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WINPOW

Rietveld refinement framework by
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The Windows graphics user interface is essentially a file handler supplied with dialog boxes to edit the various input parameters and some plot routines for display of diffraction patterns, profile functions, Fourier maps and, optionally, crystal structures. The essence of the file handler is the following: The input parameters and controls are given in an input records file, the project file (name.rec). On opening a project, this project file is copied to a parameter file (%name.par). The parameter file is used internally when editing, calculating distances, plotting, etc. The only part of WINPOW that uses the project file directly is the Rietveld refinement program. In order for new parameters to have any effect on further refinements, the parameter file has to be copied back to the project file, i.e. the project has to be updated. You can "update" using the menu item "Update" in the "Edit project menu", do "Update and Refine" in the "Refine" menu or by pressing "Apply" from a dialog box. The Rietveld program will as its main result produce a new parameter file. The new parameter file may then be examined and modified before a new update of the project file and a new refinement. It is possible and advisable to occasionally backup the parameter file. Default file names for output files are created from the project file name stripped of extension, with a leading % and an extension according to its use.

The Rietveld program is based on the LHPM1 program by R.J. Hill and C.J. Howard (ANSTO Report M122, Lucas Heights Research Laboratories, Australia, 1986). It has been extensively modified to allow for variable step data, Chebyshev polynomial background, restraints, split pseudo-Voigt profile function, asymmetry according to Finger, Cox and Jephcoat, etc.

The distances and angle calculations program and the Fourier calculations and plot programs are based on DISTAN, FORDUP and FOPLOT by J.-O. Lundgren (Uppsala University Report No. UUIC-B13-4-05, Uppsala, Sweden, 1983). Also these programs have been modernised and extensively modified to fit into the WINPOW framework.

WINPOW also make use of a general text editor. Normally Notepad from Windows is sufficient. A more able editor is Write.exe, also in the Windows or winnt/system32 directory. The full path to this or any other preferred editor should be given in the winpow.ini file. Another option is to include a crystal structure viewer. Presently Mercury 2.2 can be recommended. It can be downloaded free of charge from http://www.ccdc.cam.ac.uk/. The full path should be given in the winpow.ini file.

Input instruction and data records are for historical reasons restricted to 80 characters. The first four characters are reserved as an identifier of the instruction or data type. Record type 2 has an additional, sometimes optional, four character identifier. All input may be entered in free format, the record positions given below indicates the allowed number of positions for a variable. The record reading routine will compress the input before interpreting it, i.e. all control characters, tabs, spaces and commas are deleted and the input string is returned with just a comma between parameters. Further, the record reading routine is case insensitive as all identifiers are internally converted to upper case before being interpreted by the programs.

To install WINPOW in a Windows environment, copy the WINPOW.EXE file to your favourite Rietveld refinement program directory, copy the WINPOW.INI file to the same directory. In the INI file you can instruct the program about editor, structure plotting program, your preferred starting directory and window size etc. Locate the Notepad.exe or some other editor and specify it in the INI file. You may as well copy the WINPREP and WINEXT programs into the same directory.

Just a few more unsorted hints:

- When starting a new project, make sure all your files related to that project (powder data files, CIF-, edt-, exp-, mlt-files etc) are in the same directory. WINPOW can normally not handle a project from more than one directory, i.e. WINPOW will start by setting a default directory for the project. However, when saving a project with "Save project as" it is possible, and sometimes advisable, to change directory. Only remember that all files associated with the new project must be in this new directory.
- A refinement can be softly interrupted with a ctrl-i. In this way the ongoing cycle is finished normally, with normal updating of files, and all internal files are properly closed.
- Dragging with the mouse you can zoom the pattern plot. The full pattern is restored with F1. Using the arrow keys you can move an expanded window left or right, zoom out (up) or zoom in (down) it.
- Special positions are not treated in any special way. WINPOW uses "site occupancy factors"

(SOF), i.e. occupancy factors should normally be given as 1.0. It is the user's responsibility not to refine special coordinates and keep track of restrictions in coordinates and anisotropic thermal parameters.

