattern (**npatt**=1) and the rest of the file follows the same format as that of previous versions of ***FullProf*** for single pattern refinement.

Example:

```
NPATT  3
```

LINE 3: W_PAT (5 characters + npatt integers) (OPTIONAL, only if **NPATT** is provided**)**

Keyword **W_PAT** followed by **npatt** integers corresponding to the weight of each pattern in the refinement. The program normalises the given values in order to get 1 for the sum of all weights.

Example:

```
W_PAT  0.5 0.25  0.25
```

LINE 4: NPHASE, IDUM, IASG, NRELL, ICRYG, IOPTI, IAUTO (6 integers)

Comment line: ! Nph Dum Ias Nre Cry Opt Aut

The items of this line together with those of the next line are merged in a single line for the single patter format as:

***LINE 4*: JOBTYP, NPROF, NPHASE, NBCKGD, NEXCRG, NSCAT, NORI, IDUM, IWGT, ILOR, IASG, IRESO, ISTEP, NRELL, ICRYG, IXUNIT, ICORR IOPTI, IAUTO**
(19 integers) – Single pattern format

Comment line:!Job Npr Nph Nba Nex Nsc Nor Dum Iwg Ilo Ias Res Ste Nre Cry Uni Cor Opt Aut

NPHASE

Number of phases

IDUM

=1 If equal to 1 and some of the phases are treated with Profile Matching modes, the criterion of convergence when shifts are lower than a fraction of standard deviations is not applied.

=2 If equal to 2, the program is stopped in case of local divergence: chi2(icycle+1)> chi2(icycle)

=3 If equal to 3 the reflections near excluded regions (Tlim±wdt*FWHM) are not taken into account to calculate the Bragg R-factor. These reflections are omitted in the output files with hkl's.

If ABS(**JOBTYP**(*n_pat*))>1 (pattern calculation mode, see below) and **IDUM** is different of zero a file CODFIL.sim is generated

IASG

=0 The reordering of all reflections is performed only at the first cycle

=1 All reflections are ordered at each cycle.
(If **JBT**=2 for one phase, **IASG** is changed to 1 by the program)

NRELL

Number of parameters to be constrained within given limits. At the end of the file you must give a list of **NRELL** lines specifying the number and the limit of each parameter. This variable must be given in the case of using Montecarlo or Simulated Annealing techniques.

ICRYG

≠0 Only integrated intensity data will be given. No profile parameters are needed.
The format of the file changes slightly in the following.

=1 Refinement of single crystal data or integrated intensity powder data.

=2 No least-squares algorithm is applied. Instead a Montecarlo search of the starting configuration is performed. A selected number of parameters **NRELL** are moved within a box defined by the **NRELL** relations fixing the allowed values of the parameters. The best (lowest R-factor) NSOLU solutions are printed and the CODFIL.pcr file is updated with the best solution. This option is only efficient for a small number of parameters (3-4). The use of the next option is recommended for large number of parameters.

=3 The Simulated Annealing optimisation method is chosen. A selected number of parameters **NRELL** are moved within a box defined by the **NRELL** relations fixing the allowed values of the parameters. Different boundary conditions may be used. See below.

IOPTI

=0 The general procedures are used.

=1 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.

IAUTO

=0 The program treats the codewords as usual. The user has the total control of the numbering of parameters. The maximum number of parameters to be refined is fixed manually.

=1 The program treats the codewords of the refined parameters automatically. In this case the user may put, by hand, the codes for making constraints as usual, and just put "1.00" to inform the program that the corresponding parameter will be refined. The program will attribute automatically the codeword. In the automatic mode there is no "*holes in the matrix*" and the number of refined parameters may be different from the specified by the user in the corresponding line. The automatic mode is useful when one has to fix a parameter in the middle of many others: just put the codeword (including the multiplier) to zero. Sometimes the message "*hole in the matrix*" still appears. In such cases you have just to increase artificially the number of parameters to be refined or just put it equal to zero, or, in the worst case, suppress a large number of codewords (just leaving the multiplier 1.0). Be careful in using this option together with the automatic re-writing of the PCR-file.

[NPATT_Lines] **A line should be given for each pattern**

LINE 4n: JOBTYP, NPROF, NBCKGD, NEXCRG, NSCAT, NORI, IWGT, ILOR, IRESO, ISTEP, IXUNIT, ICORR (12 integers)
Comment line: ! Job Npr Nba Nex Nsc Nor Iwg Ilo Res Ste Uni Cor

JOBTYP(*n_pat*)
= 0 X-ray case
= 1 Neutron case (constant wavelength, nuclear and magnetic)
= 2 Pattern calculation (X-ray)
= 3 Pattern calculation (Neutron, constant wavelength)
=-1 Neutron case (T.O.F., nuclear and magnetic)
=-3 Pattern calculation (Neutron, T.O.F.)

The value of **JOBTYP**(*n_pat*) may be different for each pattern when one wants to perform combined refinements: X-ray + neutron diffraction patterns treated simultaneously.
If ABS(**JOBTYP**)>1 and **IDUM**=1 (see below) a calculated pattern is created with the name CODFIL.SIM in format corresponding to **INSTRM**(*n_pat*)=0. A Poisonian noise is added to the deterministic calculated pattern. The statistics is controlled by the value of the scale factor. This pattern corresponds to an "ideal observed" pattern and can be use for simulation purposes in order to investigate the effect of systematic errors on the structural parameters and on the reliability factors.

NPROF(*n_pat*)
Default value for selection of a normalised peak shape function. Particular values can be given for each phase, in that case the local value is used.
=0 Gaussian.
=1 Cauchy (Lorentzian).
=2 Modified 1 Lorentzian.
=3 Modified 2 Lorentzian.
=4 Tripled pseudo-Voigt.
=5 pseudo-Voigt.
=6 Pearson VII.
=7 Thompson-Cox-Hastings pseudo-Voigt convoluted with axial divergence asymmetry function (Finger, Cox & Jephcoat, J. Appl. Cryst. 27, 892, 1994).
=8 Numerical profile given in CODFIL.shp or in GLOBAL.shp.
=9 T.O.F. Convolution pseudo-Voigt with back-to-back exponential functions.
=10 T.O.F. Same as 9 but a different dependence of TOF versus d-spacing.
=11 Split pseudo-Voigt function.
=12 Pseudo-Voigt function convoluted with axial divergence asymmetry function.

NBCKGD(*n_pat*)
=0 Refine background with a polynomial function.
=1 Read background from file CODFIL.bac. The format of this file is explained in this appendix.
=2,3,...,N Linear interpolation between the N given points. If **NBCKGD**<0 but ABS(**NBCKGD**)>4 the interpolation is performed using cubic splines
=-1 Refine background with Debye-like + polynomial function.
=-2 Background treated iteratively by using a Fourier filtering technique. An extra parameter is read below. The starting background is read from file FILE.bac as for NBCKGD=1.
=-3 Read 6 additional polynomial background coefficients

NEXCRG(*n_pat*)
Number of excluded regions.

NSCAT(*n_pat*)
Number of scattering sets (zero in most cases). In the case of giving a table of values for the scattering factor and **NSCAT**>0, the program performs an internal fit in order to get the appropriate coefficients of the exponential expansion (see below) approximating the scattering factor. If **NSCAT** is negative, a linear interpolation between the values of the table is performed.

NORI(*n_pat*)
=0 Preferred orientation function No 1
=1 Preferred orientation function No 2 (March)

IWGT(*n_pat*)
=0 Standard least squares refinement
=1 Maximum likelihood refinement
=2 Unit weights

ILOR(*n_pat*)
= 0 Standard Debye-Scherrer geometry, or Bragg-Brentano if the illuminated area does not exceed the sample surface. If Bragg-Brentano geometry is used but the above condition is not fulfilled, the intensity data must be corrected for the geometric effect before attempting any refinement. A partial correction can be performed by using the parameter **SENT0**.
= 1 Flat plate PSD geometry
=-1 The Lorentz-Polarisation correction is not performed. It is supposed that the profile has been previously corrected for Lorentz-Polarisation.
=2 Transmission geometry. Flat plate with the scattering vector within the plate (Stoe geometry for X-rays)
=3 Special polarisation correction is applied even if the format of the DAT-file does not correspond to one of the synchrotron explicitly given formats (see below). This must be used for synchrotron data given in a (X, Y, Sigma) format (**INSTRM**=10).

IRESO(*n_pat*)
=0 Resolution function of the instrument is not given
≠0 The next line contains the name of the file where the instrumental resolution function is given for an instrument using as scattering variable 2θ.

This options works, at present, only for constant wavelength type of data. The profile is assumed to be a Voigt function (**NPROF**=7). 12 parameters or a table determine the resolution function. $U_i, V_i, W_i, X_i, Y_i, Z_i$ (i=1,2 for λ_1 and λ_2)
The different types of functions are:

IRESO =1
$$H_G^2 = (U_i \tan\theta + V_i)\tan\theta + Wi$$
$$H_L = X_i \tan\theta + \frac{Y_i}{\cos\theta} + Z_i$$

IRESO =2
$$H_G^2 = (U_i \tan\theta + V_i)\tan\theta + Wi$$
$$H_L = (X_i 2\theta + Y_i)2\theta + Z_i$$

IRESO =3
$$H_G^2 = (U_i 2\theta + V_i)2\theta + W_i$$
$$H_L = (X_i 2\theta + Y_i)2\theta + Z_i$$

IRESO =4 List of values 2θ, $H_G(2\theta)$, $H_L(2\theta)$
(a linear interpolation is applied for intermediate 2θ)

The format of this file is described below in this appendix.

ISTEP(*n_pat*)
=1,2,3,...,N
If **ISTEP**>1 the number of data points is reduced by a factor of ISTEP. Only those points corresponding to the new step size **ISTEP**×**STEP** (see LINE 3 below) are taken into account in the refinement. Useful for speed-up preliminary refinements.

IXUNIT(*n_pat*)
Units of the scattering variable
=0 2θ in degrees
=1 T.O.F. in micro-seconds
=2 Energy in keV.

ICORR(*n_pat*)
=0 No correction is applied
=1 A file with intensity corrections is read.
=2 A similar file is read but the coefficients of an empirical function and their standard deviations are read instead of directly the corrections.
The format of this file is described in this appendix.

[End_NPATT_Lines]

This block of lines is not given at all in the old single pattern format.

[NPATT_Lines]

LINE 5: FILEDAT(*n_pat*) **(Character)**
Comment line: ! File names of data (patterns) files

Name of the pattern files including the extension in case that is different from ".dat"

[End_NPATT_Lines]

[NPATT_Lines]

LINE 6: FILERES(*n_pat*) **(Character)**
Comment line: ! Resolution File names for Pattern #N
Name of the file with the instrumental resolution function. To be given only in the case of **IRESO** ≠0. The items in **FILERES** are read in free format. The format of this file is described below in this appendix.
The effective number of lines may be less than **NPATT**. Only the names of the files for which **IRESO**(*n_pat*)≠0 should be given.

[End_NPATT_Lines]

LINE 7: MAT, NXT, IPL1, JCIL, JSY, ISHOR (6 integers)
Comment line: ! Mat Pcr Syo Rpa Sym Sho

This line merges with the next block into a single line for the old single pattern format as:

***LINE 7*: IOT, IPL, IPC, MAT, NXT, LST1, LST2, LST3, IPL1, IPL2, INSTR, JCIL, JSY, JLKH, JFOU, ISHOR, IANAL**
(17 integers) – Single pattern format
Comment line: !Ipr Ppl Ioc Mat Pcr Ls1 Ls2 Ls3 Syo Prf Ins Rpa Sym Hkl Fou Sho Ana

MAT
=0 No action
=1 The correlation matrix is written in the file CODFIL.out
=2 The diagonal of Least Squares matrix is printed before inversion at every cycle.

NXT
=0
=1 CODFIL.pcr is re-written with updated parameters
=2 A new input file is generated conserving the old one. The new file is called CODFIL.new

IPL1
=0
=1 Symmetry operators are written in CODFIL.out. The file CODFIL.sym is also generated if **JSY**=1.

JCIL
=0
=1 Prepares the output file CODFIL.rpa. If the file exists before running the program the new data are APPENDED.
=2 Prepares file CODFIL.sav (sequential refinements) "

JSY
=0
=1 Prepares CODFIL.sym (if 1, **IPL1** must be set to 1)

ISHOR
=0
=1 Suppress the output from each cycle. Only the information from the last cycle is printed.

[NPATT_Lines]

LINE 7n: IOT, IPL, IPC, LST1, LST2, LST3, IPL2, INSTR, JLKH, JFOU, IANAL
(11 integers)
Comment line: ! Ipr Ppl Ioc Ls1 Ls2 Ls3 Prf Ins Hkl Fou Ana

Flags controlling the output of the program or the format of input data. The usual value of the flags are written in blue.

IOT(*n_pat*)
=0 No action
=1 Observed and calculated profile intensities written in CODFIL.out
=2 The files CODFILn.sub with the calculated profile of each phase are generated.
=3 As 2 but the background is added to each profile.

IPL(*n_pat*)
=0 No action
=1 Line printer plot in CODFIL.out
=2 Generates the background-file FILE.bac
=3 Puts difference pattern in file FILE.bac

IPC(*n_pat*)
=0 No action
=1 List of observed and calculated integrated intensities in CODFIL.out
=2 The reflections corresponding to the second wavelength are also written if different from the first one.

LST1(*n_pat*)
=0 No action
=1 Reflection list before starting cycles is written in CODFIL.out

LST2(*n_pat*)
=0 No action
=1 Corrected data list (profile intensities before refinement) written in CODFIL.out.
=4 In some versions of ***FullProf*** a plot of the diffraction pattern is displayed on the screen at each cycle of refinement.

LST3(*n_pat*)

=0 No action
=1 Merged reflection list written in CODFIL.out

IPL2(*n_pat*)
Generates the file CODFIL.prf containing the information to plot the observed versus calculated diffraction pattern as well as the reflection positions, etc. The output forma
=0
=1 Format suitable for ***WinPLOTR***, and other plotting programs.
=2 Format suitable for IGOR (MacOS, Windows software)
=3 Format suitable for KaleidaGraph (MacOS, Windows software) and ***WinPLOTR***.
=4 Format suitable for Picsure, Xvgr (Sun-Unix Software)

INSTRM(*n_pat*) (The detailed explanation of the formats is given in the ***FILE.dat*** section)

=0 Data supplied in free format. Up to seven comment lines are accepted. The first three real numbers found at the beginning of a line are interpreted as T_i, *step* and T_f and. The following lines after T_i, *step* and T_f must contain $NPTS=(T_f-T_i)/step+1$ values of the intensity profile. Data format of TOF raw data from Argonne are also interpreted by this value of **INSTRM**.
=1 D1A/D2B format (original Rietveld-Hewat format: the first line must be T_i, *step* and T_f
=2 D1B old format (DEC-10)
=3 Format corresponding to the ILL instruments D1B and D20.
=±4 Brookhaven synchrotron data.
4: First line: $2\theta_i$, step, $2\theta_f$ (free format). Rest of file: pairs of lines with 10 items like
Y1 Y2 ..... Y10 -- (10F8) intensities
S1 S2 ..... S10 -- " standard deviations
-4: Format given by DBWS program for synchrotron data. (Version DBW3.2S-8711)
=5 Data from GENERAL FORMAT for TWO AXIS instrument. Three lines of text followed by two lines with the items:
NPTS, TSample, Tregul, Ivari, Rmon1, Rmon2
T_i, *step*, T_f
Set of lines containing 10 items corresponding to the Intensities in format 10F8.1, up to *NPTS* points ($NPTS=(T_f-T_i)/step+1$), followed by the corresponding standard deviations in format (10f8.2) if *Ivari*=1. If *Ivari*=0 the standard deviations are calculated as

$$\sigma(y) = \sqrt{y \times \frac{Rmon1}{Rmon2}} \ .$$

=6 D1A/D2B standard format prepared by D1A(D2B)SUM (ILL), ADDET(LLB), MPDSUM (LLB) or equivalent programs.
=7 Files from D4 or D20L
=8 Data from DMC at Paul Scherrer Institute.
=9 Data of file CODFIL.uxd generated by the Socabim software on x-ray diffractometer.
=10 X, Y, Sigma format with header lines. In all cases the first six lines are considered as comments. If in the first line (left adjusted) appears the keyword XYDATA, then the following five lines are considered as the heading of the file. Among these five lines the following keywords and values have a meaning to the program:
INTER *fac_x fac_y Interpol Stepin*
TEMP *tsamp*
fac_x internal multiplier of X-values
fac_y internal multiplier of Y and Sigma-values
Interpol
=0 Variable step is used in the program
=1 The variable step data are interpolated internally to the constant step *Stepin*.
=2 Data are supplied directly at constant step

If no sigma values are provided the program assumes that $\sigma(y) = \sqrt{y}$. You can add comments to the data file if they start with the character "!" in the first position of the line. These lines are ignored by the program.

=11 Data from variable time X-ray data collection. The first four lines are considered as comments. The following lines are:

2Thetai, step, 2Thetaf Comment

(Time, Intensity) in format 5(F6, I10). The program uses the information contained in Time to normalise the observed intensities to the average time <Time> and to calculate the variance of the normalised values.

=12 The input data file conforms to GSAS standard data file.
BINTYP = LOG6, TIME_MAP and LPSD are not yet available.

JLKH(*n_pat*)
Prepares CODFIL.hkl. See the section ***Output files*** for details.

=0 No action

=1 Outputs: Code, h,k,l , $mult, d_{hkl}, 2\theta$, FWHM, I_{obs} , I_{calc} , $I_{obs} - I_{calc}$
or if ABS(**JOBTYP**)>1 : h,k,l , $mult, I_{calc}, 2\theta, d_{hkl}$

=2 Output for SIRPOW.92: h,k,l , $mult, \sin\theta/\lambda, 2\theta, FWHM, F^2, \sigma(F^2)$

=±3 Output of Real and Imaginary parts of Structure Factors: h,k,l , $mult, F_{real}, F_{imag}, 2\theta, Intensity$

=4 Output of: $h,k,l,F^2,\sigma(F^2)$.

=5 Output of: $h,k,l,mult,F_{calc},T_{hkl},d_{hkl},Q_{hkl}$

JFOU(*n_pat*)
Prepares CODFIL.fou. See the section ***Output files*** for details.

=0 No action
=1 Cambridge format
=2 SHELXS format are also in (Prepares also the file CODFILn.ins)
=3 FOURIER format (Prepares also the file CODFILn.inp)
=4 GFOURIER format (Prepares also the file CODFILn.inp)

IANALY(*n_pat*)

=0 No action
=1 Provides an analysis of the refinement at the end of the summary file CODFIL.sum.

