Abstract
A texture model suitable for use in Rietveld-refinement programs is proposed. It is based on the series expansion of the pole distribution function in symmetrized harmonics. The model was tested on a textured plate sample of Al₂O₃.

1. Introduction
The presence of texture complicates the determination and refinement of crystalline structures by X-ray or neutron diffraction on polycrystals. Making a powder sample or spinning it around one axis may only partially remove the texture or its effects. In many Rietveld-refinement programs the texture is modelled by simple formulae. In these models, discussed in detail by Dollase (1986) [who recommends the March (1932) model], the pole distribution is a function of one variable (a polar angle) and one or two parameters. The reduced number of parameters is an attractive feature, but the one-dimensional character of the pole distribution makes it useful only for textures with cylindrical sample symmetry. Moreover, these models do not take into account the crystal symmetry. From this point of view, a correct approach is that of Ahtee, Nurmela & Suortti (1989) but its validity is also limited to spun samples. The approach presented below, based on the texture theory of Bunge (1982), covers, in principle, the general case.

2. Cross section and diffracted intensity for a textured sample
The Bragg scattering cross section per unit volume of a monocrystal for a given reciprocal-lattice vector \( \mathbf{H}_i \) is given by the well known formula (see, for example, Marshall & Lovesey, 1971)

\[
\sigma_i(Q) = V^{-1} \frac{d\sigma}{d\Omega} = (2\pi)^3 |F_i|^2 v_c^{-2} \delta(Q - 2\pi H_i),
\]

where \( Q \) is the momentum transfer, \( V \) is the crystal volume, \( v_c \) is the unit-cell volume and \( F_i \) is the structure factor. For a textured polycrystal, the average unit-volume cross section can be written as

\[
\bar{\sigma}(Q) = (2\pi)^3 n_i |F_i|^2 v_c^{-2} \int \delta(Q - 2\pi \mathbf{H}_i) A(h_i, y)dy,
\]

where \( n_i \) is the multiplicity of \( \mathbf{H}_i \) and \( A(h_i, y) \) is the pole distribution (the probability of finding the unit vector \( h_i = \mathbf{H}_i/|\mathbf{H}_i| \) orientated along the unit vector \( y \) in the sample). On calculating the integral in (2), one obtains

\[
\bar{\sigma}(Q) = 2\pi n_i |F_i|^2 v_c^{-2} \mathbf{H}_i^{-2} \delta(Q - 2\pi \mathbf{H}_i) A(h_i, q),
\]

with the notation \( q = Q/Q \). Therefore, in contrast to the isotropic polycrystal case, the Bragg cross section of a textured polycrystal depends on the vector \( Q \) and not only on its modulus.

The diffracted intensity at the scattering angle \( 2\theta_j \) can be written as

\[
I_j = I(2\theta_j) \approx V \sum_i A_i \int \sigma_i(Q_j + \Delta Q) R(\Delta Q) d(\Delta Q),
\]

where \( A_i \) is the absorption factor for the peak \( \mathbf{H}_i \) and \( R(\Delta Q) \) is the resolution function for monocrystals. If one denotes by \( \Delta Q \) and \( Q_j \Delta q \) the parallel and perpendicular components of \( \Delta Q \) with respect to \( Q_j \) and takes (3) into account, (4) can be integrated over \( \Delta Q \) to yield

\[
I_j \approx 2\pi V \sum_i A_i n_i |F_i|^2 v_c^{-2} H_i^{-2} \int R(2\pi H_i - Q_j, Q_j \Delta q) \times A(h_i, q_j + \Delta q) d(\Delta q).
\]

The use of this formula in a Rietveld-refinement program is not straightforward. Incidentally, in most practical situations, the width of \( A \) is much greater than the width of \( R \) so that (5) becomes

\[
I_j \approx 2\pi V \sum_i A_i n_i |F_i|^2 v_c^{-2} H_i^{-2} R_p(2\pi H_i - Q_j) A(h_i, q_i),
\]

where \( R_p \) is the resolution function for polycrystals and \( q_i = q(2\theta_i), \theta_i \) being the Bragg angle corresponding to \( \mathbf{H}_i \). This formula differs from that for the isotropic polycrystals only by the factor \( A(h_i, q_i) \) and
can be used in a straightforward way in the Rietveld procedure if a convenient model for the pole distribution is found. Such a model is offered by the Bunge theory of texture.