- Space group symbols are assumed to be entered according to the old International Tables Vol. 1. However, new symbols like Fm-3m will be automatically transformed to Fm3m. When there is a choice of origin, the program will always assume the one with inversion at the origin. For those 20 spacegroups with an origin ambiguity, there is an optional "Change Origin" button in the Edit Phase menu, which will allow you to switch between the different origin choices.
- Do not start refining occupancy factors from zero, or splitting of special positions from exactly the special position. The derivatives usually become zero, and the program stops.
- The atomic types are entered as the atomic numbers. The form factor curve (X-rays) and scattering lengths (neutrons) are stored in the program. Also anomalous scattering factors are stored for a set of fixed wavelengths (Ta, Ag, Mo, Cu, Cr). When the wavelength does not match those wavelengths it will use interpolated values. This may be a serious problem if you have atom types which are close to their absorption edges. In order to have correct anomalous scattering factors it will be necessary to calculate them separately and enter them manually.
- It is possible to refine up to 10 different phases simultaneously. Whether or not this is advisable depends on the quality of your data and the relative amounts of the phases. Be critical! When refining more than one phase Table will calculate the weight and volume % of the phases. It is essential that temperature factors and profile parameters are comparable for the different phases otherwise this calculation becomes unreliable. Large differences in absorption coefficients between the different phases may also give unreliable results.
- There is a main output file named %file.sum. It contains 2θ-values, raw data, calculated data, refined background, weights, calculated intensities from individual phases and Bragg markers from individual phases. This file can be imported and manipulated by for example Excel to produce plots suitable for publication and other purposes.

SHORTCUTS

F1	Full pattern
F2	FWHM and peak shape vs. 2θ
F3	Horizontal tiling of the window
F4	Vertical tiling of the window
F5	Edit Files dialog
F6	Edit Controls dialog
F7	Edit Globals dialog
F8	Edit Phase 1 dialog
F9	Edit Phase 2 dialog
F10	Edit Phase 3 dialog
F12	Edit Auxiliaries dialog
Ctrl-I	Soft interrupt
Ctrl-U	Update and refine
Ctrl-B	Backup project file
Ctrl-R	Restore project file
Ctrl-D	Distance and angle calculation
Ctrl-T	Table

DIALOGS

Edit Files

- It is advisable to enter a proper project title as the title will appear on various outputs from the program.
- It is essential to specify the raw data input format so as the program can correctly read your powder diffraction data. If your file extensions are given accordingly you can easily brows for the raw data file.
- Unless you want to use special background and weighting files, the rest of the input can be left unchanged.

Edit Controls

This is the overall control of how the program will operate.

- It is advisable to start any project with the comparison option before refining. If you have no raw data for the project you have to use the calculation option.

- Some standard settings are: pseudo-Voigt profile, 5-peak asymmetry, Chebyshev background and weighting by 1/Yobs.
- Corrections: With synchrotron radiation use a polarization of 0.02. With a Guinier camera the standard angle is 45°. For autodivergence slit the standard value is 12 mm. The cylinder μR is for capillary samples and the value has to be calculated manually.
- The wavelength is by default set to CuKα1 and CuKα2 with an α2/α1 ratio of 0.5. With only one wavelength it should be entered in both places and with a ratio of 1.
- Raw data calibration should be “From File”.
- Least-squares control: No. of halfwidths in peak is by default 10, but can be increased to 25 for simple structures. With more complicated structures a too high value will result in a program halt due to “excessive peak overlap”. Try reducing this value. Diagonal damping will reduce the least-squares shifts and may dampen wild behaviour of the refinements. Convergence will normally be slower. Suitable values are in the range 1.01-1.10, 1.00 corresponds to no damping. Refining every second step will speed up initial refinements. The 2θ-step given will only affect pattern calculations. For refinements and comparisons the 2θ-step is found from the diffraction data.

Edit Globals

- Use only the constant 2θ-zero correction.
- Do not change the wavelength part. It is an option for wavelength refinements in connection with synchrotron or reactor data only.
- The number of background parameters should be determined from their standard deviations. If the actual background parameter is less than 2-3 times the standard deviation it can be omitted. Check the output in Table.

