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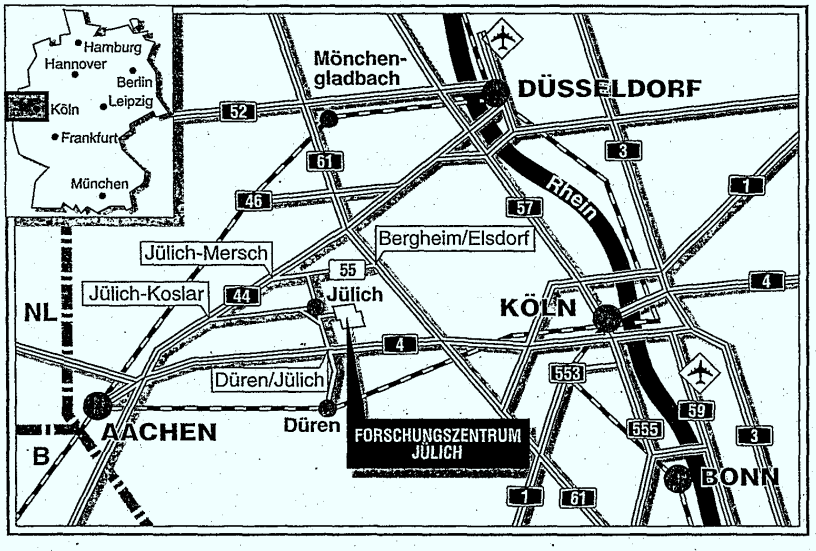

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ABSTRACT

IC-POWLS is a modified version of the computer program POWLS (POWder Least Squares) for calculation and refinement of crystallographic and magnetic structures from powder diffraction data. POWLS comprises the calculation of structure model intensities for X-ray or neutron powder diffraction. The program uses integrated intensities of individual reflections or groups of overlapping reflections as observed quantities to adjust the model parameters in a non-diagonal weighted least squares procedure. IC-POWLS has been extended for the analysis of neutron diffraction data to be simultaneously analysed for crystallographic and commensurate or incommensurate magnetic structures. The program is written in Fortran-77 and is designed to run on IBM mainframe computers, on VAX maschines or on IBM compatible personal computers.

CONTENTS

APPENDIX

1.0 Introduction

POWLS is a non-diagonal weighted least squares program for the refinement of crystal structures from X-ray as well as crystal and magnetic structures from neutron diffraction data. The program is designed for a simultaneous handling of crystallographic and magnetic structures. This program has been used routinely for the last 30 years in our as well as many outside international laboratories, many structures have been refined and many examples been published. Originally, the program was developed (Will, 1979) using refinement routines of Hamilton (1964). In the meantime the program has been repeatedly enlarged and improved (Will, Jansen & Schäfer, 1980; Will, Jansen & Schäfer, 1983), taking for example advantage of subroutines and tables partially adapted from Smith & Holomany (1978) and the ORFLS program of Busing, Martin & Levy (1962).

The POWLS program can be used at the second stage of the "two-stage method" in powder diffractometry (Will, Parrish & Huang, 1983; Jansen, Schäfer & Will, 1988, Will, 1989). The two-stage method is one of two popular approaches to analyse powder diffraction patterns; the other one is the full-pattern Rietveld method (Rietveld, 1969). At the first stage of the two-stage method, Bragg intensities are derived by decomposition of the diffraction pattern without reference to a structural model. At the second stage, these integrated intensities are used for a structure refinement analogous to the procedure in single crystal data analysis. POWLS uses a re-iterative procedure to adjust theoretical intensities, calculated from a set of model parameters, to observed integrated intensities of individual reflections, or groups of overlapping reflections. Moreover, the program allows one to treat partly overlapped reflections either as one observation or, alternatively, as a set of individual observations restricted by correlations. It is not essential by which method intensities have been obtained: by profile analysis, by individual integration or just by estimation.

The new version IC-POWLS has been extended especially with respect to magnetic structures. The program is able to handle a larger variety of magnetic structures, between them structures with commensurate and/or incommensurate lattice periodicities. Reflection indices of magnetic superlattice or satellite reflections are automatically generated by the program. The model input is based on the concept of magnetic wave vectors referring to the chemical unit cell. Enlarged commensurate structures can be handled, for example antiphase domain structures with higher order harmonics in the neutron diffraction pattern. Examples of incommensurate magnetic structure types, included in IC-POWLS, are magnetic spiral configurations and sinusoidal or square-wave amplitude modulations of magnetic moments.

The program includes four data banks stored in separate files: Symmetry information of all crystallographic space groups is supplied in "SYMPOS.TAB" (Busing, Martin & Levy, 1962) containing laue group, symmetry positions and extinction codes. Also available are X-ray scattering form factor tables for all atoms in "FORMF.TAB" (Busing, Martin & Levy, 1962), magnetic form factor tables for many magnetic 3d- and 4f-ions in "MFORMF.TAB" (Freeman & Watson, 1961; Freeman & Desclaux, 1979) and neutron nuclear scattering lengths in "SCATL.TAB" (Koester, Rauch & Seymann, 1991).

The program is written in Fortran-77 and is designed to be run on IBM mainframe computers, VAX computers or IBM compatible personal computers. When using a PC with coprocessor, the execution times of the least squares routines are comparable to working conditions on a mainframe computer. Additional PC-tools (written in Turbo Pascal) are available to display and plot model diffraction patterns using the IC-POWLS output and selected peak profiles.

2.0 Features

The main features of the program are characterized by the following keywords:

radiation	X-ray diffraction: neutron diffraction:	laboratory, synchrotron monochromatic (2θ-patterns) polychromatic (Time-of-Flight and d-spacing patterns)	
model calculation	crystal structure magnetic structure	 commensurate and incommensurate	
refinement	simultaneous refinement of crystal and magnetic structures diagonal/non-diagonal weighted least squares linear constraints		
refinement parameters	<u>structural parameters</u> neutron scatt. lengths occupation numbers positional parameters isotropic temp. param. anisotropic temp. param.	<u>magnetic parameters</u> value and direction of magnetic moment value, axis and half-cone angle of magnetic spiral amplitude and direction of modulated structure phase angles	<u>overall parameters</u> scale factor overall temp. param. preferred orientation X-ray monochromator param.
data banks	sympos: formf: scatl: mformf:	space group symmetry X-ray scattering factor tables neutron nuclear scattering lengths magnetic form factor tables	
reflections	automatic generation: read/write fundamental/satellite reflections from/to external file	fundamental (hkl) according to space group satellite/superstructure reflections: HKL (real/integer HKL referring to chemical or enlarged magnetic cell)	
auxilliary graphic programs	display of calculated diffraction patterns: (PC programs, Turbo Pascal) profile functions; hkl labeling HPGL, Postscript driver		
intentional extensions	structural incommensurate modulations: displacive and/or density modulated read symmetry elements from input file March-Dollase (1986) preferred orientation function		

3.0 Powder diffraction intensities

Calculation of integrated intensities is performed in subroutine FUNNY. The intensity I of a Bragg reflection in a powder diffraction diagram is given by:

$$I(K) = Sc * Lp(K) * To(K) * Po(K) * Mu(K) * < |F(K)|^2 > \qquad (3.1)$$

where K denotes the scattering vector. The meaning of the other symbols is:

Scaling factor *Sc*:
The scaling factor contains all factors, which are constant during a diffraction experiment, e.g. incident flux, sample volume etc.

Lorentz and polarization correction *Lp*:
The Lorentz correction (for neutrons) or Lorentz polarization correction (for X-rays) considers the distinct diffraction geometry and radiation. Calculation of *Lp* is performed in function PLOREN. Number codes "integ(3)" in the following compilation of correction factors refer to the option line (line 2) of IC-POWLS input. Symbols TT1, TT2 refer to the list of overall parameters (line 6) of IC-POWLS input. θ and d are Bragg angle and interplanar spacing, respectively.

$$Lp = \frac{1+\cos^2 2\theta \cdot \cos^m 2\theta_M}{\sin\theta \, \sin 2\theta \cdot (1+\cos^m 2\theta_M)}$$

X-ray diffraction: (Azaroff, Kaplow, Kato, Weiss, Wilson & Young (1974)
monochromator parameter $2\theta_M$,
mosaik spread parameter m:
general case: TT1=$2\theta_M$, TT2=m integ(3)=5
special case: $2\theta_M$=26.55°, m=1.7 integ(3)=0

The monochromator angle $2\theta_M$=26.55° is valid for Cu-Kα radiation. m considers the distinct effects of the mosaik distribution of the monochromator crystal, i.e. ideal crystal (m=1), real crystal (m=2), empirical value (m=1.7) (Will, Parrish & Huang, 1983).

$$Lp = \frac{1+\cos^2 2\theta \cdot \cos^2 2\theta_{M1} \cdot \cos^2 2\theta_{M2}}{\sin\theta \, \sin 2\theta \cdot (1+\cos^2 2\theta_{M1})}$$

X-ray diffraction:
two monochromators $2\theta_{M1}$ *and* $2\theta_{M2}$,
negligible mosaik spread
general case:
TT1=$2\theta_{M1}$, TT2=$2\theta_{M2}$ integ(3)=1

$$Lp = \frac{1}{\sin\theta \, \sin 2\theta}$$

neutron diffraction: (Bacon, 1975)
powder: cylindrical sample integ(3)=2

$$Lp = \frac{1}{\sin^2 2\theta}$$

neutron diffraction: (Bacon, 1975)
powder: flat sample integ(3)=3

$$Lp = \frac{1}{\sin 2\theta}$$

neutron diffraction: (Yessik, Werner & Sato, 1973)
single crystal integ(3)=4

$Lp = d^4$	*neutron diffraction, TOF d-pattern: (Schäfer, Jansen & Will, 1993)* powder: cylindrical sample integ(3)=8
$Lp = d^3$	*neutron diffraction, TOF log. scaled d-pattern: (Schäfer, Jansen & Will, 1993)* powder: cylindrical sample integ(3)=9

Overall temperature correction *To*:

$To = \exp\{-2B_{ov} (\sin\theta/\lambda)^2\}$

B_{ov} is the isotropic overall temperature parameter. λ is the wavelength of the radiation.

Preferred orientation correction *Po*:

$Po = \exp\{-P_{ov} \alpha^2\}$	preferred orientation maximum parallel to the scattering vector
$Po = \exp\{-P_{ov} (\pi/2-\alpha)^2\}$	preferred orientation maximum perpendicular to the scattering vector

P_{ov} is the preferred orientation parameter. α is the angle between scattering vector and preferred orientation normal vector.

Multiplicity factor *Mu*:

The multiplicity *Mu* is the number of degenerated, symmetry equivalent reflection planes **K** in powder diffractometry.

Structure factor quantity $|F|^2$:

$|F|^2$ depends only on the actual crystal and magnetic structure of the sample. For X-ray and nuclear neutron diffraction F is equal to the unit cell crystal structure factor (see formula 3.2). For magnetic neutron diffraction $|F|^2$ represents the (squared) component of the magnetic structure factor perpendicular to the scattering vector $\boldsymbol{K}$ (see formula (3.6)). Brackets < > indicate, that magnetic reflection intensities have to be summed over degenerated, symmetry equivalent reflections.

<u>IC-POWLS least squares overall parameters:</u>

- scaling factor: *Sc*
- overall temperature parameter: B_{ov}
- preferred orientation parameter: P_{ov}
- X-ray monochromator parameters: TT1, TT2

3.1 Crystal structure factor

The unit cell structure factor F of the crystal structure has nonzero values at fundamental reciprocal lattice points $\boldsymbol{h}$=(hkl) of the crystal structure. The structure factor for X-ray diffraction and nuclear neutron diffraction is given by:

$$F(\boldsymbol{h}) = \sum_i f_i\, t_i \exp\{2\pi i\, \boldsymbol{h}\cdot \boldsymbol{r}_i\} \tag{3.2}$$

where:

Σi sum over unit cell atoms

f_i X-ray form factor or nuclear neutron scattering length of i-th atom

t_i individual temperature correction factor of i-th atom

isotropic temperature factor: $t_i=\exp(-B_i(\sin\theta/\lambda)^2)$

B_i: isotropic individual temperature parameter

anisotropic temperature factor: $t_i=\exp(-\boldsymbol{h}^T\mathbf{B}\boldsymbol{h})$

elements $B_{ik}=B_{ki}$ of matrix **B**: anisotropic individual Debye-Waller factors

$\boldsymbol{r}_i$ positional vector of i-th atom

In order to calculate the structure factor modulus, which is done in subroutine FUNNY, the following separation is convenient:

$$|F(\boldsymbol{h})|^2 = A_h^2 + B_h^2 \tag{3.3}$$

$$A_h = \sum_i N_i/N_{r,i}\; f_i\, t_i \sum_r \cos\{2\pi\, \boldsymbol{h}\cdot \boldsymbol{r}_{i,r}\} \tag{3.4}$$

$$B_h = \sum_i N_i/N_{r,i}\; f_i\, t_i \sum_r \sin\{2\pi\, \boldsymbol{h}\cdot \boldsymbol{r}_{i,r}\} \tag{3.5}$$

where:

Σi sum over atoms within asymmetric unit, i.e. sum over atomic sites

N_i occupation number of i-th site

$N_{r,i}$ number of symmetry equivalent positons of i-th site, i.e. multiplicity of i-th site

Σr sum over $N_{r,i}$ atoms on symmetry-equivalent positions of i-th site

$\boldsymbol{r}_{i,r}$ positional vector of i-th atom on r-th symmetry equivalent position

IC-POWLS least squares atomic parameters:

- neutron scattering lenght: f_i
- occupation number: N_i
- positional parameters of site: $\boldsymbol{r}_{i,1}$=(x, y, z)
- isotropic / anisotropic individual temperature parameters: B_i or B_{ik}

3.2 Structure factor of commensurate magnetic structures

Magnetic Bragg intensities in neutron diffraction can be observed at reciprocal lattice points $K=h\pm nk$, where h is a reciprocal (fundamental) lattice vector of the crystal structure and k is the propagation vector of the magnetic structure. k has commensurate component values k=q'/q (q', q integers) and lies within the first Brillouin zone of the crystal structure. n=1,2,... denotes the order of reflection K. It is an important feature of magnetic neutron diffraction, that only magnetic moment components perpendicular to the scattering vector contribute to Bragg intensities. For magnetic structures $|F|^2$ can be expressed by: (Halpern & Johnson, 1939; Lyons, Kaplan, Dwight & Menyuk, 1962)

$$|F|^2 = |F_M(K)|^2 - |e_K \cdot F_M(K)|^2 \qquad (3.6)$$

where F_M denotes the magnetic structure factor and e_K the unit scattering vector. The magnetic structure factor $\mathbf{F}_M$ is a vector quantity and can be defined for a magnetic unit cell:

$$F_M(K) = F_o \sum_j f_j(K)\ t_j(K)\ m_j \exp\{2\pi i\ K\cdot r_j\} \qquad (3.7)$$

where

F_o	$0.27\cdot10^{-12}$ [cm] =constant; scattering amplitude for forward scattering for a single magnetic moment of 1 μ_B
Σj	sum over magnetic moments within magnetic unit cell
f_j	magnetic formfactor of j-th atom
t_j	isotropic individual temperature factor of j-th atom
m_j	magnetic moment vector of j-th atom
r_j	positional vector of j-th atom