3. Pole distribution and symmetrized spherical harmonics

In this section, we resume the theoretical background from Bunge's (1982) book on texture which is necessary for later use.

In Bunge's approach the pole distribution function \( A(h, y) \) can be written as

\[
A(h, y) = \sum_{l=0}^{\infty} \sum_{\mu=1}^{M(l)} \sum_{v=1}^{N(l)} c_\mu^v K_\mu^v(h) K_\mu^v(y). \tag{7}
\]

Here \( K_\mu^v \) and \( \tilde{K}_\mu^v \) are symmetrized spherical harmonics. They are invariant under the symmetry operations of the crystal and the sample, respectively. \( M(l) \) and \( N(l) \) are the numbers of such independent functions for given \( l \). The coefficients \( c_\mu^v \) are unknown and can be found by a least-squares procedure using a number of pole figures or, in our case, by Rietveld refinement. The pole distribution (7) is normalized to unity in \( y \) and \( h \). These unit vectors are defined in two orthogonal coordinate systems, that of the crystal, \((i, j, k)_c\), and that of the sample, \((i, j, k)_s\), by the polar and azimuthal coordinates \((\Phi, \beta)\) and \((\Psi, \gamma)\), respectively. How these coordinate systems are chosen will be clarified below.

The symmetrized harmonics can be expressed as linear combinations of ordinary spherical harmonics,

\[
\tilde{K}_\mu^v(\Psi, \gamma) = \sum_{m=-l}^{l} A_l^m K_l^m(\Psi, \gamma). \tag{8}
\]

The ordinary spherical harmonics \( K_l^m \) are defined as

\[
K_l^m(\Psi, \gamma) = (2\pi)^{-1/2} \exp (im\gamma) P_l^m(\Psi), \tag{9}
\]

\[
P_l^m(\Psi) = P_l^m(\cos \Psi) = P_l^m(x) = \left[ (l + m)! / (l - m)! \right]^{1/2} (1 - x^2)^{m/2} \left( \frac{d}{dx} \right)^m (1 - x^2)^{-m/2}.
\]

To find the coefficients \( A_l^m \) one must impose the symmetry conditions specific to the point group. Because of the Friedel-law action, only Laue groups should be considered. From the triclinic group \( C_i \) up to the cubic group \( O_h \) (Schoenflies notation), there is a maximum of four types of symmetry condition. These conditions have cumulative actions in the sense that the third condition, for instance, acts together with the first and second conditions.

(a) Any Laue group has an inversion operation that transforms \((\Psi, \gamma)\) into \((\pi - \Psi, \pi + \gamma)\). Any function \( K_l^m \)

is invariant to this transformation if

\[
l = 2l'. \tag{11}
\]

(b) If there exists an \( n \)-fold rotation axis in \( \Phi = 0 \) then \((\Psi, \gamma)\) is transformed into \((\Psi, \gamma + 2\pi/n)\). Any \( K_l^m \) is invariant to this transformation if

\[
m = m'. \tag{12}
\]

(c) One second-order axis is located at \( \gamma = 0 \). This transforms \((\Psi, \gamma)\) into \((\pi - \Psi, -\gamma)\). Except for \( K_0^0 \), the ordinary spherical harmonics are not invariant to this transformation, but the sum of two such functions with the same \(|m|\) is invariant. Then it suffices to take only two terms in (8) with the condition

\[
m = m'. \tag{13}
\]

Just as for the condition (a), the symmetrized harmonics are given by (12) but with \( m \) satisfying (13). The number \( N(l) \) of these functions together with the corresponding point groups are given in Table 1.

(c) One second-order axis is located at \( \Psi = \pi/2, \gamma = 0 \). This transforms \((\Psi, \gamma)\) into \((\pi - \Psi, -\gamma)\). Except for \( K_0^0 \), the ordinary spherical harmonics are not invariant to this transformation, but the sum of two such functions with the same \(|m|\) is invariant. Then it suffices to take only two terms in (8) with the condition

\[
m = m'. \tag{14}
\]

The symmetrized harmonics are in this case:

\[
K_l^m(\Psi, \gamma) = K_0^m(\Psi, \gamma); \tag{15a}
\]

\[
K_l^m(\Psi, \gamma) = 2^{-1/2} \left[ K_l^m(\Psi, \gamma) + K_l^m(\Psi, \gamma) \right], 1 \leq m \leq l. \tag{15b}
\]

