magnitudes and the second neighborhoods contain 41 magnitudes. Because the derivation of these neighborhoods is so similar to that given in §3 for $P2_1$, no further details for $P2_12_12_1$ are given here.

5. Concluding remarks

By embedding a given structure seminvariant T and its symmetry-related variants in appropriate structure invariants Q, one obtains the extensions of T and in this way reduces the probabilistic theory of the structure seminvariants to that of the structure invariants. Details have been described for the three-phase structure invariants in $P1$ and $P\bar{1}$, the three-phase structure seminvariants in $P2_1$, and three kinds of special three-phase structure seminvariants in $P2_12_12_1$. The method is clearly capable of extension to the structure seminvariants in general. There remains the task of deriving the associated conditional probability distributions leading to estimates of the structure seminvariants. Because the full second neighborhoods often contain so many magnitudes $|E|$, not all of which may be in the observable sphere of reflections, it will in general be necessary to derive distributions which assume as known only certain subsets of these neighborhoods. Finally, it should be pointed out that the discriminant of the structure seminvariant, a polynomial in the presumed known magnitudes $|E|$, which is easily derived, easily computed and strongly correlated with the true value of the structure seminvariant [compare, for example, the discriminant for quintets (Fortier & Hauptman, 1977)], may often serve as a substitute for the true distribution, especially in those cases when sufficiently accurate and computable forms for the latter are particularly difficult or even impossible, as yet, to derive.

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Determinantal Equations for the Scale Factor, Temperature Factors and Quantitative Chemical Contents of the Unit Cell

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A class of determinantal equations for the scale factor, the temperature factors and quantitative chemical contents of the unit cell is derived assuming non-penetrating atoms but without making use of statistical arguments. A new method for the determination of the scale and Debye–Waller factors is developed on the basis of these equations and applied to the structure factors of $Al(OH)_3$, giving results with errors of about 2%.

The various methods of structure analysis require the knowledge of the moduli of a sufficient number of Fourier coefficients of the scattering density function of the crystal to be analysed and a more or less complete knowledge of the form factors of the atoms present in its elementary cell.

Except for the scale factor and the temperature

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factors, the required quantities are usually obtained with the help of physical laws from the routine experiments which precede structure analysis. For the determination of the scale factor and Debye–Waller factor additional assumptions of a statistical kind are made (Wilson, 1942).

If we assume that the atoms of a crystal do not interpenetrate, we can derive a system of equations for the determination of the scale factor, the temperature factors and the numbers of atoms of different kinds in the unit cell without making use of statistical arguments. This system of equations is derived in a similar way to the equations of Sayre (1952) and Woolfson (1958) by making use of a special class of locally defined mappings of the scattering-density function, which are closely related to those generating the convolution-type structure factor equations (Rothbauer, 1975, 1976, 1977*a*,*b*).

The equation

The derivative of the scattering density

$$\rho(\mathbf{x}) = \frac{1}{V}\sum_{\mathbf{m}} F(\mathbf{m},\rho)\exp(-2\pi i\mathbf{m}.\mathbf{x})$$

along an arbitrary vector **v** is

$$\mathrm{d}\rho(\mathbf{x})/\mathrm{d}\mathbf{v} = \frac{1}{V}\sum_{\mathbf{m}}(-2\pi i\mathbf{m}.\mathbf{v})F(\mathbf{m},\rho)\exp(-2\pi i\mathbf{m}.\mathbf{x}),$$

where $F(\mathbf{m},\rho)$ is the structure factor of ρ at reciprocal-lattice point **m**. If D* is a differential operator, representing a linear combination of direction derivatives of different order along different directions, $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3 \ldots$, we have

$$\mathrm{D}^*\rho(\mathbf{x}) = \frac{1}{V}\sum_{\mathbf{m}} G(\mathbf{m})F(\mathbf{m},\rho)\exp(-2\pi i\mathbf{m}.\mathbf{x}),$$

where $G(\mathbf{m})$ is a polynomial of the scalar products, $\mathbf{m}.\mathbf{v}_1$, $\mathbf{m}.\mathbf{v}_2$, ..., and hence a polynomial of the coefficients m_1, m_2, m_3 of **m**.