In order to calculate the magnetic structure factor, which is done in subroutine MAGFUN, it is convenient to separate $\mathbf{F}_M$ into components:

$$F_M = (A_x+A_y+A_z) + i\ (B_x+B_y+B_z) \qquad (3.8)$$

with components for X=x,y,z along crystal axes

$$A_X = F_o \sum_i N_i/(N_{r,i}\ N_s)\ f_i\ t_i\ m_{o,i} \sum_r \sum_s e_{X,i,r,s} \cos\{2\pi K\cdot r_{i,r,s}\} \qquad (3.9)$$

$$B_X = F_o \sum_i N_i/(N_{r,i}\ N_s)\ f_i\ t_i\ m_{o,i} \sum_r \sum_s e_{X,i,r,s} \sin\{2\pi K\cdot r_{i,r,s}\} \qquad (3.10)$$

where:

Σi	sum over magnetic atoms in asymmetric unit of the chemical cell
N_i	occupation number of i-th site in one chemical cell
$N_{r,i}$	multiplicity of i-th site of symmetry equivalent atoms within chemical cell
N_s	number of chemical unit cells within magnetic unit cell
$m_{o,i}$	magnitude of magnetic moment $m_{i,1,1}=m_{o,i}\ e_{i,1,1}$
Σr	sum over $N_{r,i}$ symmetry equivalent magnetic atom positions of i-th site within chemical cell
Σs	sum over N_s chemical cells of the magnetic cell

$\boldsymbol{m}_{i,r,s}$ $= m_{o,i}\, \boldsymbol{e}_{i,r,s} = m_{o,i}(\boldsymbol{e}_{x,i,r,s} + \boldsymbol{e}_{y,i,r,s} + \boldsymbol{e}_{z,i,r,s})$:
magnetic moment vector on the r-th equivalent position in the s-th chemical cell

$\boldsymbol{e}_{i,r,s}$ unit vector of of magnetic moment $\boldsymbol{m}_{i,r,s}$

$\boldsymbol{e}_{X,i,r,s}$ X(=x,y,z)-component of i-th magn. moment unit vector $\boldsymbol{e}_{i,r,s}$ along cell axis direction

$\boldsymbol{m}_{X,i,r,s}$ $= |m_{o,i}\, \boldsymbol{e}_{X,i,1,1}|$: X-component of i-th magnetic moment $\boldsymbol{m}_{i,r,s}$

$\boldsymbol{r}_{i,r,s}$ positional vector of i-th magnetic moment on the r-th equivalent position in the s-th chemical cell

In formulas (3.9) and (3.10), occupation numbers N_i are divided by the total number of magnetic atoms $N_{r,i} \cdot N_s$ on site i, in order to take account on different unit cell volumes of crystal and magnetic unit cell. Mutual orientations between symmetry equivalent magnetic moments are defined by magnetic rotation matrices. The direction of the magnetic moment $\boldsymbol{m}_{i,r,s}$ on the r-th equivalent position of the s-th chemical unit cell is connected to the unit vector $\boldsymbol{e}_{i,1,1}$ of a first magnetic moment:

$$\boldsymbol{e}_{i,r,s} \quad ROT_{i,r,s} * \boldsymbol{e}_{i,1,1} \tag{3.11}$$

where $ROT_{i,r,s}$ is a magnetic rotation matrix. On line(s) 7 of IC-POWLS input, magnetic moments $\boldsymbol{m}_{i,1,1} = m_{o,i}\, \boldsymbol{e}_{i,1,1}$ are specified by giving either: (a) $m_{o,i}$ and angles of $\boldsymbol{m}_{i,1,1}$ to crystal axes or: (b) components $m_{X,i,1,1}$ (X=x, y, z). Rotation matrices are to be defined on line(s) 8 of IC-POWLS input, either by giving spin sequences or full rotation matrices.

IC-POWLS least squares magnetic parameters:

- magnetic moment value: m_o
- magnetic moment direction: φ_c, δ_a
  - φ_c: angle between moment vector and c-axis
  - δ_a: angle between projection of moment vector on ab-plane and a-axis

or alternatively:

- magnetic moment vector components: m_x, m_y, m_z

3.3 Structure factors of incommensurate magnetic structures

Magnetic structures can have periodicities, which are incommensurate with the underlying crystal lattice. Incommensurate structures are characterized by magnetic superstructure reflections $\boldsymbol{K}=\boldsymbol{h}\pm n\boldsymbol{k}$, which are called satellite reflections of fundamental peaks $\boldsymbol{h}$. The magnetic propagation vector $\boldsymbol{k}$ has non-rational components and will be at any point of the Brillouin zone. n is the order of satellites. Only first order fourier components (n=1) are observed for the most frequent observed incommensurate structures: spiral structures and sinusoidal structures. In general, there is no magnetic unit cell for incommensurate structures. The structure factor $\boldsymbol{F}_M$ (and hence the quantity $|F|^2$ in equation (3.6)) of incommensurate structures can be calculated using the fourier components of the moment distribution: (see for example Lyons, Kaplan, Dwight & Menyuk, 1962)

$$\boldsymbol{F}_M(\boldsymbol{K}) = F_o \sum_i f_i(\boldsymbol{K})\; t_i(\boldsymbol{K})\; \boldsymbol{m}_k^i \exp\{\, 2\pi i\, (\boldsymbol{K}+\boldsymbol{k}) \cdot \boldsymbol{r}_i \,\} \tag{3.12}$$

where the sum Σi is now over magnetic atoms of the chemical cell. $\boldsymbol{m}_k^i$ is the complex

fourier component of i-th magnetic moment. Of course, equation (3.12) can be used to calculate structure factors of commensurate structures as well, since incommensurate structures include commensurate structure types. For many purposes it is more convenient to define a magnetic unit cell and to use actual magnetic moment vectors instead of fourier components. Accordingly IC-POWLS does not use the general formula (3.12) to calculate magnetic structure factors; structure factors of incommensurate structures are to be calculated by one of the following approaches:

1. The incommensurate periodicity is approximated by a commensurate periodicity by defining rational components k=q'/q (q', q integers) of the propagation vector **k** ("quasi-commensurate structure"). Structure factors are calculated using the general formulas (3.6–3.10) of commensurate magnetic structures. Lattice parameters and positional parameters of atoms refer to the chemical cell.
   For isolated cases this procedure may suffer from the disadvantage, that a large magnetic cell has to be defined in order to have an acceptable approximation of the periodicity. As a consequence the number of magnetic atoms to be included in the calculation will be very large. For magnetic spiral structures or amplitude modulated structures IC-POWLS generates rotation matrices $ROT_{i,r,s}$ (see equation 3.11) for all magnetic atoms within the magnetic unit cell, using the phase angle $\alpha=2\pi \boldsymbol{k}\cdot\boldsymbol{r}_{i,r,s}$ and a given set of magnetic rotation matrices $ROT_{i,r,1}$ of a first chemical cell.

2. For regular incommensurate modulations of magnetic moments, fourier component expressions can be used to derive special structure factor quantities $|F|^2$ for spiral structures, sinusoidal structures etc., starting from the general formulas (3.6) and (3.12). Only parameters of magnetic atoms within the chemical cell have to be specified. The disadvantage with respect to the 1. method is, that these special expressions for $|F|^2$ can not be used to calculate composite structures, which have, for example, helical and sinusoidal modulation components.

In the following, special structure factor quantities $|F|^2$ are given for the most important incommensurate structures: a) the conical spiral and b) the amplitude (sinusoidal, square-wave) modulated structure.

a) conical spiral: (Fig. 1)
A conical spiral is described by: magnetic moment value m_0, half-cone angle β, propagation vector $\boldsymbol{k}$ and spiral axis $\boldsymbol{w}$. The helical, incommensurate moment component $m_0 \sin(\beta)$ rotates around the spiral axis when moving in direction of the propagation vector $\boldsymbol{k}$. The helical component gives rise to satellite reflections $(hkl)^{\pm}$. The commensurate, ferromagnetic moment component $m_0 \cos(\beta)$, which is oriented parallel to the spiral axis $\boldsymbol{w}$, gives rise to magnetic intensities at fundamental reciprocal lattice points coinciding with nuclear Bragg peaks. The structure factor is given by

$$|F|^2 = \sin^2 \omega \; | \; F_o \sum_i f_i \, t_i \, m_{o,i} \cos\beta_i \exp\{2\pi i \, \boldsymbol{h}\cdot\boldsymbol{r}_i\} \; |^2 \qquad (3.13)$$

for the ferromagnetic, fundamental Bragg peaks and by

$$|F^{\pm}|^2 = \frac{1 + \cos^2 \omega}{4} \left| F_o \sum_i f_i \, t_i \, m_{o,i} \sin\beta_i \exp\{2\pi i \boldsymbol{h}\cdot\boldsymbol{r}_i \; i\phi_i\} \right|^2 \qquad (3.14)$$

for the incommensurate magnetic satellite peaks. The meaning of the symbols is:

ω	angle between scattering vector $\boldsymbol{K}$ and spiral axis $\boldsymbol{w}$
F_o	$0.27 \cdot 10^{-12}$ [cm]=constant
Σi	sum over magnetic moments in chemical unit cell
β_i	half cone angle of i-th spiral
f_i	magnetic form factor of i-th atom
t_i	isotropic individual temperature factor of i-th atom
$m_{o,i}$	magnetic moment value of i-th atom
$\boldsymbol{r}_i$	positional vector of i-th atom
ϕ_i	phase angle of i-th atom in chemical cell

Remarks concerning the structure factor formulas (3.13) and (3.14):

1. Different magnetic spiral components i must have the same spiral axis direction w.
2. Phase shifts ϕ_i between spiral components can be refined.
3. Formula (3.14) does not apply for a spiral with turn angle $\alpha=\pi$, since (3.14) was obtained by averaging over perpendicular helical moment component directions $\boldsymbol{u}$ and $\boldsymbol{v}$ (Fig. 1).
4. Magnetic moments, belonging to the same Bravais lattice (i.e. related by a lattice vector translation), must have the same phase angles ϕ_i. One of the phase angles of i-th site is arbitrary.

IC-POWLS least squares parameters of the spiral structure:

- magnetic moment magnitude: m_o
- spiral axis direction: φ_c, δ_a
- half-cone angle: β
- phase angle parameters ϕ

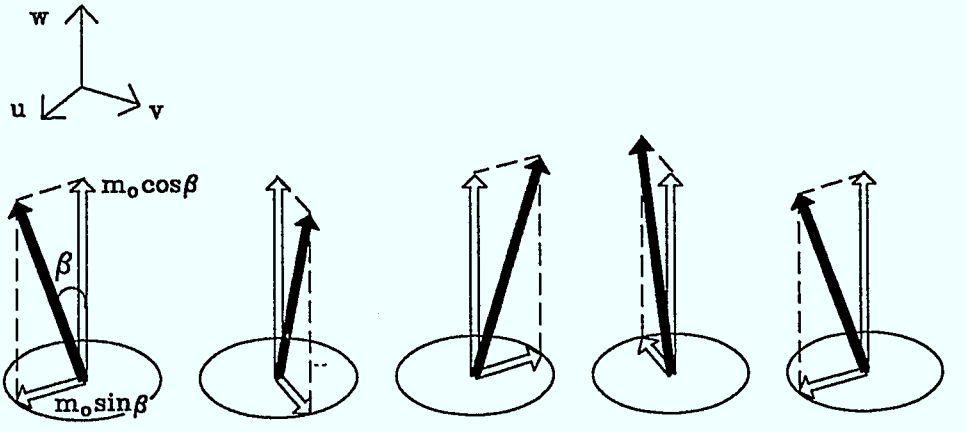

Fig. 1 Schematic representation of a conical spiral. Separation of the magnetic moment vector into ferromagnetic component (parallel $\boldsymbol{w}$) and spiral component ($\boldsymbol{u}$-$\boldsymbol{v}$-plane) perpendicular to the spiral axis w.

b) amplitude modulated structure: (Fig. 2)

An amplitude modulated structure is described by: magnetic moment amplitude A_k and magnetic moment direction (or polarization) $\boldsymbol{u}$. The most simple types of modulations are sine-wave (sinusoidal) modulations and square-wave (or antiphase domain) modulations. The structure factors are given by

$$|F^{\pm}|^2 = \frac{\sin^2 \omega}{4} \left| F_o \sum_i f_i\, t_i\, A_{k,i} \exp\{2\pi i\, \boldsymbol{h}\cdot\boldsymbol{r}_i \mp i\phi_i\} \right|^2 \qquad (3.15)$$

for the sinusoidal structure and by

$$|F^{\pm n}|^2 = \left(\frac{4}{n\pi}\right)^2 \frac{\sin^2 \omega}{4} \left| F_o \sum_i f_i\, t_i\, A_{k,i} \exp\{2\pi i\, \boldsymbol{h}\cdot\boldsymbol{r}_i \mp i\phi_i\} \right|^2 \qquad (3.16)$$

for the square-wave modulated structure. The meaning of the symbols is:

n	order of satellite peak (n=1, 3, 5, etc.)
ω	angle between scattering vector $\boldsymbol{K}$ and moment direction $\boldsymbol{u}$
F_o	$0.27 \cdot 10^{-12}$ [cm]= constant
Σi	sum over atoms within chemical unit cell
f_i	magnetic form factor of i-th atom
t_i	isotropic individual temperature factor of i-th atom
$A_{k,i}$	amplitude of modulation
$\boldsymbol{r}_i$	positional vector of i-th atom
ϕ_i	phase angle of i-th atom within chemical cell

Remarks concerning the structure factor formulas (3.15) and (3.16):

1. Different modulation components i must have the same moment direction $\boldsymbol{u}$.
2. Phase shift ϕ_i between different modulation components can be refined.
3. Magnetic moments, belonging to the same Bravais lattice, must have the same phase angles ϕ_i. One of the phase angles of i-th site is arbitrary.

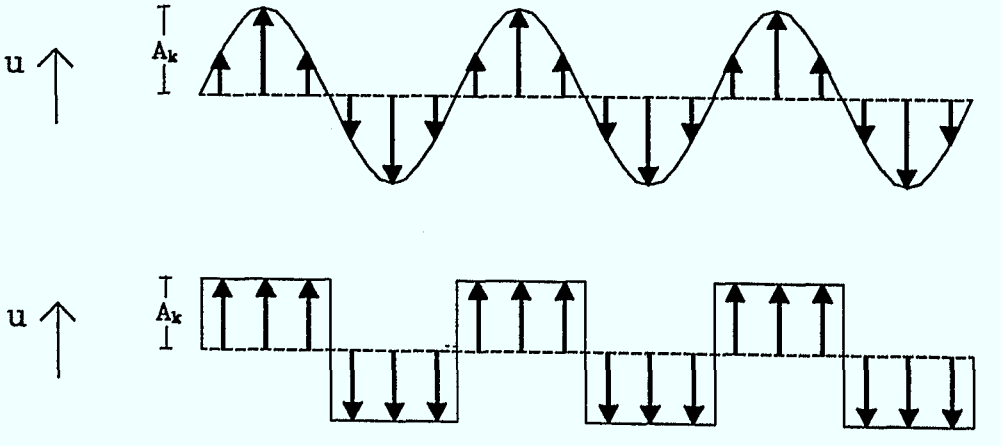

Fig. 2 Transverse sine-modulated structure (above) and squared-up structure (below).