The number \( N(l) \) for the corresponding point groups is given in Table 2.
(d) For the cubic groups, a third-order axis exists along the cube diagonal. This axis transforms $(\Psi, 0)$ into $(\pi/2, \Psi)$. More than two terms must be kept in (8) to ensure invariance under this transformation. For the group $T_d$, one can write (8), with conditions (a), (b) and (c) accounted for, as
\[
K_{2l}(\Psi, \gamma) = \sum_{m=0}^{l} B_{2l}^{2m} \cos (2m\gamma) P_{2l}^{2m}(\Psi)
\]
with the notation
\[
B_{2l}^{2m} = A_{2l}^{2m} \quad \text{and} \quad B_{2l}^{2m} = 2^{-1/2} A_{2l}^{2m}.
\]
By using the Fourier transform of $P_{2l}^{2m}$,
\[
P_{2l}^{2m}(\Psi) = \sum_{s=0}^{l} a_{2l}^{2m} \cos (2s\Psi),
\]
and by imposing the condition that (16) is invariant to the transformation from $(\Psi, 0)$ to $(\pi/2, \Psi)$, one obtains a linear homogeneous system for the coefficients $B$:
\[
\sum_{m=0}^{l} B_{2l}^{2m} \left[ a_{2l}^{2m} - \sum_{s=0}^{l} (-1)^{s} a_{2l}^{2s} \cos (2s\Psi) \right] = 0.
\]
The system has a trivial solution for $l' = 1$, one solution for $l' = 2$ and two independent solutions for $l' = 3$. These are:
\[
K_{1}^{0}(\Psi, \gamma) = 0.3046972 P_{0}(\Psi) + 0.3641828 \cos (2\gamma) P_{1}(\Psi),
\]
\[
K_{1}^{0}(\Psi, \gamma) = -0.1410474 P_{0}(\Psi) + 0.527751 \cos (3\gamma) P_{1}(\Psi),
\]
\[
K_{1}^{0}(\Psi, \gamma) = -0.4678013 \cos (2\gamma) P_{1}(\Psi) + 0.3153915 \cos (6\gamma) P_{1}(\Psi).
\]

# Table 3. An 'abacus' giving the pole distribution function for the noncubic symmetries

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<tr>
<th>Group</th>
<th>$C_{1}$</th>
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For any index $2l$, all filled positions in this table fulfilling the relation $0 \leq m \leq 2l$ must be considered. $c$ represents the cosine term and $s$ the sine term of (2.3). For further details, refer to the text.

\[
R_{l}(\Phi, \beta) = \begin{cases} 
0.3046972 P_{0}(\Psi) + 0.3641828 \cos (2\gamma) P_{1}(\Psi) & \text{for cubic symmetry}, \\
0.1410474 P_{0}(\Psi) + 0.527751 \cos (3\gamma) P_{1}(\Psi) & \text{for cubic symmetry}, \\
0.4678013 \cos (2\gamma) P_{1}(\Psi) + 0.3153915 \cos (6\gamma) P_{1}(\Psi) & \text{for cubic symmetry}, \\
\end{cases}
\]

but for noncubic symmetry they are equal to
\[
\cos (m\beta) P_{n}^{m}(\Phi) \quad \text{or} \quad \sin (m\beta) P_{n}^{m}(\Phi).
\]

Let us denote these two functions by the symbols $c$ and $s$ respectively. Table 3 uses these symbols and allows the pole distribution function for any noncubic group to be written straightforwardly. If, for example, the symmetry is $D_{3d}$, we have:
\[
R_{1}^{D}(\Phi, \beta) = P_{0}^{1}(\Phi); \quad R_{2}^{D}(\Phi, \beta) = P_{0}^{2}(\Phi);
\]
\[
R_{3}^{D}(\Phi, \beta) = \sin (3\beta) P_{1}^{3}(\Phi); \quad R_{4}^{D}(\Phi, \beta) = P_{0}^{4}(\Phi);
\]
\[
R_{5}^{D}(\Phi, \beta) = \sin (3\beta) P_{2}^{5}(\Phi); \quad R_{6}^{D}(\Phi, \beta) = \cos (6\beta) P_{0}^{6}(\Phi)
\]
and so on. The numbers $N(2l)$ and $M(2l)$ (given in the Tables 1 and 2) are identical only if the sample symmetry and the crystal symmetry are the same. But for cylindrical sample symmetry, $N(2l) = 1$ and $R_{1}^{D}(\Psi, \gamma) = P_{0}^{1}(\Psi)$, as shown by the last row of Table 3. Finally, the number $L$ in (22) is determined by successive refinements starting with $L = 1$. If in a given refinement with $L = L_{0}$ all fitted parameters $t_{2l}^{m}_{\alpha}$ take insignificant values, then $L = L_{0} - 1$.