[End_NPATT_Lines]

[NPATT_Lines] **[Only if ICRYG=0]**
[2θ]
LINE 8: LAMBDA1, LAMBDA2, RATIO, BKPOS, WDT, CTHM, TMV, RLIM, RKK (9 reals)
Comment line:!lambda1 lambda2 Ratio Bkpos Wdt Cthm muR AsyLim Rpolarz -> Patt #N [T.O.F or Energy dispersive]
LINE 8: BKPOS, WDT, IABSCOR (2 reals, 1 integer)
Comment line:!Bkpos Wdt Iabscor for Pattern# N

LAMDA1(*n_pat*)
wavelength λ_1

LAMDA2(*n_pat*)

wavelength λ_2 (=λ_1 for monochromatic beam)

RATIO(*n_pat*)
Intensity ratio I_2 / I_1
If **RATIO** < 0 the parameters U,V,W (see below) for the second wavelength are read separately.

BKPOS(*n_pat*)
Origin of polynomial for background (in 2θ degrees or μseconds for TOF)

WDT(*n_pat*)
Width (range) of calculated profile of a single Bragg reflection in units of FWHM (typically 4 for Gaussian and 20-30 for Lorentzian, 4-5 for TOF). The value of the peak shape function is set to zero for ABS(x) > **WDT** × FWHM, with x=T_i-T_h.

CTHM(*n_pat*)
Coefficient for monochromator polarisation correction. See Mathematical section.

TMV(*n_pat*)
Absorption correction coefficient μR, used only for refinement on cylindrical samples and flat samples with symmetrical θ-2θ scanning (the scattering vector lying within the sample plane).

μ = effective absorption coefficient
R = radius or thickness of the sample

RLIM(*n_pat*)
Peaks below this 2θ limit are corrected for asymmetry.

RKK(*n_pat*)
Polarisation factor (synchrotron, **ILOR**=3)
Fraction of mosaic-crystal (transmission geometry, **ILOR**=2)

IABSCOR(*n_pat*)

Type of absorption correction for T.O.F. data

=1 Flat plate perpendicular to the incident beam
=2 Cylindrical sample
=3 Exponential correction $Abs = \exp[-c\lambda^2]$

[End_NPATT_Lines]

LINE 9: MCYCLE, EPS, RELAX(4) (1 integer - 5 reals)
Comment line: !NCY Eps R_at R_an R_pr R_gl

This line merges with the next block into a single line for the old single pattern format as:
***LINE 9*: MCYCLE, EPS, RELAX(4), THMIN, STEP, THMAX, ALPSD, SENT0**
(1 integer, 10 reals) – Single pattern format
Comment line: ! NCY Eps R_at R_an R_pr R_gl Thmin Step Thmax PSD Sent0
Comment line: ! NCY Eps R_at R_an R_pr R_gl TOF-min <Step> TOF-max
Comment line: ! NCY Eps R_at R_an R_pr R_gl Emin <Step> Emax

MCYCLE
Number of cycles of refinement

EPS
Forced termination when *shifts* < **EPS** × e.s.d. A reasonable value is **EPS**=0.2 or lower.

RELAX
The four relaxation factors for shifts :

1. Atomic parameters: co-ordinates, magnetic moments, site occupancies and isotropic displacement (temperature) factors
2. Anisotropic displacement (temperature) factors
3. Profile parameters, asymmetry, overall displacement (temperature), cell constants, preferred orientation parameters, strains, size, propagation vectors & user-supplied parameters.
4. Global parameters, zero-shift, background, displacement and transparency.

[NPATT_Lines]

LINE 9n: THMIN, STEP, THMAX, ALPSD, SENT0 (5 reals)
Comment line:! Thmin Step Thmax PSD Sent0 -> Patt #N
[T.O.F]
LINE 9n: THMIN, STEP, THMAX (3 reals)
Comment line:! TOF-min <Step> TOF-max PSD Sent0 -> Patt# N
[Energy dispersive]
LINE 9n: THMIN, STEP, THMAX (3 reals)
Comment line:! Emin <Step> Emax -> Patt# N

THMIN(*n_pat*)
Starting angle 2θ /TOF/Energy for calculated pattern in degrees/micro-seconds/keV. For normal refinement the triplet **THMIN, STEP, THMAX** is superseded by reading the provided file with profile intensities.

STEP(*n_pat*)
Step size in degrees 2θ /micro-seconds/keV

THMAX(*n_pat*)
Ending angle 2θ /TOF/Energy for calculated pattern in degrees/micro-seconds/keV

ALPSD(*n_pat*)
Incident beam angle at sample surface in degrees

SENT0(*n_pat*)
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:

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

[End_NPATT_Lines]

[NPATT_Lines] **[only if ICRYG=0]**

LINE 10: POS, BCK (2 reals)(NBCKGD(*n_pat*) **Lines, to be given only if NBCKGD**(*n_pat*)**≠0)**
Comment line:!2Theta/TOF/E(Kev) Background for Pattern #N

If **NBCKGD**(*n_pat*) > 2 or **NBCKGD**(*n_pat*) <-3, there are ABS(**NBCKGD**) lines with:
POS(*n_pat*)
Position in degrees/micro-seconds/keV

BCK(*n_pat*)
Background counts at this position

If **NBCKGD**(*n_pat*) > 0 linear interpolation
If **NBCKGD**(*n_pat*) < 0 cubic splines interpolation

LINE 11: ALOW, AHIGH (2 reals)(NEXCRG(*n_pat*) **lines, to be given only if NEXCRG**(*n_pat*)**≠0)**
Comment line:!Excluded regions (LowT HighT) for Pattern #N

If **NEXCRG**(*n_pat*) > 0, enter limits of excluded regions :

ALOW(*n_pat*)
Low scattering variable bound in degrees/micro-seconds/keV

AHIGH(*n_pat*)
High scattering variable bound in degrees/micro-seconds/keV

[End_NPATT_Lines]

[NPATT_Lines] **(optional lines, to be given only if NSCAT**(*n_pat*)**≠0)**
LINE 12: NAM, DFP, DFPP, ITY (Character A4 - 2 reals - 1 integer) (NSCAT(*n_pat*) **Lines)**
Comment line: ! Additional scattering factor for Pattern #N

NSCAT(*n_pat*) sets of lines (needed only if you wish to enter your own scattering length or form factor instead of using the values stored in internal table; scattering factors and anomalous dispersion corrections incorporated in the program.

NAM
Symbol identifying this set (left justified). This symbol is converted to lower case for X-ray diffraction global data.

DFP
Df' or Neutron Scattering length *b*

DFPP
Df'' (ignored in the neutron case)

ITY
=1 Indicates that you are giving a magnetic form factor
=0 And and **JOBTYP**=1 or 3 (neutron case) THE NEXT LINE MUST NOT BE GIVEN. You are just giving the Fermi length of the species **NAM** in **DFP**.
=2 Indicates that you are giving just Df' and Df'' and the program will use tabulated coefficients for the sinθ/λ dependent part of *f* (X-rays). The name **NAM** must correspond in this case to a valid tabulated name (See Notes(1, 2) below). At variance with the name used for determining the scattering factor in the description of atoms, the chemical symbol used in **NAM** must be LOWER CASE. This is the most simple way of giving anomalous dispersion parameters for synchrotron data.

LINE 12b: (to be given only if ITY≠0)
A1, B1, A2, B2, A3, B3, A4, B4,C (9 reals) or
A, a, B, b, C, c, D (7 reals) or
A, B (2 reals)

- One line of the form *A1,B1,A2,B2,A3,B3,A4,B4,C* giving the coefficients for the analytic approximation to the X-ray form factor *f*. The expression is the following:

$$f(\frac{\sin\theta}{\lambda}) = \sum_{i=1}^{4} a_i \exp\{-b_i(\frac{\sin\theta}{\lambda})^2\} + c$$

- Or one line of the form *A,a,B,b,C,c,D* giving the coefficients for the analytic approximation to the magnetic form factor *f* (P.J. Brown, Vol C new ed. ITC) similar to the above one but with the sum extended to 3 terms only.
- Or a set of lines of the form : $sin\theta/\lambda$ - *f*. The set is terminated by a line with *-100* in first position.

If the first form is desired, A2 must not be zero.

Note: Scattering length, X-rays and magnetic form factors are stored in internal tables. To use them you must give the "name" of the scatterer using UPPER CASE chemical symbols (scattering length), chemical species (e.g. CU+2, for the X-rays form factor of Cu^{2+}) or M followed by the chemical symbol and formal charge state (e.g. MNI2, for magnetic form factor of Ni^{2+}). These names are given in lines 11-4 behind the atom name (see below). In the case of giving user supplied Df' and Df'' the chemical symbol is converted to LOWER CASE. For X-ray diffraction the form factors symbols behind the atom name could be given either in LOWER or UPPER case.
If the magnetic form factors of the rare earths are to be used, two options exist.

Example:
MHO3: magnetic form factor of Ho^{3+} as $\langle j_0 \rangle$
JHO3: magnetic form factor of Ho^{3+} as $\langle j_0 \rangle + c_2 \langle j_2 \rangle$
where c_2 has been calculated using the dipolar approximation. Seven coefficients A,a,B,b,C,c,D are used for approximating $\langle j_0 \rangle + c_2 \langle j_2 \rangle$.

Note: If a table is supplied and **NSCAT**(*n_pat*)> 0 the program performs an internal fit to NINE coefficients and this could fails. If you want a linear interpolation **NSCAT**(*n_pat*) must be negative and the list is given as:

1000.0× $2sin\theta/\lambda$ - *f*

[End_NPATT_Lines]

LINE 13: MAXS (1 integer)
Comment line: Maxs !Number of refined parameters

MAXS
Number of parameters varied. In case of using **IAUTO** =1 the program determines automatically the number of parameters to be refined.

[NPATT_Lines] **[Only if ICRYG=0]**

LINE 14: ZER, FLGZER, SYCOS, FLCOS, SYSIN, FLSIN, LAMBDA, FLAMBDA, IGLMORE (8 reals - 1 integer)
Comment line:! Zero Code Sycos Code Sysin Code Lambda Code More -> Patt #N

[T.O.F]
LINE 14: ZER, FLGZER, DTT1, FDTT1, DTT2, FDTT2, TOFTET (7 reals)
Comment line:! Zero Code Dtt1 Code Dtt2 Code 2SinTh -> Patt #N

[Energy dispersive]
LINE 14: ZER, FLGZER, STE1, FSTE1, STE2, FSTE2, TOFTET (7 reals)
Comment line:! Zero Code StE1 Code StE2 Code 2SinTh -> Patt #N

ZER(*n_pat*)

Zero point for T (in degrees/microseconds/keV): $T_{True} = T_{Exp} - ZER$

FLGZER(*n_pat*)
Codeword for zero-shift

SYCOS(*n_pat*)
Systematic 2θ shift with $cos\theta$ dependence. Sample displacement in θ - 2θ diffractometers

FLCOS(*n_pat*)
Codeword for **SYCOS**

SYSIN(*n_pat*)
Systematic 2θ shift with $sin2\theta$ dependence. Sample transparency coefficient in θ-2θ diffractometers

FLSIN(*n_pat*)
Codeword for **SYSIN**

LAMBDA(*n_pat*)
Wavelength to be refined (only a single wavelength can be refined)

FLAMBDA(*n_pat*)
Codeword for **LAMBDA**.
Cell parameters should be fixed if wavelength is to be refined.

DTT1(*n_pat*), **DTT2**(*n_pat*)
The TOF position of a reflection, for **NPROF**(*n_pat*)= 9, with d-spacing *d* is calculated using the formula:

TOF = **ZER** + **DTT1** *d* + **DTT2** d^2

The component of thee TOF position of a reflection, for **NPROF**(*n_pat*)= 10, with d-spacing *d* for the region of epithermal neutrons (**DTT2** is not used) is calculated using the formula:

TOF_e = **ZER** + **DTT1** *d*

See next line to see the calculation of the TOF position when **NPROF**(*n_pat*)= 10.

FDTT1(*n_pat*), **FDTT2**(*n_pat*)
Codewords for **DTT1, DTT2**

TOFTET(*n_pat*)
Value of $2\sin\theta$ for the detector bank. Used for obtaining the wavelengths and for Lorentz factor correction.

IGLMORE(*n_pat*)
If different from zero the following line is read

LINE 15: **P0, CP0, CP, CCP, TAU, CTAU (5 reals, to be given only if IGLMORE≠0)**
Comment line:! P0 Cod_P0 Cp Cod_Cp Tau Cod_Tau

Micro-absorption coefficients and codes (only used if **ILOR**(*n_pat*)=0 and **JOBTYP**(*n_pat*)=0 or 2). Only valid for Bragg-Brentano geometry.
The value of the parameters correspond to the variables in the following formula:

$$P(\mathbf{h}) = P_0 + C_p \frac{\tau}{\sin\theta_{\mathbf{h}}}\left(1 - \frac{\tau}{\sin\theta_{\mathbf{h}}}\right)$$

See Mathematical section for details.

P0(*n_pat*), value of P_0 ; **CP0**(*n_pat*), codeword of P_0

CP(*n_pat*), value of C_p; **CCP**(*n_pat*), codeword of C_p
TAU(*n_pat*), value of τ; **CTAU**(*n_pat*), codeword of τ.

[T.O.F.]
LINE 16: **ZERt, DTT1t, DTT2t, XCROSS, WCROSS (5 reals) (OPTIONAL, to be given only if IXUNIT(*n_pat*)=1 and NPROF(*n_pat*)=10)**
Comment line: ! Zerot/Code Dtt1t/Code Dtt2t/Code x-cross/Code Width/Code

This line corresponds to the formulation, by Jason Hodges, of the TOF versus d-spacing that divides the spectrum in three parts depending on the neutron energy. The epithermal (fastest neutrons), crossover (intermediate) and thermal regions. It is supposed that in the previous line the parameters allowing the calculation of TOF as a function of d-spacing correspond to epithermal neutrons. In this line the parameters controlling the thermal and crossover regions. See Mathematical section for details.

ZERt(*n_pat*)
Zero shift for thermal neutrons
DTT1t(*n_pat*)
Coefficient 1 for d-spacing calculation
DTT2t(*n_pat*)
Coefficient 2 for d-spacing calculation
XCROSS(*n_pat*)
Position of the centre of the crossover region
WCROSS (*n_pat*)
Width of the crossover region

The component of the TOF position of a reflection, for **NPROF**(*n_pat*)= 10, with d-spacing *d* for the region of thermal neutrons is calculated using the formula:

$$TOF_t = \mathbf{ZERt} + \mathbf{DTT1t}\ d - \mathbf{DTT2t}\ d^{-1}$$

The position of a Bragg reflection (in microseconds TOF) is finally calculated using the expressions:

$$n_{cross} = 0.5\ erfc(\mathbf{WCROSS}\ (\mathbf{XCROSS}\text{-}d^{-1}))$$

$$TOF = n_{cross}\ TOF_e + (1\text{-}n_{cross})\ TOF_t$$

Where *erfc* is the complementary error function.

LINE 16b: **CZERt, CDTT1t, CDTT2t, Cx-cross, CWIDTH (5 reals) (OPTIONAL)**
Codewords of the previous parameters.

LINE 17: BACK1, BACK2, BACK3, BACK4, BACK5, BACK6
FBACK1,FBACK2,FBACK3,FBACK4,FBACK5,FBACK6
BACK7, BACK8, BACK9, BACK10, BACK11, BACK12
FBACK7,FBACK8,FBACK9,FBACK10,FBACK11,FBACK12 [NBCKGD=-3]
Comment line:! Background coefficients/Codes for Pattern #N

FWINDOW [NBCKGD=-2]
Comment line:! Window for Fourier Filter for Pattern #N

BACK7, BACK8, BACK9, BACK10, BACK11, BACK12
FBACK7,FBACK8,FBACK9,FBACK10,FBACK11,FBACK12
Bc1, Bc2, Bc3, Bc4, Bc5, Bc6
CBc1, CBc2, CBc3, CBc4, CBc5, CBc6
D1, D2, D3, D4, D5, D6

CD1, CD2, CD3, CD4, CD5, CD6 [NBCKGD=-1]
Comment line:! Additional Background coefficients/Codes for Pattern #N

BACK1, BACK2, BACK3, BACK4, BACK5, BACK6
FBACK1,FBACK2,FBACK3,FBACK4,FBACK5,FBACK6 [NBCKGD=0]
Comment line:! Background coefficients/Codes for Pattern #N

BACK1, BACK2, BACK3, BACK4
FBACK1,FBACK2,FBACK3,FBACK4 [NBCKGD=1]
Comment line:! Background Trans_coefficients/Codes for Pattern #N

BACK(i, *n_pat*)
Background coefficients (see Mathematical section)

FBACK(i, *n_pat*)
Codewords for background coefficients

FWINDOW(*n_pat*)
Window for Fourier filtering. 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!).
The starting background is read from file FILE.bac as in the case **NBCKGD**=1. But, at variance with the case **NBCKGD** =1, the file FILE.bac is re-written at the end of the session.

Note: If **NBCKGD**=1 (background read from file), BACK1 cannot be zero. Only four coefficients are needed if such a case.

[End_NPATT_Lines]

[LOOP OVER PHASES] ***Include lines 18 to 46.***

LINE 18: PHSNM (Character)

PHSNM
Name of phase

LINE 19: NATOM, NDIC, {NMAGC or NANGL}, JBT, ISYM, ISTR, IFURT, ATZ, NVK, IMORE
(7 integers - 1 real - 2 integers)
Comment line: !Nat Dis Mom Jbt Isy Str Furth ATZ Nvk More
or
Comment line: !Nat Dis Ang Jbt Isy Str Furth ATZ Nvk More

This line merges with the next block into a single line for the single pattern format as:
***LINE 19*: NATOM, NDIC, {NMAGC or NANGL}, PREF(3), JBT, IRF, ISYM, ISTR, IFURT, ATZ, NVK, NPRO, IMORE**
(3 integer, 3 reals, 5 integers, 1 real, 3 integers) – Single pattern format
Comment line: ! Nat Dis Mom Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nvk Npr More
Comment line: ! Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nvk Npr More

NATOM
Number of atoms in asymmetric unit. The total number of atoms for all phases cannot be greater than NATS

NDIC
Number of distance constraints

NANGL
Number of angle constraints

NMAGC
Number of magnetic moment constraints

JBT

= 0 The phase is treated with the Rietveld Method, then refining a given structural model.

= 1 The phase is treated with the Rietveld Method and it is considered as pure magnetic. Only magnetic atoms are required. In order to obtain the correct values of the magnetic moments the scale factor and structural parameters must be constrained to have the same values (except a multiplying factor defined by the user) that their crystallographic counterpart. See note on magnetic refinements. The three extra parameters characterising the atomic magnetic moments corresponds to components (in Bohr magnetons) along the crystallographic axes.

=-1 As 1 but the three extra parameters characterising the atomic magnetic moments corresponds to the value of M (in Bohr magnetons) the spherical Φ angle with X axis and the spherical Θ angle with Z axis. This mode works only if the Z axis is perpendicular to the XY plane. (for monoclinic space groups the Laue Class *1 1 2/m* is required).