The structure factor of $\mathrm{D}^*\rho$ is then given by

$$F(\mathbf{h},\mathrm{D}^*\rho) = G(\mathbf{h})F(\mathbf{h},\rho). \qquad (1)$$

If we denote the complex conjugate of ρ by $\bar{\rho}$ we obtain

$$\bar{\rho}(\mathbf{x}) = \frac{1}{V}\sum_{\mathbf{m}} \bar{F}(\mathbf{m},\rho)\exp(2\pi i\mathbf{m}.\mathbf{x})$$

$$= \frac{1}{V}\sum_{\mathbf{m}} \bar{F}(-\mathbf{m},\rho)\exp(-2\pi i\mathbf{m}.\mathbf{x})$$

and hence

$$F(\mathbf{h},\bar{\rho}) = \bar{F}(-\mathbf{h},\rho),$$

and applying (1)

$$F(\mathbf{h},\overline{\mathrm{D}^*\rho}) = \bar{G}(-\mathbf{h})\bar{F}(-\mathbf{h},\rho). \qquad (2)$$

If ρ_1 and ρ_2 are density functions of the same translational periodicity we have

$$F(\mathbf{h},\rho_1\rho_2) = \frac{1}{V}\sum_{\mathbf{m}} F(\mathbf{m},\rho_1)F(\mathbf{h}-\mathbf{m},\rho_2). \qquad (3)$$

Using (1) and (2) it follows that

$$F(\mathbf{h},\mathrm{D}_1^*\rho\overline{\mathrm{D}_2^*\rho})$$

$$= \frac{1}{V}\sum_{\mathbf{m}} G_1(\mathbf{m})\overline{G_2}(\mathbf{m}-\mathbf{h})F(\mathbf{m},\rho)\bar{F}(\mathbf{m}-\mathbf{h},\rho). \qquad (4)$$

The Fourier summation of the periodically repeated scattering-density function of the νth atom of the μth kind with position $\mathbf{x}_{\mu\nu}$ in the elementary cell is

$$\rho_{\mu\nu}(\mathbf{x}) = \frac{1}{V}\sum_{\mathbf{m}} F(\mathbf{m},\rho_\mu)t_{\mu\nu}(\mathbf{m})$$

$$\exp[-2\pi i\mathbf{m}.(\mathbf{x}-\mathbf{x}_{\mu\nu})] \qquad (5)$$

where $F(\mathbf{m},\rho_\mu)$ is the form factor of the atoms of the μth kind at rest at lattice point **m**, and $t_{\mu\nu}(\mathbf{m})$ is the temperature factor of the νth atom of the μth kind.

We then have

$$F(\mathbf{h},\rho_{\mu\nu}) = F(\mathbf{h},\rho_\mu)t_{\mu\nu}(\mathbf{h})\exp(2\pi i\mathbf{h}.\mathbf{x}_{\mu\nu})$$

and by the application of (1) and (2)

$$F(\mathbf{h},\mathrm{D}^*\rho_{\mu\nu}) = G(\mathbf{h})F(\mathbf{h},\rho_\mu)t_{\mu\nu}(\mathbf{h})\exp(2\pi i\mathbf{h}.\mathbf{x}_{\mu\nu})$$

$$F(\mathbf{h},\overline{\mathrm{D}^*\rho_{\mu\nu}}) = \bar{G}(-\mathbf{h})\bar{F}(-\mathbf{h},\rho_\mu)\bar{t}_{\mu\nu}(-\mathbf{h})\exp(2\pi i\mathbf{h}.\mathbf{x}_{\mu\nu}).$$