## 5. Coordinate systems and calculation of $(\Phi, \beta)$ and $(\Psi, \gamma)$

The choice of the crystal and sample coordinate systems is imposed by the construction of the symmetrized spherical harmonics for the groups having symmetry higher than triclinic: the axis $k$ must be along the $n$th-order axis and $i$ along a second-order axis, if any exists. For the crystal coordinate system, these two conditions are fulfilled if we take
\[
i_{i} = a_{0}/a_{0}, \quad k_{c} = c_{0}^{*}/c_{0}. \quad j_{c} = (k_{c} \times i_{i})
\]
for all crystallographic systems except for the monoclinic second setting and the trigonal first
setting. In these cases one should take:

\[ i = c_0/c_0; \quad k = b_0/b_0 \]  

(monoclinic 2);  

\[ i = (a_0 - b_0)/|a_0 - b_0|; \quad k = (a_0 + b_0 + c_0)/|a_0 + b_0 + c_0| \]  

(trigonal 1);  

\( a_0, b_0, c_0 \) being the basis vectors of the unit cell.

With these choices, \( \Phi \) and \( \beta \) are obtained by elementary calculations from

\[ \cos \Phi = h \cdot k; \quad \tan \beta = h \cdot j/h \cdot i. \]  

(25)

The dependence of these angles on the Miller indices and lattice parameters is given explicitly in the Appendix for all systems and settings.

In the sample coordinate system, the unit vectors \( i, j, k \) are oriented along the most probable corresponding unit vectors \( i', j', k' \) if the sample and crystal have the same symmetry. Generally, the sample coordinate system imposed by symmetry may not coincide with the sample system \( I, J, K \) imposed by the sample geometrical form. If one denotes by \( \xi, \eta, \zeta \) the Euler angles that transform \( I, J, K \) into \( i, j, k \), and \( (\Psi_q, \gamma_q) \) as the angular coordinates of \( q \) in the first system, it is easy to show that:

\[ \cos \Psi = \cos \eta \cos \Psi_q - \sin \eta \sin \Psi_q \sin (\gamma_q - \xi); \]  

\[ \tan \gamma = \left[ -\sin \Psi_q \cos (\gamma_q - \xi) \sin \zeta \right. \right. \left. \sin \Psi_q \sin (\gamma_q - \xi) \cos \eta \cos \zeta \right. \right. \left. + \cos \Psi_q \sin \eta \cos \zeta \right. \right. \left. \times [\sin \Psi_q \cos (\gamma_q - \xi) \cos \zeta \right. \right. \left. + \sin \Psi_q \sin (\gamma_q - \xi) \cos \eta \sin \zeta \right. \right. \left. + \cos \Psi_q \sin \eta \sin \zeta \right]^{-1}. \]  

(26a)

If one knows some information about the texture, for example, two orthogonal crystal directions oriented preferentially along two orthogonal sample directions, then the angles \( \xi, \eta, \zeta \) can be calculated beforehand (see Appendix). If not, these angles must be taken as free parameters in the Rietveld refinement.

The angle \( \eta \) is in fact the angle between the \( n \)-fold axis of the sample \( k_n \) and the \( K \) axis. If the sample symmetry is cylindrical around \( K (n = \infty, k_n || K) \) then \( \eta = 0 \) and \( \Psi = \Psi_q \). The \( \infty \)-fold axis \( k \) being, in this case, the only unambiguously defined direction in the sample, the vectors \( i', j' \) are not defined and consequently \( \xi \) and \( \zeta \) have no meaning.

6. Implementation of the texture model in Rietveld programs

The texture model described above was introduced into a Rietveld-type program written specially for a curved-monochromator focusing neutron diffractometer (A. D. Stoica, M. Popovici, N. C. Popa, F. Constantin & M. Ion, in preparation). The focusing is achieved in a large angular range by using thin plate samples normal to the scattering plane, making an angle \( x \) with the incident beam and rotated around the vertical axis as a function of \( 20 \). The sample system \( (I, J, K) \) is taken with \( K \) normal to the plate surface and \( I \) vertical along the sample surface. With this choice, the coordinates of \( q \) are

\[ \Psi_q = x - \theta; \quad \gamma_q = \left[ 2 - \text{sign}(x - \theta) \right] \pi/2. \]  

(27)

These coordinates together with the corresponding functions \( R_{2i}^\phi(\Phi, \beta) \) are calculated beforehand in an additional program for the set of reflections used in the Rietveld refinement.