= 2 Profile Matching mode with constant scale factor.

=-2 As 2 but instead of intensity the modulus of the structure factor is given in the CODFILn.hkl file

= 3 Profile Matching mode with constant relative intensities for the current phase. The scale factor can be refined. In this case **IRF**(*n_pat*) must be equal to 2, see below.

=-3 As 3 but instead of intensity the modulus of the structure factor in absolute units (effective number of electrons for X-rays/ units of 10^{-12} cm for neutrons) is given in the CODFILn.hkl file. This structure factor is given for the non-centrosymmetric part of the primitive cell, so for a centrosymmetric space group with a centred lattice the structure factor to be read is:

$$F_{reduced} = F_{conventional} / (Nlat \cdot Icen)$$

where *Nlat* is the multiplicity of the conventional cell and *Icen*=1 for non-centrosymmetric space groups and *Icen*=2 for centrosymmetric space groups.

= 4 The intensities of nuclear reflections are calculated from a routine handling Rigid body groups.

= 5 The intensities of magnetic reflections are calculated from a routine handling conical magnetic structures in real space.

=+10/-10 The phase can contain nuclear and magnetic contributions STFAC is called for reflections with no propagation vector associated and CALMAG is called for satellite reflections. CALMAG is also called for fundamental reflections if there is no propagation vector given but the number of magnetic symmetry matrices (**NMAGR**, see below)is greater than 0. The negative value indicates spherical components for magnetic parameters. For this case the atom parameters are input in a slightly different format.

=+15/-15 The phase is treated as a commensurate modulated crystal structure. All the input propagation vectors and also **k**=(0,0,0) are identified to be magnetic and/or structural by the reading subroutine. All nuclear contributions at reflections without propagation vectors, fundamental reflections of the basic structure, and reflections associated to a modulation propagation vector, superstructure reflections, are calculated by MOD_STFAC. Magnetic contributions are added, if necessary, calling the subroutine CALMAG as in the case of **JBT**=+10/-10. The negative value indicates spherical components for magnetic parameters. This value of **JBT** implies the use of a specific format for atom parameters.

ISYM

=0 The symmetry operators are generated automatically from the space group symbol.

=+/-1 The symmetry operators are read below. In the case of a pure magnetic phase **ISYM** must be always equal to 1 or 2.

=2 The basis functions of the irreducible representations of the propagation vector group are read instead of symmetry operators. At present this works only for a pure magnetic phase.

For **JBT**=10 with magnetic contribution **ISYM** could be 0 but a comment starting with "Mag" should be given after the space group symbol.

Note: For Profile Matching mode 2, **IRF** can be 0 in the first run. In that case, a CODFILn.hkl file is generated and **IRF** is set to 2 in the new CODFIL.pcr file. The file is updated at each run in the case of **JBT** =2. Of course **ISYM** must be 0.
If for a phase **IRF**≤0 and **ISYM**=1, the reflections are generated from the symbol given in the place reserved for the space group. In that case, a file CODFILn.hkl is generated with the relevant (non-zero) reflections and proper multiplicities for the particular model described by user-given symmetry operators. In addition the calculated intensities are F^2 (corrected for multiplicity, scale and LP-factor) in absolute units. This file can be used as an input file to accelerate the calculations. The program does not use the intensities in new runs reading this generated file.

The contain of this generated file, apart from the features described above, is:
No k-vectors ⇒ *h k l m* F^2(calc) F^2(obs)

k-vectors ⇒ *h k l nv m* F^2(calc) F^2(obs) *hr kr lr*
with obvious meaning.

ISTR

=0 If strain or/and size parameters are used, they are those corresponding to selected models

=1 The generalised formulation of strains parameters will be used for this phase.
If **ISTRAINMOD**≠0 a quartic form in reciprocal space is used (see below)

=-1 Options **1** and **2** simultaneously. The size parameters of the quadratic form are read before the strain parameters.

=2 The generalised formulation of size parameters will be used for this phase.
Quadratic form in reciprocal space. Only special options of strains with **ISTRAINMOD**≠0 can be used together with this size option.

=3 The generalised formulation of strain *and* size parameters will be used for this phase.

IFURT

Number of further parameters defined by user, to be used with user supplied subroutines. The default is the number of parameters defining the TLS for rigid body groups. It should be used only when **JBT**=4.

ATZ

Coefficient to calculate the weight percentage of the phase.

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

Z: Number of formula units per cell, M_w= molecular weight

f: Used to transform the site multiplicities used on line 11-41 to their true values. For a stoichiometric phase *f*=1 if these multiplicities are calculated by dividing the Wyckoff multiplicity *m* of the site by the general multiplicity *M*. Otherwise *f*=*Occ*.*M*/*m*, where *Occ*. is the occupation number given in LINE 25.

t: Is the 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), this factor is nearly 1 (in such case $ATZ=Z.M_w.f^2$). The Brindley coefficient is directly read in one of the following lines.

NVK

Number of propagation vectors. If **NVK** < 0 the vector **-k** is added to the list.

IMORE

If different from 0 the LINE 19-1 is read

LINE 19-1: JVIEW, JDIST, JHELIX, JSOL, JMOM, JTER (6 integers)
(to be given only if IMORE≠0)
Comment line: !Jvi Jdi Hel Sol Mom Ter

This line merges with some items of the next block into a single line for the old single pattern format as:
***LINE 19-1*: JVIEW, JDIST, JHELIX, JSOL, JMOM, JTER, BRINL, RMUA, RMUB, RMUC, JTYP (to be given only if IMORE≠0)**
(6 integers, 4 reals, 1 integer) – Single pattern format
Comment line: ! Jvi Jdi Hel Sol Mom Ter Brind RMua RMub RMuc Jtyp

JVIEW

=1 A file suitable for SCHAKAL is generated

=2 A file suitable for STRUPLO is generated (The extension of the file is in both cases ".sch")

=11 If **JBT**=2 a file CODFIL*n*.int with a list of overlapped peak clusters is output. Useful as input file for working with integrated intensities in further processing using **IRF**=4 and/or **ICRYG**=1, 2, 3 (Least Squares, Montecarlo or Simulated Annealing optimisation).

JDIST

=1 Creates a file called CODFIL*n*.atm with all atoms within a primitive unit cell for a magnetic phase. The number *n* corresponds to the number of the current phase. If **JBT**=10 only the list of magnetic atoms is generated.

=-1 For a magnetic phase creates a file called CODFIL*n*.atm with a format suitable for further processing with the program **MOMENT**.

=2 As 1 but, for a crystal structure, all atoms inside the conventional cell are generated.
If **JBT**=15 then the output is slightly different. It gives the co-ordinates of all the atoms calculated from the average structure, displacement parameters, and symmetry relations in a multiple cell defined by the user, after all the atom parameters and before scale factors. The user has to provide the rotational part transforming the average structure basis vectors into the multiple cell basis and a translation part giving the shift of the origin of the multiple cell in the conventional cell setting (see below).

=3 Distance and angle calculations will be performed for the current phase. Bond Valence calculations may also be performed. The output is in the file CODFIL*n*.dis. An additional file helping to create strings for soft constraints is output. This file has a fixed name: "dconstr*n*.hlp".

=4 Only Bond Valence calculations are output to the file CODFIL*n*.dis for the current phase.

JHELIX

=0 No action

=1 The real and imaginary components of the Fourier coefficient of a magnetic atom are constrained to be orthogonal. The factor 1/2 is also included. This constraint may be unstable because is applied *a posteriori*. (see Mathematical section).

JSOL

=0 No action

=1 Additional *hkl*-dependent shifts parameters are read.

JMOM

Unused at present

JTER

Unused at present

LINE 19-2: JCONTR(1:NPATT) (NPATT integers)

Comment line: !Contributions (0/1) of this phase to the #N Pattern

JCONTR

=0 The current phase *does not* contributes to the pattern

=1 The current phase contributes to the pattern

Example (it is supposed that we are dealing with 5 diffraction patterns simultaneously):

```
0  1  1  0  1
```

The meaning of the list is that the current phase only contributes to patterns number 2, 3 and 5.

[NPATT_Lines] ***This set of lines should not be given at all for the old single pattern format***

LINE 19-3: IRF, NPRO, JTYP (3 reals)[Only if JCONTR(n_pat)≠0]

Comment line:! Irf Npr Jtyp for Pattern #N

IRF(*n_pat*)

= 0 The list of reflections for this phase is automatically generated from the space group symbol

= 1 The list *h, k , l, Mult* is read from file CODFIL*n*.hkl (where *n* is the ordinal number of the current phase)

=-1 The satellite reflections are generated automatically from the given space group symbol

= 2 The list *h, k, l, Mult, Intensity* (or Structure Factor if **JBT**=-3) is read from file CODFIL*n*.hkl.

= 3 The list *h, k, l, Mult,* F_{real}, F_{imag} is read from file CODFIL*n*.hkl. In this case, the structure factor read is added to that calculated from the supplied atoms. This is useful for simplifying the calculation of structure factors for intercalated compounds (rigid host).

=4,-4 A list of integrated intensities is given as observations for the current phase (In the case of **ICRYG**≠0 this is mandatory)

The file CODFIL*n*.hkl can also be named as HKL*n*.hkl, or CODFIL.int in the case **ICRYG**≠0.

The format of CODFIL*n*.hkl files is described in this appendix in the paragraph

NPRO(*n_pat*)
Integer indicating the peak shape function for the present phase (see LINE 4n). If **NPRO**=0, the default value of **NPROF** is taken.

JTYP(*n_pat*)
Job type for the current phase. Allows the refinement of heterogeneous data (Same values as the global variable **JOBTYP** in LINE 4n). For the moment is only useful for **IRF**=4.

LINE 19-4: PREF(3), BRINL, RMUA, RMUB, RMUC (7 reals) [Only if JCONTR(n_pat)≠0]

Comment line:! Pr1 Pr2 Pr3 Brind Rmua Rmub Rmuc for Pattern #N

PREF(*n_pat*)
Preferred orientation direction in reciprocal space. Three components.

BRINL(*n_pat*)
Brindley coefficient

RMUA(*n_pat*)
Used when **IRF**=4. If **RMUA**=0.0 the program puts **RMUA**=1.0 internally. 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**.

RMUB(*n_pat*)
If **IRF**=4, **RMUB** is a factor for excluding reflections: only the reflections verifying the constraint: $G_{obs} \geq$ **RMUB** $\times\sigma(G_{obs})$, are considered in the refinement. G_{obs} is the integrated intensity, structure factor or structure factor squared of the current reflection.
If **JVIEW**=11 and **JBT**=2 and **IRF**≠4 see note below.

RMUC(*n_pat*)
If **IRF**=4 and **RMUC**>0.9 the weights are divided by the reduced χ^2 of the precedent cycle (not tested!) for integrated intensity refinements (**IRF**=4).
If **JVIEW**=11 and **JBT**=2 and **IRF**≠4 see note below.

Note: If **JVIEW**=11 and **JBT**=2 the parameters **RMUB** and **RMUC** are used to control whether two consecutive reflections belongs to a same cluster. This is only for IRF different from 4/-4. The rule is the following:

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

$T(i+1)-T(i) < 0.5\times(H(i)+H(i+1)) \times$**RMUB**

or

$T(i+1)-T(i) < 0.5\times(H(i)+H(i+1))$ and $G(i+1) < G_{sum}\times$**RMUC**

$G(i)$ 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, the program uses the values **RMUB**=1.0 and **RMUC**=0.2.

[End_NPATT_Lines]

From here up to the end of the PCR-file the old single pattern format coincides with the format for multiple patterns. The only prescription to take into account is that **NPATT**=1 in the loops depending on the number of patterns.

LINE 20: DIS_MAX, ANG_MAX, BVS (2 reals - Character) [Optional, only if JDIST=3, 4]

Comment line: ! Max_dst(dist) (angles) Bond-Valence Calc

DIS_MAX

Maximum distance between atoms to output in file CODFILn.dis.

ANG_MAX

Maximum distance between atoms to output angles in file CODFILn.dis. If ANG_MAX=0 no angle calculations are performed.

BVS

If this character variable is equal to BVS then Bond Valence calculations are performed and the results output to file CODFILn.dis. The LINE 21 is then read.

LINE 21: N_CATIONS, N_ANIONS, TOLERANCE (2 integers - 1 real) [Optional, only if JDIST=3, 4 and BVS=BVS]

Comment line: ! N_cations N_anions Tolerance(%) / Name cations/ and Anions

N_CATIONS

Number of cations

N_ANIONS

Number of anions

TOLERANCE

Tolerance for the ionic radius in percentage. Two atoms are considered as bonded if their distance is less than the sum of their respective ionic radius augmented by the value of **TOLERANCE**. The explicit expression for considering two atoms as bonded is:

$Distance(Atom_1, Atom_2) \leq (R(Atom_1)+R(Atom_2))\times(1+0.01\times$ **TOLERANCE**$)$

If **TOLERANCE**=0 the program takes **TOLERANCE**=20.

LINE 21-1: CATIONS (Character) (N_CATIONS)

CATIONS

Symbols of the cations in uppercase and putting the sign of the charge before the valence.

Example for three cations:

```
CU+2    Y+3    BA+2
```

The chemical species are numbered sequentially, so: Cu^{2+} is the species number 1, Y^{3+} is the species number 2 and Ba^{2+} is the species number 3. This numbering is important to identify the chemical nature of the atoms in the asymmetric unit.

LINE 21-2: ANIONS (Character) (N_ANIONS)

ANIONS
Symbols of the anions in uppercase and putting the sign of the charge before the valence.
Example for two anions:

```
O-2   CL-1
```

O^{2-} is the species number 4 and Cl^{-} is the species number 5.

LINE 22: SYMB, Comment (Character A20, A60)

SYMB
Space group symbol must be given in the first 20 positions of the line.
Examples:

```
P 63/m              <- Space Group Symbol
P 21 21 21           Magnetic symmetry follows
```

If **SYMB** starts with the keyword HALL, the program expects to read the Hall symbol of the space group instead of the conventional Hermann-Mauguin symbol.
Example:

```
HALL   -P 4 2a
```

Comment
Only needed for **JBT**=+10/-10. The comment must start after the position number 20 in the line.

Note: At present rhombohedral space groups must be given in the hexagonal description. Do not forget blanks between symmetry operators corresponding to different directions. It is advisable to check the Laue symmetry and symmetry operators in the output file especially for those space groups for which alternative origins are shown in the International Tables. By default the program uses the setting with the inversion centre at the origin. Upper and/or lower case characters can be used. If you find that for a non standard space group symbol the operators of the space group do not correspond to what you expect (the program has selected another origin!), you have to change the setting (another symbol) or give your own symmetry operators (see above **ISYM**). For cubic space groups you may use either the old notation, e.g. `F d 3 m` or the new notation of the International Tables: `F d -3 m`. The space group symbol must be given even in the case that you are giving your own symmetry operators. The reflections (if they are not read from file) will be generated according to the space group symbol.
A comment can be put after column 20. If this comment starts with the keyword "Mag" (without quotes) then the following line is read if **JBT**=10 or **JBT**=15.

LINE 23: TIME_REV (NS+1 integers) [Optional, only for JBT=±10, Comment = Mag]
Comment line: ! Time Reversal Operations on Crystal Space Group

NS is the number of independent symmetry operators given in file CODFIL.out for the crystallographic space group. **TIME_REV**(*i*)=-1 if time reversal is associated to operator "*i*" for magnetic symmetry, otherwise is equal to 1. The order of operators is the same as in CODFIL.out, so a first run is needed for knowing the list of crystallographic symmetry operators. For centrosymmetric groups **TIME_REV**(NS+1) tells the program if time reversal is associated (-1) or not (1) to the inversion operator. This last item should be given only for centrosymmetric space groups.

This approach assumes that the magnetic symmetry belongs to the family of the crystallographic space group. However the user can treat the problem using subgroups of the space group (making the appropriate constraints in the atomic positions) when needed.

Example:

```
P 6/m m m           Magnetic symmetry below
! Time Reversal Operations on Crystal Space Group
1  1  1  1  1  1 -1 -1 -1 -1 -1 -1  1
```

LINE 23-1: **MLTG, ICET, NLAUE, NMAGR (4 integers)** **[If ISYM≠0]**
Comment line: ! Nsym Cen Laue MagMat
MLTG, ICET, NLAUE, NEDPR, NMAGR (5 integers) **[If ISYM≠0, JBT=15]**
Comment line: ! Nsym Cen Laue DepMat MagMat
MLTG, ICET, NLAUE, IREPS, NBASIS (5 integers) **[If ISYM=-2, JBT=±1]**
Comment line: ! Nsym Cen Laue Ireps N_Bas

MLTG
Number or symmetry operators given below.

ICET
= 1 Non centrosymmetric structure
= 2 Centrosymmetric structure

NLAUE
Integer corresponding to the following Laue classes:

1: -1
2: 2/m
3: mmm
4: 4/m
5: 4/mmm
6: -3 R
7: -3m R
8: -3
9: -3m1
10: -31m
11: 6/m
12: 6/mmm
13: m3
14: m3m

This number is only used for checking the symmetry operators given by users. For a phase described in a hexagonal basis one should put **NLAUE**=6,7...12, even if the space group symbol used for generating the reflections is of different symmetry.

NMAGR
Number of magnetic rotation matrices for each symmetry operator.

NDEPR
Number of atomic displacement rotation matrices for each symmetry operator. This item is given only if **JBT**=15.

IREPS
Number of irreducible representations. The representations themselves must not be given. The user must provide the components of atomic basis functions (constant vectors) corresponding to the irreducible representations of the propagation vector group. Given only if **ISYM**=-2.
If **IREPS** is given a negative value, complex basis functions will be provided, that is the real an imaginary components of the atomic basis functions.

NBASIS
Number of atomic basis functions: constant vectors of three components referred to the conventional unit cell. This number corresponds to the maximum number of free coefficients that can be refined. At present **NBASIS** ≤ 9

LINE 23-2: ICOMPL (up to 9 integers) [OPTIONAL. Only given if ISYM=-2]
Comment line: ! Real(0)-Imaginary(1) indicator for Ci
(ICOMPL(i), i=1, **NBASIS)**
Flags indicating if the coefficient of the linear combination of atomic basis functions is real or pure imaginary. See Mathematical section for details.