Using equation (4) this implies

$$F(\mathbf{h},\mathrm{D}_1^*\rho_{\mu\nu}\overline{\mathrm{D}_2^*\rho_{\mu\nu}})$$

$$= \frac{1}{V}\sum_{\mathbf{m}} G_1(\mathbf{m})\bar{G}_2(\mathbf{m}-\mathbf{h})F(\mathbf{m},\rho_\mu)$$

$$\times \bar{F}(\mathbf{m}-\mathbf{h},\rho_\mu)$$

$$\times t_{\mu\nu}(\mathbf{m})\bar{t}_{\mu\nu}(\mathbf{m}-\mathbf{h})\exp(2\pi i\mathbf{h}.\mathbf{x}_{\mu\nu}). \qquad (6)$$

Now, let p be the number of types of atom present in the crystal and $q(\mu)$ the number of atoms of the μth type, then

$$\rho(\mathbf{x}) = \sum_{\mu=1}^{p}\sum_{\nu=1}^{q(\mu)} \rho_{\mu\nu}(\mathbf{x})$$

represents the scattering-density function of the crystal. Because of the local character of the mapping,

$$\Gamma(\rho) = \mathrm{D}_1^*\rho\overline{\mathrm{D}_2^*\rho},$$

of the scattering-density function we may conclude

$$\mathrm{D}_1^*\rho\overline{\mathrm{D}_2^*\rho} = \sum_{\mu=1}^{p}\sum_{\nu=1}^{q(\mu)} \mathrm{D}_1^*\rho_{\mu\nu}\overline{\mathrm{D}_2^*\rho_{\mu\nu}} \qquad (7)$$

providing the atoms of the structure do not interpenetrate. Taking the Fourier transform of (7) we have

$$F(\mathbf{h}, \mathrm{D}_1^*\rho\overline{\mathrm{D}_2^*\rho}) = \sum_{\mu=1}^{p}\sum_{\nu=1}^{q(\mu)} F(\mathbf{h}, \mathrm{D}_1^*\rho_{\mu\nu}\overline{\mathrm{D}_2^*\rho_{\mu\nu}})$$

and by inserting equation (4) and (6) we obtain a system of equations

$$0 = \sum_{\mathbf{m}} G_1(\mathbf{m})\bar{G}_2(\mathbf{m}-\mathbf{h}) \Bigg[F(\mathbf{m},\rho)\bar{F}(\mathbf{m}-\mathbf{h},\rho) - \sum_{\mu=1}^{p} F(\mathbf{m},\rho_\mu)\bar{F}(\mathbf{m}-\mathbf{h},\rho_\mu) \times \sum_{\nu=1}^{q(\mu)} t_{\mu\nu}(\mathbf{m})\bar{t}_{\mu\nu}(\mathbf{m}-\mathbf{h}) \exp(2\pi i\mathbf{h}.\mathbf{x}_{\mu\nu}) \Bigg]$$

labelled by the polynomials G_1 and G_2, representing differential operators D_1^* and D_2^*.

We may obviously define $G_1(\mathbf{m})$ and $G_2(\mathbf{m})$ more generally, without altering the derived equations, by requiring only that the basis (German: Träger) of the Fourier transform of $G(\mathbf{m})F(\mathbf{m},\rho_\mu)$ is not more extensive than that of ρ_μ, $\mu = 1, 2, \ldots, p$.

Applying the derived equations for the case of point scatterers we have to replace the $G(\mathbf{m})$ functions by the form factors $F(\mathbf{m},\gamma)$ of arbitrary density functions γ no more extensive than a sphere with diameter equal to the minimum distance of the scatterers (Rothbauer, 1977*a*).

We notice that the class of functions which represents allowed $G(\mathbf{m})$'s is very restricted.

As we can use any polynomial of degree N in the variables m_1, m_2, m_3 as a $G(\mathbf{m})$ function if the $\rho_\mu(\mathbf{x})$, $\mu = 1, 2, \ldots p$ are N times differentiable, we may approximate any piece-wise continuous single-valued function of $\mathbf{m}$ in the range of reciprocal space covered by experiment with arbitrary accuracy by an allowed $G(\mathbf{m})$ function if N is sufficiently large.