The Rietveld program including this texture model was tested on a diffraction diagram measured on a rectangular plate of \( \text{Al}_2\text{O}_3 \), 0.7 mm thick and 65 mm wide, over the \( 2\theta \) range from 20 to 123° with a step of 4°. For \( \lambda = 1.3282 \) Å the diagram contains 73 peaks in this range. No information about the texture was available but the sample history suggested that the symmetry \( C_{x,y} \) could be assumed. In this case, the pole distribution function becomes (taking account of the fact that the crystal symmetry is \( D_{3d} \))

\[ A(\Phi, \beta, \Psi) = 1 + t_{11}^2 P_{20}^2(\Phi)P_{20}^2(\Psi) \]

\[ + [t_{12}^1 P_{20}^2(\Phi) + t_{22}^1 \sin (3\beta)P_{30}^3(\Phi)]P_{20}^2(\Psi) \]

\[ + [t_{10}^2 P_{20}^2(\Phi) + t_{20}^2 \sin (3\beta)P_{30}^3(\Phi)] \]

\[ + t_{31}^3 \cos (6\beta)P_{20}^2(\Phi)]P_{20}^2(\Psi) + \cdots. \]  

(28)

The structural parameters of \( \text{Al}_2\text{O}_3 \) were fixed in the early stages of the refinement to the values reported by Jorgensen & Rotella (1982). The best fit with the texture parameters fixed to zero (no texture at all) gave a Gauss standard deviation \( (\chi^2/\text{degree of freedom}) = 3.6 \). The relative discrepancy between measured and computed intensities was up to 100% for many peaks. Further refinements were performed using (28) for the pole distribution with \( L = 2, 3 \) and 4. The standard-deviation values were 1.56, 1.53 and 1.53, respectively. All fitted values of \( t_{11}^1 \) were insignificant at the 0.95 confidence level, so \( L \) was fixed at 3. Finally, the structural parameters were set free together with the texture parameters. The results of the refinement are shown in Table 4 and Fig. 1(a). The values of the structural parameters are in good agreement with those of Jorgensen & Rotella (1982) (given in square brackets) but our precision is lower. This is due to our poorer statistics: only 760 counts were obtained for the highest peak (the diagram was measured at the 2 MW reactor in Bucharest). This fact (not an
Table 4. The results of the Rietveld refinement of a neutron diffraction pattern collected on an Al₂O₃ plate sample using the present model for texture

Structural parameters obtained by Jørgensen & Rotella (1982) are given in square brackets and those obtained without texture correction are given in braces.

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<td>[0.068 (23)]</td>
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Inaccuracy of the model also explains the relatively high values of the reliability factors, as confirmed by Fig. 1(a). For comparison, Fig. 1(b) shows the fit obtained using the texture model of March (1932) and in Fig. 1(c) the fit with no texture correction at all. In this last case we obtained inaccurate atom coordinates and unphysical thermal parameters (the values in braces in Table 4). Finally, Fig. 2 shows the pole distribution for a number of reciprocal vectors \( \mathbf{H}_{ijh} \), calculated using the values of \( t_{ijh} \) obtained from the Rietveld refinement. It is seen that the planes \((hhh)\) are preferentially oriented parallel to the plate surface. This result differs from that reported by Lutterotti & Scardi (1990), who used the March model for the texture in \( \text{Al}_2\text{O}_3 \).

7. Concluding remarks

It is suggested that the texture model presented in this work could be successfully used in Rietveld-refinement programs for samples with weak and medium textures. For strong texture many terms must be retained in the series expansion of the pole distribution to ensure series convergence. Their number increases rapidly with the index \( l \), especially for low-symmetry groups. For instance, at \( l = 4 \) there are 81 terms for the triclinic group \( C_i \), 25 for the monoclinic group \( C_{2h} \) and 9 for the orthorhombic \( D_{2h} \). The addition of such large numbers of nonstructural parameters would drastically decrease the performance of the Rietveld procedure. It may be possible to construct another model with a reasonable number of parameters capable of describing strong textures while still accounting for the sample and crystal symmetries.