LINE 24: MLTG × (1+NMAGR+NDEPR) ISYM≠-2
or
MLTG × (1+ABS(**IREPS)) or MLTG × (1+2 ×** ABS(**IREPS)) ISYM=-2**

lines of the form:

If ISYM=1 the symmetry operators are given in numeric form:
Remark: NDEPR is always 0 if JBT ≠ 15

Comment line :

```
!S11 S12 S13  T1    S21 S22 S23  T2    S31 S32 S33  T3
!M11 M12 M13  M21 M22 M23  M31 M32 M33     Ph
!D11 D12 D13  D21 D22 D23  D31 D32 D33     Ph
```
(If **JBT**=±15)

MLTG blocks of the form:

```
S11 S12 S13  T1  S21 S22 S23  T2  S31 S32 S33  T3     (3(3Int,1real))
D11 D12 D13   D21 D22 D23   D31 D32 D33 .Phase        (9Int,1real)
                                                    NDEPR lines
R11 R12 R13   R21 R22 R23   R31 R32 R33 .Phase        (9Int,1real)
                                                    NMAGR lines
```

If ISYM=-1 the symmetry operators are given in alpha-numeric form:

Example (the displacement operator is given only if **JBT**=±15):

```
!
SYMM   X,Y,Z
MSYM   U,V,W, 0.0
DSYM   U,V,W, 0.0
!
SYMM   X+1/2,-y, Z
MSYM  -U,  V,-W, 0.0
DSYM   u,-v, w, 0.5
!
SYMM   -x,-y,-Z
MSYM    U, V, W, 0.0
DSYM   U,-V,W, 0.0
. . . . . . . . . . .
```

The symbols U,V,W (lower or capital case) are used for the Fourier components of the magnetic moments/displacement vectors along X,Y,Z. The numerical value following the MSYM/DSYM operator is the magnetic/displacement phase in units of 2π.

If ISYM=-2 the basis functions of the irreducible representations of the propagation vector group are read in the following form:

The keyword BASR precedes the list of 3-components vectors corresponding to the real part of the atomic basis functions. A list of 3×**NBASIS** real numbers should be given in the same line. In the case of negative **IREPS**, the keyword BASI precedes the list of 3×**NBASIS** real numbers corresponding to the imaginary components of the atomic basis functions.

Example for **MLTG**=4, **IREPS**=-1 and **NBASIS**=3:

```
!
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+1/2,-y, z
BASR   0 0 0   0 0 0   0 0  0
BASI  -1 0 0   0 1 0   0 0 -1
!
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+1/2,y,-z
BASR   0 0 0   0 0 0   0 0  0
BASI  -1 0 0   0 1 0   0 0 -1
```

INPUT FORMAT OF ATOM PARAMETERS FOR JBT≠±10, ±15

LINE 25: Several lines for each of the N atoms depending on the value of the variable N_Type. In the following the refinement codewords for a variable adopts the same name as the variable preceded by the character C.

For X-ray or nuclear Neutron scattering [JBT=0]:
LINE 25-1:LABEL, NTYP, X, Y, Z, B, OC, IOPIN, IOPFIN, N_Type, N_Species
(2A4, 5 reals, 4 integers)
Comment line : !Atom Typ X Y Z Biso Occ In Fin N_t Spc / Codes

Structural model supplied by user (Rigid body refinement) [JBT=4,-4]:
LINE 25-1: LABEL, NTYP, P1, P2, P3, P4, P5, P6, P7, P8 (2A4, 8 reals)
Comment line : !Atom Typ p1 p2 p3 p4 p5 p6 p7 p8
! p9 p1 p11 p12 p13 p14 p15 p16

Parameters defined by user in STRMOD. At present for Rigid Body Groups.

For magnetic Neutron scattering [JBT=1]:
LINE 25-1: LABEL, NTYP, IMAGR, IK, X, Y, Z, B, OC, RX, RY, RZ
(2A4, 2 integers, 8 reals)
Comment line : !Atom Typ Mag Vek X Y Z Biso Occ Rx Ry Rz
! Ix Iy Iz beta11 beta22 beta33 MagPh

For magnetic Neutron scattering [JBT=-1]:
LINE 25-1: LABEL, NTYP, IMAGR, IK, X, Y, Z, B, OC, RM, RPHI, RTHET
(2A4, 2 integers, 8 reals)
Comment line : ! Atom Typ Mag Vek X Y Z Biso Occ Rm Rphi Rtheta'
! Im Iphi Itheta beta11 beta22 beta33 MagPh

For magnetic Neutron scattering [JBT=-1 and ISYM=-2], (Coefficients for basis functions)**:**
LINE 25-1: LABEL, NTYP, IMAGR, IK, X, Y, Z, B, OC, C1, C2, C3
(2A4, 2 integers, 8 reals)
Comment line : ! Atom Typ Mag Vek X Y Z Biso Occ C1 C2 C3
! C4 C5 C6 C7 C8 C9 MagPh

Magnetic model supplied by user. At present conical structures in real space [JBT=5,-5]:
LINE 25-1: LABEL, NTYP, IMAGR, IK, P1, P2, P3, P4, P5, P6, P7, P8
(2A4,2 integers, 8 reals)
Comment line : !Atom Typ Mag Vek X Y Z Biso Occ Mom beta Phase
! Phi & Theta of Cone-axis + unused params

LABEL
Identification characters for atom or object.

NTYP
Link to scattering data of the atom: either **NAM** from LINE 12 or chemical symbol and valence to access internal table (use only upper case letters). See notes given in LINE 12b. Also a series of special form factors are available with refinable parameters. For using this option **NTYP** should be equal to one of the following words: SPHS, SPHE, SASH, ELLI,

DISK, TORE (not available yet), FUD1, FUD2, FUD3, FUD4 are dummy symbols that may be introduced for special form-factor refinements, the code calculating the form-factor must be included in the subroutine Form_Factor. In case of special form-factor the content of the variable **LABEL** must start with the chemical symbol to normalise the scattering density. See Mathematical section for details.

IMAGR
Ordinal number of the magnetic rotation matrices applied to the magnetic moment of the atom. To be given only in the case of a magnetic phase

IK
Number of the propagation vector to which the atom contributes. If **IK**=0 the atom is used for all the propagation vectors in the calculation of structure factor. If **IK**<0 the atom contributes to **VK**(abs(**IK**)) and to the vector **VK**(abs(**IK**)+**NVK**/2)

X, Y, Z
Fractional atomic coordinates

B
Isotropic displacement (temperature) parameter in $Å^2$

OC
Occupation number i.e. chemical occupancy × site multiplicity (can be normalised to the multiplicity of the general position of the group).

IOPIN, IOPFIN
Ordinal number of first and last symmetry operator applied to the atom, apart from the identity which must always be the first one.
Useful to describe pseudo-symmetries. This option is normally used when the user supply their own list of symmetry operators (**ISYM**=1).Be careful with multiplicity of reflections!. It is suggested that the users supply also their list of reflections. If **IOPIN**=**IOPFIN**=0 all the symmetry operators are applied. Only used for crystallographic structures.

N_Type
=0 Isotropic atom. No anisotropic temperature factors are given.
=2 Anisotropic atom. The anisotropic temperature factors should be given below.
=4 The form-factor of this atom is calculated using a special subroutine and refinable parameters should be given below (under test!)

N_Species
Number of the chemical specie. Used for Bond Valence calculations, see LINE 21 for details.

RX, RY, RZ
Components along the crystallographic axis of the magnetic moments, in units of Bohr magnetons.

RM, RPHI, RTHET
In the case **JBT**=-1 these three parameters correspond to the spherical components of the magnetic moment **M**, in the following order: (μ, ϕ, θ). μ: magnitude of the Fourier component of magnetic moment, ϕ and θ are spherical angles of vector **M** (see note on magnetic refinements).

If the magnetic phase is incommensurate or described in the crystallographic cell with the help of a propagation vector, these components (**RX, RY, RZ** or **RM, RPHI, RTHET**) are actually the real part of the Fourier component of the magnetic moment of the atom ($\mathbf{S_k}$).

LINE 25-2: CX, CY, CZ, CB, CN, CRX , CRY , CRZ (8 reals)

Codewords for fractional atomic co-ordinates, isotropic displacement (temperature) parameter, occupation number and magnetic moment components.

If JBT=4,-4/5,-5 the codewords are CP1, CP2, CP3, CP4, CP5, CP6, CP7, CP8

For X-ray or nuclear Neutron scattering [JBT=0]:
LINE 25-3: B11, B22, B33, B12, B13, B23 (7 reals)[For N_typ=2]
Comment line : ! beta11 beta22 beta33 beta12 beta13 beta23 /Codes
B11, B22, B33, B12, B13, B23

Anisotropic displacement (temperature) parameters (β_{ij})

For X-ray or nuclear Neutron scattering [JBT=0] and special form-factor [For N_typ=4]:
LINE 25-3: f1 f2 f3 f4 f5 f6 f7 (7 reals)
LINE 25-4: Cf1 Cf2 Cf3 Cf4 Cf5 Cf6 Cf7 (7 reals)
LINE 25-5: f8 f9 f10 f11 f12 f13 f14 (7 reals)
LINE 25-6: Cf8 Cf9 Cf10 Cf11 Cf12 Cf13 Cf14 (7 reals)
Comment line : ! Form-factor refinable parameters

The parameters **f1** to **f14** are used for describing the form-factor of the current object and the corresponding codewords **Cf1-Cf14**. The meaning of the coefficients is explained in Mathematical section.

In the particular case of **NTYP** =SASH, the following items must be included:
LINE 25-7: SASH-type, Ncoeff, Matrix (1 character, 1 integer, 9 reals)
LINE 25-8: lmp(3, 12) (3× Ncoeff, or 2× Ncoeff, integers)

The meaning of the different items is the following:

SASH-type
Label indicating if real spherical harmonics (**SASH-type** =ylmp) or cubic harmonics (**SASH-type** =klj) are used to describe the scattering density.

Ncoeff
Number of coefficients used in the description of the scattering density.

Matrix
Matrix transforming the crystallographic Cartesian axes to the local Cartesian axes for the representative position of the molecular centre. If not given, the program uses the identity matrix.

lmp(3, 12)
List of real spherical harmonics indices: **Ncoeff** triplets (l, m, p) for **SASH-type** =ylmp, or
List of cubic harmonics indices: **Ncoeff** pairs (l, j) for **SASH-type** = klj.

The form-factor corresponding to **NTYP** =SASH is well adapted to nearly free molecular rotations. For a molecule with N atoms rotating around its centre of mass (supposed to be in a particular crystallographic site) the molecular form factor is given by:

$$f(\mathbf{Q}) = 4\pi \sum_{slmp} c^{s}_{lmp} i^{l} j_{l}(Qr_{s}) b_{s} y_{lmp}(\theta,\varphi)$$

or

$$f(\mathbf{Q}) = 4\pi \sum_{slj} c^{s}_{lj} i^{l} j_{l}(Qr_{s}) b_{s} K_{lj}(\theta,\varphi)$$

Where the index *s* runs from 1 to N and corresponds to N spherical shells. $j_l(x)$ is the spherical Bessel function of order *l*. $K_{lj}(\theta,\varphi)$ and $y_{lmp}(\theta,\varphi)$ and are the cubic harmonics and the real spherical harmonics, respectively, as defined in M. Kara and K. Kurki-Suonio, *Acta Cryst* **37**, 201 (1981). b_s is the scattering length (or X-ray scattering factor). The coefficients c_{lj}^s and c_{lmp}^s are free parameters.

In ***FullProf*** the form-factor **NTYP** =SASH corresponds to just *one shell* (a particular value of *s*). For a complete molecule the user must provide a number of SASH objects equal to the number of spherical shells characterising the molecule. The first parameter in the list (**f1, f2, f3, …**) corresponds to the value of the spherical shell radius: **f1**=*r*, the second parameter is the number of atoms of the chemical species given by **LABEL,** within the spherical shell. The coefficients (**f3, f4, f5, …f14**) correspond to the free parameters c_{lj}^s or c_{lmp}^s of the current shell in the order specified by the list **lmp(3, 12)**. The first coefficient **f3** corresponds to the free rotator term *l*=*m*=0 (or *l*=*j*=0) and should, normally, be fixed to 1. The user must provide the list (*l, m, p*)/(*l, j*) in ascending order on *l* according to the local site symmetry. See Table 2 in the above reference.

Example:

For X-ray or nuclear Neutron scattering [JBT=4], Rigid Body constraints:
LINE 25-3: P9, P10, P11, P12, P13, P14, P15 (7 reals)

Parameters defined by user in STRMOD. At present the parameters correspond to the Rigid Body constraints. The meaning of the parameters is explained in the Rigid Body Refinements section.

For magnetic Neutron scattering [JBT=1]:
LINE 25-3: IX, IY, IZ, B11, B22, B33, Mphas (7 reals)

For magnetic Neutron scattering [JBT=-1]:
LINE 25-3: IM, IPHI, ITHET, B11, B22, B33, Mphas (7 reals)

For magnetic Neutron scattering [JBT=-1, ISYM=-2]:
LINE 25-3: C4, C5, C6, C7, C8, C9, Mphas (7 reals)

If JBT=±5: P9, P10, P11, P13, P14, P15, P12

Parameters defined by user in MAGMOD. At present the parameters correspond to the treatment of conical structures in real space.

IX, IY, IZ
Imaginary components of the Fourier coefficient of magnetic moment:

IM, IPHI, ITHET
Spherical components as for real components.

C4, C5, C6, C7, C8, C9
Coefficients of the linear combinations of basis functions.

B11, B22, B33
Diagonal part of anisotropic temperature factors

Mphas
Magnetic phase of the atom in units of 2π (see Mathematical section)

The units of **IX, IY, IZ** and **IM** are in Bohr magnetons. The angles **IPHI, ITHET** are in degrees, the vector corresponding to the Fourier component of the magnetic moments is defined as (see Mathematical section):

$$\mathbf{S_k}=1/2\ (\mathbf{R_k}+i\ \mathbf{I_k})\ \exp(-2\pi\ i\ \mathbf{Mphas})$$

The components of the real, $\mathbf{R_k}$, and imaginary, $\mathbf{I_k}$, parts are given with respect to a basis of unit vectors along the crystallographic unit cell.

If **JHELIX**=1 (see LINE) the third component **IZ** is calculated by the program in order to have an imaginary vector orthogonal to the real vector ($\mathbf{R_k}\cdot\mathbf{I_k}$ =0). If **JBT**<0, then the ϕ-angle of the imaginary part is calculated by the program for keeping the orthogonal constraint.

For magnetic Neutron scattering [JBT=1]:
LINE 25-4: CIX, CIY, CIZ, CB11, CB22, CB23, CMphas (7 reals)
For magnetic Neutron scattering [JBT=-1]:
LINE 25-4: CIM, CIPHI, CITHET, CB11, CB22, CB23, CMphas (7 reals)
For magnetic Neutron scattering [JBT=-1, ISYM=-2]:
LINE 25-4: CC4, CC5, CC6, CC7, CC8, CC9, CMphas (7 reals)

Codewords for variables: **IX, IY, IZ, IM, IPHI, ITHET, C4, C5, C6, C7, C8, C9, B11, B22, B23.**

If JBT=4,-4 the codewords are CP9, CP10, CP11, CP12, CP13, CP14, CP15

INPUT FORMAT OF ATOM PARAMETERS FOR JBT=±10, ±15

For X-rays or nuclear + magnetic Neutron scattering JBT=±10:
LINE 25-1: LABEL, NTYP, IMAGR, IK, X, Y, Z, B, OC N_type N_species (a)
(2a4,2 integers,5 reals,2 integers)
LINE 25-2: CX, CY, CZ, CB, COC (b) (5 reals)

LINE 25-3: RX RY RZ IX IY IZ Mphas (c) (7 reals)
LINE 25-4: CRX CRY CRZ CIX CIY CIZ CMPhas (d) (7 reals)

LINE 25-3: RM RPHI RTHET IM IPHI ITHET Mphas (c) (7 reals)
LINE 25-4: CRM CRPHI CRTHET CIM CIPHI CITHET CMPhas (d) (7 reals)

LINE 25-3: C1 C2 C3 C4 C5 C6 Mphas (c) (7 reals)
LINE 25-4: CC1 CC2 CC3 CC4 CC5 CC6 CMPhas (d) (7 reals)

LINE 25-5: B11 B22 B33 B12 B13 B23 (e) (6 reals)
LINE 25-6: CB11 CB22 CB33 CB12 CB13 CB23 (f) (6 reals)

LINE 25-7: f1 f2 f3 f4 f5 f6 f7 (g) (7 reals)
LINE 25-8: Cf1 Cf2 Cf3 Cf4 Cf5 Cf6 Cf7 (h) (7 reals)
LINE 25-9: f8 f9 f10 f11 f12 f13 f14 (i) (7 reals)
LINE 25-10: Cf8 Cf9 Cf10 Cf11 Cf12 Cf13 Cf14 (j) (7 reals)

Comment lines : !Atom Typ Mag Vek X Y Z Biso Occ N_type Spc
!Line below:Codes
or
! Rx Ry Rz Ix Iy Iz MagPh
!Line below:Codes
or
! Rm Rphi Rtheta Im Rphi Rtheta MagPh
!Line below:Codes
or
! C1 C2 C3 C4 C5 C6 MagPh
!Line below:Codes
or

! beta11 beta22 beta33 beta12 beta13 beta23 /Line below:Codes
or
! Form-factor refinable parameters

If **N_type** = 0 Only lines (a) and (b) need to be given
If **N_type** = 1 give the lines (a), (b), (c) and (d)
If **N_type** = 2 give the lines (a), (b), (e) and (f)
If **N_type** = 3 give the lines from (a) to (f)
if **N_type** = 4 give the lines (a), (b), (g),(h),(i) and (j) (special form-factor)

This input could be also used for X-rays, in such case **IMAGR** and **IK** should be zero for all the atoms and **JOBTYP** or **JTYP**(n)=0. In such case the space group symbol can be used for generation of reflections and symmetry operators.
For a phase with magnetic contributions **NTYP** should be equal to the magnetic form factor symbol. The program extracts internally the Fermi length symbol from **NTYP**. If there are magnetic contributions the symmetry should be controlled by the user (**ISYM**=±1,-2) and the magnetic part should be described with the formalism of propagation vectors, the magnetic contribution is calculated only for the satellite reflections. If fundamental reflections have magnetic contribution the propagation vector **k**=(0,0,0) must be included explicitly if there are other propagation vectors. If the magnetic cell is the same as the chemical cell propagation vectors are not needed.
The symmetry operators must belong to the group of the propagation vector $G_{\mathbf{k}}$, so some atoms need, in general, to be repeated for the rest of positions not generated by $G_{\mathbf{k}}$.

For X-rays or nuclear + magnetic Neutron scattering (Modulated structures) JBT=±15:
At present only rational components of the propagation vectors are allowed. The calculation of the structure factor is exact.