IC-POWLS least squares parameters of the amplitude modulated structure:

- magnetic moment amplitude: A_k
- magnetic moment amplitude direction: φ_c, δ_a (see p. 7)
- phase angle parameters: ϕ

or alternatively:

- magnetic moment amplitude: ($A_{k,x}$, $A_{k,y}$, $A_{k,z}$)
- phase angle parameters: ϕ

Model intensities for both, spiral structure and amplitude modulated structures, are calculated in subroutine MAGFUN. It is convenient, to have the following separation of structure factor terms of equations (3.13)–(3.16):

$$| F_o \sum_j f_j\, t_j\, M_j \exp\{2\pi i\, \boldsymbol{h}\cdot\boldsymbol{r}_j \mp i\phi_j\} |^2 = A_h^2 + B_h^2 \qquad (3.17)$$

$$A_h = F_o \sum_i N_i/N_{r,i}\; f_i\, t_i \sum_r M_{i,r} \cos\{2\pi\, \boldsymbol{h}\cdot \boldsymbol{r}_{i,r} \mp \phi_i\} \qquad (3.18)$$

$$B_h = F_o \sum_i N_i/N_{r,i}\; f_i\, t_i \sum_r M_{i,r} \sin\{2\pi\, \boldsymbol{h}\cdot \boldsymbol{r}_{i,r} \mp \phi_i\} \qquad (3.19)$$

Σj sum over atoms in chemical unit cell

Σi sum over atoms in asymmetric unit

N_i occupation number of i-th site

$N_{r,i}$ multiplicity of i-th site

Σr sum over $N_{r,i}$ symmetry equivalent magnetic atoms of i-th site

$M_{i,r}$ magnetic moment magnitude (spiral structure: $m_0 \cos\beta$, $m_0 \sin\beta$) or magnetic moment amplitude (amplitude modulated structure: A_k).

$\phi_{i,r}$ phase angle of i-th atom on r-th equivalent position

4.0 Least squares procedure

The actual refinement routines in (IC-)POWLS are those originally developed by Hamilton (1964). The refinement is carried out on any general observed quantity **G**, which is a vector or a one-column matrix with n components g_i. Observations **G** are to be approximated by a vector C with components c_i, which are calculated from a set of parameters **P** with m < n components p_j. The function to be minimized is given by:

$$\boldsymbol{R}^T\, \boldsymbol{W}\, \boldsymbol{R} = \mathit{MINIMUM} \qquad (4.1)$$

W is a weight matrix, being proportional to the inverted variance-covariance error matrix of **G**. **R** represents the vector of residuals of observed and calculated quantities. The superscript T denotes a transposed matrix. The components of **R** are given by:

$$r_i = g_i - c_i(\boldsymbol{P}) \qquad (4.2)$$

Minimization of (4.1) is a general non-linear least squares problem. (IC-)POWLS reduces the non-linear problem to a linear form by using a Taylor series expansion. The solution of the non-linear problem is then approached by several re-iterative linear least squares cycles. The formulation of the linearization is as follows: We assume, that the original parameter vector **P** can be replaced by a better parameter set **P'** obeying the equation:

$$r'_i = g_i - c_i(P') \tag{4.3}$$

The components r'_i form a new residual vector **R'** < **R**. The mathematical problem now is to find the parameter adjustment vector **X** given by

$$X = P' - P \tag{4.4}$$

Thereby, the first order Taylor expansion of c_i about the point **P** gives

$$c_i(P') = c_i(P) + \sum_j a_{ij} \cdot x_j \tag{4.5}$$

The coefficients a_{ij} define the matrix **A** of partial derivatives with elements

$$a_{ij} = \partial c_i / \partial p_j \tag{4.6}$$

Referring to equation (4.2) and (4.3) the linearization can be expressed in matrix notation by

$$R = A \cdot X + R' \tag{4.7}$$

This is an overdetermined system of linear equations, which can be handled by a least squares formalism meeting the requirements of equation (4.1). This procedure, described for example by Hamilton (1964), leads to the solution **X** of parameter improvements:

$$(A^T W A)\ X = A^T W R \tag{4.8}$$

This is the matrix equation formed and solved by (IC-)POWLS. Since the Taylor series expansion (4.5) is only valid for small parameter increments x_j, several refinement cycles will be necessary to find the "best parameter set" **P**.

In structure refinements with (IC-)POWLS the parameter vector **P** contains crystal structure parameters (scattering length, occupation number, positional parameters, individual temperature factor), overall parameters (scaling, overall temperature, preferred orientation factor) and magnetic structure parameters (magnetic moment magnitude, direction of magnetic moment). For the first refinement cycle in (IC-)POWLS, a set of starting parameters **P** is choosen as close as possible to the true values. The matrix **A** of partial derivatives a_{ij} is calculated by changing the parameters to be varied one by one by small increments dp_j and forming a neighbouring set of intensities I'^{calc}. The derivatives are then calculated in routine MAIN by:

$$a_{ij} = (I'^{calc}_i - I^{calc}_i) / dp_j \tag{4.9}$$

Initial parameter increments for the first cycle are defined by dp_j=0.001 per default. Some of the starting parameter increments dp_j may be specified by the user in the input file. For the ensuing refinement cycles, the program calculates parameter increments dp_j=0.1*sigma(p_j) from the standard deviations of **P** determined at each cycle.

Observed quantities **G** in (IC-)POWLS are generally integrated intensities $\mathbf{I}^{obs}$. The calculated quantities **C** are intensities $\mathbf{I}^{calc}$ which are calculated in subroutine FUNNY using formula (3.1). The residual **R** is given by:

$$R = I^{obs} - I^{calc} \tag{4.10}$$

The connection between observed and calculated intensities has to be specified by the user, either by giving the hkl-numbers (generated by the program) or by specifying the 2θ- or d-value range of those reflections hkl, which may contribute to a given observation $\mathbf{I}_i^{obs}$. Observations are read by subroutine ROBS. Error margins of observed intensities and correlations between overlapping reflections are processed to calculate the weight matrix **W** (in ROBS). **W** is equal to the inverse of the variance-covariance matrix, which contains the squared estimated standart deviations of $\mathbf{I}_i^{obs}$ as diagonal elements and correlations between intensities as off-diagonal elements. Error margins and correlations may be specified by the user to perform a non-diagonal weighted least squares refinement with subroutine WEAST. If not given by the user, error margins of intensities are assumed to be equal to the square root of $\mathbf{I}_i^{obs}$ and correlations are zero per default. In the latter case the program performs a diagonal weighted least squares refinement in subroutine DWEAST.

The matrix $\mathbf{N} = \mathbf{A}^T\mathbf{W}\mathbf{A}$ and the vector $\mathbf{Y} = \mathbf{A}^T\mathbf{W}\mathbf{R}$ of the normal equations (4.8) are calculated in (D)WEAST. For solving the equation $\mathbf{N}\mathbf{X} = \mathbf{Y}$, a matrix inversion **N** to $\mathbf{N}^{-1}$ is performed in subroutine SMI50. The matrix of the parameter adjustments is obtained by $\mathbf{X} = \mathbf{N}^{-1}\mathbf{Y}$.

5.0 R-values

The goodness of the least squares structure refinement is defined by a weighted R-value R_w:

$$R_w = \left(\frac{(I^{obs} - I^{calc})^T \, W \, (I^{obs} - I^{calc})}{(I^{obs})^T \, W \, (I^{obs})} \right)^{1/2} \tag{5.1}$$

A further traditional criterion for the reliability of the least squares solution is the absolute 'linear' R-value based on unit weights, known as *R-Bragg*:

$$R_{Bragg} = \frac{\sum_{j=1}^{n} |I_j^{obs} - I_j^{calc}|}{\sum_{j=1}^{n} |I_j^{obs}|} \tag{5.2}$$

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Appendix

A1.0 Hardware and software environment

IC-POWLS is written in Standard Fortran 77 including some common extensions[1]. In our laboratory the program is run on three systems[2]:
1. IBM mainframe computer
2. IBM compatible PC (80x86)
3. VAX computer
At present, the program has the temporary name ICPW, which stands for "InCommensurate PoWls".

1. IBM mainframe: (VS-Fortran compiler)

The name of the program source code is ICPW FORTRAN. The following files are needed to run the program:

ICPW EXEC	batch file to run the program
ICPW TEXT	executable code
SYMPOS TAB	table with crystal symmetry information
FORMF TAB	table of X-ray form factor values
SCATL TAB	table of coherent neutron scattering lengthes
MFORMF TAB	table of magnetic form factor values
<*name* HKL *mode*>	hkl-reflection list

The program is started with: ICPW *name type mode*
where "*name type mode*" is the IC-POWLS input. If the hkl-read option is selected[3], the reflection file "*name* HKL *mode*" must exist.

The program creates the following files:

name OPOWLS *mode*	IC-POWLS output
name NPOWLS *mode*	in case of refinements: new input with updated parameters
name HKL *mode*	hkl-reflection list, in case of hkl-write option[3]

The mainframe version uses emulations of MS-Fortran routines (GETARG, GETTIM) and emulations of VAX-Fortran routines (SECNDS, TIME, JINT, JFIX)

---

[1] integer*, real* variable declarations; names with more than 6 characters; !-comment; enddo statement

[2] .true. value has to be assigned to the corresponding variable IBM, PC or VAX in subroutine OPENIO

[3] see control switches (line 2) of IC-POWLS input

2. IBM compatible PC (MS-Fortran compiler)

The program source code has been segmented into four parts: MAIN, PREPAR, MAGINP, FUNNY. The following files must be in the same directory to run the program:

ICPW.EXE	executable program (380 kbyte with present variable dimensions)
SYMPOS.TAB	table with crystal symmetry information
FORMF.TAB	table of X-ray form factor values
SCATL.TAB	table of coherent neutron scattering lengthes
MFORMF.TAB	table of magnetic form factor values

The program is started with: ICPW *input.ext* < *hkl.ext* >
where parameter "*input.ext*" is the IC-POWLS input. If the hkl-read or hkl-write option has been selected[3], the reflection file "*hkl.ext*" may be given as second parameter. Per default, the name of the reflection list is "*input*.HKL"

The program creates the following files:

input.OPO	IC-POWLS output file
input.NPO	in case of refinements: new input with updated parameter values
hkl.ext	reflection list, in case of hkl-write option[3] (default name: *input*.HKL)

The PC-version uses emulations of VAX-Fortran routines (SECNDS, TIME, JINT, JFIX).

3. VAX computer (VAX-Fortran compiler)

The name of the program source code is ICPW.FORTRAN. The following files must be in the same directory to run the program:

ICPW.EXE	executable program
SYMPOS.TAB	table with crystal symmetry information
FORMF.TAB	table of X-ray form factor values
SCATL.TAB	table of coherent neutron scattering lengthes
MFORMF.TAB	table of magnetic form factor values
<POWLS.HKL>	hkl reflection list

The program is started with: RUN ICPW
The name of the IC-POWLS input is "POWLS.IN". If the hkl-read option has been selected[3], the reflection file "POWLS.HKL" must exist.

The program creates the following files:

POWLS.OUT	POWLS output file
POWLS.NEW	in case of refinements: new input with updated parameter values
POWLS.HKL	hkl-reflection list, in case of hkl-write option[3]

The VAX-version uses an emulation of MS-Fortran routine GETARG.

A2.0 Input description

Overview on input lines:

Lines marked with '#' are optional.

Line 1:	**Title**
Line 2:	**Control switches**
Line 3:	**Crystallographic unit cell**
Line 4:	**Symmetry: Space group and extinctions**
Line(s) 5:	**Atomic parameters**
Line(s) 6:	**Overall parameters**
Blank line	
# Line(s) 7:	**Magnetic parameters**
# Blank line	
# Line(s) 8:	**Magnetic propagation vector and rotation matrices**
# Blank line	
# Line(s) 9:	**X-ray/ magnetic form factor tables**
# Blank line	
Line(s) 10	**Observations**
Blank line	
Line(s) 11	**Parameter refinement switches**

List of symbols and abbreviations:

P	parameter vector with components P_i, i=1, ... , NP
p_i	subset of parameter vector (i=1, ... , np) corresponding to a single atom or magnetic moment of the asymmetric unit
mp	pointer to magnetic model description
$\mathbf{m}=(m_x, m_y, m_z)$	magnetic moment vector; components along crystal axes
m_o	magnetic moment magnitude
A_k	magnetic moment amplitude
u	moment direction unit vector of amplitude modulation
w	spiral axis unit vector
φ_c	angle between vector and c-axis
δ_a	angle between ab-projection of vector and a-axis
$\mathbf{k}=(k_x, k_y, k_z)$	magnetic propagation vector
q_x, q_y, q_z	number of chemical cells along crystal axes within the magnetic unit cell
$N_s=q_x q_y q_z$	total number of chemical unit cells within magnetic unit cell
N_r	number of equivalent site positions in chemical unit cell
$\mathbf{r}_{r,s}$	positional vector of the r-th equivalent atom in the s-th chemical unit cell
ϕ	phase angle of magnetic moment
$ROT_{r,s}$	magnetic rotation matrix of the r-th equivalent atom in the s-th chemical unit cell
c_i	'+', 'n' or '–' symbol
nt	number of form factor tables
nat	number of atoms in asymmetric unit
nov	number of overall parameters
nmat	number of magnetic atoms in asymmetric unit
C	commensurate magnetic structure
IC	incommensurate magnetic structure
< >	indicates optional input entries

General rules:

- Input line with "*" in col.1 is a *comment line.*
- Entries on input line following "!" are ignored.
- Input on line may not exceed col.80.

Line 1: Title

alphanumeric text

Line 2: Control switches (free format)

integ(1) < *integ*(2) < . . . *integ*(24) > >

Entries integ(i) are integer codes or integer numbers. Per default integ(i)=0. A question mark (?) anywhere on the line forces the program to display the list of control switches.

integ(1) > 0 number of atoms in asymmetric unit

integ(2)
- > 0 number of X-ray form factor tables to be read from file "FORMF.TAB" (see line 9)
- = 0 neutron diffraction (no X-ray form factor table)
- < 0 number of X-ray form factor tables to be supplied on line(s) 9

integ(3) Lorentz and polarization (Lp) correction code (definitions see Chapter 3.1)
- = 0 Lp-correction for X-rays for one monochromator: M=26.55°, m=1.7
- = 1 Lp-correction for X-rays (general) for two monochromators: TT1=M1, TT2=M2 (see line 6)
- = 2 Lp-correction for neutrons powder: cylindrical sample
- = 3 Lp-correction for neutrons powder: flat sample
- = 4 Lp-correction for neutrons single crystal
- = 5 Lp-correction for X-rays for one monochromator: TT1=M, TT2=m (see line 6)
- = 6 ...
- = 7 ...
- = 8 Lp-correction for neutrons powder: cylindrical sample (Time-of-Flight d-pattern)
- = 9 Lp-correction for neutrons powder: cylindrical sample (Time-of-Flight logarithmic scaled d-pattern)

integ(4)
- = 0 isotropic thermal motion (see line 5)
- = 1 anisotropic thermal motion (see line 5)

integ(5) Miller index h
integ(6) Miller index k
integ(7) Miller index l

preferred orientation direction. If all indices are ≥0, then preferred orientation maximum is at planes of indexed zone. Else maximum is at indexed plane.

integ(8)	< 0	least squares with unit weights
	$= 0$	least squares with diagonal weighting scheme
	> 0	least squares with non-diagonal weighting scheme
integ(9)		background value for calculation of standard deviations for observations being supplied without sigma(obs). sigma = sqrt{I(obs) + integ(9)}
integ(10)	$= 0$	no matrix output
	$\neq 0$	matrix output of parameter correlations
integ(11)		number of refinement cycles
	≥ 0	least squares parameters selected by parameter-switch line (line 11) =0: number of refinement cycles = number of parameter-switch lines
	< 0	least squares parameters selected by parameter-switch block (lines 11). Linear constraints between parameter may be specified.
integ(12)	$= 0$	calculation of X-ray or neutron nuclear intensities
	$\neq 0$	calculation of neutron nuclear and magnetic intensities
integ(13)	< 0	write hkl reflections to external file =–1: only fundamental =–2: only satellite else: fundamental and satellite
	$= 0$	ignore hkl-file
	> 0	read hkl reflections from external file =+1: only fundamental =+2: only satellite else: fundamental and satellite
integ(14)	$= 0$	space group hkl index generator on
	$\neq 0$	space group hkl index generator off
integ(15)		intensity threshold value in [0.1 %]. hkl reflections with starting model intensities below this threshold value are omitted.
integ(16)		
.		
.		(free for user's application)
.		
integ(24)		

Line 3: Crystallographic unit cell (free format)

R_1/SY	R_2	R_3	. .	R_9	R_{10}

R_i is of real type, SY is of character*2 type.