Edit Phase

- When starting a new project, make sure all parameters, spacegroup etc is correctly interpreted by the program.
- Preferred orientation: It is possible to use two different directions, but unless special reasons use only one.
- In order to refine a parameter write 1 in the small refinement codeword box to the right of the actual parameter, or below in case of atomic parameters. Parameters can be coupled by adding a number multiplied by 10. For example, to couple the x- and y- coordinates of an atom, use the codeword 11 in the x- and y-codeword boxes. If you want to couple some other parameters you have to add 20 and so on. In the case of coupled unit cell refinements as for the a- and b-axes in the tetragonal and hexagonal cells and the a-, b- and c-axes in the cubic cells you also have to give a coupled codeword.
- The atomic occupancy factor, g, is assumed to be a site occupancy factor, i.e. it will normally be 1. If you have mixed occupancies and are entering two or more atoms in the same position, the occupancy factors have to be adjusted accordingly. Remember that when refining the coordinates, occupancies, g:s, and temperature factors, B:s, of such a set of atoms, the coordinates, occupancies and B-factors should be coupled.
- The program does not treat atoms in special positions in any special way. It is the user’s responsibility to ensure that only refinable coordinates are refined and coordinates are coupled appropriately. Consult International Tables Volume I or Volume A for your spacegroup.

INPUT FOR THE REFINEMENT PROGRAM

Record 1 Title. Optional. Default: UNTITLED

Pos.	Parameter	Comments
1- 4	ID	'TITL'
11-78	TEXT	Job title

Record set 2. File names. The default name for output files is the input records file name stripped of path and extension, and a leading % added.

Record 2.1 Input diffraction pattern file. Necessary for comparisons and refinements.

Pos.	Parameter	Comments
1- 4	ID	'PWDT'
11-70	FILE	Diffraction pattern file name

Record 2.2 Input background data file. If given it will be subtracted from the diffraction pattern with a factor given on the FRMT record.

Pos.	Parameter	Comments
1- 4	ID	'PWBG'
11-70	FILE	Background pattern file name

Record 2.3 Input weighting data file. Must be included if IWT = 2 on record 4.

Pos.	Parameter	Comments
1- 4	ID	'PWWG'
11-70	FILE	Weighting data file name

Record 2.4 Output list file. Optional. Default extension is 'OUT'.

Pos.	Parameter	Comments
1- 4	ID	'PWUT'
11-70	FILE	Output file name

Record 2.5 Output parameter file. Optional. Default extension is 'PAR'.

Pos.	Parameter	Comments
1- 4	ID	'PWPR'
11-70	FILE	Output parameter file name

Record 2.6 Pattern summary file. Optional. Default extension is 'SUM'.

Pos.	Parameter	Comments
1- 4	ID	'PWSM'
11-70	FILE	Pattern summary file name

Record 2.7 Output Fourier file. Optional. Default extension is 'FOU'.

Pos.	Parameter	Comments
1- 4	ID	'PWFO'
11-70	FILE	Output Fourier file name

Record 3 Input data format. Optional.

Pos.	Parameter	Comments
1- 4	ID	'FRMT'
11-15	FRMT	1 – dat (standard format) 2 -- udf (Philips) 3 – xrdml (Panalytical) 4 – gdf (Huber) 5 – xy (standard format) 6 – xyw (standard format) 7 – epf (ESRF) 8 – txt (Bruker)
16-25	BKGF	Background subtraction factor

Record 4 Control record.

Pos.	Parameter	Comments
1- 4	ID	'JOBT'
11-15	JOBTYP	0 - X-ray data 1 - Neutron data 2 - X-ray pattern calculation 3 - Neutron pattern calculation 4 - X-ray pattern comparison, generates Fourier file, raw data file must be included 5 - Neutron pattern comparisin, generates Fourier file, raw data file must be included
16-20	NPROF	Profile function 1 - Pseudo-Voigt 2 - Pearson VII 3 - Voigt 4 - Pseudo-Voigt including five peaks asymmetry 5 - Voigt including five peaks asymmetry 6 - Split pseudo-Voigt 7 - Asymmetry according to Finger, Cox and Jephcoat
21-25	NPHASE	Number of phases
26-30	NBCKGR	Background function type -1 - Chebyshev type I 0 - Polynomial of order -1 to 4
31-35	NEXCRG	Number of excluded regions (max 30)
36-40	NSCAT	Number of scattering sets. If given as zero, the scattering factor types on the XYZ records will be interpreted as atomic numbers
41-45	IWT	Weighting scheme 0 - w = 1/Yobs 1 - w = 1/Ycalc (after first cycle) 2 - w = 1/weight from file
46-50	NINC	Only every NINT:th intensity data point is used in the refinements. The used intensities are the averages of the NINC points.