LINE 25-1: LABEL, NTYP, IMAGR, IK, X, Y, Z, B, OC N_type Ndvk (a)
(2a4,2 integers,5 reals,2 integers)
LINE 25-2: CX, CY, CZ, CB, COC (b) (5 reals)

LINE 25-3: RX RY RZ IX IY IZ Mphas (c) (7 reals)
LINE 25-4: CRX CRY CRZ CIX CIY CIZ CMPhas (d) (7 reals)

LINE 25-3: RM RPHI RTHET IM IPHI ITHET Mphas (c) (7 reals)
LINE 25-4: CRM CRPHI CRTHET CIM CIPHI CITHET CMPhas (d) (7 reals)

Ndvk pairs of lines:
LINE 25-3: Dx Dy Dz Dxi Dyi Dzi DPhas Dep Dvek (c) (7 reals)
LINE 25-4: CDx CDy CDz CDxi CDyi CDzi CDPhas (d) (7 reals)

LINE 25-5: B11 B22 B33 B12 B13 B23 (e) (6 reals)
LINE 25-6: CB11 CB22 CB33 CB12 CB13 CB23 (f) (6 reals)

LINE 25-7: f1 f2 f3 f4 f5 f6 f7 (g) (7 reals)
LINE 25-8: Cf1 Cf2 Cf3 Cf4 Cf5 Cf6 Cf7 (h) (7 reals)
LINE 25-9: f8 f9 f10 f11 f12 f13 f14 (i) (7 reals)
LINE 25-10: Cf8 Cf9 Cf10 Cf11 Cf12 Cf13 Cf14 (j) (7 reals)

Comment lines : !Atom Typ Mag Vek X Y Z Biso Occ N_type Nki
!Line below:Codes
or
! Rx Ry Rz Ix Iy Iz MagPh Dep Dvek
!Line below:Codes
or
! Rm Rphi Rtheta Im Rphi Rtheta MagPh Dep Dvek

!Line below:Codes
or
! beta11 beta22 beta33 beta12 beta13 beta23 /Line below:Codes
or
! Form-factor refinable parameters

If **N_type** = 0 Only lines (a) and (b) need to be given
If **N_type** = 1 give the lines (a), (b), (c) and (d)
If **N_type** = 2 give the lines (a), (b), (e) and (f)
If **N_type** = 3 give the lines from (a) to (f)
if **N_type** = 4 give the lines (a), (b), (g),(h),(i) and (j) (special form-factor)

The symmetry operators must belong to the group of the propagation vector $G_{\mathbf{k}}$, so some atoms need, in general, to be repeated for the rest of positions not generated by $G_{\mathbf{k}}$.

[If ABS**(IRF)=4]**

LINE 26: SC1, SC2, SC3, SC4, SC5, SC6 (6 reals)
Comment line:! Scale Factors
Comment line:! Sc1 Sc2 Sc3 Sc4 Sc5 Sc6

SC1, SC2, SC3, SC4, SC5, SC6
Scale factor for different domains or for heterogeneous integrated intensity data. For powder data only the first scale factor is used

LINE 26-1: CSC1, CSC2, CSC3, CSC4, CSC5, CSC6 (6 reals)

Codewords of the scale factors

LINE 27: EXT1, EXT2, EXT3, EXT4, EXT5, EXT6, EXT7 (7 reals)
Comment line:! Extintion Parameters
Comment line:! Ext1 Ext2 Ext3 Ext4 Ext5 Ext6 Ext7

EXT1, EXT2, EXT3, EXT4, EXT5, EXT6, EXT7
Extinction parameters

At present only the first extinction parameter is used for single crystal work.

LINE 27-1: CEXT1, CEXT2, CEXT3, CEXT4, CEXT5, CEXT6, CEXT7 (7 reals)

Codewords of the extinction parameters

LINE 29: a, b, c, alpha, beta, gamma (6 reals)
Comment line:! a b c alpha beta gamma

Cell parameters in Å an angles in degrees

LINE 29-1: ca, cb, cc, cd, ce, cf (6 reals)

Codewords for cell constants. They must be equal to zero if there is no powder profile to be refined simultaneously with the integrated intensity data.

LINE 30: Par1...Par5 (5 reals)

Comment line:! Not yet used parameters

LINE 30-1: **cpar1,...,cpar5** **(5 reals)**

[End If ABS**(IRF)=4]**

START OF PROFILE PARAMETERS FOR EACH PATTERN

[NPATT_Lines] **[Only if JCONTR≠0, and** ABS**(IRF)≠4]**

LINE 26: **SCALE, SHAPE1, BOV, STR1, STR2, STR3, ISTRAINMOD**
(6 reals – 1 integer)
Comment line:! Scale Shape1 Bov Str1 Str2 Str3 Strain-Model
[T.O.F]
LINE 26: **SCALE, EXTINC, BOV, STR1, STR2, STR3, ISTRAINMOD**
Comment line:! Scale Extinc Bov Str1 Str2 Str3 Strain-Model

SCALE(*n_pat*)
Scale factor

SHAPE1(*n_pat*)
Profile shape parameter
E.g.: η_0 for **NPROF**=4,5 but not for **NPROF**=7, in which case it is not used.
m_0 for **NPROF**=6

EXTINC(*n_pat*)
Extinction parameter for powders

BOV(*n_pat*)
Overall isotropic displacement (temperature) factor in in $Å^2$

STR1(*n_pat*), **STR2**(*n_pat*), **STR3**(*n_pat*)
Strain parameters, defined through the subroutine STRAIN (see Microstructure in ***FullProf*** section)
If **ISTR**=1 set these values to 0.0

ISTRAINMOD(*n_pat*)
Integer to select a particular model for strains in subroutine STRAIN. This variable depends on the pattern, but, to be consistent it should normally be the same for all patterns to which the current phase is contributing.

LINE 26-1: **CSCALE, CSHAPE1, CBOV, CSTR1, CSTR2, CSTR3** **(6 reals)**
LINE 26-1: **CSCALE, CEXTI, CBOV, CSTR1, CSTR2, CSTR3** **(6 reals)**

CSCALE, CSHAPE1, CBOV, CEXTI
Codewords for scale factor, shape parameter, extinction, and overall temperature factor.

CSTR1, CSTR2, CSTR3
Codeword for strain parameters, if **ISTR**=1 set these values to 0.0

LINE 27: **U, V, W, X, Y, IG, SZ, ISIZEMOD** **(7 reals – 1 integer)** **[If NPRO≠11]**

Comment line:! U V W X Y GauSiz LorSiz Size-Model

LINE 27: **UL, VL, WL, XL, Y, IG, SZ, ISIZEMOD (7 reals – 1 integer)** **[If NPRO=11]**

Comment line:! U1 V1 W1 X1 Y GauSiz LorSiz Size-Model

[T.O.F]

LINE 27: **SIG2, SIG1, SIG0, Xt, Yt, Z1, Z0, ISIZEMOD**

Comment line:! Sig-2 Sig-1 Sig-0 Xt Yt Z1 Zo Size-Model

U(*n_pat*), **V**(*n_pat*), **W**(*n_pat*)
Half-width parameters (normally characterising the instrumental resolution function).

UL(*n_pat*), **VL**(*n_pat*), **WL**(*n_pat*)
Left Half-width parameters for split pseudo-Voigt profile **NPRO**=11.

X(*n_pat*)
Lorentzian isotropic strain parameter for **NPRO**=7.

Y(*n_pat*)
Lorentzian isotropic size parameter for **NPRO**=7.

DST(STR) (*n_pat*)
Anisotropic Gaussian contribution of micro-strain. It is calculated in subroutine STRAIN as a function of **ISTRAINMOD** and/or **ISTR**. If **ISTR**=1 and **ISTRAINMOD** ≠ 0 then the notation of P. Stephens is used. DST depends on **STR1**, **STR2**,...parameters and *hkl*. See Mathematical section for details.

IG(*n_pat*)
Isotropic size parameter of Gaussian character.

F(SZ) (*n_pat*)
Anisotropic Lorentzian contribution of particle size. The function F is calculated in subroutine SIZEF and depend on parameter **SZ** and *hkl*. Different F-functions are selected by **ISIZEMOD**.

Sig2(*n_pat*), **Sig1**(*n_pat*), **Sig0**(*n_pat*)

The variance of the Gaussian component of the peak shape in TOF neutrons is given by:

$$\sigma^2 = (Sig2 + GSIZ)d^4 + (Sig1 + DST)d^2 + Sig0$$

where *d* is the d-spacing in angstroms
Units: **Sig2** (microsecs/Å^2)^2
Sig1 (microsecs/Å^2)
Sig0 (microsecs^2)

Xt, Yt
Not used at present

Z1(*n_pat*)
GSIZ : Gaussian isotropic size component (microsecs/Å^2)^2, this parameter cannot be refined simultaneously with **Sig-2**.

Z0
Not used at present

ISIZEMOD(*n_pat*)
Integer to select a particular model for F(**SZ**) in subroutine SIZEF.

LINE 27-1: **CU, CV, CW, CX, CY, CIG, CSZ** **(7 reals)**
[T.O.F]
LINE 27-1: **CSIG-2, CSIG-1, CSIG-0, CXt, CYt, CZ1, CZ0**

Codewords for the FWHM (or shape) parameters

LINE 27-2: **Ur, Vr, Wr, Eta0r, Xr** **(5 reals)** **[Only if NPRO=11]**
Comment line:! Ur Vr Wr Eta0r Xr

Ur(*n_pat*), **Vr**(*n_pat*), **Wr**(*n_pat*), **Eta0r**(*n_pat*), **Xr**(*n_pat*)
FWHM and shape parameters for the right part of the split pseudo-Voigt function. This function is similar to **NPROF**=5 but the left (x<0) and right (x>0) parts of the profile have different U,V,W,eta0 and X parameters. Additional shape parameters are also read.

LINE 27-3: **CUr, CVr, CWr, CEta0r, CXr** **(5 reals)** **[Only if NPRO=11]**

Codewords for the FWHM and shape parameters

LINE 29: **a, b, c, alpha, beta, gamma** **(6 reals)**
Comment line:! a b c alpha beta gamma

a(*n_pat*), **b**(*n_pat*), **c**(*n_pat*), **alpha**(*n_pat*), **beta**(*n_pat*), **gamma**(*n_pat*)
Cell parameters in Å an angles in degrees. If all diffraction patterns are well calibrated the cell constants should be the same for all patterns, and therefore the cell parameters should be constrained to be the same for all patterns.

LINE 29-1: **ca, cb, cc, cd, ce, cf** **(6 reals)**

Codewords for cell constants A, B, C, D, E and F defined by :

$$\frac{1}{d^2} = Ah^2 + Bk^2 + Cl^2 + Dkl + Ehl + Fhk$$

Note that these codewords do not refer directly to the cell parameters; for instance, in the hexagonal system, the last codeword CF must be the same as CA and CB.

LINE 30: **G1, G2, PA1, PA2, PA3, PA4** **(6 reals)**
Comment line:! Pref1 Pref2 Asy1 Asy2 Asy3 Asy4
LINE 30: **G1, G2, PA1, PA2, PA3, PA4, S_L, D_L** **(8 reals)** **[For NPRO=7]**
Comment line:! Pref1 Pref2 Asy1 Asy2 Asy3 Asy4 S_L D_L
[T.O.F]
LINE 30: **G1, G2, ALPH0, BETA0, ALPHA1, BETA1**
Comment line:! Pref1 Pref2 alph0 beta0 alpha1 beta1

G1(*n_pat*), **G2**(*n_pat*)
Preferred orientation parameters (see Mathematical section)
- when **NORI** = 0, **G1** = 0 means no preferred orientation
- when **NORI** = 1, **G1** = 1 means no preferred orientation

PA1(*n_pat*), **PA2**(*n_pat*), **PA3**(*n_pat*), **PA4**(*n_pat*)
Asymmetry parameters applied to angles below **RLIM** (given on LINE 8)

S_L(*n_pat*), **D_L**(*n_pat*)

Asymmetry parameters corresponding to the L. Finger formulation of the axial divergence.

ALPH0(*n_pat*), **BETA0**(*n_pat*), **ALPH1**(*n_pat*), **BETA1**(*n_pat*)
Parameters defining the variation of the exponential decay function with d-spacing.

For **NPRO**=9

- Fast decay: $\alpha = \alpha_0 + \alpha_1/d$
- Slow decay: $\beta = \beta_0 + \beta_1/d^4$

For **NPRO**=10, the parameters **ALPH0, BETA0, ALPHA1, BETA1** correspond to the epithermal component of the neutron spectrum. In this case the TOF peak positions and decay parameters versus d-pacing are calculated using the following expressions:

$$TOF_e = \mathbf{ZER} + \mathbf{DTT1}\ d$$
$$TOF_t = \mathbf{ZERt} + \mathbf{DTT1t}\ d - \mathbf{DTT2t}\ d^{-1}$$
$$n_{cross} = 0.5\ erfc(\mathbf{WCROSS}\ (\mathbf{XCROSS}\text{-}d^{-1}))$$
$$TOF = n_{cross}\ TOF_e + (1\text{-}n_{cross})\ TOF_t$$

Where *erfc* is the complementary error function.

- Fast and slow decay for epithermal component: $\alpha_e = \alpha_{e0} + \alpha_{e1}\ d$, $\beta_e = \beta_{e0} + \beta_{e1}\ d$
- Fast and slow decay for thermal component: $\alpha_t = \alpha_{t0} - \alpha_{t1}\ d^{-1}$, $\beta_t = \beta_{t0} - \beta_{t1}\ d^{-1}$

The final fast and slow decay parameters are calculated like the case of TOF peak positions:

$$\alpha = n_{cross}\ \alpha_e + (1\text{-}n_{cross})\ \alpha_t$$
$$\beta = n_{cross}\ \beta_e + (1\text{-}n_{cross})\ \beta_t$$

The parameters for calculating the thermal fast and slow decay functions are read in LINE 31.

LINE 30-1: CG1, CG2, CPA1, CPA2, CPA3, CPA4 (6 reals)
LINE 30-1: CG1, CG2, CPA1, CPA2, CPA3, CPA4, CS_L, CD_L (8 reals) [For NPRO=7]

[T.O.F]
LINE 30-1: CG1, CG2, CALPH0, CBETA0, CALPHA1, CBETA1

CG1, CG2
Codewords for preferred orientation parameters

CPA1, CPA2, CPA3, CPA4, CS_L, CD_L
Codewords for asymmetry parameters

CALPH0, CBETA0, CALPH1, CBETA1
Codewords of the decay parameters for TOF.

[T.O.F]
LINE 31: ALPH0T, BETA0T, ALPH1T, BETA1T (4 reals)[If NPRO=10]
Comment line:! alph0t beta0t alph1t beta1t

ALPH0T(*n_pat*), **BETA0T**(*n_pat*), **ALPH1T**(*n_pat*), **BETA1T**(*n_pat*)
Parameters defining the variation of the exponential decay functions with d-spacing for the thermal component of the neutron spectrum. Only given for **NPRO**=10. See LINE 30 for the expressions used to calculate the final α and β decay parameters.

LINE 31-1: CALPH0T, CBETA0T, CALPH1T, CBETA1T (4 reals)[If NPRO=10]

Codewords for the exponential decay parameters for TOF.

LINE 32: **U2, V2, W2** **(3 reals)** **[If RATIO < 0]**
Comment line:! Additional U,V,W parameters for Lambda2

U2(*n_pat*)**, V2**(*n_pat*)**, W2**(*n_pat*)
Parameters for the second wavelength present in the diffraction pattern.

LINE 32-1: **CU2, CV2, CW2** **(3 reals)** **[If RATIO < 0]**

Codewords of the additional U,V,W parameters

LINE 33: **SHP1, CSHP1, SHP2, CSHP2** **(4 reals)** **[NPROF=4, >7]**
Comment line:! Additional Shape Parameters
[TOF]
LINE 33: **ABS1, CABS1, ABS2, CABS2** **(4 reals)**
Comment line:! Absorption Correction Parameters

For **NPRO**=11 (split pseudo-Voigt) the additional shape parameters correspond to the additional contribution to the FWHM for the Left (L) and Right (R) part of the profile for 2θ<90° and 2θ>90° respectively.

$$addFWHM^2(L) = Shp1/\tan^2 2\theta$$
$$addFWHM^2(R) = Shp2/\tan^2 2\theta$$

For **NPRO**=12 (Convoluted pseudo-Voigt with L. Finger axial divergence asymmetry)
- **SHP1**(*n_pat*)= **S_L** is source width/detector distance
- **SHP2**(*n_pat*)= **D_L** is detector width/detector distance

The parameters **S_L** and **D_L** play the role of asymmetry parameters, they are used only for reflections below 2θ = **RLIM**.

CSHP1, CSHP2 are the codewords of the shape parameters.

ABS1(*n_pat*)**, ABS2**(*n_pat*)
Absorption correction parameters
CABS1, CABS2
Codewords

The physical meaning of these parameters depend on the function selected by **IABSCOR** in LINE 8.

START hkl-DEPENDENT SHIFT PARAMETERS

LINE 34: **SHF1, SHF2, SHF3, ISHIF** **(3 reals- 1 integer)** **[If JSOL≠0]**
Comment line:! Shift1 Shift2 Shift3 ModS

SHF1(*n_pat*)**, SHF2**(*n_pat*)**, SHF3**(*n_pat*)
hkl-dependent shift parameters.

These parameters are defined by the user through the subroutines SHIFHKL, where a particular model for displacement of Bragg reflections is built for each value of **ISHIF**.

ISHIF(*n_pat*)
Model for shifts.

LINE 34-1: CSHF1, CSHF2, CSHF3 (3 reals) [IF JSOL≠0]

Codewords for *hkl*-dependent shift parameters.

LINE 35: Sh1, Sh2, Sh3 (3 reals) [IF JSOL≠0, ISHIF =±1]
Comment line:! Shift-cos(1) or Shift-sin(-1) axis

[Sh1,Sh2,Sh3]
Is the vector defining the "shift axis". Should be the same for all patterns.
The position of the reflection is displaced according to the expressions:

$$T_S = T_B + \textbf{Shift1} \times cos\phi$$
$$T_S = T_B + \textbf{Shift1} \times sin\phi$$

Where ϕ is the angle between the reciprocal vector [*hkl*]* and the direct vector **[Sh1,Sh2,Sh3]**

LINE 35-1: n1, n2, n3, n4, n5, Shift, CShift (5 integers, 2 reals) [IF JSOL≠0, ISHIF <-1]
Comment line: ! Shift integers (n1.h + n2.k + n3.l = n4.n + n5) Shift-par Code

Set of ABS(**ISHIF**) (≤10) lines, defining rules to be satisfied by reflections undergoing shifts with respect to the theoretical Bragg position, due to some kind of defects: stacking and twin faults.

n1, n2, n3, n4, n5
Are set of integers that should be the same for all patterns. If the Miller indices of the reflection satisfy the relation:

$$\textbf{n1}\ H + \textbf{n2}\ K + \textbf{n3}\ L = \textbf{n4}\ n + \textbf{n5}$$

The position of the reflection is displaced according to the expressions:

$$2\theta_S = 2\theta_B + 2\ \textbf{Shift}\ d^2\ tan\theta \times 10^{-2} \quad (2\theta \text{ space})$$
$$TOF_S = TOF_B - \textbf{Shift}\ d^3\ \textbf{Dtt1} \times 10^{-2} \quad (\text{T.O.F. space})$$
$$E_S = E_B - \textbf{Shift}/(2d)\ \textbf{Dtt1} \times 10^{-2} \quad (\text{Energy space})$$

LINE 35-2: Set of parameters for a general shift formulation up to quartic form in *hkl*. The parameters of a phase may be different for each pattern (*n_pat*).