R_1 radiation wavelength [Å]

SY only for X-rays: alternative input of radiation wavelength by radiation symbol:

	SY= MO, CU, NI, CO, FE, CR or AG
R_2, R_3, R_4	lattice constants a, b, c either in [Å] (R_i>1.0) or in [$Å^{-1}$] (R_i<1.0)
R_5, R_6, R_7	unit cell angles alpha, beta, gamma either in degrees (R_i>1.0) or as cosines (R_i<1.0)
R_8	Minimum value of reflection range, either d-value or 2theta, dependent on R_9
R_9	Maximum value of reflection range in 2theta If R_9=0., then R_8 is minimum d-value
R_{10}	zero point shift [degrees] of whole diagram

Line 4: Symmetry: Space group and extinctions (free format)

SPACE < *LAUE* > < I_1 > . . . < I_{13} >

Entries are of integer type:

SPACE	space group number according to Int. Tables for X-ray Crystallogr. (second setting, if SPACE is preceeded by a minus sign)
LAUE	Laue group indication (number code in appendix A4.0) default: Laue group according to space group Reflection indices (hkl) and corresponding multiplicities are generated according to the Laue group. LAUE rules the powder averaging of equivalent magnetic reflections.
I_1 ... I_{13}	Nonextinction indication (number codes in Appendix A5.0) default: LAUE=0: I_i according to general site of space group LAUE≠0: no extinctions

Line(s) 5: Atomic parameters

One line for each of nat (=integ(1)) atoms in asymmetric unit:

p-ident p_1/*SY* p_2 . . . p_6 < *mp* >

Col.1-8 is reserved for the atom-identification string "p-ident", containing alphanumeric text. The rest of line has free format. Atomic parameters p_k are of real type; SY is of character*2 type.

p_1	scattering length (f_i) [10^{-12} cm] for neutrons (if integ(2)=0) form factor table number for X-rays (if integ(2)≠0; see line 9)
SY	only for neutrons: alternative input of scattering length chemical element symbol of atom; the scattering length of SY is read from file "SCATL.TAB" (values taken from Koester, Rauch & Seymann (1991))
p_2	occupation number (N) of atom site
p_3, p_4, p_5	fractional x-, y-, z-coordinate of atom
p_6	isotropic temperature factor (B_i in $Å^2$) of atom
mp	pointer to magnetic model: mp=1., 2. etc (see lines 7–9) default: mp=0.

optional (if integ(4)=1 on line 2): a second line for each atom containing anisotropic temperature parameters:

B_{11} B_{12} B_{13} B_{22} B_{23} B_{33}

Line(s) 6: Overall parameters

One line for each of nov=0–5 overall parameters:

po-ident po < dpo >

Col.1-8 is reserved for the overall parameter identification string "po-ident", containing alphanumeric text. The rest of line has free format. The overall parameter po and the corresponding starting parameter increment dpo are of real type. Per default: dpo=0.001.

The program expects the following sequence of overall-parameter lines:
1. scaling factor (Sc) (default: po=1.)
2. overall temperature parameter (B_{ov}) (default: po=0.)
3. preferred orientation parameter (P_{ov}) (default: po=0.)

only for X-rays: (integ(3)=1 or integ(3)=5 on line 2)
4. monochromator parameter (TT1) (default: po=0.)
5. monochromator parameter (TT2) (default: po=0.)

Overall parameter line(s) is (are) ended by a *blank line.*

blank line

Magnetic input:
The magnetic input comprises:
line(s) 7: magnetic descriptors and model parameters
line(s) 8: propagation vectors, spin sequences/rotation matrices
line(s) 9: optional: magnetic form factor values (if not read from "MFORMF.TAB")
Lines 7, 8 and 9 are separated by blank lines:

Important note:
The magnetic intensities depend on the Laue group indicator LAUE (see line 4), which rules the powder averaging over degenerated, equivalent magnetic reflections. No powder averaging is performed for LAUE=1.

Line(s) 7: Magnetic descriptors and model parameters

to be supplied if: a) line 2; integ(12)≠0 ("magnetic calculation on")
b) line 5; mp≠0 ("magnetic pointer found")

tab/sy <typ <ord <mom <con <hkl <rot <all>...> </> p_1 <p_2 ... p_{np}>

optional:

</> dp_1 < dp_2 ... dp_{np} >

For each pointer mp, specified on line(s) 5, one line must be supplied to specify *magnetic descriptors* in the *descriptor segment* (col.1–15) and *magnetic model parameters* p_i in the *parameter segment* (col.16–80). Optionally, for each pointer mp a second line can be supplied, containing a blank segment (col.1–15) and a parameter segment (col.16-80). Th, to specify the starting *magnetic parameter increments* dp_i. Per default, parameter increments are

dp_i=0.001. Alternatively, line segments can be separated by a *slash (/) separator*: The slash separator finishes the descriptor (or blank) segment and can be positioned anywhere on the line.

Descriptor segment: (col.1–15 or terminated by "/"; free format)
Entries are integer codes and/or character string keywords. An entry may be specified by giving either the integer code or a corresponding keyword. Whereas integer codes must follow the defined sequence, keywords can be positioned anywhere in the descriptor segment. "?" in col.1 forces the program to display a table of descriptor segment entries. The meaning of the entries is as follows:

Entry	Code	Keyword	Meaning
tab/	integer pointer	"TAB="sy	magnetic form factor table
sy	sy: character*2		tab: pointer to table on line(s) 9
			sy: chemical element symbol, pointing to form factor table in "MFORMF.TAB"

The external file "MFORMF.TAB" contains calculated form factor values for 3d-Elements (Freeman & Watson, 1961) and rare earth ions R^{3+} (Freeman & Desclaux, 1979). The 'tab/sy' entry must not be omittet. The element symbol 'sy' must be the first entry on line, if it is not preceded by keyword 'TAB='.

typ	typ: integer code		type of magnetic structure
	typ=0 (default)	"C"	magn. cell = chem. cell (C): **k**=(000)
	typ=+1	"MC"	magn. cell > chem. cell (C): **k**≠(000)
	typ=+2	"SP..."	spiral structure (IC)
	typ=–2	"XSP..."	spiral structure (C)
	typ=+3	"SI..."	sinusoidal structure (IC)
	typ=–3	"XSI..."	sinusoidal structure (C)
	typ=+4	"SQ..."	squared-up structure (IC)
	typ=–4	"XSQ..."	squared-up structure (C)
	typ=±5	"US", "XUS"	to be defined by user

The program displays a list of available 'typ' codes, if an unknown 'typ' code is given. C-structures are calculated according to structure factor formulas (3.6–3.10). IC-structures are calculated according to formulas (3.13–(3.16).

ord	integer value		order of satellites
	ord=1 (default)		±1
	ord=–1	"FIRST"	0, ±1
	ord=–3	"THIRD"	0, ±1, ±2, ±3
	ord>0		±1, ±3, ±5, ..., ±ord
	ord<0		0, ±1, ±2, ±3, ..., ±ord

If two or more magnetic atoms with different pointers mp have the same propagation vector (see line 8), the satellite order is $\max(ord_1, \ldots, ord_p)$.

mom	integer pointer		pointer to subset of magnetic parameters $[p_1, \ldots, p_{np}]_{mom}$
	default: mom=mp		
	mom>0 (default)	"MPD"	magnetic moment given by: m_o, φ_c, δ_a
	mom<0	"XYZ"	magnetic moment given by: m_x, m_y, m_z

For most applications, specification of pointers "mom" others than the default pointers "mp" will not be necessary. A non-default pointer may be used to limit the number of model parameters, for example if two magnetic atoms must have the same magnetic parameter subset.

con integer code configurational symmetry

con=0 (default)	"H&J"	

Intensity calculation of commensurate magnetic structures are performed according to Halpern & Johnsons (1939) general formulas (see chapter 3.2). Powder averaging over degenerated magnetic reflections is done automatically according to the laue group indicator LAUE (line 4). If the configurational magnetic symmetry is not obvious, it is recommended to use laue indicator LAUE=1.
(For reasons of completeness, structure factor expressions for uniaxial and cubic configurational symmetry (not given in the text in chapter 3.0) are implemented and can be selected with:

con=1	"UNI"	uniaxial configurational symmetry
con=2	"CUB"	cubic configurational symmetry)

hkl integer code (HKL) index definition

hkl=0 (default)	"SHKL"	satellite hkl: (HKL)=(h±k_x, k±k_y, l±k_z)
hkl≠0	"MHKL"	only for commensurate structures: k_i=1/q_i magn. cell hkl: (HKL)=(h/q_x, k/q_y, l/q_z)

Magnetic reflection indices are generated only from those fundamental reflections, which are within the reflection range limits specified on line 3. As a consequence, the set of magnetic superstructure reflections (may not be, but) can be incomplete for the 2θ- (d-) value range limits given on line 3! 2θ- and d-value limits, up to which the list of magnetic reflections are complete, is given in the IC-POWLS output.

rot integer code input manner of magnetic rotation matrices on line(s) 8

rot=0 (default)	"SSQ"	spin sequences
rot≠0	"FUL"	full rotation matrix per moment

all integer code omit multiple generated magnetic reflections:

all=0 (default)		yes
all≠0	"all"	no

For all=0, the surplus of generated reflections is listet in the IC-POWLS output following the regular hkl-reflection list. For all≠0, the regular reflection list may contain a given reflection more than once, or the list may contain an equivalent plane of that given reflection.

Parameter segment: (col.16–80 or preceded by "/"; free format)
Entries are of real type. The subset $p_1, \ldots, p_{np}$ of the parameter vector **P** defines the magnetic moment vector $\mathbf{m}_{1,1}$ (magnitude in μ_B) of magnetic phase component "mp". The meaning of parameters depends on the actual magnetic structure type 'typ' and the sign of the 'mom'-pointer as given in the following table:

MAGNETIC MOMENT PARAMETERS [$p_1 \cdots p_{np}$] of mp					
	'typ' code	'typ' keyword	np	'mom' > 0 "MPD"	'mom' < 0 "XYZ"
commensurate k=(000)	0	C	3	magnetic moment m $p_1\ p_2\ p_3 = m_o\ \varphi_c\ \delta_a$	magnetic moment m $p_1\ p_2\ p_3 = m_x\ m_y\ m_z$
commensurate k≠(000)	+1	MC	3	magnetic moment m $p_1\ p_2\ p_3 = m_o\ \varphi_c\ \delta_a$	magnetic moment m $p_1\ p_2\ p_3 = m_x\ m_y\ m_z$
incommensurate spiral	+2	SP...	4	moment magnitude $p_1 = m_o$ spiral axis w $p_2\ p_3 = \varphi_c\ \delta_a$ half cone angle $p_4 = \beta$ [1]	spiral axis w $p_1\ p_2\ p_3 = w_x\ w_y\ w_z$ (moment magnitude m_o = length(w)) half cone angle $p_4 = \beta$ [1]
commensurate spiral (only orthog. systems)	–2	XSP...	7	moment magnitude $p_1 = m_o$ spiral axis w $p_2\ p_3 = \varphi_c\ \delta_a$ half cone angle $p_4 = \beta$ [1] moment direction 1. cell $p_5\ p_6$ [2] p_7 [3] = 0 $\varphi_c\ \delta_a$	spiral axis w $p_1\ p_2\ p_3 = w_x\ w_y\ w_z$ (moment magnitude m_o = length(w)) half cone angle $p_4 = \beta$ [1] moment direction 1. cell $p_5\ p_6\ p_7 = m_x\ m_y\ m_z$
sinusoidal incommensurate commensurate	+3 –3	SI... XSI...	3	magnetic moment amplitude A_k u $p_1\ p_2\ p_3 = A_k\ \varphi_c\ \delta_a$	magnetic moment amplitude A_k u $p_1\ p_2\ p_3 = A_{k,x}\ A_{k,y}\ A_{k,z}$
squared-up incommensurate commensurate	+4 –4	SQ... XSQ...	3	magnetic moment m $p_1\ p_2\ p_3 = m_o\ \varphi_c\ \delta_a$	magnetic moment m $p_1\ p_2\ p_3 = m_x\ m_y\ m_z$
to be user defined Incommensurate Commensurate	+5 -5	US... XUS...	6	magnetic moment m $p_1\ p_2\ p_3 = m_o\ \varphi_c\ \delta_a$ $p_4\ p_5\ p_6$ to be def. in: subroutine "amplitude" subroutine "rotate"	magnetic moment m $p_1\ p_2\ p_3 = m_x\ m_y\ m_z$ $p_4\ p_5\ p_6$ to be def. in: subroutine "amplitude" subroutine "rotate"

Default values p_i=0 except: [1] p_4=90. [2] p_6=p_2+90. [3] p_7=p_3

For incommensurate (IC) magnetic structure types, phase angles ϕ [°] between magnetic moments within the chemical unit cell may be specified and refined (e.g. phase shift between two magnetic spirals). N_r phase angle parameters can be specified on the parameter segment following the moment vector parameters (N_r=number of symmetry equivalent atoms within chemical cell). The magnetic parameters of "mp" are: $p_1 \cdots p_{np}\ p_{np+1} \cdots p_{np'}$ with np'=np+N_r. The ordinal sequence of phase angle parameters $p_{np+1} \cdots p_{np'}$ (i.e. the numeration of symmetry positions of the site) is determined by the program and must be taken from a trial IC-POWLS output. Per default, all phase angle parameters are zero. Phase differences between magnetic moments of the same Bravais lattice are fully determined by the propagation vector, i.e. phase angles must have the same value. One of the N_r phase angles is arbitrary, since intensities depend on relative phase shifts.

The magnetic parameter line(s) is (are) ended by a *blank line.*

blank line

Line(s) 8: Magnetic propagation vector and rotation matrices

to be supplied if: a) line 2; integ(12)≠0 ("magnetic calculation on")
b) line 5; mp≠0 ("magnetic pointer found")

For each pointer mp the program expects: 1. propagation vector line
2. line(s) with spin sequences or rotation matrices.

1. propagation vector line: (free format)
1st version: commensurate or incommensurate propagation vector

k_x k_y k_z $<q_x\ q_y\ q_z>$

Real entries k_x, k_y, k_z are components of the propagation vector. For a commensurate structure type with an enlarged magnetic unit cell with respect to the chemical cell, real entries q_x, q_y, q_z may be specified, to denote the number of chemical unit cells along crystal axes (i.e. the magnetic unit cell contains $N_s=q_x*q_y*q_z$ chemical cells). Per default: q_i=anint($1/k_i$).

2nd version: commensurate propagation vector

q'_x/q_x q'_y/q_y q'_z/q_z

Integer entries q'_i and q_i are nominators and denominators to define the propagation vector components $k_i=q'_i/q_i$.

Notes: – a propagation vector **k**=(0, 0, 0) may be omited if typ=0 or 'C' (see line 7).
– 1st and 2nd input version can be mixed.