Record 5 Output control. Default 0, 0

Pos.	Parameter	Comments
1- 4	ID	'UTPT'
11-15	IOT	Integrated intensities and Bragg R-value < 0 - print every nth reflection = 0 - No printing > 0 - Print maximum n reflections
16-20	ICOR	= 0 - No printing of correlations > 0 - Print correlation larger than ICOR %.

Record 6 Wavelengths. Default: 1.5406, 1.5444, 0.5

Pos.	Parameter	Comments
1- 4	ID	'ELAM'
11-20	LAMD(1)	Shortest
21-30	LAMD(2)	Longest
31-40	RATIO	Intensity ratio LAMD(2)/LAMD(1)

Record 7 Control record.

Pos.	Parameter	Comments
1- 4	ID	'RLIM'
11-20	WDT	Width of calculated profile in units of FWHM
21-30	CTHM	Coefficient in formula for polarization correction. Ignored for neutron data.
31-40	TMV	Value for μ*R for cylindrical absorption correction
41-50	RLIM	Peaks below this angle are corrected for asymmetry according to Rietvelds original model. Ignored for NPROF = 4, 5 and 6.
51-60	SYNPOL	Synchrotron polarization factor
61-70	GUINIER	Guinier tangent angle
71-80	AUTODIV	Autodivergence slit correction. Enter beam footprint in mm.

Record 8 Least-squares control record.

Pos.	Parameter	Comments
1- 4	ID	'RELX'
11-15	MCYCLE	Number of least-squares cycles
16-20	EPS	Run terminates when all parameter shifts are < EPS*Φ
21-25	RELX1	Relaxation on coordinates and occupancy factors.
26-30	RELX2	Relaxation on thermal parameters: Overall, isotropic and anisotropic temperature factor coefficients.
31-35	RELX3	Relaxation on profile parameters: Peak width, peak shape, assymmetry, axial divergence, preferred orientation.
36-40	RELX4	Relaxation on other parameters.
41-50	THMIN	Starting angle for pattern
51-60	STEP	Pattern step size. Only valid with pattern calculation.
61-70	THMAX	Finishing angle for pattern

Record 9 Damping factor. Multiplies the diagonal elements of the L.S. matrix before inversion. Default: 1.

Pos.	Parameter	Comments
1- 4	ID	'DAMP'
11-20	DIDAMP	Factor to multiply the diagonal elements.

Record set 10 Parameter limits.

Record 10.1 Optional. A refined parameter above or below a limit will be reset to the limiting value. The derivatives of the parameter will be zeroed in the following L.S. cycle. Upper and lower limits can be used simultaneously on the same parameter. Maximum 50 limits. The parameter number must correspond to an explicit parameter number in Record set 17. The reset is triggered by the first occurrence of the parameter.

Pos.	Parameter	Comments
1- 4	ID	'LIMP'
11-15	LIMPAR	Number of the parameter to be limited. A positive value means an upper limit, a negative number means a lower limit.
15-25	PARLIM	Parameter limit. Do not put occupancy or scale factor limits to zero.

Record 10.2 Optional. Blocking instructions. When one parameter is below a specific value, the refinement of another parameter may be stopped. The derivatives of the parameter will be zeroed in the following L.S.

Pos.	Parameter	Comments
1- 4	ID	'BLOK'
11-15	LBLOK	Controlling parameter
16-25	BLOK	Parameter value
26-30	KBLOK	Parameter to block

Record 11 Excluded regions. NEXCRG records.

Pos.	Parameter	Comments
1- 4	ID	'EXRG'
11-18	ALOW	Low angle bound
19-26	AHIGH	High angle bound

Record set 12 Optional. Scattering factors/lengths. NSCAT sets. If NSCAT is given as zero, the scattering factor types given on the XYZ records will be interpreted as atomic numbers. X-ray scattering factors for neutral atoms with dispersion corrections and neutron scattering lengths are stored in the program. When the identifier on Record 12.1 is correctly given (first upper case and second lower case character), the stored scattering factors will be used. If, in addition, FP = 0 on record 12.1, also the stored X-ray dispersion corrections or neutron scattering lengths will be used. In any case, only Record 12.1 is needed for neutron data. The scattering factor for O^{2-} from Hovestreydt (1983) can be applied if 'Ow' (or atomic number 99) is used as identifier.