Such a fitted polynomial will not necessarily be useful in practice because it may increase with increasing $\mathbf{m}^2$ so quickly outside the range covered by experiment, that the termination errors in the above equation may be serious.

For practical applications we will therefore have to impose further restrictions on the $G(\mathbf{m})$ functions. We will return to this point at the end of the paper, when a numerical example will be given.

For the case $\mathbf{h} = \mathbf{0}$ the above system of equations does not depend on the phases of the structure factors and the coordinates of the atoms:

$$0 = \sum_{\mathbf{m}} G_1(\mathbf{m})\bar{G}_2(\mathbf{m}) \Bigg[F(\mathbf{m},\rho)\bar{F}(\mathbf{m},\rho) - \sum_{\mu=1}^{p} F(\mathbf{m},\rho_\mu)\bar{F}(\mathbf{m},\rho_\mu) \sum_{\nu=1}^{q(\mu)} t_{\mu\nu}(\mathbf{m})\bar{t}_{\mu\nu}(\mathbf{m}) \Bigg]. \quad (8)$$

We may formally describe (8) by saying that the height of the origin peak in a weighted Patterson synthesis is equal to the sum of the squares of the similarly weighted temperature-corrected atomic scattering factors. However, we cannot develop the properties of the allowed weighting functions $G(\mathbf{m})$ on the basis of this interpretation. To derive these properties we are forced to make use of the fact that the atoms do not interpenetrate, a proposition which is not necessary in order to calculate the Patterson function.

Special cases

We may express $t_{\mu\nu}(\mathbf{m})$, to a first approximation, by

$$t_{\mu\nu}(\mathbf{m}) = \exp(-\mathbf{m}.\boldsymbol{\beta}_{\mu\nu}\mathbf{m}), \quad (9)$$

where $\boldsymbol{\beta}_{\mu\nu}$ is a positive definite symmetric tensor (Cochran, 1954; Rollett & Davies, 1955; Waser, 1955). If we approximately describe the thermal movement of all the atoms of the μth kind by a single tensor $\boldsymbol{\beta}_\mu$ we have

$$\sum_{\nu=1}^{q(\mu)} t_{\mu\nu}(\mathbf{m})\bar{t}_{\mu\nu}(\mathbf{m}) = q(\mu)\exp(-2\mathbf{m}.\boldsymbol{\beta}_\mu\mathbf{m}). \quad (10)$$

Let $I(\mathbf{m})$ be the experimentally determined relative intensity at lattice point $\mathbf{m}$ and s be the scale factor independent of $\mathbf{m}$; then

$$F(\mathbf{m},\rho)\bar{F}(\mathbf{m},\rho) = sI(\mathbf{m}). \quad (11)$$

Inserting (10) and (11) into (8) and taking the usual symbol $f_\mu(\mathbf{m})$ instead of $F(\mathbf{m},\rho_\mu)$ for the form factors of the atoms of the μth kind, one obtains the system of equations

$$0 = \sum_{\mathbf{m}} G_1(\mathbf{m})\bar{G}_2(\mathbf{m}) \Bigg[sI(\mathbf{m}) - \sum_{\mu=1}^{p} f_\mu(\mathbf{m})\bar{f}_\mu(\mathbf{m})q(\mu)\exp(-2\mathbf{m}.\boldsymbol{\beta}_\mu\mathbf{m}) \Bigg] \quad (12)$$

from which the scale factor s, the temperature tensors $\boldsymbol{\beta}_\mu$, $\mu = 1, 2, \ldots, p$, and the chemical contents of the elementary cell described by $q(\mu)$, $\mu = i, 2, \ldots, p$, can be derived.

It is beyond the scope of this paper to present a method by which the system of equations can be solved. We restrict ourselves here to the derivation of the system of equations (8) and (12), using the proposition of non-penetrating atoms, and to the discussion of the allowed weight functions $G(\mathbf{m})$.