2. line(s) with spin sequences or rotation matrices: (free format)
Symmetry equivalent positions of an atom with magnetic moment $\mathbf{m}_{1,1}$ are generated by the program using space group symmetries. To define mutual orientations of magnetic moments, rotation matrices for all symmetry equivalent positions have to be specified. The magnetic moment vector $\mathbf{m}_{r,s}$ in the r-th equivalent position of the s-th chemical unit cell is connected to $\mathbf{m}_{1,1}$ by:

$$m_{r,s} = ROT_{r,s} * m_{1,1}$$

where ROT is a magnetic rotation matrix with components:

$$ROT = \begin{pmatrix} r_{11} & r_{12} & r_{13} \\ r_{21} & r_{22} & r_{23} \\ r_{31} & r_{32} & r_{33} \end{pmatrix}$$

In order to condense the input of rotation matrices, sequences of characters c_i='+' (=+1), c_i='n' (=0) and c_i='−' (=−1)) may be specified. These sequences are called "spin sequences". A spin sequence element '$c_xc_yc_z$' (no intervening blanks) stands for a rotation matrix:

$$ROT = \begin{pmatrix} c_x & 0 & 0 \\ 0 & c_y & 0 \\ 0 & 0 & c_z \end{pmatrix}$$

Both collinear and non-collinear magnetic structures can be defined with spin sequences. The program allows input of both spin sequences or full rotation matrices.

Spin sequences for N_r equivalent positions within the chemical cell are given on one line: (free format); ('rot'=0 or 'SSQ' on line 7, default)

$c_x^1 <c_y^1 <c_z^1>>$ $c_x^2 <c_y^2 <c_z^2>>$ . . . $c_x^{Nr} <c_y^{Nr} <c_z^{Nr}>>$	1 *line for* N_r *elements*

c_i^j stand for the sign of the j-th magnetic atom of the site. Elements of different atoms are separated by blanks. Since the ordinal sequence of N_r equivalent atoms is determined automatically by the program, the numeration j=1, ..., N_r of spin sequence elements must be taken from a trial IC-POWLS output. Per default: c_x^j='+', $c_y^j=c_x^j$, $c_z^j=c_y^j$.

Full rotation matrices can be specified instead of spin sequences. There is one line for each rotation matrix: (9 real entries in free format); ('rot'≠0 or 'FUL' on line 7)

r_{11}^1 r_{12}^1 r_{13}^1 r_{21}^1 r_{22}^1 r_{23}^1 r_{31}^1 r_{32}^1 r_{33}^1	
.	
.	N_r *lines for* N_r *rotation matrices*
.	
r_{11}^{Nr} r_{12}^{Nr} r_{13}^{Nr} r_{21}^{Nr} r_{22}^{Nr} r_{23}^{Nr} r_{31}^{Nr} r_{32}^{Nr} r_{33}^{Nr}	

To calculate magnetic intensities of a commensurate magnetic structure the program needs rotation matrices of all magnetic moments inside the magnetic unit cell. The N_r*N_s matrices can be specified by the user. Instead of specifying the total set of matrices, default rotation matrices $ROT_{r,s}$ can be generated by the program. If the lines 8 contain only one set of N_r spin sequences/rotation matrices $ROT_{r,1}$ for a single chemical cell, the program calculates default rotation matrices $ROT_{r,s}$ using the phase angle $\alpha=2\pi\mathbf{k}\mathbf{r}_{r,s}$, as indicated in the following table. ROT(α) is a rotation matrix with turn angle α around the spiral axis.

	typ	keyword	default spin sequences/ rotation matrices $ROT_{r,s}$=	further input of rotation matrices possible
commens. spiral (IC) sinus. (IC) squared (IC)	0 2 3 4	C SP SI SQ	no further matrices	---
commens. k≠(000)	+1	MC	sign[cosα]*$ROT_{r,1}$	spin sequ.: N_s lines, each with N_r entries rot. matr.: N_s*N_r lines, each with 9 entries
spiral (C)	−2	XSP	ROT(α) * $ROT_{r,1}$ only orthogonal systems	---
sinus. (C)	−3	XSI	cosα * $ROT_{r,1}$	---
squared (C)	−4	XSQ	sign[cosα] * $ROT_{r,1}$	---

Lines 8 are terminated by a *blank line.*

blank line

Line(s) 9: X-ray/ magnetic form factor tables (free format)

to be supplied if:

X-rays	a)	line 2; integ(2)≠0	("number of X-ray tables")
	b)	line 5; p_1≠0	("X-ray form factor table pointer")
neutrons	a)	line 2; integ(12)≠0	("magnetic calculation on")
	b)	line 5; mp≠0	("magnetic pointer found")
	c)	line 7; 'tab' integer code found	

1st version (only for X-rays): read form factor table from file "FORMF.TAB" (integ(2)>0)

IT_1 IT_2 . . . IT_{nt} /

Integer entries IT_i are number codes of form factor table arrays. nt is the total number of tables. Entries are terminated with a slash (/). Entry p_1 on line 5 refers to the p_1-th table on line. The connection between number codes IT_i and form factor tables in "FORMF.TAB" is given in appendix A5.0.

2nd version: read form factor table from input lines

X-rays:	for integ(2) < 0; for each table pointer p_1 on line 5
neutrons:	for each 'tab' integer pointer on line 7

S_1 S_2 . . . S_k /

Sequence of real type entries S_j: form factor values S_j in steps of 0.05 in $\sin\theta/\lambda$ starting with S_1 for $\sin/\lambda$=0.0. The maximum number of entries per table is k=32. For k<j<32: S_j=0. Each table can be shared over several lines. Each table starts with a new line and is terminated by a slash (/).

Form factor table lines are terminated by a *blank line.*

blank line

Now the structure model is completely described. With this input the program may be started for the calculation of the structure model. The output will provide a numbered (hkl)-list with calculated intensities.

Line(s) 10 Observations

Observed intensities may be specified by different input versions. These versions differ in the way, how hkl-reflection indices are connected to an observed integrated intensity I_k^{obs}. The type of input version is automatically identified by the program by checking the sign of the second entry on lines. Input versions must not be mixed.

1st version (old version): (Format: 2F9,10I3,2X 6I3)
one line for each observation I_k^{obs}

I_k^{obs}	$< sigma_k >$	$n_{k,1} \ldots n_{k,m}$	$< cor_{k,1} \ldots cor_{k,6} >$

col.	1–8:		observed integrated intensity I_k^{obs}
col.	9–16:		optional: standart deviation $sigma_k$ of observation; default: $sigma_k$=sqrt(I_k^{obs})
col.	17–19:	$n_{k,1}$	plane number(s) $n_{k,m}$ in (hkl)-reflection list due to the starting
col.	20–22:	$n_{k,2}$	structure model (see IC-POWLS output). $n_{k,m}$ indicate those reflections, which contribute to observation I_k^{obs}. Maximum: m=10.
	.		
	.		
	.		
col.	44–46:	$n_{k,m}$	
col.	49–51:	$cor_{k,1}$	optional: percentage correlations $cor_{k,i}$ to subsequent observations
col.	52–54:	$cor_{k,2}$	I_{k+i}^{obs} (i=1, 6).
	.		default: $cor_{k,i}$=0
	.		
	.		
col.	64–66:	$cor_{k,6}$	

2nd version: (free format, real entries)
one line for each observation I_k^{obs}, lines in arbitrary order

$< xb_k >$	$-xe_k$	I_k^{obs}	$< sigma_k >$	$< cor_{k,1} \ldots cor_{k,6} >$

xb_k $-xe_k$	2θ- or d-value range limits of reflections. xb and xe denote begin and end of the k-th range respectively. All model-hkl within limits are considered to contribute to observation I_k^{obs}. Default value of xb_k is xb_k=xe_{k-1}. xe_k must be preceeded by a minus sign (without intervening blank), i.e. $-xe_k$ is a negative number. x stands for 2θ-values if R9≠0 on line 3. x stands for d-values if R9=0 on line 3.
I_k^{obs}	observed intensity
$sigma_k$	optional: estimated error of observation; default $sigma_k$=sqrt(I_k^{obs})
$cor_{k,i}$	optional: percentage correlations $cor_{k,i}$ to following observations I_{k+i}^{obs} (i=1,6) default: $cor_{k,i}$=0

When starting the program at this point, a comparative list of model intensities and observations is printed out. No refinement is performed.

Observation lines are ended by a *blank line.*

blank line

Line(s) 11 Parameter refinement switches

There are two input versions to select the parameters to be refined, i.e. the least squares parameters. The type of parameter-switch input depends on the sign of integ(11) ("number of refinement cycles", line 2).

1st version (old version): integ(11) ≥ 0: Line of parameter switches
(Format: 80I1): one line of parameter switches for one refinement cycle

$isel_1$ $isel_2$ . . . $isel_N$ ($isel_i$ = 0 *or* 1)

Switch $isel_i$ (integer*1, i≤80) in col.i corresponds to parameter P_i of the parameter vector. N is the length of the parameter vector.
$isel_i$=0 (or blank) parameter P_i is not refined
$isel_i$=1 parameter P_i is refined

Lines with parameter switches, selecting identical or different sets of parameters for successive refinement cycles, follow each other without intervening blank lines. The total number of refinement cycles (ncyc) depends on integ(11) and the number of parameter-switch lines (nline):
integ(11)=0 ncyc = nline
integ(11)>0 ncyc = integ(11); if integ(11) > nline, integ(11)–nline refinement cycles are performed according to the final line of parameter switches.

2nd version: integ(11)<0: Block of parameter switches
Linear constraints between parameters

sel_1 . . sel_6 *1st atom parameter switches*
. .
. .
sel_1 . . sel_6 *nat–th atom parameter switches*
sel *1st overall parameter switch*
. .
. .
sel *nov–th overall parameter switch*
blank line
sel_1 . . sel_{np} *1st magnetic atom parameter switches*
. .
. .
sel_1 . . sel_{np} *nmat–th magnetic atom parameter switches*

nat=integ(1): number of atoms in asymmetric unit; nov: number of overall parameters
nmat: number of magnetic atoms in asymmetric unit
The block of parameter refinement switches complies with the parameter block of the starting model parameters (lines 5, 6 and 7). For each parameter of the parameter block, the propram

expects a corresponding entry sel_i, which may be a parameter-switch or a character string, defining linear constraints between parameters:

sel_i is a numerical entry:	sel_i=0: corresponding parameter is not refined $sel_i \neq 0$: corresponding parameter is refined
sel_i is a character string containing "/PJ/":	corresponding parameter (increment) is constrained to other parameters (increments). Unconstrained parameters are designated by "X/PJ/" (X=a,A,m,M, see below).

A character string, containing non-numerical characters, is ignored, unless it contains /PJ/. The number of refinement cycles is ncyc=integ(11).

Linear constraints can be defined between parameters or parameter increments. The character string of linear constraints must not contain intervening blanks. The dependence of the constrained parameter (increment) on unconstrained parameters (or increments) (d)P_j can be specified as follows:

$$<b> \; <+> \; <\sum_j> \; <a_j> \; <*> \; <X>/PJ/$$

b constant value (default: b=0)
a_j coefficient of parameter P_j (default: a_j=1.)
+, * plus, multiplication operator
X lowercase or uppercase letter (default: X=A)
X=a, A indicates atomic parameter
X=m, M indicates magnetic parameter
Lowercase letter "a" or "m" indicates constraints between parameter increments. Uppercase letter "A" or "M" indicates constraints between parameters. If a string sel_i of linear contraints contains both lower- and uppercase letters, parameter increments are constrained.
/PJ/ parameter pointer of P_j
1st version: /j/ integer j points to j-th component P_j of the parameter vector
2nd version: /i,k/ integers i,k point to the i-th atomic (magnetic) parameter (p_i) of the k-th (magnetic) atom.

Brackets "(", ")" are ignored and may be used to define more decipherable entries sel_i. With the present setting of the program variable dimensions (see chapter A7.0), the sum can contain up to mc=10 unconstrained parameters P_j.

Examples:	"/5/" or "A/5/"	parameter is equal to parameter P_5 of the parameter vector
	"A/5,1/"	parameter is equal to 5-th parameter of 1st atom
	"m/1,3/*(–1.)"	parameter increment is inversely constrained to the parameter increment of the 1st magnetic parameter of the 3rd magnetic atom.

The present setting of the program variable dimensions (see chapter A7.0) allows a total of mc=10 constrained functions to be defined. Further constrained functions and non-linear constraints can be defined in subroutine PATCH using Fortran statements.

A2.1 Input example: Quartz (X-ray diffraction)

```
QUARTZ COLLECTED WITH A GRAPHITE MONOCHROMATOR  (Will et al, 1983)
  2  2  0  1  0  0  1  1
CU      4.91329 4.91329 5.40483 90.     90.     120.            100.
 154
SI      2.      3.      .4697   .0      .1666667
.0093   .0039   -.00001 .0078   -.00002 .0049
O       1.      6.      .4135   .2669   .2857667
.0190   .0106   -.0025  .0144   -.0035  .0083
SCALE           1.      .001
OTEMP           .0      .001
PREFOR          .0      .001

 21 34/

    2932      62  1
   14110     122  2  3
    1034      45  4
     927      43  5  6
     465      38  7
     699      41  8
     486      38  9 10
    1830      70 11                                  -48
      35      60 12
     557      39 13 14                               -24
     212      34 15 16
      31      32 17
    1313      48 18 19
     226      35 20
      59      11 21
     823      45 22 23                               -19  2
     947      62 24 25                               -36
     568      50 26 27
     283      35 28 29
     409      37 30 31
     223      34 32
     428      53 33 34                               -43
      95      51 35
     335      53 36                                  -41
     389      55 37
     273      35 38 39
      37      32 40 41
       3      31 42
      36      32 43 44
     451      38 45 46
      83      32 47
     205      34 48 49
     151      33 50 51
     234      35 52 53
     210      34 54

  1  111  1  1111111111 0
  1  111  1  1111111111 0
```

A2.2 Input example: $HoNiC_2$ (magnetic neutron diffraction)

```
HoNiC2   temperature difference pattern 1.9K-4.6K  (Yakinthos et al, 1994)
  4  0  2  0  0  0  0  0  0  0 -2  1  2  1  0
1.250    3.530   4.486   6.014   90.     90.     90.    0.0      32.
  38  1
Ho1        0.0000  2.0000  0.0000  0.0000  0.0000  0.0000  1.0
Ho2        0.0000  2.0000  0.0000  0.0000  0.0000  0.0000  2.0
Ni         0.0000  2.0000  0.5000  0.0000  0.6120  0.0000  0.0
C          0.0000  4.0000  0.5000  0.1530  0.3020  0.0000  0.0
SCAL            21.30   0.40
TEMP             0.0

HO 1/         3.8978   90.0    0.0     ! magn. parameters 1st magn atom
HO SINUS/     8.0      40.0    12.     ! magn. parameters 2nd magn atom

0. 0. 1.                               ! propagation vector 1st magn atom
+ +
0.5  0.33  0.86                        ! propagation vector 2nd magn atom
+ +

11.5 -12.0      8375                   ! 1st observation
14.6 -15.0      9158
15.0 -15.5      6168
15.8 -16.2      4746
17.4 -18.2      3358
23.5 -23.8      4369
25.6 -26.3      1046
26.3 -26.9      1380
28.5 -29.       2003
     -30.       1351
     -31.       1938                   ! last observation

Ho1      0.0  0.0  0.0  0.0  0.0  0.0   parameter switches
Ho2      0.0  0.0  0.0  0.0  0.0  0.0   atomic parameters
Ni       0.0  0.0  0.0  0.0  0.0  0.0
C        0.0  0.0  0.0  0.0  0.0  0.0
SCALE      0.                           parameter switches
TEMP       0.                           overall parameters

Ho1       1.0  0.0  0.0                  parameter switches
Ho2       1.0  1.0  1.0                  magnetic parameters
```