Record 12.1 X-ray dispersion correction factors or neutron scattering length. Record type 2.

Pos.	Parameter	Comments
1- 4	ID	'ANOM'
11-14	NAM	Identifier
21-30	FP	Real part or neutron scattering length. Optional
31-40	FPP	Imaginary part. Optional

Record 12.2 X-ray scattering factors. Record type 2. Optional.

Pos.	Parameter	Comments
1- 4	ID	'AXTB'
11-14	NAM	Optional identifier
21-30	A1	
31-40	A2	
41-50	A3	
51-60	A4	

Record 12.3 X-ray scattering factors. Record type 2.

Pos.	Parameter	Comments
1- 4	ID	'BXTB'
11-14	NAM	Optional identifier
21-30	B1	
31-40	B2	
41-50	B3	
51-60	B4	

Record 12.4 X-ray scattering factors. Record type 2.

Pos.	Parameter	Comments
1- 4	ID	'CXTB'
11-14	NAM	Optional identifier
21-30	C	

Record set 13 Detector calibration constants.

Record 13.1 Calibration type.

Pos.	Parameter	Comments
1- 4	ID	'ICLT'
11-15	ICALTP	-1 - Cubic spline calibration 0 - Read from data file 1 - Polynomial calibration (standard data)

Record 13.2 Cubic spline coefficients. If ICALTP = 0

Pos.	Parameter	Comments
1- 4	ID	'SPLX'
11-26	SPLX	
27-42	SPLY	
43-58	SPLP	

Record 13.3 Polynomial coefficients. If NCALTP = 1. Two records. With standard data: First coefficient for starting 22, and second for 22-increment.

Pos.	Parameter	Comments
1- 4	ID	'POLY'
11-24	POL(I)	Totally ten coefficients

Record 14 Display chosen refined parameters with e.s.d. and shift on the screen after each cycle. Maximum 14 parameters. The parameter number must correspond to an explicit parameter number in Record set 17. Optional.

Pos.	Parameter	Comments
1- 4	ID	'DSPL'
11-15	NDSPL	Parameter number to be displayed.

Record set 15 Restraints. Optional. Restraints may be given as single distances, regular tetrahedral groups, and/or regular octahedral groups. In the case of octahedral group, the ligands must be given as "trans"-pairs. The restraints are most conveniently set up in the restraints dialog in the edit parameters dialog.

Record 15.1 Overall restraints weight.

Pos.	Parameter	Comments
1- 4	ID	'WRES'
11-20	WOVRL	Overall weight

Record 15.2 Central atom, distance and weight.

Pos.	Parameter	Comments
1- 4	ID	'CRES'
11-14	CA	Central atom identifier
21-30	W2	Weight for distance. Normally $\Phi(\text{distance})^{-2}$.
31-40	D1	Central atom to ligand distance

Record 15.3 Ligand list. One, four or six atoms.

Pos.	Parameter	Comments
1- 4	ID	'LRES'
11-14	L1	Ligand identifier
15-20	N1	Translation relative unit cell 555, symmetry operation number
22-25	L2	given as tttsss (c.f. ORTEP)
26-31	N2	
etc		

Record set 16 Phase specific information. NPHASE sets

Record 16.1 Phase identifier.

Pos.	Parameter	Comments
1- 4	ID	'PHTI'
11-80	PHSNM	Phase identifier

Record 16.2 Number of atoms and preferred orientation.

Pos.	Parameter	Comments
1- 4	ID	'PHNA'
11-15	NATOM	Number of atoms of this phase
16-20	H	Miller indices of preferred orientation direction 1
21-25	K	
26-30	L	
31-35	H	Miller indices of Voigt vector
36-40	K	
41-45	L	
46-50	H	Miller indices of preferred orientation direction 2
51-55	K	
56-60	L	

Record 16.3 Space group.

Pos.	Parameter	Comments
1- 4	ID	'SPGR'
11-30	SYMB	Space group symbol in the old Hermann-Mauguin notation, e.g. P 21 21 21, P -3, P 63/M, F d d d, F m -3 m. N.B. the spaces.