To demonstrate the usefulness of the system of equations (8) and (12) we will give the description of a new method for the determination of the scale and Debye–Waller factor on the basis of the previous considerations.

Before we do this, we will discuss some further simplifications. In most cases the $q(\mu)$ can be determined from a quantitative chemical analysis, a knowledge of the lattice constants and the density of the crystal, so that

$$I_\mu(\mathbf{m}) = f_\mu(\mathbf{m})\bar{f}_\mu(\mathbf{m})q(\mu) \tag{13}$$

is a quantity which can be derived independently of the intensity measurements. We can therefore use the following system of equations:

$$0 = \sum_{\mathbf{m}} G_1(\mathbf{m})\bar{G}_2(\mathbf{m}) \left[sI(\mathbf{m}) - \sum_{\mu=1}^{p} I_\mu(\mathbf{m}) \exp(-2\mathbf{m}.\boldsymbol{\beta}_\mu\mathbf{m}) \right] \tag{14}$$

for the determination of the scale factor s and the temperature tensors $\boldsymbol{\beta}_\mu$, $\mu = 1, 2, \ldots, p$.

The special case $G_1(\mathbf{m})\bar{G}_2(\mathbf{m}) = 1$ of these equations has been derived by Kartha (1953), Krogh-Moe (1956) and Norman (1957).

The description of the thermal motion (9) and the assumption that the thermally enlarged scattering density functions of the atoms of the crystals do not penetrate each other are approximations, therefore (14) is also an approximation. However, as the penetration occurs only in the outer parts of the atoms, with low scattering density, the resulting errors should be small.

If we want to use only one tensor $\boldsymbol{\beta}$ for the description of the thermal movement of all atoms of the crystal we obtain from (14):

$$0 = \sum_{\mathbf{m}} G_1(\mathbf{m})\bar{G}_2(\mathbf{m}) \left[sI(\mathbf{m}) - \exp(-2\mathbf{m}.\boldsymbol{\beta}\mathbf{m}) \sum_{\mu=1}^{p} I_\mu(\mathbf{m}) \right]. \tag{15}$$

If one tensor $\boldsymbol{\beta}$ is sufficient for the description of the thermal motion of all atoms, we may derive a system of equations for the determination of s and $\boldsymbol{\beta}$ which differs from (15). By leaving the temperature factors $t_{\mu\nu}(\mathbf{m})$ out of the previous treatment and assuming that ρ is the scattering density function of a hypothetical crystal, with atoms at rest, (7) is more strictly valid. The intensities of the hypothetical crystal are derived from those of the real crystal by multiplying with the factor $\exp(2\mathbf{m}.\boldsymbol{\beta}\mathbf{m})$. This leads to

$$0 = \sum_{\mathbf{m}} G_1(\mathbf{m})\bar{G}_2(\mathbf{m}) \left[sI(\mathbf{m}) \exp(2\mathbf{m}.\boldsymbol{\beta}\mathbf{m}) - \sum_{\mu=1}^{p} I_\mu(\mathbf{m}) \right]. \tag{16}$$

To the most simple description of the thermal movement, given by the Debye–Waller factor B, corresponds an isotropic movement of all the atoms of the structure, so that we have instead of (9)

$$t_{\mu\nu}(\mathbf{m}) = \exp(-B\mathbf{m}^2/4),$$

where B is a number independent of μ and ν. (15) and (16) then become

$$0 = \sum_{\mathbf{m}} G_1(\mathbf{m})\bar{G}_2(\mathbf{m}) \left[sI(\mathbf{m}) - \exp(-B\mathbf{m}^2/2) \sum_{\mu=1}^{p} I_\mu(\mathbf{m}) \right], \tag{17}$$

$$0 = \sum_{\mathbf{m}} G_1(\mathbf{m})\bar{G}_2(\mathbf{m}) \left[sI(\mathbf{m}) \exp(B\mathbf{m}^2/2) - \sum_{\mu=1}^{p} I_\mu(\mathbf{m}) \right], \tag{18}$$

respectively.