The position of the reflection is displaced according to the expressions:

$$2\theta_S = 2\theta_B + 2\ S_{\mathbf{h}}\ d^2\ tan\theta \times 10^{-2} \quad (2\theta \text{ space})$$
$$TOF_S = TOF_B - S_{\mathbf{h}}\ d^3\ \textbf{Dtt1} \times 10^{-2} \quad (\text{T.O.F. space})$$
$$E_S = E_B - S_{\mathbf{h}}/(2d)\ \textbf{Dtt1} \times 10^{-2} \quad (\text{Energy space})$$

The expression used for calculating the scalar $S_{\mathbf{h}}$ for reflection **h** is given by:

$$S_{\mathbf{h}} = \sum_{\{H+K+L=2\}} D2_{HKL}\, h^H k^K l^L + \sum_{\{H+K+L=4\}} D4_{HKL}\, h^H k^K l^L$$

Comment lines are directly the names of the variables as given below.
[ISHIF =101] Laue class: -1

D2_200, D2_020, D2_002, D2_011, D2_101, D2_110 (6 reals)
CD2_200, CD2_020, CD2_002, CD2_011, CD2_101, CD2_110 (6 reals)

D4_400, D4_040, D4_004, D4_220, D4_202 (5 reals)
CD4_400, CD4_040, CD4_004, CD4_220, CD4_202 (5 reals)
D4_022, D4_211, D4_121, D4_112, D4_301 (5 reals)
CD4_022, CD4_211, CD4_121, CD4_112, CD4_301 (5 reals)
D4_301, D4_130, D4_103, D4_013, D4_031 (5 reals)

CD4_301, CD4_130, CD4_103, CD4_013, CD4_031 **(5 reals)**

[ISHIF =102] Laue class: ***1 2/m 1***

D2_200, D2_020, D2_002, D2_101	**(4 reals)**
CD2_200, CD2_020, CD2_002, CD2_101	**(4 reals)**
D4_400, D4_040, D4_004, D4_220, D4_202	**(5 reals)**
CD4_400, CD4_040, CD4_004, CD4_220, CD4_202	**(5 reals)**
D4_022, D4_121, D4_301, D4_103	**(5 reals)**
CD4_022, CD4_121, CD4_301, CD4_103	**(5 reals)**

[ISHIF =-102] Laue class: ***1 1 2/m***

D2_200, D2_020, D2_002, D2_110	**(4 reals)**
CD2_200, CD2_020, CD2_002, CD2_110	**(4 reals)**
D4_400, D4_040, D4_004, D4_220, D4_202	**(5 reals)**
CD4_400, CD4_040, CD4_004, CD4_220, CD4_202	**(5 reals)**
D4_022, D4_112, D4_310, D4_130	**(5 reals)**
CD4_022, CD4_112, CD4_310, CD4_130	**(5 reals)**

[ISHIF =103] Laue class: ***mmm***

D2_200, D2_020, D2_002	**(4 reals)**
CD2_200, CD2_020, CD2_002	**(4 reals)**
D4_400, D4_040, D4_004, D4_220, D4_202, D4_022	**(6 reals)**
CD4_400, CD4_040, CD4_004, CD4_220, CD4_202, CD4_022	**(6 reals)**

[ISHIF =104, 105] Laue classes: ***4/m, 4/mmm***

D2_200, D2_002	**(2 reals)**
CD2_200, CD2_002	**(2 reals)**
D4_400, D4_004, D4_220, D4_202	**(4 reals)**
CD4_400, CD4_004, CD4_220, CD4_202	**(4 reals)**

[ISHIF =106, 107] Laue classes: ***-3 R, -3m R***

D2_200, D2_002	**(2 reals)**
CD2_200, CD2_002	**(2 reals)**
D4_400, D4_004, D4_112, D4_211	**(4 reals)**
CD4_400, CD4_004, CD4_112, CD4_211	**(4 reals)**

[ISHIF =108, 109, 110, 111, 112] Laue classes: ***-3 H, -3m1, -31m, 6/m, 6/mmm***

D2_200, D2_002	**(2 reals)**
CD2_200, CD2_002	**(2 reals)**
D4_400, D4_004, D4_112	**(3 reals)**
CD4_400, CD4_004, CD4_112	**(3 reals)**

[ISHIF =113, 114] Laue classes: ***m3, m3m***

D2_200	**(1 real)**
CD2_200	**(1 real)**
D4_400, D4_220	**(2 reals)**
CD4_400, CD4_220	**(2 reals)**

END hkl-DEPENDENT SHIFT PARAMETERS

START ADDITIONAL ANISOTROPIC SIZE PARAMETERS

LINE 36: Sz1, Sz2, Sz3 (3 reals) [If ISIZEMOD =±1]
Comment line:! Platelet-Needle vector (Size)

[Sz1,Sz2,Sz3]
Is the vector defining the platelets. Must be the same for all patterns.

LINE 37: n1, n2, n3, n4, n5, SZ, CSZ (5 integers, 2 reals) [If ISIZEMOD <-1]
Comment line:! Size-Broadening (n1.h + n2.k + n3.l=n n4 +/- n5) Size-par Code

Set of ABS(**ISIZEMOD**) (≤9) lines, defining rules to be satisfied by reflections undergoing selective "size-like" broadening due to some kind of defects (anti-phase domains, …).

n1, n2, n3, n4, n5
Are set of integers that should be the same for all patterns. If the Miller indices of the reflection satisfy the relation:

$$\mathbf{n1}\ H + \mathbf{n2}\ K + \mathbf{n3}\ L = \mathbf{n4}\ n + \mathbf{n5}$$

The Lorentzian broadening of the reflection is given by the expressions:

$H_L = 0.360\ \mathbf{SZ}\ \lambda/cos\theta\ /\pi^2$	(2θ space)
$H_L = (2/\pi)\ \mathbf{SZ}\ d^5\ \mathbf{Dtt1} \times 10^{-3}$	(T.O.F. space)
$H_L = \mathbf{SZ}/(2d)\ \mathbf{Dtt1} \times 10^{-3}$	(Energy space)

The following lines correspond to anisotropic Lorentzian size broadening modelled using Spherical Harmonics.
Comment lines are directly the names of the variables as given below.

[ISIZEMOD =15] Laue class: *2/m*

Y00, Y22+, Y22-, Y20, Y44+, Y44-	**(6 reals)**
CY00, CY22+, CY22-, CY20, CY44+, CY44-	**(6 reals)**
Y42+, Y42-, Y40	**(3 reals)**
CY42+, CY42-, CY40	**(3 reals)**

[ISIZEMOD =16] Laue class: *-3 m H*

Y00, Y20, Y40, Y43-, Y60, Y63-	**(6 reals)**
CY00, CY20, CY40, CY43-, CY60, CY63-	**(6 reals)**
Y66+	**(1 real)**
CY66+	**(1 real)**

[ISIZEMOD =17] Laue classes: *m3, m3m*. Cubic harmonics, for *m3m* K62=0.

K00, K41, K61, K62, K81	**(5 reals)**
CK00, CK41, CK61, CK62, CK81	**(5 reals)**

[ISIZEMOD =18] Laue class: *mmm*

Y00, Y20, Y22+, Y40, Y42+, Y44+	**(6 reals)**
CY00, CY20, CY22+, CY40, CY42+, CY44+	**(6 reals)**

[ISIZEMOD =19] Laue classes: *6/m*, 6/*mmm*. For 6/*mmm* Y66-=0.

Y00, Y20, Y40, Y60, Y66+, Y66- **(6 reals)**
CY00, CY20, CY40, CY60, CY66+, CY66- **(6 reals)**

[ISIZEMOD =20] Laue class: *-3 H.*

Y00, Y20, Y40, Y43-, Y43+ **(5 reals)**
CY00, CY20, CY40, CY43-, CY43+ **(5 reals)**

[ISIZEMOD =21] Laue classes: *4/m, 4/mmm.* For *4/mmm* Y44-=0 and Y64=0.

Y00, Y20, Y40, Y44+, Y44-, Y60 **(6 reals)**
CY00, CY20, CY40, CY44+, CY44-, CY60 **(6 reals)**
Y64+, Y64- **(2 reals)**
CY64+, CY64- **(2 reals)**

[ISIZEMOD =22] Laue class: *-1.*

Y00, Y20, Y21+, Y21-, Y22+, Y22- **(6 reals)**
CY00, CY20, CY21+, CY21-, CY22+, CY22- **(6 reals)**

END ADDITIONAL ANISOTROPIC SIZE PARAMETERS

START ADDITIONAL ANISOTROPIC STRAIN AND SIZE PARAMETERS

LINE 38: St1, St2, St3 (3 reals) [If ISTRAINMOD=7]
Comment line:! Axial vector Microstrain

[St1,St2,St3]
Is the vector defining the axial microstrain.

LINE 39:STR4, STR5, STR6, STR7, STR8 (5 reals) [If ISTRAINMOD>8 and ISTR=0]
Comment line:! 5 additional strain parameters (IstrainModel>8)

STR4, STR5, STR6, STR7, STR8
Additional strain parameters. Their meaning depend on the particular value of **ISTRAINMOD**.

LINE 39-1: CSTR4, CSTR5, CSTR6, CSTR7, CSTR8 (5 reals)

Codewords for the additional strain parameters only if **ISTRAINMOD** > 8 and **ISTR**=0.

LINE 40: SZ1, SZ2, SZ3, SZ4, SZ5, SZ6 (6 reals) [If ISTR=-1, 2, 3]
Comment line! Generalised size parameters (quadratic form):

Coefficients of the quadratic form:

$$DSIZ = k_s \times d^2 \times (\mathbf{SZ1}\, h^2 + \mathbf{SZ2}\, k^2 + \mathbf{SZ3}\, l^2 + \mathbf{SZ4}\, kl + \mathbf{SZ5}\, hl + \mathbf{SZ6}\, hk)$$

Where k_s is defined as:

$k_s = 360/\pi^2 \times \lambda\ 10^{-3}$ (2θ space)
$k_s = 2/\pi \times \mathbf{DTT1}\ 10^{-3}$ (TOF and Energy space)

The FWHM of the Lorentzian size broadening is given by the expression:

$H_L = DSIZ/\cos\theta$ (2θ space)
$H_L = DSIZ\ d^2$ (TOF space)

LINE 40-1: CSZ1, CSZ2, CSZ3, CSZ4, CSZ5, CSZ6 (6 reals) [If ISTR=-1, 2, 3]
Codewords of the size parameters (quadratic form).

LINE 41:

The following items correspond to anisotropic strain broadening modelled using a quartic form in reciprocal space. This correspond to an interpretation of the strains as due to static fluctuations and correlations between metric parameters [see J. Rodríguez-Carvajal, M.T. Fernandez-Díaz and J.L. Martínez, *J. Phys: Condensed Matter* **3**, 3215 (1991)]. The notation used is that of P. Stephens [Peter W. Stephens, *J. Appl. Cryst.* **32**, 281 (1999)].

$$DST = \sum_{\{H+K+L=4\}} S_{HKL} h^H k^K l^L$$

A maximum of 15 parameters can be given. The input for the different Laue classes is given below.
Comment lines are directly the names of the variables as given below.

[ABS(ISTR)=1 and ISTRAINMOD =1] Laue class: *-1*

S_400, S_040, S_004, S_220, S_202 (5 reals)
CS_400, CS_040, CS_004, CS_220, CS_202 (5 reals)
S_022, S_211, S_121, S_112, S_301 (5 reals)
CS_022, CS_211, CS_121, CS_112, CS_301 (5 reals)
S_301, S_130, S_103, S_013, S_031 (5 reals)
CS_301, CS_130, CS_103, CS_013, CS_031 (5 reals)

[ABS(ISTR)=1 and ISTRAINMOD =2] Laue class: *1 2/m 1*

S_400, S_040, S_004, S_220, S_202 (5 reals)
CS_400, CS_040, CS_004, CS_220, CS_202 (5 reals)
S_022, S_121, S_301, S_103 (4 reals)
CS_022, CS_121, CS_301, CS_103 (4 reals)

[ABS(ISTR)=1 and ISTRAINMOD =-2] Laue class: *1 1 2/m*

S_400, S_040, S_004, S_220, S_202 (5 reals)
CS_400, CS_040, CS_004, CS_220, CS_202 (5 reals)
S_022, S_112, S_310, S_130 (4 reals)
CS_022, CS_112, CS_310, CS_130 (4 reals)

[ABS(ISTR)=1 and ISTRAINMOD = 3] Laue class: *mmm*

S_400, S_040, S_004, S_220, S_202, S_022 (6 reals)
CS_400, CS_040, CS_004, CS_220, CS_202, CS_022 (6 reals)

[ABS(ISTR)=1 and ISTRAINMOD = 4, 5] Laue classes: *4/m, 4/mmm*

S_400, S_004, S_220, S_202 (4 reals)
CS_400, CS_004, CS_220, CS_202 (4 reals)

[ABS(ISTR)=1 and ISTRAINMOD = 6, 7] Laue classes: *-3 R, -3m R*

S_400, S_004, S_112, S_211 (4 reals)

CS_400, CS_004, CS_112, CS_211 **(4 reals)**

[ABS(ISTR)=1 and ISTRAINMOD = 8, 9, 10, 11, 12] Laue classes: *-3, -3m1, -31m, 6/m, 6/mmm*

S_400, S_004, S_112 **(3 reals)**
CS_400, CS_004, CS_112 **(3 reals)**

[ABS(ISTR)=1 and ISTRAINMOD = 13, 14] Laue classes: *m3, m3m*

S_400, S_220 **(2 reals)**
CS_400, CS_220 **(2 reals)**

The following block of lines correspond to another formulation of the strain parameters
[ISTR=1 and **ISTRAINMOD=0, or ISTR=3]**
(STR(i), i=4, 15) (Two blocks of 6/6 reals)
Comment line:! 12 Additional strain parameters:

This block of strain parameters correspond to the following format.
STR4, STR5, STR6, STR7, STR8, STR9 **(6 reals)**
CSTR4, CSTR5, CSTR6, CSTR7, CSTR8, CSTR9 **(6 reals)**
STR10, STR11, STR12, STR13, STR14, STR15 **(6 reals)**
CSTR10, CSTR11, CSTR12, CSTR13, CSTR14, CSTR15 **(6 reals)**

See Mathematical section for explanation.

The following line is read only if **NPRO** ≥ 7 and **ISTRAINMOD≠0** or. **ISTR=**1 or **ISTR=**3.
LINE 42: XI, CXI (2 reals)
Comment line: ! Lorentzian strain coeff.+ code

END OF ADDITIONAL ANISOTROPIC STRAIN AND SIZE PARAMETERS

LINE 43: NAMEPAR, VALUEPAR, CODEPAR (IFURT Lines) [If IFURT ≠0]
Comment line:! Futher parameters

NAMEPAR
Character A4. Name of the parameter given by the user.

VALUEPAR
Value of the parameter

CODEPAR
Codeword of the parameter

[End_NPATT_Lines] **[End if JCONTR≠0, and** ABS**(IRF)≠4]**

LINE 44: PVK / CPVK (3 reals / 3 reals)(ABS**(NVK) pairs of Lines) [If NVK≠0]**
Comment line:! Propagation vectors

PVKX, PVKY, PVKZ,
Components of **k** in reciprocal lattice units.

CPVKX, CPVKY, CPVKZ,
Codewords of the component of **k**.

LINE 45: CATOD1, CATOD2, ITnum, T1, T2, T3, Dist, Sigma (2A4, 1 integer, 5 reals) (NDIC Lines) [If NDIC≠0]

Comment line:! Soft distance constraints:

CATOD1, CATOD2
Names of the atoms to be constrained. They must coincide with labels (**LABEL** in LINE 25) in the asymmetric unit (see **LABEL** in LINE 25).

ITnum
Integer for selecting the rotation part of the symmetry operator to be applied to the coordinates of the atom **CATOD2** given as representative in the asymmetric unit.

(T1, T2, T3)
Translation part of the above symmetry operator

Dist
Value of the required distance in angstroms (Å).

Sigma
Standard deviation of the distance.

The numbering of symmetry operators to be given in distance constraints conditions correspond to the listed values of **Itnum** in the tables below. If combination with a centre of symmetry is needed the value must be entered as negative.

Non-hexagonal frames

ITnum	Symmetry symbol		Rotation matrix
(1)	1	-->	(x, y, z)
(2)	2 (0, 0, z)	-->	(-x,-y, z)
(3)	2 (0, y, 0)	-->	(-x, y,-z)
(4)	2 (x, 0, 0)	-->	(x,-y,-z)
(5)	3+ (x, x, x)	-->	(z, x, y)
(6)	3+ (-x, x,-x)	-->	(z,-x,-y)
(7)	3+ (x,-x,-x)	-->	(-z,-x, y)
(8)	3+ (-x,-x, x)	-->	(-z, x,-y)
(9)	3- (x, x, x)	-->	(y, z, x)
(10)	3- (x,-x,-x)	-->	(-y, z,-x)
(11)	3- (-x,-x, x)	-->	(y,-z,-x)
(12)	3- (-x, x,-x)	-->	(-y,-z, x)
(13)	2 (x, x, 0)	-->	(y, x,-z)
(14)	2 (x,-x, 0)	-->	(-y,-x,-z)
(15)	4- (0, 0, z)	-->	(y,-x, z)
(16)	4+ (0, 0, z)	-->	(-y, x, z)
(17)	4- (x, 0, 0)	-->	(x, z,-y)
(18)	2 (0, y, y)	-->	(-x, z, y)
(19)	2 (0, y,-y)	-->	(-x,-z,-y)
(20)	4+ (x, 0, 0)	-->	(x,-z, y)
(21)	4+ (0, y, 0)	-->	(z, y,-x)
(22)	2 (x, 0, x)	-->	(z,-y, x)
(23)	4- (0, y, 0)	-->	(-z, y, x)
(24)	2 (-x, 0, x)	-->	(-z,-y,-x)

Hexagonal frames

ITnum	Symmetry symbol		Rotation matrix
(25)	1	-->	(x , y, z)

```
(26)  3+ ( 0, 0, z) --> (  -y, x-y, z)
(27)  3- ( 0, 0, z) --> (-x+y,-x  , z)
(28)   2 ( 0, 0, z) --> (-x  ,  -y, z)
(29)  6- ( 0, 0, z) --> (   y,-x+y, z)
(30)  6+ ( 0, 0, z) --> ( x-y, x  , z)
(31)   2 ( x, x, 0) --> (   y, x  ,-z)
(32)   2 ( x, 0, 0) --> ( x-y,  -y,-z)
(33)   2 ( 0, y, 0) --> (-x  ,-x+y,-z)
(34)   2 ( x,-x, 0) --> (  -y,-x  ,-z)
(35)   2 ( x,2x, 0) --> (-x+y,   y,-z)
(36)   2 (2x, x, 0) --> ( x  , x-y,-z)
```

The string representing a distance soft constraint may be obtained after a run with fixed parameters asking for output a distance file CODFIL*n*.dis, another file called "dconstr*n*.hlp" is automatically generated. After editing this file, the user may paste into the file CODFIL.pcr the desired strings and modify them as wished.