Record set 17 Codewords. NPHASE sets

The parameters are mapped to the elements of the normal matrix internally. It is in most cases only necessary to enter '1.' for a parameter to be refined. A zero value means that a parameter is not refined. Codewords are all optional, and will be treated as zeros when not given. For parameters that are refined coupled, are limited by the 'LIMP' instruction or displayed by the 'DSPL' option, it is necessary to enter codewords as: SIGN(A)*(10*P+ABS(A)), where P is the parameter number and A is the factor by which the parameter shift will be multiplied before use. The shifts are also multiplied by a relaxation factor (RELXn) before being applied to the parameter. All records are optional. When a record is missing the corresponding parameters will not be refined. If 5000 is added to the absolute codeword, the parameter will be updated based on the shift of parameter P.

Record 17.1 Codeword for scale factor and overall temperature factor coefficient. Default: 0, 0.

Pos.	Parameter	Comments
1- 4	ID	'CSCA'
11-20	CS	Codeword for scale factor
21-30	CQ	Codeword for overall temperature factor

Record 17.2 Codewords for unit cell parameters. Default: 0, 0, 0, 0, 0, 0.

Pos.	Parameter	Comments
1- 4	ID	'CCEL'
11-20	CA	Codeword for a
21-30	CB	Codeword for b
31-40	CC	Codeword for c
41-50	CD	Codeword for ∀
51-60	CE	Codeword for ∃
61-70	CC	Codeword for (

Record 17.3 Codeword for FWHM parameters. Default: 0, 0, 0, 0, 0, 0.

Pos.	Parameter	Comments
1- 4	ID	'CHWT'
11-20	CU	
21-30	CV	
31-40	CW	
41-50	CUR	Right side parameters if NPROF=6
51-60	CVR	"
61-70	CWR	"

Record 17.4 Codewords for preferred orientation and asymmetry. Default: 0, 0.

Pos.	Parameter	Comments
1- 4	ID	'CASY'
11-20	CP1	Codeword for preferred orientation 1
21-30	CAS	Codeword for asymmetry (not to be used if NPROF = 6 or 7)
11-20	CP2	Codeword for preferred orientation 2

Record 17.5 Codeword for peak shape. Default: 0, 0, 0, 0, 0, 0.

Pos.	Parameter	Comments
1- 4	ID	'CPKS'
11-20	CG1	CG1 is the only one necessary if NPROF = 3 and 5
21-30	CG2	
31-40	CG3	CG3 should not be released for NPROF = 2
41-50	CGR1	Right side parameters if NPROF=6
51-60	CGR2	"
61-70	CGR3	"

Record 17.6 Codeword for atomic parameters. NATOM records. Default: 0, 0, 0, 0, 0.

Pos.	Parameter	Comments
1- 4	ID	'CXYZ'
11-20	CX	Codeword for x
21-30	CY	Codeword for y
31-40	CZ	Codeword for z
41-50	CG	Codeword for g
51-60	CB	Codeword for Biso

Record 17.7 Codewords for anisotropic temperature factor coefficients. Optinal. If used it should be included for all atoms. NATOM records.

Pos.	Parameter	Comments
1- 4	ID	'CBET'
11-20	CB11	Codeword for B11
etc		

Record set 18 Codewords for global parameters.

Record 18.1 Codeword for 22-zero shift. Default: 0, 0.

Pos.	Parameter	Comments
1- 4	ID	'CZET'
11-20	FLGZR0	Codeword for 22-constant shift
21-30	FLGZR1	Codeword for cos(22)shift

Record 18.2 Codeword for axial divergence parameters. If NPROF = 7.

Pos.	Parameter	Comments
1- 4	ID	'CAXI'
11-20	CSL	Source size / sample-detector distance ratio
21-30	CDL	Detector size / sample-detector distance ratio

Record 18.3 Codeword for background parameters. Five records. Default: 0, 0, 0, 0, 0.

Pos.	Parameter	Comments
1- 4	ID	'CBKG'
11-20	FBKG	Codewords for background parameters. Five
21-30	FBKG	codewords on each records.
31-40	FBKG	-1 to 4 for polynomial background function
41-50	FBKG	0 to 24 for Chebyshev background function
51-60	FBKG	

Record set 19 Refinable parameters. NPHASE sets.

Record 19.1 Scale factor. Default: 1.0, 0.0

Pos.	Parameter	Comments
1- 4	ID	'SCAL'
11-20	SCALE	Scale factor
21-30	BOVR	Overall temperature factor coefficient

Record 19.2 Cell dimensions.