Calculation of scale and Debye–Waller factors

We may formally describe the Wilson (1942) statistics by G functions and (17). The reciprocal space is divided into N spherical shells separated by the spheres $\mathbf{m}^2 = c_j$, $j = 1, 2, \ldots, N$, $0 < c_1 < c_2 < \ldots < c_N$, and $G_{j1}(\mathbf{m})\bar{G}_{j2}(\mathbf{m})$ is defined to be equal to 1 inside the jth shell and equal to 0 outside. In this way one gets N determinantal equations of type (17) from which the Wilson plot is derived.

As the bases of the Fourier transforms of $G_{jk}(\mathbf{m})F(\mathbf{m},\rho_\mu)$ are in this case more extensive than the bases of ρ_μ, we cannot completely see from this point of view how the statistical method works (see also Harker, 1953; Magdoff, Crick & Luzzati, 1956).

We may approximate the $G(\mathbf{m})$ functions of the Wilson statistics with arbitrary accuracy by polynomials, which are allowed G functions, in the range of reciprocal space covered by experiment, but these polynomials are not necessarily optimal ones, because they may increase so quickly with $\mathbf{m}^2$ that the termination errors are serious.

Applying (14) to (18) one is forced to cut off the series somewhere, so that one has to work with functions $G(\mathbf{m})$, which disappear if $\mathbf{m}^2$ exceeds a certain limit and which are therefore not allowed in a strict sense. For practical applications one must therefore take into account the termination of the series. This can be done by choosing G functions, such that the essential part of the Fourier transform of $G(\mathbf{m})F(\mathbf{m},\rho_\mu)$, $\mu = 1, 2, \ldots, p$, is not more extensive than the basis of ρ_μ if one terminates the series.

Appropriate approximations of G functions for (17) and (18) in the range of $\mathbf{m}^2$ which is usually covered by experiment are obviously given by $\exp(b\mathbf{m}^2/4)$ if $b \geq 0$ is in the range of observed Debye–Waller factors, so that the function reduces the effect of thermal motion and does not enlarge the essential parts of the bases of the ρ_μ.

Accordingly exp ($\mathbf{m}.\boldsymbol{\alpha}\mathbf{m}$) with positive definite tensors $\boldsymbol{\alpha}$ will be suitable for insertion into (14), (15) and (16).

One should then not interpret (8), (12) or (14) as a difference of two sums over the points of reciprocal lattice, terminated at different values of $\mathbf{m}^2$. Using similar arguments as in the Wilson statistics, one may estimate that the rest of the series of the two terms of the difference (minuend and the subtrahend) will approximately annihilate each other if one terminates both in the same way.

We denote by K the absolute intensity of the origin of reciprocal space:

$$K = sI(\mathbf{0}) = F(\mathbf{0})\bar{F}(\mathbf{0}).$$

From (13) we have

$$K = \sum_{\mu,\nu=1}^{p} q(\mu)q(\nu)f_\mu(\mathbf{0})\bar{f}_\nu(\mathbf{0}). \tag{19}$$

Setting

$$J(\mathbf{m}) = \sum_{\mu=1}^{p} I_\mu(\mathbf{m}) \tag{20}$$

and inserting (19), (20) into (17) and solving for s we obtain, with the choosen approximation $G_1(\mathbf{m})\bar{G}_2(\mathbf{m}) = \exp(b\mathbf{m}^2/2)$,

$$s = \frac{\left\{ \sum\limits_{\mathbf{m}} \exp[(b-B)\mathbf{m}^2/2]J(\mathbf{m}) - K \right\}}{\left[\sum\limits_{\mathbf{m}\neq\mathbf{0}} \exp(b\mathbf{m}^2/2)I(\mathbf{m}) \right]}. \tag{21}$$

For every value of b, (21) describes s as a function of B and hence a curve in an s, B diagram. The intersection of two curves of this kind for two different values of b gives a solution for the scale factor and Debye–Waller factor.