LINE 45-1: CATOD1, CATOD2, CATOD3, ITnum1, ITnum2, T1, T2, T3, t1, t2, t3, Angl, Sigma
(3A4, 2 integer, 8 reals) (NANGL Lines) [If NANGL≠0]
Comment line:! Soft angle constraints:

CATOD1, CATOD2, CATOD3
Names of the atoms to be constrained. They must coincide with labels (**LABEL** in LINE 25) in the asymmetric unit (see **LABEL** in LINE 25).
The central atom for angle constraints is the atom **CATOD2**.

ITnum1
Integer for selecting the rotation part of the symmetry operator to be applied to the coordinates of the atom **CATOD2** given as representative in the asymmetric unit.

ITnum2
Integer for selecting the rotation part of the symmetry operator to be applied to the coordinates of the atom **CATOD3** given as representative in the asymmetric unit.

(T1, T2, T3)
Translation part of the symmetry operator indexed by **ITnum1**.

(t1, t2, t3)
Translation part of the symmetry operator indexed by **Itnum2**.

Angl
Value of the required angle in degrees.

Sigma
Standard deviation of the angle.

As in the case of distance constraints, the string representing an angle soft constraint may be obtained from the file "dconstr*n*.hlp" (remember to put **ANG_MAX**≠0, see LINE 20). After editing this file, the user may paste into the file CODFIL.pcr the desired strings and modify them as wished.

LINE 46: CATOM, Moment, Sigma (A2, 2 reals) (NMAGC Lines) [If NMAGC ≠0]
Comment line:! Soft moments constrains

CATOM
Two letters equal to the two first character of the label of atoms in asymmetric unit which are constrained.

Moment
Value of the required magnetic moment.

Sigma
Standard deviation of **Moment**. It does not work with incommensurate magnetic structures.

[END LOOP OVER PHASES]

LINE 47: NUMPAR, LowLIMIT, HighLIMIT, Step, IBOUND, NAMPAR
(1 integer, 2 reals, 1 integer, character) (NRELL Lines) [If NRELL≠0]
Comment line:! Limits for selected parameters
or
Comment line:! Limits for selected parameters (+ steps & BoundCond for SA) **[If ICRYG=3]**

NUMPAR
Is the "number" of the parameter to be constrained within the limits specified by the interval [**LowLIMIT, HighLIMIT**] (**NUMPAR**=INT(CODEWORD/10)). For a proper use of this option one has to put limits to the variable appearing for the first time (from top to bottom in the CODFIL.pcr file) with the wished parameter code, this must have a positive sign and a unit multiplier; only then the constraints established by using the same codeword will work.

LowLIMIT
Smallest admissible value of the parameter number **NUMPAR**.

HighLIMIT
Highest admissible value of the parameter number **NUMPAR**.

Step
Only used if **ICRYG** = 3 (Simulated Annealing job). Value of the maximum allowed variation of the parameter number **NUMPAR** in order to generate a new configuration. A configuration means a set of **NRELL** values of the selected parameters within the box defined by the limits. The change in a single parameter generates a new configuration. If $\mathbf{PAR}_{old}$ is the current value of the parameter, the new configuration is generated by modifying the value of the parameter as $\mathbf{PAR}_{new} = \mathbf{PAR}_{old} + \mathbf{Step}\ (2 \times \mathrm{RND} - 1.0)$, where RND is a random number between 0 and 1.

IBOUND
Integer to select the type of boundary conditions for the parameter number **NUMPAR**.
If **IBOUND**=0 the boundaries are treated as hard, e.g. if $\mathbf{PAR}_{new}$ exceed the higher limit, then the value is set to the limit: $\mathbf{PAR}_{new} = \mathbf{HighLIMIT}$.
If **IBOUND**=1 the boundaries are treated as periodic, e.g. if $\mathbf{PAR}_{new}$ exceed the higher limit, then the value is calculated as: $\mathbf{PAR}_{new}$ (corrected) = $\mathbf{PAR}_{new} - (\mathbf{HighLIMIT} - \mathbf{LowLIMIT})$.

NAMPAR
Name given by the user to the parameter number **NUMPAR**.

LINE 48: NCONF, NSOLU, NREFLEX, NSCALEF (4 integers) [If ICRYG =2]
Comment line:! Nconf Nsolu Num_Ref Nscalef

This option is a crude Montecarlo way of searching a starting configuration suitable for further refinement using LSQ. A configuration means a set of **NRELL** values of the selected parameters within the box defined by the limits in LINE 47, here the **Step** value is not used. The program tries at random **NCONF** configurations and select the best **NSOLU** solutions (lower R-factors) using the first **NREFLEX** reflections of the file CODFILn.hkl or CODFIL.int. If **NSCALEF** is different from zero, then the scale factor used in the program is obtained from the relation:

$$\sum I_{obs} = Scale \sum I_{calc}$$

Note: The constraints established with the coding of parameters have the same meaning as with least-squares(LS). In LSQ refinement, or in Montecarlo search, two variables having codes `xx1.00` and `xx0.5` means that the shift applied to the second variable is half the shift applied to the first one irrespective of their initial values. Remember the prescription given in LINE 47.

LINE 49: **T_INI, ANNEAL, ACCEPT, NUMTEMPS, NUMTHCYC, INITCONF**
(3 reals - 3 integers) **[If ICRYG =3]**
Comment line:! T_ini Anneal Accept NumTemps NumThCyc InitConf

The parameters given in this line and the next two lines are specific to the Simulated Annealing algorithm for optimising a crystal and/or magnetic structure using integrated intensities. This method may be used for *solving* crystal structures when more efficient methods (like direct methods) fail. It may be used always for magnetic structure determination when simple trial an error (even using symmetry analysis) fail.

T_INI
Starting temperature in the Simulated Annealing procedure. Arbitrary value, the user should experiment with different values for each problem. A good starting point is a temperature for which the percentage of accepted configurations in the first Montecarlo cycle is of the order of 80-90%.

ANNEAL
Value of the constant needed for reducing the temperature for the next Montecarlo cycle. Normally 0.9 is a good value.

ACCEPT
Lowest percentage of accepted configurations to consider the algorithm has converged. In case of using **NALGOR**=0,1 (see below) the meaning of **ACCEPT** is the value of the lowest admissible average step, i.e. the program stops if $\langle$**Step**$\rangle \leq$ **ACCEPT**.

NUMTEMPS
Maximum number of temperatures.
The program stops after running the algorithm for **NUMTEMPS** temperatures irrespective of the convergence criterion based on **ACCEPT**.

NUMTHCYC
Number of Montecarlo cycles to be excluded from the calculation of averages. Normally 0.

INITCONF
Flag for select the treatment of the initial configuration. If **INITCONF**=0 the initial configuration is totally random. If **INITCONF**=1, the initial configuration is the one given by the values of the parameters in the PCR-file. This last option is useful when one tries to optimise an already good starting configuration, by controlling the box limits and the steps.

LINE 49-1: **NCYCLM, NSOLU, NREFLEX, NSCALEF, NALGOR**
(5 integers) **[If ICRYG =3]**
Comment line:! NCyclm Nsolu Num_Ref Nscalef NAlgor

NCYCLM
Number of Montecarlo cycles per temperature. A Montecarlo cycle corresponds to the change of all the free parameters one by one. **NCYCLM** must be at least 10 to 20 (or more!) times the number of free parameters. This is crucial for the success of the algorithm, however the user should experiment with this number. Remember that run time increases proportional to the value of **NREFLEX** $\times$ **NCYCLM** $\times$ **NUMTEMPS** $\times$ **NRELL**.

NSOLU
Number of solutions to be stored. Due to the nature of the Simulated Annealing algorithm this number should be fixed to 1.

NREFLEX
The program uses the first **NREFLEX** reflections of the file CODFILn.hkl or CODFIL.int

NSCALEF
If different from zero the scale factor used in the program is obtained from the relation:

$$\sum I_{obs} = Scale \sum I_{calc}$$

NALGOR
Flag to select the type of algorithm to be applied.

=0 The Corana algorithm is selected. This algorithm do not use fixed steps for moving the parameters defining the configuration, instead the program starts by using then whole interval as initial step for all parameters and then adapt progressively their values in order to maintain an approximate rate of accepted configurations between two pre-set values (40% and 60% in our case).

=1 The Corana algorithm is selected using as initial steps, instead of the whole interval, the steps given in LINE 47.

=2 The conventional algorithm is selected using the fixed steps as given in LINE 47.

LINE 49-2: ISWAP, MCOMPL (2 integers) [If ICRYG =3]
Comment line: ! ISwap Var-Real/Imag

ISWAP
Flag to allow interchange of atoms in the Simulated Annealing algorithm. If **ISWAP**≠0 the program enter into a procedure of interchanging pairs of atoms each **ISWAP** Montecarlo cycles. The new configurations are accepted only if the cost function is reduced. For magnetic structures this flag has to be fixed to zero.

MCOMPL

Number of coefficients C_i to be switched between real or pure imaginary in magnetic structure determination when the irreducible representations of the propagation vector group are used.

LINE 49-3: (CPL(i), i=1,MCOMPL) (MCOMPL integers) [If ICRYG =3 and ISYM=-2]
Comment line: ! Coefficients for Real/Imag switch

Flags to indicate if the coefficient **Ci** (see LINE) will be switched, **CPL(i)**=1, or will remain fixed, **CPL(i)**=0, in the Simulated Annealing algorithm.

LINE 50: ISCALE, IDIF (2 integers) [If IPL =1] *[NPATT_Lines]*
Comment line:! Iscale Idif → Pattern #N

ISCALE
Counts per character position for observed and calculated curves on line printer plot

IDIF
Counts per character for difference curve

LINE 51: THET1, THET2 (2 reals) [If JCIL =2]
Comment line:! 2Th1 2Th2

The reflection list between these angles is saved in the file CODFIL.sav

CODFIL.shp or global.shp

File providing a numerical table for calculating the peak shape and its derivative. This option is useful only in very special cases where the peak shape characteristic of a given instrument is not possible to be fitted with one of the peak shape analytical functions provided by ***FullProf***.

The peak shape should be given in a normalised form $P(x)$ where the variable $x \in [x_1, x_2]$ is chosen to give a FWHM=1 and the area is 1, so $\int_{x_1}^{x_2} P(x)dx = 1$. That allows the use of the conventional U,V,and W parameters for defining the FWHM as a function of angle.
The format of this file is the following:

- Line1: Any comment
- Line2: *Np8, nupr,* $2\theta_1$, $2\theta_2$, ... $2\theta_{nupr}$
  - *Np8*: Number of points
  - *nupr*: Number of different profiles
  - $2\theta_j$: Angle to which profile *j* is best adapted

The rest of the lines are columns with x, $P_1(x)$, $P_1'(x)$, $P_2(x)$, $P_2'(x)$, … $P_{nupr}(x)$, $P_{nupr}'(x)$ in free format. $P_j'(x)$ is the derivative of $P_j(x)$ with respect to x. The profile of a reflection situated between $2\theta_j$ and $2\theta_{j+1}$ is linearly interpolated between the profiles $P_j(x)$ and $P_{j+1}(x)$.

CODFIL.cor / cor.cor

The format of this file depends on the value of the input variable **ICORR.**

ICORR=1

The file CODFIL.cor (or cor.cor) starts with a comment and follows with a list of pairs: a simple list of scattering variable and correction values.

TITLE ...
Scattering variable (T) ***Value of the correction***
" "
....

Data are read in free format. For peaks between points provided in the CODFIL.cor file, the correction is linearly interpolated.
Example:

```
This is my correction FILE for integrated intensities
10.0        1.3
20.0        1.1
30.0        1.0
40.0        0.9
80.0        0.8
120.0       0.7
```

The intensity of a reflection at scattering variable T=40 is assumed to be I_{calc} *0.9.

ICORR=2

The file contains the coefficients of an empirical function and their standard deviations. The format is:

TITLE ...
ITYCORR, ITYFUNC, NPCORR
Coefficient ***Sigma(Coefficient)***
.....
(NPCORR lines)

ITYCORR

=1 Corrections are applied to the integrated intensities. Standard deviations must not be given.

=2 Corrections are applied to the observed profile. The corrected observed profile and their variance are obtained as:

$$y_{corr} = y_{obs} / cor$$
$$\sigma^2_{y_{corr}} = (\sigma^2_{y_{obs}} / cor^2) + (\sigma^2_{cor} / y^2_{obs})$$

NPCORR

Number of coefficients of the empirical function.

ITYFUNC

=1 Polynomial function:

$$cor = \sum_{i=1}^{npcorr} coeff\,(i)\, T^{(i-1)}$$

=2 Exponential + Maxwellian for TOF raw data

$$cor = coeff(1) + coeff(2)\exp(-coeff(3)/T^2)/T^5 + \\ + \sum_{i=4}^{npcorr,2} coeff(i)\exp(-coeff(i+1)\,T^2)$$

MYRESOL.irf

This file is read only when **IRESO**≠0. The name of the file is stored in the character variable **FILERES= *MYRESOL.irf***. All items are read in free format.

This options works, at present, only for constant wavelength type of data. The profile is assumed to be a Voigt function (**NPROF**=7). 12 parameters or a table determine the resolution function. The parameters are $U_i, V_i, W_i, X_i, Y_i, Z_i$ (i=1,2 for λ_1 and λ_2)

The different types of functions are:

IRESO =1
$$H_G^2 = (U_i \tan\theta + V_i)\tan\theta + Wi$$
$$H_L = X_i \tan\theta + \frac{Y_i}{\cos\theta} + Z_i$$

IRESO =2
$$H_G^2 = (U_i \tan\theta + V_i)\tan\theta + Wi$$
$$H_L = (X_i 2\theta + Y_i)2\theta + Z_i$$

IRESO =3
$$H_G^2 = (U_i 2\theta + V_i)2\theta + W_i$$
$$H_L = (X_i 2\theta + Y_i)2\theta + Z_i$$

IRESO =4 List of values 2θ, $H_G(2\theta)$, $H_L(2\theta)$

(a linear interpolation is applied for intermediate 2θ)

The first line is considered as a title

For **IRESO**=1,2,3 the 12 parameters U_i, V_i, W_i, X_i, Y_i and Z_i are read from lines 2 and 3 (see the above line for the available instrumental functions).
Example:

```
Resolution function of MyXrayDiffractometer
0.00802 -0.00936  0.01024 0.0029   0.0  0.0     ! U1,V1...
0.00774 -0.00552  0.00814 0.0000   0.0  0.0     ! U2,V2...
```

For **IRESO** =4, the file **FILERES** starts with a line containing the title followed by a line with the number of points (NPOINS) where the instrumental Gaussian and Lorentzian FWHM are given. NPOINS lines follow containing the three items: 2θ, H_G and H_L. The Bragg peaks of the diffraction pattern must be between 2θ(1) and 2θ(NPOINS) For this case the same resolution function is applied to both wavelengths. The maximum number of NPOINS is 60.

FILE.dat

The format of this file, containing the input profile intensity data, depends on the value of the variable **INSTRM**. The different formats are described here in more detail than was described in the explanation of the **INSTRM** variable within the PCR-file.

When adequate a small piece of Fortran code, without specifying tests and writings, is provided in order to help users understand how the program reads the data. The module containing the procedures for reading profile intensity files in ***FullProf*** is available on request to the author. The important variables are the following: the variable `n_pat` indexes the pattern; `thmin`, `step` and `thmax` correspond to the initial value of the scattering variable (2θ, TOF, Energy); `npts` is the number of channels in the diffraction pattern; `y` is the profile intensity; `var` is the variance of the intensities; `txv` contains the values of the scattering variable for each channel.

INSTRM =0

Data supplied in free format. Up to seven comment lines are accepted. The first three real numbers found at the beginning of a line are interpreted as T_i, *step* and T_f and. The following lines after T_i, *step* and T_f must contain $NPTS=(T_f-T_i)/step+1$ values of the intensity profile. Data format of TOF raw data from Argonne are also interpreted by this value of **INSTRM**.