Pos.	Parameter	Comments
1- 4	ID	'CELL'
11-20	ACEL	a in Å
21-30	BCEL	b in Å
31-40	CCEL	c in Å
41-50	ALCEL	∀ in deg.
51-60	BECEL	∃ in deg.
61-70	GACEL	(in deg.

Record 19.3 FWHM parameters. Default: 0.0,0.0,0.03,0.0,0.0,0.03

Pos.	Parameter	Comments
1- 4	ID	'HWTH'
11-20	U	Coefficients in the expression for FWHM:
21-30	V	$(FWHM)^2 = U*\tan^2 2 + V*\tan 2 + W.$ This is the total
31-40	W	peak FWHM for NPROF = 1, 2, 4 and 6, but only for the Gaussian component for NPROF = 3 and 5
41-50	UR	Coefficients for the right hand side. If NPROF = 6
51-60	VR	"
61-70	WR	"

Record 19.4 Preferred orientation and asymmetry parameters. Default: 1.0,0.0

Pos.	Parameter	Comments
1- 4	ID	'ASYM'
11-20	PREF1	Preferred orientation parameter 1
21-30	ASYM	Asymmetry parameter
31-40	PREF2	Preferred orientation parameter 2

Record 19.5 Peak shape parameters. Default: 0.5,0.0,0.0,0.5,0.0,0.0

Pos.	Parameter	Comments
1- 4	ID	'PKSH'
11-20	G1	Parameters of the peak shape function:
21-30	G2	$(= (_1 + (_2*2 2 + (_3*(2 2)^2$
31-40	G3	
41-50	GR1	Coefficients for the right hand side. If NPROF = 6
51-60	GR2	"
61-70	GR3	"

Record 19.6 Atomic coordinates. NATOM records. Record type 2.

Pos.	Parameter	Comments
1- 4	ID	'XYZ '
11-14	ATOM	Atom identifier
18-20	ITBL	Atomic number or scattering factor set
21-30	X	Fractional coordinates
31-40	Y	"
41-50	Z	"
51-60	G	Site occupancy factor
61-70	BISO	Isotropic temperature factor coefficient

Record 19.7 Anisotropic temperature factor coefficients. NATOM records. Record type 2.
Optional. If used with one atom, it should be included for all.

Pos.	Parameter	Comments
1- 4	ID	'BETA'
11-14	ATOM	Atom identifier
21-30	B11	Anisotropic temperature factor coefficients
31-40	B22	
41-50	B33	
51-60	B12	
61-70	B13	
71-80	B23	

Record set 20 Global parameters

Record 20.1 2θ-zero shift. Default: 0.0,0.0

Pos.	Parameter	Comments
1- 4	ID	'ZETT'
11-20	ZER0	2θ-constant shift
21-30	ZER1	cos(2θ)shift

Record 20.2 Axial divergence parameters. If NPROF = 7. Default: 0.0,0.0

Pos.	Parameter	Comments
1- 4	ID	'AXID'
11-20	SL	Source size / sample-detector distance ratio
21-30	DL	Detector size / sample-detector distance ratio Note that if a Guinier angle is given on Record 7, the sample-detector distance will automatically be corrected.

Record 20.3 Background parameters. Five records. Default: 0.0, ... ,0.0

Pos.	Parameter	Comments
1- 4	ID	'BKGR'
11-20	BKG	Polynomials: Σ (B(i)*(2θ)^i), i = -1, 4
21-30	BKG	Chebyshev: Order 0 to 24
31-40	BKG	
41-50	BKG	
51-60	BKG	

INPUT FOR DISTANCES AND ANGLES CALCULATIONS

Record 1 Calculation range. Default: 3., 2., 0., 0.,

Pos.	Parameter	Comments
1- 4	ID	'DIST'
11-20	DMAX	Maximum distance to calculate
21-30	AMAX	Maximum distance for angle calculation (#DMAX)
31-40	DMIN	Minimum distance to calculate
41-50	AMIN	Minimum distance for angle calculation

The results are written on a file with the default name plus extension 'DIS'.

INPUT FOR FOURIER CALCULATIONS

Record 1 Control record. Default: 6, 500, 0, 2000., 2., 0., -2.