A2.3 Output example: $HoNiC_2$ (magnetic neutron diffraction)

```
HoNiC2   temperature difference pattern 1.9K-4.6K  (Yakinthos et al, 1994)

NO. OF ATOMS IN ASSYM. UNIT.  4          PREF. ORIENTATION (HKL).. 0 0 0
NO. XRAY FORM FACTOR TABLES.  0          VERSION OF WEIGHTING SCHEME.  0
VERSION OF LP-CORRECTION....  2          BACKGROUND .................  0
ANISOTROPIC TEMP. FACTOR.... NO          MATRIX OUTPUT.............. NO

NUMBER OF REFINEMENT CYCLES   2          MAGNETIC CALCULATIONS ......YES
HKL WRITTEN TO FILE .......  NO          HKL READ FROM FILE ........ YES


WAVELENGTH =1.25000
2 THETA RANGE FROM    .00 TO  32.00 DEGREE

CELL                                     RECIPROCAL CELL

A     3.5300                             A*      .2833
B     4.4860                             B*      .2229
C     6.0140                             C*      .1663
ALPHA  90.00                             ALPHA*  90.00
BETA   90.00                             BETA*   90.00
GAMMA  90.00                             GAMMA*  90.00


SPACE GROUP   38          NUMBER OF GENERAL POSITIONS    8
SPECIAL LAUE GROUP   1
SPECIAL EXTINCTION CODE   9 0 0 0 0 0 0 0 0 0 0 0 0

ATOM       SF        OC         X         Y         Z         B        PTR
Ho1      .00000   2.00000    .00000    .00000    .00000    .0000    1.00
Ho2      .00000   2.00000    .00000    .00000    .00000    .0000    2.00
Ni       .00000   2.00000    .50000    .00000    .61200    .0000     .00
C        .00000   4.00000    .50000    .15300    .30200    .0000     .00

SCAL       21.3000                      TEMP         .0000


MAGNETIC PARAMETERS        MOM      PHI      DEL
HO 1                     3.898   90.000     .000
HO SINUS                 8.000   40.000   12.000


//////////////////////////////////////////////////////////////////////////////
* MAGNETIC  Ho1 ATOM Nr. 1:
*
* FORM FACTOR TABLE  "HO  "  READ FROM "MFORMF TAB"
* MODEL PARAMETERS 1-3: MOMENT, PHI C, DELTA A  (MAGNETIC MOMENT VECTOR)
*
* PROPAGATION VECTOR:     .000  .000 1.000
*
*        x       y       z     sm  spin
* 1    .00000  .00000  .00000      +++
* 2    .00000  .50000  .50000      ---
//////////////////////////////////////////////////////////////////////////////


//////////////////////////////////////////////////////////////////////////////
* MAGNETIC  Ho2 ATOM Nr. 2: SINUSOIDAL MODULATION
*
* FORM FACTOR TABLE  "HO  "  READ FROM "MFORMF TAB"
* MODEL PARAMETERS 1-3: MOMENT, PHI C, DELTA A  (MAX MAGNETIC MOMENT VECTOR)
*
* PROPAGATION VECTOR:     .500  .330  .860
*
*        x       y       z     sm  spin
* 1    .00000  .00000  .00000   4  +
* 2    .00000  .50000  .50000   4  +
//////////////////////////////////////////////////////////////////////////////
```

FORM FACTOR TABLES

TABLE NO. 1 READ FROM FILE HO (3+) Freeman (1979), JMMM 12 p.11

1.000	.989	.959	.913	.853	.786	.714	.641
.571	.503	.442	.388	.333	.290	.246	.213
.179	.153	.127	.109	.090	.076	.062	.052
.042	.000	.000	.000	.000	.000	.000	.000

CALCULATED FUNDAMENTAL INTENSITIES FROM STARTING PARAMETERS

PLANE 2THETA D H K L M LP |Fnuc| Inuc

no fundamental hkl in reflection list

CALCULATED SATELLITE INTENSITIES FROM STARTING PARAMETERS

HKL DEFINITION TAU= 1: (H K L) + S * (.000 .000 1.000)
HKL DEFINITION TAU= 2: (H K L) + S * (.500 .330 .860)

HKL READ FROM FILE

PLANE	2 THETA	D	H	K	L	S	TAU	M	LP	|Fmag|	Imag
1	11.57	6.19982	0	0	1	-1	2	2	49.452	.00	.0
2	11.57	6.19982	1	0	1	-1	2	2	49.452	.00	.0
3	11.93	6.01400	0	0	0	1	1	2	46.547	2.04	8250.4
4	14.88	4.82742	0	1	1	-1	2	2	30.082	2.00	5112.7
5	14.88	4.82742	1	1	1	-1	2	2	30.082	1.63	3404.0
6	15.39	4.66643	0	0	0	1	2	2	28.126	.48	273.2
7	15.39	4.66643	1	0	0	-1	2	2	28.126	2.03	4960.0
8	16.02	4.48600	0	1	1	-1	1	2	26.013	2.00	4411.4
9	17.82	4.03547	0	0	2	-1	2	2	21.099	1.99	3553.3
10	17.82	4.03547	1	0	2	-1	2	2	21.099	.86	661.7
11	18.02	3.98986	0	1	0	-1	2	2	20.631	.00	.0
12	18.02	3.98986	1	1	0	-1	2	2	20.631	.00	.0
13	20.02	3.59582	0	1	0	-1	1	2	16.806	.00	.0
14	20.02	3.59582	0	1	0	1	1	2	16.806	.00	.0
15	20.14	3.57368	0	1	2	-1	2	2	16.603	.00	.0
16	20.14	3.57368	1	1	2	-1	2	2	16.603	.00	.0
17	20.40	3.53000	1	0	1	-1	1	2	16.206	.00	.0
18	23.69	3.04432	1	0	0	1	1	2	12.121	.95	469.5
19	23.69	3.04432	1	0	0	-1	1	2	12.121	.95	469.5
20	23.76	3.03583	0	-1	1	-1	2	2	12.055	1.82	1699.7
21	23.76	3.03583	1	-1	1	-1	2	2	12.055	1.89	1836.9
22	23.99	3.00700	0	0	1	1	1	2	11.832	.00	.0
23	25.13	2.87329	-1	0	1	1	2	2	10.827	.00	.0
24	25.13	2.87329	0	0	1	1	2	2	10.827	.00	.0
25	25.88	2.79061	0	1	0	1	2	2	10.228	.00	.0
26	25.88	2.79061	-1	1	0	1	2	2	10.228	.00	.0
27	26.04	2.77411	-1	1	1	-1	1	2	10.110	1.14	559.9
28	26.04	2.77411	1	1	1	-1	1	2	10.110	1.14	559.9
29	26.85	2.69169	0	-1	1	1	2	2	9.534	1.06	460.3
30	26.85	2.69169	-1	-1	1	1	2	2	9.534	1.76	1262.0
31	27.43	2.63620	0	-1	2	-1	2	2	9.156	.00	.0
32	27.43	2.63620	1	-1	2	-1	2	2	9.156	.00	.0
33	28.22	2.56416	0	0	3	-1	2	2	8.678	.00	.0
34	28.22	2.56416	1	0	3	-1	2	2	8.678	.00	.0
35	28.73	2.51904	1	1	0	1	1	2	8.384	.00	.0
36	28.73	2.51904	1	1	0	-1	1	2	8.384	.00	.0
37	28.73	2.51904	-1	1	0	-1	1	2	8.384	.00	.0
38	28.73	2.51904	-1	1	0	1	1	2	8.384	.00	.0
39	28.88	2.50636	0	2	1	-1	2	2	8.303	.00	.0
40	28.88	2.50636	1	2	1	-1	2	2	8.303	.00	.0

41	28.98	2.49777	0	-1	1	1	1	2	8.248	1.79	1127.8
42	28.98	2.49777	0	1	1	1	1	2	8.248	1.79	1127.8
43	29.78	2.43260	0	1	3	-1	2	2	7.838	1.58	838.2
44	29.78	2.43260	1	1	3	-1	2	2	7.838	.68	153.5
45	30.67	2.36296	1	2	0	-1	2	2	7.411	1.80	1025.4
46	30.67	2.36296	0	2	0	-1	2	2	7.411	1.69	902.8
47	31.32	2.31547	2	0	1	-1	2	2	7.127	.00	.0
48	31.32	2.31547	-1	0	1	-1	2	2	7.127	.00	.0
49	31.69	2.28907	-1	0	1	1	1	2	6.972	.00	.0
50	31.69	2.28907	1	0	1	1	1	2	6.972	.00	.0

LIST OF MULTIPLE GENERATED (REJECTED) SATELLITE-HKL

*	DSTAR=0		0	0	1	-1	1	
*	16.02	4.48600	0	-1	1	-1	1	2
*	20.40	3.53000	-1	0	1	-1	1	2
*	11.93	6.01400	0	0	2	-1	1	2
*	26.04	2.77411	1	-1	1	-1	1	2
*	26.04	2.77411	-1	-1	1	-1	1	2
*	20.02	3.59582	0	1	2	-1	1	2
*	20.02	3.59582	0	-1	2	-1	1	2
*	23.69	3.04432	1	0	2	-1	1	2
*	23.69	3.04432	-1	0	2	-1	1	2
*	28.73	2.51904	1	1	2	-1	1	2
*	28.73	2.51904	-1	1	2	-1	1	2
*	28.73	2.51904	1	-1	2	-1	1	2
*	28.73	2.51904	-1	-1	2	-1	1	2
*	23.99	3.00700	0	0	3	-1	1	2
*	28.98	2.49777	0	1	3	-1	1	2
*	28.98	2.49777	0	-1	3	-1	1	2
*	31.69	2.28907	1	0	3	-1	1	2
*	31.69	2.28907	-1	0	3	-1	1	2

OBSERVED PEAKS AND MILLER PLANES UNDER EACH PEAK

PEAK	PLANE NO	2THETA RANGE	I(CALC)	I(OBS)	SIGMA
1	1 ... 3	11.50 ... 12.00	8250	8375	91
2	4 ... 5	14.60 ... 15.00	8516	9158	95
3	6 ... 7	15.00 ... 15.50	5233	6168	78
4	8 ... 8	15.80 ... 16.20	4411	4746	68
5	9 ... 12	17.40 ... 18.20	4215	3358	57
6	18 ... 21	23.50 ... 23.80	4475	4369	66
7	25 ... 28	25.60 ... 26.30	1119	1046	32
8	29 ... 30	26.30 ... 26.90	1722	1380	37
9	35 ... 42	28.50 ... 29.00	2255	2003	44
10	43 ... 44	29.00 ... 30.00	991	1351	36
11	45 ... 46	30.00 ... 31.00	1928	1938	44

THE NUMBER OF OBSERVED PEAKS INCLUDED IS 11

THE NUMBER OF PLANES PROCESSED IN FUNNY IS 46

NO	I(CALC)	I(OBS)	NO	I(CALC)	I(OBS)	NO	I(CALC)	I(OBS)	NO	I(CALC)	I(OBS)
1	8250.	8375.	2	8517.	9158.	3	5233.	6168.	4	4411.	4746.
5	4215.	3358.	6	4476.	4369.	7	1120.	1046.	8	1722.	1380.
9	2256.	2003.	10	992.	1351.	11	1928.	1938.			

R - VALUE = .0920 (BASED ON UNWEIGHTED ABSOLUTE RESIDUALS)

NUMBER CODES, VALUES AND STARTING INCREMENTS OF PARAMETERS

CODE NO	PARAMETER	VALUE	INCREMENT
1	SF Ho1	.0000	.0010
2	OC Ho1	2.0000	.0010
3	X Ho1	.0000	.0010
4	Y Ho1	.0000	.0010
5	Z Ho1	.0000	.0010
6	B Ho1	.0000	.0010
7	SF Ho2	.0000	.0010
8	OC Ho2	2.0000	.0010
9	X Ho2	.0000	.0010
10	Y Ho2	.0000	.0010
11	Z Ho2	.0000	.0010
12	B Ho2	.0000	.0010
13	SF Ni	.0000	.0010
14	OC Ni	2.0000	.0010
15	X Ni	.5000	.0010
16	Y Ni	.0000	.0010
17	Z Ni	.6120	.0010
18	B Ni	.0000	.0010
19	SF C	.0000	.0010
20	OC C	4.0000	.0010
21	X C	.5000	.0010
22	Y C	.1530	.0010
23	Z C	.3020	.0010
24	B C	.0000	.0010
25	SCAL	21.3000	.0010
26	TEMP	.0000	.0010
27	MOM Ho1	3.8978	.0010
28	PHI Ho1	90.0000	.0010
29	DEL Ho1	.0000	.0010
30	MOM Ho2	8.0000	.0010
31	PHI Ho2	40.0000	.0010
32	DEL Ho2	12.0000	.0010

STRUCTURE FACTOR AND LEAST SQUARES PROGRAM FOR OVERLAPPING POWDER DATA.

HoNiC2 (temperature difference pattern data 1.9K-4.6K)

LEAST SQUARES. CYCLE 1 OF 2 CYCLES.

REF$		PARAMETER	OLD VALUE	CHANGE	NEW VALUE	SIGMA
NO	1	SF Ho1	.00000	.00000	.00000	.00000
NO	2	OC Ho1	2.00000	.00000	2.00000	.00000
NO	3	X Ho1	.00000	.00000	.00000	.00000
NO	4	Y Ho1	.00000	.00000	.00000	.00000
NO	5	Z Ho1	.00000	.00000	.00000	.00000
NO	6	B Ho1	.00000	.00000	.00000	.00000
NO	7	SF Ho2	.00000	.00000	.00000	.00000
NO	8	OC Ho2	2.00000	.00000	2.00000	.00000
NO	9	X Ho2	.00000	.00000	.00000	.00000
NO	10	Y Ho2	.00000	.00000	.00000	.00000
NO	11	Z Ho2	.00000	.00000	.00000	.00000
NO	12	B Ho2	.00000	.00000	.00000	.00000
NO	13	SF Ni	.00000	.00000	.00000	.00000
NO	14	OC Ni	2.00000	.00000	2.00000	.00000
NO	15	X Ni	.50000	.00000	.50000	.00000
NO	16	Y Ni	.00000	.00000	.00000	.00000
NO	17	Z Ni	.61200	.00000	.61200	.00000
NO	18	B Ni	.00000	.00000	.00000	.00000
NO	19	SF C	.00000	.00000	.00000	.00000
NO	20	OC C	4.00000	.00000	4.00000	.00000
NO	21	X C	.50000	.00000	.50000	.00000
NO	22	Y C	.15300	.00000	.15300	.00000
NO	23	Z C	.30200	.00000	.30200	.00000
NO	24	B C	.00000	.00000	.00000	.00000
NO	25	SCAL	21.30000	.00000	21.30000	.00000
NO	26	TEMP	.00000	.00000	.00000	.00000
YES	27	MOM Ho1	3.89780	.00196	3.89976	.05525

NO	28	PHI Ho1	90.00000	.00000	90.00000	.00000
NO	29	DEL Ho1	.00000	.00000	.00000	.00000
YES	30	MOM Ho2	8.00000	.08208	8.08208	.09120
YES	31	PHI Ho2	40.00000	.55890	40.55890	2.74965
YES	32	DEL Ho2	12.00000	-26.78706	-14.78706	4.57031

NO	I(CALC)	I(OBS)	NO	I(CALC)	I(OBS)	NO	I(CALC)	I(OBS)	NO	I(CALC)	I(OBS)
1	8259.	8375.	2	9050.	9158.	3	6455.	6168.	4	4416.	4746.
5	3558.	3358.	6	4405.	4369.	7	1121.	1046.	8	1326.	1380.
9	2258.	2003.	10	1351.	1351.	11	1669.	1938.			