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APPENDIX
Polar and azimuthal angles $\Phi, \beta$; Euler angles $\xi, \eta, \zeta$

Let us denote by $a_0, b_0, c_0, \alpha_0, \beta_0, \gamma_0$ the unit-cell parameters (with * denoting the reciprocal cell). The angles $\Phi$ and $\beta$ [see (24), (25)] are:

\[
\cos \Phi = (ha_0^* \cos \beta_0^* + kb_0^* \cos \alpha_0^* + lc_0^*)/H
\]
(for triclinic)

\[
\cos \Phi = l/c_0^* H
\]
(for monoclinic 1 (first setting), orthorhombic, trigonal 2, tetragonal, hexagonal)

\[
\cos \Phi = k/b_0^* H
\]
(for monoclinic 2)

\[
\cos \Phi = l/a_0^* H
\]
(for cubic)

\[
\cos \Phi = (h + k + l)/{a_0H[3(1 + 2 \cos \alpha_0)]^{1/2}}
\]
(for trigonal 1)

\[
\beta = \arctan2(kb_0^* \cos \eta_0, h_0 \cos \eta_0 - k_0 \sin \eta_0)
\]
(for triclinic, monoclinic 1)

\[
\beta = \arctan2(hc_0/a_0^* - l \cos \beta_0, l \sin \beta_0)
\]
(for monoclinic 2)

\[
\beta = \arctan2(kc_0, hc_0)
\]
(for orthorhombic)

\[
\beta = \arctan2[h + k - 2l, 3^{1/2}(h - k)]
\]
(for trigonal 1)

\[
\beta = \arctan2(h + 2k, 3^{1/2}h)
\]
(for trigonal 2, hexagonal)

\[
\beta = \arctan2(k, h)
\]
(for cubic).

Let us suppose that the vector $H_0 = h_0a_0^* + k_0b_0^* + l_0c_0^*$ preferentially oriented along $K$ and $R_0 = u_0a_0 + v_0b_0 + w_0c_0$ preferentially oriented along $\cos \delta I + \sin \delta J (H_0 \cdot R_0 = 0)$. The Euler angles $\xi, \eta, \zeta$ transforming $I, J, K$ into $i_0, j_0, k_0$ (see §5) are

\[
\xi = \delta + \arctan2[p \sin \eta - (m \sin \zeta + n \cos \zeta) \cos \eta, m \cos \zeta - n \sin \zeta],
\]
where

\[
\cos \eta = (h_0a_0^* \cos \beta_0^* + k_0b_0^* \cos \alpha_0^* + l_0c_0^*)/H_0;
\]

\[
\zeta = \arctan2(h_0 \sin \gamma_0, k_0a_0/b_0 - h_0 \cos \gamma_0);
\]

\[
m = u_0a_0 + v_0b_0 \cos \gamma_0 + w_0c_0 \cos \beta_0;
\]

\[
n = v_0b_0 \sin \gamma_0 - w_0c_0 \sin \beta_0 \cos \alpha_0;
\]

\[
p = w_0/c_0^*
\]
(for all classes except for monoclinic 2 and trigonal 1)

\[
\cos \eta = k_0/H_0b_0^*;
\]

\[
\zeta = \arctan2(l_0 \sin \beta_0, h_0c_0/a_0 - l_0 \cos \beta_0);
\]

\[
m = u_0a_0 \cos \beta_0 + w_0c_0;
\]

\[
n = u_0a_0 \sin \beta_0;
\]

\[
p = v_0/b_0^*
\]
(for monoclinic 2)

\[
\cos \eta = (h_0 + k_0 + l_0)/{H_0a_0[3(1 + 2 \cos \alpha_0)]^{1/2}};
\]

\[
\zeta = \arctan2[3^{1/2}(h_0 - k_0), h_0 + k_0 - 2l_0];
\]

\[
m = a_0(1 - \cos \alpha_0)^{1/2}(u_0 - v_0)/2^{1/2};
\]

\[
n = a_0(1 - \cos \alpha_0)^{1/2}(u_0 + v_0 - 2w_0)/6^{1/2};
\]

\[
p = a_0(1 + 2 \cos \alpha_0)^{1/2}(u_0 + v_0 + w_0)/3^{1/2}
\]
(for trigonal 1).

References