The following piece of Fortran is used for reading intensity data for **INSTRM** =0:

```
line_da=0
DO
   line_da=line_da+1
   IF(line_da > 7) GO TO 99999
   READ(i_dat,'(a)',END=99998) aline
   IF(aline(1:4) == 'BANK') THEN
     READ(aline(5:41),*) inum,npts(n_pat)
     READ(aline(47:90),*) thmin(n_pat),step(n_pat)
     thmax(n_pat)=thmin(n_pat)+(npts(n_pat)-1)*step(n_pat)
   ELSE
     READ(aline,*,iostat=ier)thmin(n_pat),step(n_pat),thmax(n_pat)
     if(ier /= 0) cycle
     npts(n_pat) = (thmax(n_pat)-thmin(n_pat))/step(n_pat)+1.5
   END IF
   IF(npts(n_pat) < 4) THEN
     IF(line_da < 7) CYCLE
     GO TO 99999
   END IF
END DO
READ(i_dat,*,END=99998,ERR=99999)(y(i,n_pat),i=1,npts(n_pat))
```

INSTRM =1

D1A/D2B format (original Rietveld-Hewat format: the first line must be T_i, *step* and T_f
The following piece of Fortran is used in ***FullProf*** for reading intensity data for **INSTRM** =1:

```
READ(i_dat,*,END=99998,ERR=99999)thmin(n_pat),step(n_pat),thmax(n_pat)
npts(n_pat) = (thmax(n_pat)-thmin(n_pat))/step(n_pat)+1.5
READ(i_dat,3,END=99998,ERR=99999)(iww(i,n_pat),y(i,n_pat),i=1,npts(n_pat))
DO i=1,npts(n_pat)
  IF (y(i,n_pat) <= 0.00001) y(i,n_pat) = 1.0
  IF (iww(i,n_pat) == 0) iww(i,n_pat) = 1
  var(i,n_pat) = y(i,n_pat)/REAL(iww(i,n_pat))
  txv(i,n_pat)= thmin(n_pat)+(i-1)*step(n_pat)
END DO
```

INSTRM =2

D1B old ILL format (DEC-10). The code for reading this format is:

```
READ(i_dat,5,END=99998,ERR=99999)date
READ(i_dat,5,END=99998,ERR=99999)txt1
READ(i_dat,*,END=99998,ERR=99999)io,numor(n_pat)
tsamp(n_pat) = REAL(numor(n_pat))
inum = 1
READ(i_dat,5,END=99998,ERR=99999)txt2
READ(i_dat,5,END=99998,ERR=99999)txt3
j = 0
READ(i_dat,'(f7.3,10f6.0)',END=99998,ERR=99999) a1,(y(j+no,n_pat),no=1,10)
j = j+10
DO i=2,40
  READ(i_dat,'(f7.3,10f6.0)',END=99998,ERR=99999)(y(j+no,n_pat),no=1,10)
  j = j+10
END DO
y(1,n_pat)   = y(2,n_pat)
y(400,n_pat) = y(399,n_pat)
thmin(n_pat) = 2.0*a1
step(n_pat)  = 0.2
npts(n_pat)  = 400
thmax(n_pat) = thmin(n_pat)+399*step(n_pat)
DO i=1,npts(n_pat)
  var(i,n_pat) = y(i,n_pat)
  txv(i,n_pat)= thmin(n_pat)+(i-1)*step(n_pat)
END DO
```

INSTRM =3

Format corresponding to the ILL instruments D1B and D20.
The code for reading the files corresponding to these instruments is:

```
READ(i_dat,11,END=99998,ERR=99999)nset
READ(i_dat,'(1x,a,2X,a,2X,a)',END=99998,ERR=99999)jdate,noexp,txt1
READ(i_dat,'(i3,1X,i6,1X,i4)  ',END=99998,ERR=99999)nset1,numor(n_pat),nsumad
READ(i_dat,'(f13.0,f9.0,1X,10(f8.3,1X))  ',END=99998,ERR=99999)  &
    xm,ti,x0,ome,chi,phi,tr1,tr2,step(n_pat),tset,tcons,tsamp(n_pat)
thmin(n_pat) = x0
READ(i_dat,'(i4,a)',ERR=99999) npts(n_pat),txt1
j = 0
npunt = nint(REAL(npts(n_pat))/10.)
thmax(n_pat) = thmin(n_pat)+(npts(n_pat)-1)*step(n_pat)
DO i=1,npunt
  READ(i_dat,19,END=99998,ERR=99999)(iww(j+no,n_pat),y(j+no,n_pat),no=1,10)
  j = j+10
END DO
READ(i_dat,20,END=99998,ERR=99999)inum
DO i=1,npts(n_pat)
  IF (y(i,n_pat) <= 0.00001) y(i,n_pat) = 1.0
  IF (iww(i,n_pat) <= 0) iww(i,n_pat) = 1
  var(i,n_pat) = y(i,n_pat)/REAL(iww(i,n_pat))
  txv(i,n_pat)= thmin(n_pat)+(i-1)*step(n_pat)
END DO
```

INSTRM =±4

Brookhaven synchrotron.

4: First line: $2\theta_i$, step, $2\theta_f$ (free format). Rest of file: pairs of lines with 10 items like
Y1 Y2 ..... Y10 -- (10F8) intensities
S1 S2 ..... S10 -- " standard deviations
-4: Format given by DBWS program for synchrotron data. (Version DBW3.2S-8711)

The Fortran code for **INSTRM** = **4** is:

```
READ(i_dat,*,END=99998,ERR=99999)thmin(n_pat),step(n_pat),thmax(n_pat)
npts(n_pat) = (thmax(n_pat)-thmin(n_pat))/step(n_pat)+1.5
nlines = npts(n_pat)/10+1
j = 0
DO i=1,nlines
  READ(i_dat,23,END=99998,ERR=99999)(y(j+no,n_pat),no=1,10)
  READ(i_dat,24,END=99998,ERR=99999)(var(j+no,n_pat),no=1,10)
  j = j+10
END DO
var(1,n_pat) = var(1,n_pat)**2
txv(1,n_pat)=thmin(n_pat)
DO i=2,npts(n_pat)
  IF (  y(i,n_pat) < 0.00001) y(i,n_pat) = y(i-1,n_pat)
  IF (var(i,n_pat) < 0.00001) var(i,n_pat) = 1.0
  var(i,n_pat) = var(i,n_pat)**2
  cnorm(n_pat)=cnorm(n_pat)+var(i,n_pat)/y(i,n_pat)
  txv(i,n_pat)= thmin(n_pat)+(i-1)*step(n_pat)
END DO
```

INSTRM =**5**

Data from GENERAL FORMAT for TWO AXIS instrument. Three lines of text followed by two lines with the items:

NPTS, *TSample*, *Tregul*, *Ivari*, *Rmon1*, *Rmon2*
T_i, *step*, T_f

Set of lines containing 10 items corresponding to the Intensities in format 10F8.1, up to *NPTS* points (*NPTS*=(T_f–T_i)/*step+1*), followed by the corresponding standard deviations in format (10f8.2) if *Ivari*=1. If *Ivari*=0 the standard deviations are calculated as

$$\sigma(y) = \sqrt{y \times \frac{Rmon1}{Rmon2}}\ .$$

The following Fortran code read the data corresponding to this format:

```
READ(i_dat,'(A)',ERR=99999)txt1
READ(i_dat,'(A)',ERR=99999)txt2
READ(i_dat,'(A)',ERR=99999)txt3
READ(i_dat,'(I6,1X,2F10.3,i5,2f10.1)',ERR=99999)  &
    npts(n_pat),tsamp(n_pat),treg,ivari,rmon1,rmon2
READ(i_dat,'(3F10.0)',ERR=99999)thmin(n_pat),step(n_pat),thmax(n_pat)
READ(i_dat,'(10F8.1)',ERR=99999)(y(i,n_pat),i=1,npts(n_pat))
READ(i_dat,*,ERR=99999)(y(i,n_pat),i=1,npts(n_pat))
IF(ivari /= 0) THEN          !IVARI
  READ(i_dat,'(10F8.2)',ERR=99999)(var(i,n_pat),i=1,npts(n_pat))
  READ(i_dat,*,ERR=99999)(var(i,n_pat),i=1,npts(n_pat))
  cnorm(n_pat)=0.0
  DO i=1,npts(n_pat)
    IF(y(i,n_pat) < 0.0001) y(i,n_pat)=0.0001
    var(i,n_pat)=var(i,n_pat)*var(i,n_pat)
    IF(var(i,n_pat) < 0.000001) var(i,n_pat)=1.0
    txv(i,n_pat)= thmin(n_pat)+(i-1)*step(n_pat)
    cnorm(n_pat)=cnorm(n_pat)+var(i,n_pat)/y(i,n_pat)
  END DO
  cnorm(n_pat)=cnorm(n_pat)/REAL(npts(n_pat))
ELSE                         !IVARI
  IF(rmon1 > 1.0 .AND. rmon2 > 1.0) THEN
    cnorm(n_pat)=rmon1/rmon2
  ELSE
    cnorm(n_pat)=1.0
  END IF
  DO i=1,npts(n_pat)
```

```
    var(i,n_pat)=y(i,n_pat)*cnorm(n_pat)
    txv(i,n_pat)= thmin(n_pat)+(i-1)*step(n_pat)
  END DO
END IF                          !IVARI
```

INSTRM =6

D1A/D2B standard format prepared by D1A(D2B)SUM (ILL), ADDET(LLB), MPDSUM (LLB) or equivalent programs. The Fortran code reading this kind of file is:

```
READ(i_dat,'(A)',ERR=99999) txt1
READ(i_dat,'(16x,F8.3)',ERR=99999) step(n_pat)
READ(i_dat,'(F8.3)',ERR=99999)thmin(n_pat)
READ(i_dat,'(2F8.0)',ERR=99999) rmoni,rmoniold
IF(rmoniold < 1.) THEN
  cnorm(n_pat)=1.00
  rmoniold=rmoni
ELSE
  cnorm(n_pat)=rmoni/rmoniold
END IF
npunt = nint(18./step(n_pat))
j=0
DO i=1,npunt
  READ(i_dat,3,ERR=99999)(iww(j+no,n_pat),y(j+no,n_pat),no=1,10)
  IF(ABS(y(j+1,n_pat)+1000.) < 1.e-03) EXIT
  j = j+10
END DO
j=j-10
npts(n_pat)=j
thmax(n_pat) = thmin(n_pat)+(npts(n_pat)-1)*step(n_pat)
DO   i=1,npts(n_pat)
  IF (y(i,n_pat) <= 0.00001) y(i,n_pat) = 1.0
  IF (iww(i,n_pat) == 0) iww(i,n_pat) = 1
  var(i,n_pat) = cnorm(n_pat)*y(i,n_pat)/REAL(iww(i,n_pat))
  txv(i,n_pat)= thmin(n_pat)+(i-1)*step(n_pat)
END DO
```

INSTRM =7

Files from D4 or D20L. The Fortran code reading this kind of file is:

```
READ(i_dat,'(I5,1X,F5.0,1X,A72)',ERR=99999)npts(n_pat),tsamp(n_pat),txt1
READ(i_dat,'(5(F7.2,1X,F8.1,1X,F5.1))',ERR=99999)  &
    (txv(i,n_pat),y(i,n_pat),var(i,n_pat),i=1,npts(n_pat))
iconstep(n_pat)=0
cnorm(n_pat)=0.0
step(n_pat)=txv(2,n_pat)-txv(1,n_pat)
thmin(n_pat)=txv(1,n_pat)
thmax(n_pat)=txv(npts(n_pat),n_pat)
DO i=1,npts(n_pat)
  var(i,n_pat)=0.5*var(i,n_pat)*var(i,n_pat)
END DO
```

INSTRM =8

Data from DMC at Paul Scherrer Institute. The Fortran code reading this kind of file is:

```
READ(i_dat,'(A)',ERR=99999)txt1
READ(i_dat,'(A)',ERR=99999)txt2
READ(i_dat,*,ERR=99999) thmin(n_pat),step(n_pat),thmax(n_pat)
npts(n_pat) = (thmax(n_pat) - thmin(n_pat))/step(n_pat) + 1.005
READ(i_dat,'(10F8.0)', ERR=99999)  (y(i,n_pat),i=1,npts(n_pat))
READ(i_dat,'(10F8.0)', ERR=99999)  (var(i,n_pat),i=1,npts(n_pat))
DO i=1,npts(n_pat)
  var(i,n_pat) = var(i,n_pat)*var(i,n_pat)
  txv(i,n_pat)= thmin(n_pat)+(i-1)*step(n_pat)
END DO
```

INSTRM =9

Data of file CODFIL.uxd generated by the Socabim software on x-rays diffractometer.

INSTRM =10

X, Y, Sigma format with header lines. In all cases the first 6 lines are considered as comments. If in the first line (left adjusted) appears the keyword XYDATA, then the following 5 lines are considered as the heading of the file. Among these 5 lines the following keywords and values have a meaning to the program:

INTER *fac_x fac_y Interpol Stepin*

TEMP *tsamp*

fac_x internal multiplier of X-values

fac_y internal multiplier of Y and Sigma-values

Interpol

=0 Variable step is used in the program

=1 The variable step data are interpolated internally to the constant step *Stepin*.

=2 Data are supplied directly at constant step

If no sigma values are provided the program assumes that $\sigma(y) = \sqrt{y}$. You can add comments to the data file if they start with the character ! in the first position of the line. These lines are ignored by the program.

The Fortran code reading this type of file is too long to be reproduced here.

INSTRM =11

Data from variable time X-ray data collection. The first four lines are considered as comments The following lines are:

2Thetai, step, 2Thetaf Comment

(Time, Intensity) in format 5(F6, I10). The program uses the information contained in Time to normalise the observed intensities to the average time <Time> and to calculate the variance of the normalised values. The Fortran code reading this type of file is reproduced below:

```
 READ(i_dat,'(A)',ERR=99999)txt1                    !1
 READ(i_dat,'(A)',ERR=99999)txt2                    !2
 READ(i_dat,'(A)',ERR=99999)txt3                    !3
 READ(i_dat,'(A)',ERR=99999)txt4                    !4
 READ(i_dat,*,ERR=99999)thmin(n_pat),step(n_pat),thmax(n_pat)
 npts(n_pat) = (thmax(n_pat)-thmin(n_pat))/step(n_pat)+1.5
 READ(i_dat,'(5(F6.0,F10.0))',ERR=99999)(bk(i,n_pat),y(i,n_pat),i=1,npts(n_pat))
!Normalize data to constant time
 cnorma=0.0
 DO i=1,npts(n_pat)
   IF(bk(i,n_pat) < 1.0E-06)CALL stop_cond(' Zero time in *.DAT ',1)
   cnorma=cnorma+bk(i,n_pat)
   txv(i,n_pat)= thmin(n_pat)+(i-1)*step(n_pat)
 END DO
 cnorma=cnorma/REAL(npts(n_pat))
 DO i=1,npts(n_pat)
   y(i,n_pat)=y(i,n_pat)*cnorma/bk(i,n_pat)
   var(i,n_pat)=y(i,n_pat)
   bk(i,n_pat)=0.0
 END DO
```

INSTRM =12

The input data file conforms to GSAS standard data file.

BINTYP = LOG6, TIME_MAP and LPSD are not yet available.

The subroutine reading GSAS formats is available on request.

CODFILn.hkl, CODFIL.int or HKLn.hkl

The format of CODFIL*n*.hkl files is the following:

For ABS(**IRF**(*n_pat*))<4:

The first two lines are read as titles (characters) The rest of the lines consist of the following items:

1) No propagation vectors

```
h   k   l    m                   (IRF=1)         (free format)
h   k   l    m  Coeff            (IRF=1 & JSOL=1)(    "      )
h   k   l    m  Intensity (or F) (IRF=2)         (    "      )
h   k   l    m  Freal Fimag      (IRF=3)         (    "      )
```

2) **NVK** propagation vectors
In the third line you have to give the number of propagation vectors in format (32x, i2), then you give **NVK** lines with: *nv* K_1 K_2 K_3 , where *nv* is the ordinal number of **k** and K_i are the components of **k** in free format.

The rest of lines contain the following sets of items:

```
h   k   l   nv   m                   (IRF=1)         (free format)
h   k   l   nv   m  COEFF           (IRF=1 & JSOL=1)(    "      )
h   k   l   nv   m  Intensity (or F) (IRF=2)         (    "      )
h   k   l   nv   m  Freal Fimag      (IRF=3)         (    "      )
```

Note: The generated files when JBT=2,3 may content additional items that are not used by ***FullProf***. These items (sigma, angle, FWHM) can be used by other programs. The case **IRF**=1 and **JSOL**=1 is to be used when shifts of Bragg reflections are observed and a model for it () is known. The user must provide the value of the coefficient COEFF for each reflection.

For ABS(**IRF**(*n_pat*))=4:

- The first line is considered as a **TITLE**
- In the second line the format of the intensity data to be read below is given.
  Example: (3i4,2f10.2,i4,3f8.4)
  Do not forget parentheses. The program expect to read *h, k, l,* F^2, $\sigma(F^2)$, *code*, and three angles (or coefficients for extinction calculations) in the case of no propagation vectors. The format must be provided for all items even if some of them (particularly the *code* and the three final items) are not provided.
- **R_lambda**(n), **Itypdata**, **ipow**(n)
  This third line is read in free format, the three items must be given. The meaning of the three items is:

  R_lambda(n)
  Wavelength for phase n

  Itypdata
  = 0 Square of structure factors (F^2) and $\sigma(F^2)$ are input.
  = 1 Structure factors (F) and $\sigma(F)$ are input. These quantities are transformed internally to case **Itypdata**=0 (F^2 and $\sigma(F^2)$).

  Ipow(n)
  = 0 Single crystal observations.
  = 1 Twinned single crystal observations. At present up to 6 *hkl*'s can contribute to a single observation.

= 2 Powder integrated intensities. In this case cluster of peaks can be given. For this case **Itypdata** is irrelevant.

- **cmono**, **rkks**
  This fourth line is optional (to be given only for X-rays and **Ipow**=2). The items correspond to variables **CTHM** and **RKK** for monochromator polarisation correction.

The rest of lines correspond to the list of integrated intensities or structure factors. The particular set of items to be read depends on whether there are propagation vectors given or not.

1) No propagation vectors. The set of items read by the program is:
h k l G_{obs}, $\sigma(G_{obs})$ *code* c_1 c_2 c_3

2) Propagation vectors
In the third/fourth line you have to give the number of propagation vectors N_{ok} that must be equal to **NVK**, then you give **NVK** lines with: *nv* K_1 K_2 K_3 , where *nv* is the ordinal number of **k** and K_i are the components of **k** in free format.

The rest of lines contain the following sets of items:

h k l nv G_{obs}, $\sigma(G_{obs})$ *code* c_1 c_2 c_3

The format of the data corresponds to that given explicitly in line 2 of the CODFIL*n*.hkl file. No data reduction is performed. The program expects to be provided with an independent set of reflections. The integer *nv* is the ordinal number of the propagation vector corresponding to the current observation *hkl*. G_{obs} and $\sigma(G_{obs})$ have different meanings depending on the value of **Itypdata** and **Ipow**:

Ipow
=0 **Itypdata**= 0 $\Rightarrow G_{obs}=F^2$
= 1 $\Rightarrow G_{obs}=F$
=1 As above but if $G_{obs}<0$ the reflection contributes to the next positive observation.
=2 $G_{obs}=\Sigma\{jLpF^2\}$: Sums of powder integrated intensities

cod: code for reflections indicating the scale factor number to be applied (for twinned crystals or inhomogeneous data).
If **Ipow**=2 and **NVK**≠0 *cod* is the multiplicity of the reflection.
If **Ipow**=2 and **NVK**=0 the multiplicity is automatically calculated using the symmetry operators generated from the symbol of the space group.

For IRF=4
c_1, c_2, c_3: Not yet used (but they are read!) (coefficients for extinction corrections)

For IRF=-4
c_1, c_2: Real and Imaginary part of the partial calculated structure factor or the reflection. The program will add this contribution to the structure factor calculated with the given atoms: $\Rightarrow F_{tot}= F + F_p= (A+ i B) + (c_1+ i c_2)$. See comments for **IRF**=3.

Examples:

```
Twinned Orthorhombic crystal with two domains
                                          (a,b,c) (b,a,c)
          h  k  l    Gobs    Sigma   cod
          ..........................
          2  0  0     -1.0     0.0     2
```

```
  0  2  0   3221.0   12.1     1
  3  1  1     -1.0    0.0     2
  1  3  1   1221.0    8.2     1

   Powder cluster of peaks

1  1  1     23.2    0.4     1  Isolated peak
.............................
5  3  1     -1.0    0.0     1  Cluster of peaks: four
3  4  2     -1.0    0.0     1  independent reflections
4  4  1     -1.0    0.0     1    contribute to
5  0  3    832.1    9.4     1 <- this observation
```