R - VALUE = .0395 (BASED ON UNWEIGHTED ABSOLUTE RESIDUALS)

STRUCTURE FACTOR AND LEAST SQUARES PROGRAM FOR OVERLAPPING POWDER DATA.

HoNiC2 (temperature difference pattern data 1.9K-4.6K)

LEAST SQUARES. CYCLE 2 OF 2 CYCLES.

REF$		PARAMETER		OLD VALUE	CHANGE	NEW VALUE	SIGMA
NO	1	SF	Ho1	.00000	.00000	.00000	.00000
NO	2	OC	Ho1	2.00000	.00000	2.00000	.00000
NO	3	X	Ho1	.00000	.00000	.00000	.00000
NO	4	Y	Ho1	.00000	.00000	.00000	.00000
NO	5	Z	Ho1	.00000	.00000	.00000	.00000
NO	6	B	Ho1	.00000	.00000	.00000	.00000
NO	7	SF	Ho2	.00000	.00000	.00000	.00000
NO	8	OC	Ho2	2.00000	.00000	2.00000	.00000
NO	9	X	Ho2	.00000	.00000	.00000	.00000
NO	10	Y	Ho2	.00000	.00000	.00000	.00000
NO	11	Z	Ho2	.00000	.00000	.00000	.00000
NO	12	B	Ho2	.00000	.00000	.00000	.00000
NO	13	SF	Ni	.00000	.00000	.00000	.00000
NO	14	OC	Ni	2.00000	.00000	2.00000	.00000
NO	15	X	Ni	.50000	.00000	.50000	.00000
NO	16	Y	Ni	.00000	.00000	.00000	.00000
NO	17	Z	Ni	.61200	.00000	.61200	.00000
NO	18	B	Ni	.00000	.00000	.00000	.00000
NO	19	SF	C	.00000	.00000	.00000	.00000
NO	20	OC	C	4.00000	.00000	4.00000	.00000
NO	21	X	C	.50000	.00000	.50000	.00000
NO	22	Y	C	.15300	.00000	.15300	.00000
NO	23	Z	C	.30200	.00000	.30200	.00000
NO	24	B	C	.00000	.00000	.00000	.00000
NO	25	SCAL		21.30000	.00000	21.30000	.00000
NO	26	TEMP		.00000	.00000	.00000	.00000
YES	27	MOM	Ho1	3.89976	.00398	3.90374	.06071
NO	28	PHI	Ho1	90.00000	.00000	90.00000	.00000
NO	29	DEL	Ho1	.00000	.00000	.00000	.00000
YES	30	MOM	Ho2	8.08208	-.01553	8.06656	.09919
YES	31	PHI	Ho2	40.55890	-1.69522	38.86368	2.72287
YES	32	DEL	Ho2	-14.78706	3.85040	-10.93666	3.95748

NO	I(CALC)	I(OBS)	NO	I(CALC)	I(OBS)	NO	I(CALC)	I(OBS)	NO	I(CALC)	I(OBS)
1	8276.	8375.	2	9109.	9158.	3	6227.	6168.	4	4425.	4746.
5	3578.	3358.	6	4463.	4369.	7	1123.	1046.	8	1340.	1380.
9	2263.	2003.	10	1258.	1351.	11	1723.	1938.			

R - VALUE = .0348 (BASED ON UNWEIGHTED ABSOLUTE RESIDUALS)

STRUCTURE FACTOR AND LEAST SQUARES PROGRAM FOR OVERLAPPING POWDER DATA.

HoNiC2 (temperature difference pattern data 1.9K-4.6K)

FUNCTIONS OF INTENSITIES

PEAK	PLANE	NO	2THETA	RANGE	I(CALC)	I(OBS)	DELTA	DELTA/SIGMA
1	1...	3	11.50...	12.00	8275.54	8375.00	99.46	1.09
2	4...	5	14.60...	15.00	9109.16	9158.00	48.84	.51
3	6...	7	15.00...	15.50	6226.57	6168.00	-58.57	-.75
4	8...	8	15.80...	16.20	4424.88	4746.00	321.12	4.66
5	9...	12	17.40...	18.20	3577.89	3358.00	-219.89	-3.79
6	18...	21	23.50...	23.80	4463.48	4369.00	-94.48	-1.43
7	25...	28	25.60...	26.30	1123.12	1046.00	-77.12	-2.38
8	29...	30	26.30...	26.90	1340.10	1380.00	39.90	1.07
9	35...	42	28.50...	29.00	2262.54	2003.00	-259.54	-5.80
10	43...	44	29.00...	30.00	1257.78	1351.00	93.22	2.54
11	45...	46	30.00...	31.00	1722.52	1938.00	215.48	4.89

R - VALUE = .0503 (WEIGHTED SQUARED RESIDUALS, WITHOUT CORRELATIONS)
R - VALUE = .0503 (WEIGHTED SQUARED RESIDUALS, CORRELATIONS INCLUDED)

INTENSITIES ABOVE ARE CALCULATED WITH THE FOLLOWING PARAMETER VALUES

PARAMETER	DESCRIPTION	VALUE	SIGMA
1	SF Ho1	.0000	
2	OC Ho1	2.0000	
3	X Ho1	.0000	
4	Y Ho1	.0000	
5	Z Ho1	.0000	
6	B Ho1	.0000	
7	SF Ho2	.0000	
8	OC Ho2	2.0000	
9	X Ho2	.0000	
10	Y Ho2	.0000	
11	Z Ho2	.0000	
12	B Ho2	.0000	
13	SF Ni	.0000	
14	OC Ni	2.0000	
15	X Ni	.5000	
16	Y Ni	.0000	
17	Z Ni	.6120	
18	B Ni	.0000	
19	SF C	.0000	
20	OC C	4.0000	
21	X C	.5000	
22	Y C	.1530	
23	Z C	.3020	
24	B C	.0000	
25	SCAL	21.3000	
26	TEMP	.0000	
27	MOM Ho1	3.9037	.0607
28	PHI Ho1	90.0000	
29	DEL Ho1	.0000	
30	MOM Ho2	8.0666	.0992
31	PHI Ho2	38.8637	2.7229
32	DEL Ho2	-10.9367	3.9575

A3.0 hkl-file input description

hkl reflections can be written to and read from an external file "hklfile.ext" (see integ(13), line 2 of IC-POWLS input). One line is expected for each hkl: (free format)

icode h k l < sign < mult >>

icode	integer	icode=1: fundamental reflection icode=2: superstructure reflection
h	integer	fundamental reflection index h
k	integer	fundamental reflection index k
l	integer	fundamental reflection index l
sign	integer or real	optional: order of reflection sign=0 (default) (fundamental reflection) sign=±1, ±2, ±3, ... (superstructure reflection)
mult	integer or real	optional: multiplicity of reflection per default, the multiplicity is determined by the program according to the laue group indicator LAUE (line 4 of IC-POWLS input).

'*' or 'c' in col.1 denotes a comment line. Reflections hkl are ordered on d-values, if written to external file.

IC-POWLS generates superstructure reflections using fundamental (h, k, l). There are two versions of magnetic HKL definition:

1. Magnetic satellite-reflections HKL:
   "hkl"=0 or "SHKL" (line 7 of IC-POWLS input)

   (H, K, L)=(h, k, l) + sign * (k_x, k_y, k_z)

   where (k_x, k_y, k_z) denotes the magnetic propagation vector.

2. Alternative definiton of reflections HKL for a commensurate magnetic unit cell with cell axes $q_x a$, $q_y b$, $q_z c$ (a, b, c are lattice constants of the chemical cell):
   "hkl"≠0 or "hkl"="MHKL" (line 7 of IC-POWLS input)

   (H, K, L)=(h/q_x, k/q_y, l/q_z)

   Magnetic reflections HKL are generated only for sign=0.

A4.0 Number codes of Laue group and nonextinction indicators

The code word LAUE (line 4 of POWLS input) is interpreted as follows:

LAUE = 1	Laue group –1	
LAUE = 2	Laue group 2/m	(y axis unique)
LAUE = 3	Laue group 2/m	(z axis unique)
LAUE = 4	Laue group mmm	
LAUE = 5	Laue group 4/m	
LAUE = 6	Laue group 4/mmm	
LAUE = 7	Laue group m3	
LAUE = 8	Laue group m3m	
LAUE = 9	Laue group –3	(rhombohedral axes)
LAUE =10	Laue group –3m	(rhombohedral axes)
LAUE =11	Laue group –3	(hexagonal axes)
LAUE =12	Laue group –3m1	(hexagonal axes)
LAUE =13	Laue group 6/m	
LAUE =14	Laue group 6/mmm	
LAUE =15	Laue group –31m	(hexagonal axes)

The nonextinction code words I1 to I13 are interpreted as follows:

I1 is code word for lattice type as follows

I1 = 0	P primitive	no conditions
1	A centered	k+l=2n
2	B centered	h+l=2n
3	C centered	h+k=2n
4	F centered	h+k, k+l, l+h=2n
5	I centered	h+k+l=2n
6	R obverse	–h+k+l=3n
7	R reverse	h–k+l=3n
8	H hexagonal	h–k=3n
9	same as 0	

I2 is code word for (hk0)

I2 = 0	no conditions	
1	a glide	h=2n
2	b glide	k=2n
3	n glide	h+k=2n
4	d glide	h+k=4n (h=2n, k=2n)

I3 is code word for (h01)

I3 = 0	no conditions	
1	a glide	h=2n
2	c glide	l=2n
3	n glide	h+l=2n
4	d glide	h+l=4n (h=2n, l=2n)

I4 is code word for (0kl)

I4 =	0	no conditions	
	1	b glide	k=2n
	2	c glide	l=2n
	3	n glide	k+l=2n
	4	d glide	k+l=4n (k=2n, l=2n)

I5 is code word for (hhl)

I5 =	0	no conditions	
	1	c(n) glide	l=2n
	2	d glide	2h+l=4n

I6 is code word for (h–hl)

I6 =	0	no conditions	
	1	c(n) glide	l=2n
	2	d glide	2h+l=4n

I7 is code word for (hkh)

I7 =	0	no conditions	
	1	b(n) glide	k=2n
	2	d glide	2h+k=4n

I8 is code word for (hk–h)

I8 =	0	no conditions	
	1	b(n) glide	k=2n
	2	d glide	2h+k=4n

I9 is code word for (hkk)

I9 =	0	no conditions	
	1	a(n) glide	h=2n
	2	d glide	h+2k=4n

I10 is code word for (hk–k)

I10=	0	no conditions	
	1	a(n) glide	h=2n

I11 is code word for (h00)

I11=	0	no conditions	
	1	2(1) or 4(2) screw	h=2n
	2	4(1) or 4(3) screw	h=4n

I12 is code word for (0k0)

I12=	0	no conditions	
	1	2(1) or 4(2) screw	k=2n
	2	4(1) or 4(3) screw	k=4n

I13 is code word for (00l)

I13=	0	no conditions	
	1	2(1) or 4(2) screw	l=2n
	2	3(1), 3(2), 6(2) or 6(4) screw	l=3n
	3	4(1) or 4(3) screw	l=4n
	4	6(1) or 6(5) screw	l=6n

A5.0 Number codes of X-ray form factor tables

Atom	Origin	Code	Atom	Origin	Code
H	SCF	1	V+1	SCF	57
H–1	SCF	2	V+2	SCF	58
HE	SCF	3	V+3	SCF	59
HE–1	SCF	4	CR	SCF	60
LI	SCF	5	CR+1	SCF	61
LI+1	SCF	6	CR+2	SCF	62
LI–1	SCF	7	CR+3	SCF	63
BE	SCF	8	MN	SCF	64
BE+1	SCF	9	MN+1	SCF	65
BE+2	SCF	10	MN+2	SCF	66
B	SCF	11	MN+3	SCF	67
B+1	SCF	12	MN+4	SCF	68
B+2	SCF	13	FE	SCF	69
B+3	SCF	14	FE+1	SCF	70
C	SCF	15	FE+2	SCF	71
C+3	SCF	16	FE+3	SCF	72
C+4	SCF	17	FE+4	SCF	73
N	SCF	18	CO	SCF	74
N+3	SCF	19	CO+1	SCF	75
N+4	SCF	20	CO+2	SCF	76
O	SCF	21	CO+3	SCF	77
OX–2	SUZK	22	NI	SCF	78
OH–1	SUZK	23	NI+1	SCF	79
H20	SUZK	24	NI+2	SCF	80
F-1	SCF	25	NI+3	SCF	81
NE	SCF	26	CU	SCF	82
NA	SCF	27	CU+1	SCF	83
NA+1	SCF	28	CU+2	SCF	84
MG	SCF	29	CU+3	SCF	85
MG+2	SCF	30	ZN	SCF	86
AL	SCF	31	ZN+2	SCF	87
AL+2	SCF	32	GA	SCF	88
AL+3	SCF	33	GA+1	SCF	89
SI	SCF	34	GA+3	SCF	90
SI+4	SCF	35	GE	SCF	91
P	SCF	36	GE+2	SCF	92
S	SCF	37	GE+4	SCF	93
S-1	SCF	38	CA	TFDS	94
S-2	SCF	39	CA+1	TFDS	95
CL	SCF	40	CA+2	TFDS	96
CL–1	SCF	41	SC	TFDS	97
A	SCF	42	SC+1	TFDS	98
K	SCF	43	SC+2	TFDS	99
K+1	SCF	44	SC+3	TFDS	100
CA	SCF	45	TI	TFDS	101
CA+1	SCF	45	TI+1	TFDS	102
CA+2	SCF	47	TI+2	TFDS	103
SC	SCF	48	TI+3	TFDS	104
SC+1	SCF	49	V	TFDS	105
SC+2	SCF	50	V+1	TFDS	106
SC+3	SCF	51	V+2	TFDS	107
TI	SCF	52	V+3	TFDS	108
TI+1	SCF	53	CR	TFDS	109
TI+2	SCF	54	CR+1	TFDS	110
TI+3	SCF	55	CR+2	TFDS	111
V	SCF	56	CR+3	TFDS	112

Atom	Origin	Code	Atom	Origin	Code
MN	TFDS	113	SB	TFDS	168
MN+1	TFDS	114	TE	TFDS	169
MN+2	TFDS	115	I	TFDS	170
MN+3	TFDS	116	XE	TFDS	171
MN+4	TFDS	117	CS	TFDS	172
FE	TFDS	118	BA	TFDS	173
FE+1	TFDS	119	LA	TFDS	174
FE+2	TFDS	120	CE	TFDS	175
FE+3	TFDS	121	PR	TFDS	176
FE+4	TFDS	122	ND	TFDS	177
CO	TFDS	123	PM	TFDS	178
CO+1	TFDS	124	SM	TFDS	179
CO+2	TFDS	125	EU	TFDS	180
CO+3	TFDS	126	GD	TFDS	181
NI	TFDS	127	TB	TFDS	182
NI+1	TFDS	128	DY	TFDS	183
NI+2	TFDS	129	HO	TFDS	184
NI+3	TFDS	130	ER	TFDS	185
CU	TFDS	131	TM	TFDS	186
CU+1	TFDS	132	YB	TFDS	187
CU+2	TFDS	133	LU	TFDS	188
CU+3	TFDS	134	HF	TFDS	189
ZN	TFDS	135	TA	TFDS	190
ZN+2	TFDS	136	W	TFDS	191
GA	TFDS	137	RE	TFDS	192
GA+1	TFDS	138	OS	TFDS	193
GA+3	TFDS	139	IR	TFDS	194
GE	TFDS	140	PT	TFDS	195
GE+2	TFDS	141	AU	TFDS	196
GE+4	TFDS	142	AU+1	TFDS	197
AS	TFDS	143	HG	TFDS	198
AS+1	TFDS	144	HG+2	TFDS	199
AS+2	TFDS	145	TL	TFDS	200
AS+3	TFDS	146	TL+1	TFDS	201
SE	TFDS	147	TL+3	TFDS	202
BR	TFDS	148	PB	TFDS	203
KR	TFDS	149	PB+3	TFDS	204
RB	TFDS	150	BI	TFDS	205
RB+1	TFDS	151	PO	TFDS	206
SR	TFDS	152	AT	TFDS	207
Y	TFDS	153	RN	TFDS	208
ZR	TFDS	154	FR	TFDS	209
ZR+4	TFDS	155	RA	TFDS	210
NB	TFDS	156	AC	TFDS	211
MO	TFDS	157	TH	TFDS	212
MC+1	TFDS	158	PA	TFDS	213
TC	TFDS	159	U	TFDS	214
RU	TFDS	160	NP	TFDS	215
RH	TFDS	161	PU	TFDS	216
PD	TFDS	162	AM	TFDS	217
AG	TFDS	163	CM	TFDS	218
AG+1	TFDS	164	BK	TFDS	219
CD	TFDS	165	CF	TFDS	220
IN	TFDS	166	ES	TFDS	221
SN	TFDS	167			