Pos.	Param.	Comments	
1- 4	ID	'FORD'	
11-15	NTYPE	2	Patterson (Fo**2)
		3	Patterson (Fc**2)
		4	Fobs synthesis with Fcalc signs
		5	Fcal synthesis
		6	Difference synthesis
16-20	NSCAN(1)	Scan level for positive peak scan.	
21-25	NSCAN(2)	Scan level for negative peak scan.	
26-35	F000	F(000) for correct scaling of Fourier syntheses of NTYPE = 2, 3, 4 and 5	
36-45	SINMAX	Maximum $\sin 2/8$ to be included.	
46-55	SINMIN	Minimum $\sin 2/8$ to be included.	
56-65	RSIG	Minimum F**2 to be included expressed as RSIG*Φ(F**2)	

Record 2 Fourier summation limits. Default: -.04,.1.04,-.04,.1.04,-.04,.1.04'

Pos.	Param.	Comments
1- 4	ID	'FLIM'
11-20	XMIN	Limits of Fourier summation grid in
21-30	XMAX	fractional coordinates. The program
31-40	YMIN	will automatically create a grid of
41-50	YMAX	maximum 28*28*28 grid points with
51-60	ZMIN	a separation of an even multiple of 0.01
61-70	ZMAX	

Record 3 Plot title. Optional. Default = Project title

Pos.	Param.	Comments
1- 4	ID	'PTIT'
11-50	PTIT	Plot title

Record set 4 Atom coordinates. Optional. N.B. These coordinates will not be symmetry transformed.
Record ID = 'PXYZ'. Standard atom format. Maximum 50 atoms.
Atoms will be included in the Fourier maps if the distance to the shown plane is less than 2.0 Å.
O if the atom is in the plane (less than 0.03 Å from the plane) or
O-/+ if the atom is below/above the plane

The results from the peak search will be displayed. The found peak positions may be copied into the parameter file and directly used in for instance a distance and angle calculation. To include a new position in the refinements, add it to the coordinate list, and to the codeword list (CXYZ) and increase the number of atoms in that phase (PHNA, Rec. 16.2). The peak positions are written in a file with default name and extension .PRM. The plot data (for FOPLOT) is written in a file with extension 'PLO'. This file actually contains the full 3D Fourier map.

INPUT FOR TABLE PROGRAM

Record 1 Table formats. Default: 4, 1, 4, 1

Pos.	Parameter	Comments
1- 4	ID	'TABL'
11-15	NDC	No. of decimals in coordinate
16-20	NDGB	No. of decimals in occupancy and isotropic temperature factor
21-25	NDBE	No. of decimals in anisotropic temperature factor coefficients
26-30	IBTYP	Temperature factor type: 1 = beta:s, 2 = U:s

The results are written on a file with the default name plus extension ‘TAB’.

MULTIPLE REFINEMENTS

MLT - run a set of rec-files through WINPOW

Create a text file containing a list of the names of the individual rec-files. Save the file using “mlt” as file extension. Open this mlt-file in WINPOW and start refinements. The mlt-file can be edited using “edit all”. N.B. update will be necessary for the changes to take effect. After refinements the program will ask if you want to update the files. You can update individual files, all files or none. (Make sure the “Notes” window is active before responding.) Rerunning the mlt-file will now be from the updated rec-files. N.B. If you run Table or Distan you will obtain the results from all the rec-files in one output file.

EXP - expansion of for example a temperature run

With a large number of data sets with small structural changes in between, it is practical to be able to start the next refinement with parameters from the previous. Again, create a text file, now with the extension “exp”. It should contain for each refinement the rec-file name (even if it does not yet exist), the lines in the rec-file that need to be changed from the previous rec-file, plus one blank line:

```
pz35b_450.rec
TITL      PbNb2O6 pz35b 450
PWDT      pz35b_450_bgs.xy
PWWG      pz35b_450.xy
```

Starting WINPOW with such an exp-file will always start from the first rec-file and then apply the same set of parameters to the following rec-files. If your data contain abrupt changes, phase transitions etc, it is likely that this procedure will screw up. In this case the exp-file should be split up into several files, each for data sets containing reasonable changes.

EDT - multiple refinements with changes of parameters

If you want to introduce changes like locking parameters for all data sets, these can be introduced in an edt-file. Like before, create a text file with the extension “edt”. It should contain the rec-file name, the lines that you want to change and a blank line for each data set.

```
BaCuSi_095.rec
PKSH         0.35
CPKS         0.00
```

Now refinements will start from existing rec-files and work very much like with a mlt-files.