A6.0 Source code description

A6.1 List of routines

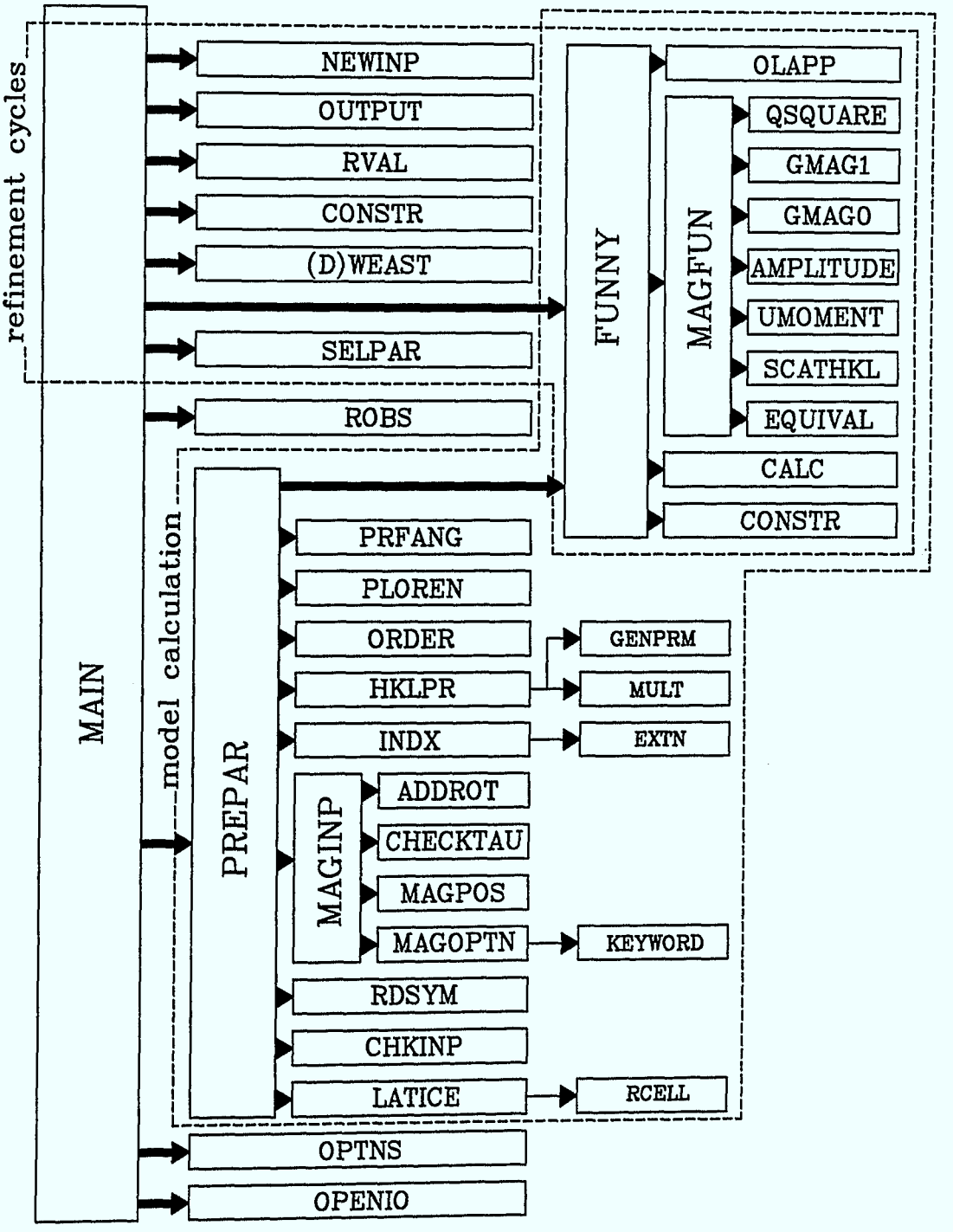

Fig. 3: Block diagram of IC-POWLS routines

List in alphabetic order; called external routines in brackets:

ABSM	calculates magnitude of magnetic moment from components m_x, m_y, m_z.
ADDROT	reads magnetic rotation matrices or prints default rotation matrices (SPNDIR, UMOMENT, ROTATE, TPHI, LTAU, XT)
AMPLITUDE	calculates prefactor for incommensurate (IC) magnetic structures. The prefactors depend on the individual type of magnetic structure (spiral, sine wave etc)
BACKIN	backspace in input file while ignoring comment lines ('*' in 1st col.)
CALC	calculates sum of nuclear structure factor over symmetric positions; applies anisotropic temperature factor corrections (XT)
CHECKP	checks if an atom is already in list of equivalent magnetic atoms, while generating magnetic atoms (XT)
CHECKTAU	checks during magnetic input if propagation vector is already in list of propagation vectors; sets up table "nstrtab". Entries of this table mark those magnetic atoms, which have the same propagation vector and therefore do interfere. (COMBINE)
CHKINP	checks input file; determines sort of observation range indication, number refinement cycles etc
COMBINE	checks if two magnetic structure models may be combined, i.e. if the structure factor amplitudes do interfere in case of identical propagation vectors
CONSTR	applies constraints between model parameters; linear constraints are defined either in the parameter-switch block of POWLS input or by Fortran code in subroutine PATCH.
DSDS	calculates square of reciprocal lattice vector
DWEAST	determines weighted least squares solution using diagonal weights (SMI50)
EQUALHKL	checks if a reflection $(hkl)_1$ is equal to another reflection $(hkl)_2$ or one of the symmetry eqivalent reflections of $(hkl)_2$ (EQUIVAL)
EQCYCL	generates all cyclic permutations of hkl triple
EQEXCH	generates new hkl by exchanging two indices
EQSIGN	generates hkl in different octants of reciprocal lattice
EQUIVAL	generates list of equivalent magnetic reflections according to laue group (EQSIGN, EQEXCH, EQCYCL)
EXTN	eliminates hkl reflections due to systematic structural extinctions
FUNNY	calculates model intensities of reflections from parameter vector (CONSTR, CALC, MAGFUN, OLAPP)
FUNHKL	checks if fundamental reflection intensity is calculated
GENPRM	assignes hkl parameters to magnetic reflections during generation: satellite order, numbering of propagation vectors, code for q^2 calculation (DSDS)
GETARG	PC: gets command line parameters; else: dummy routine
GETTIM	emulation of VAX routine; clock for IBM mainframe and PC

GMAG0	calculates sum of magnetic structure factor over equivalent atoms (only chemical cell) (XT)
GMAG1	calculates sum of magnetic structure factor over equivalent atoms (magnetic unit cell) (XT, TPHI, ROTATE)
HKLOMIT	rejects multiple generated magnetic hkl (EQUALHKL, MULT)
HKLPR	determines multiplicity of reflections; generates magnetic hkl reflections, reads (writes) reflections from (to) external file (MULT, GENPRM, ORDER)
ICONT	interpretes entry of parameter switch block as refinement switch or linear constrained function
INDX	generates fundamental (nuclear) hkl indices according to the laue group indicator (EXTN)
IPARSE	list directed read of integers
IPE	returns number of magnetic parameters np given in IC-POWLS input
IPPH	returns number of magnetic phase angle parameters given in IC-POWLS input
JINT	emulation of VAX routine; converts integer/real to long integer
KEYWORD	checks magnetic input for keyword on magnetic descriptor segment (UPCASE)
KEYWORD2	blockdata subroutine of magnetic structure type keywords (cphdat: keyword; mpardat: number of magnetic moment parameters; icldat: code for q^2 calculation in routine qsquare)
LATICE	reads wavelength, lattice parameters and reflection limits, calculates reciprocal cell (RCELL)
LCHAR	checks if string contains a letter
LENS	determines length of string ignoring leading and trailing blanks
LTAU	checks if input line contains components of magnetic propagation vector instead of rotation matrices
MAGFUN	calculates magnetic intensities from magnetic parameters (EQUIVAL, SCATHKL, UMOMENT, AMPLITUDE, GMAG0, GMAG1, QSQUARE, IPE, IPPH)
MAIN	main program; loop of least-squares refinement cycles (MESSAG, OPENIO, OPTNS, PREPAR, ROBS, OLAPP, RVAL, SELPAR, FUNNY, WEAST, DWEAST, CONSTR, OUTPUT, NEWINP)
MESSAG	displays message on screen
MAGINP	reads and prepares magnetic structure model (MAGOPTN, PATCH, MAGPOS, PRINFO, LTAU CHECKTAU, SPNDIR, ADDROT, IPE, IPPH, BACKIN)
MAGOPTN	reads and interpretes magnetic descriptor segment of magnetic atom (KEYWORD)
MAGPOS	determines list of symmetry equivalent magnetic atoms within crystallographic unit cell (CHECKP)
MULT	determines multiplicity of reflection according to laue group
NEWINP	generates new IC-POWLS input file with new parameter vector (IPE)

OLAPP	determines sum of overlapping model reflections, which contribute to a single observation
OPENIO	open files for I/O (GETARG)
OPTNS	reads and interpretes option line 2 of IC-POWLS input
ORDER	orders hkl reflection list on decreasing d-values
OUTPUT	print current parameters, R-values and final parameters (PRINTM)
PARSE	list directed read of reals
PATCH	dummy routine; can be used to include Fortran code to constrain model parameters
PLOREN	calculates Lorentz (and polarization) correction factor for reflection hkl
PREPAR	reads starting model, form factor tables and gives a list of theoretical intensities from starting model parameters (MESSAG, LATICE, CHKINP, RDSYM, PATCH, PLOREN, PRFANG, RDSCAT, MAGINP, INDX, ORDER, HKLPR, FUNNY, THRESH)
PRFANG	calculates preferred orientation angle α
PRINFO	prints info about magnetic structure model
PRINTM	prints magnetic moment magnitude, calculated from the final parameter vector (ABSM, IPE)
QSQUARE	calculates square of magnetic structure factor P^2 and magnetic cross section $P^2-(eP)^2$ (DSDS)
RCELL	calculates reciprocal lattice
RDMIX	list directed read of entries of mixed data type
RDSCAT	reads scattering length from file "SCAT.TAB"
RDSCR	reads rotation matrix from scratch file
RDSYM	reads crystal symmetry information from data base "SYMPOS.TAB"
READIN	reads a line from IC-POWLS input
READSIN	reads a line from parameter-switch block of IC-POWLS input
ROBS	reads observed intensities, error margins and correlations of intensities from input file (MESSAG, OLAPP, SMI50)
ROTATE	sets up rotation matrix of magnetic atom (RDSCR)
RVAL	calculates R-values
SCATHKL	calculates scattering vector (DSDS)
SECNDS	emulation of VAX routine; gets seconds from system
SELPAR	reads and interpretes LSQ parameter switches (READSIN, ICONT)
SMI50	symmetric matrix inversion
SPNDIR	interpretes element of spin sequence ("+"=+1, "n"=0 (paramagnetic), "–"=–1)
SUBSTR	breaks string into substrings
THRESH	rejects model reflections hkl with intensities lower than integ(15)*0.1 % of maximum intensity
TIME	emulation of VAX routine; gets time from system
TPHI	calculates phase difference according to propagation vector: $\alpha=2\pi\mathbf{k}\,\mathbf{r}$

UMOMENT	calculates magnitude and direction cosines of magnetic moment vector; calculates moment magnitude and direction cosines of spiral axis vector from model parameters (ABSM)
UPCASE	converts mixed-case string into uppercase string
WEAST	determines weighted least squares solution using non-diagonal weights (SMI50)
XT	determines symmetry positions of atom from space group symmetries

A6.2 Implementing new modulation types

In order to include new types of magnetic moment modulations, the following IC-POWLS routines must be modified:

1. Data assignment in subroutine KEYWORD2:
   To define a new integer 'typ' code "i" (see line 7 in chapter A2.0), the following data are required:

cphdat(i+10)	'typ' keyword (see line 7, A2.0)
mpardat(i+10)	number of model parameters np (without phase angles ϕ)
icldat(i+10)	q^2-square code which determines the kind of structure factor calculation:
	=0,3: general formula $\|F\|^2$-$\|eF\|^2$ (see chapter 3.2)
	=1: uniaxial config. symmetry
	=2: cubic config. symmetry
	=4: incommensurate structure A(K)*$\|F\|^2$; e.g. A(K)=sinω/4 for sinusoidal structure (see chapter 3.3)

2. a) Commensurate structure (typ<0):
   Prescription of the generation of magnetic rotation matrices $ROT_{r,s}$ is to be defined in subroutine ROTATE, for example using the phase angle $\alpha=2\pi \mathbf{k}\,\mathbf{r}_{r,s}$. Rotation matrices $ROT_{r,s}$ are used to calculate the magnetic unit cell structure factor (see chapter 3.2).

   b) Incommensurate structure (typ>0):
   A(**K**), which depends on the scattering vector **K**, are to be defined in function AMPLITUDE. Structure factor formulas (3.13)–(3.16), and hence A(**K**), were derived using the fourier components of the modulations.

A7.0 Present values of variable dimensions and I/O units

Present values of variable dimensions:

ipr	100	maximum number of model parameters
iq	20	maximum number of least squares parameters
ihk	400	maximum number of reflections
iob	60	maximum number of observations
iat	15	maximum number of atoms/form factor tables
iar	48	maximum number of equivalent atoms
mc	10	maximum number of linear constraints
		maximum number of independent parameters in linear constraints
ip	10	maximum number of magnetic atoms in asymmetric unit
mnat	32	maximum number of equivalent magnetic atoms within chemical unit cell
ip1	2	maximum number of magnetic atoms in asymmetric unit for structure type (1, MC), if the input file contains all rotation matrices
irot	15	maximum number of chemical unit cells within magnetic unit cell for structure type (+1, MC), if the input file contains all rotation matrices

Dimensions ipr, iq, ihk etc are symbolic names of Fortran parameter statements. Therefore variable dimension can be easily increased by changing the parameter statement values in all subroutines.

Input/output units used by the program:

symmetry tables	: isymt	=1	(file)
x-ray form factor tables	: ifmt	=2	(file)
input	: in	=3	(file)
printed output	: iout	=4	(file)
display output	:	=*	(display)
new input	: inew	=7	(file)
dump	:	=77	(scratch file: rotation matrices
dump	:	=88	(scratch file: rejected hkl
dump	:	=89	(scratch file: error message
dump	:	=99	(scratch file: newinp
hkl list in/out	: ihkls	=10	(file)
nucl. scatt. lengthes	: iscat	=11	
magn. form factor tables	: imfmt	=12	

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