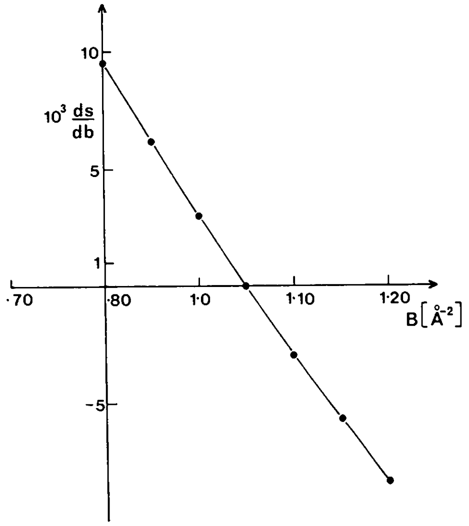

Fig. 1. The dependence of $\partial s/\partial b$ on B for $b = 0$ with a series termination of $(\sin\theta)/\lambda = 0{\cdot}70$ Å^{-1}.

Two curves in an infinitesimal neighbourhood with b values b and $b + \mathrm{d}b$ intersect where the derivative $\partial s/\partial b$ of (21) disappears. We find

$$\begin{aligned}\partial s/\partial b = \Bigg[& \sum_{\mathbf{m}} (\mathbf{m}^2/2)\exp[(b-B)\mathbf{m}^2/2]J(\mathbf{m}) \\ & \times \sum_{\mathbf{m}\neq\mathbf{0}} \exp(b\mathbf{m}^2/2)I(\mathbf{m}) \\ & - \left\{ \sum_{\mathbf{m}} \exp[(b-B)\mathbf{m}^2/2]J(\mathbf{m}) - K \right\} \\ & \times \sum_{\mathbf{m}\neq\mathbf{0}} (\mathbf{m}^2/2)\exp(b\mathbf{m}^2/2)I(\mathbf{m}) \Bigg] \\ & \div \left[\sum_{\mathbf{m}\neq\mathbf{0}} \exp(b\mathbf{m}^2/2)I(\mathbf{m}) \right]^2 \end{aligned} \tag{22}$$

and hence the determinantal equation

$$\begin{aligned} 0 = & \sum_{\mathbf{m}} (\mathbf{m}^2/2)\exp[(b-B)\mathbf{m}^2/2]J(\mathbf{m}) \\ & \times \sum_{\mathbf{m}\neq\mathbf{0}} \exp(b\mathbf{m}^2/2)I(\mathbf{m}) \\ & - \left\{ \sum_{\mathbf{m}} \exp[(b-B)\mathbf{m}^2/2]J(\mathbf{m}) - K \right\} \\ & \times \left[\sum_{\mathbf{m}\neq\mathbf{0}} (\mathbf{m}^2/2)\exp(b\mathbf{m}^2/2)I(\mathbf{m}) \right] \end{aligned} \tag{23}$$

for the Debye–Waller factor B.

For each value of b a solution for the temperature factor B and the scale factor s may be derived from (23) and (21). To keep the termination errors low it seems desirable to use both equations with $b = 0$.

For a numerical example the structure factors of bayerite, Al(OH)$_3$ (Rothbauer, Zigan & O'Daniel, 1967), calculated with $B = 1$ and $s = 1$, were chosen. Fig. 1 shows the dependence of $\partial s/\partial b$, (22), on B for $b = 0$ with a series termination of $(\sin\theta)/\lambda = 0{\cdot}70$ Å^{-1}. The intersection with the B axis gives the Debye–Waller factor 1·05 Å^{-2}. Inserting this number together with $b = 0$ into the right-hand side of (21) gives the scale factor 0·98. These estimates are within 5 and 2%, respectively, of the theoretical values.

The calculations were repeated, terminating the series at $(\sin\theta)/\lambda = 0{\cdot}65$ and $0{\cdot}60$ Å^{-1}. The results are given in Table 1. The corresponding Wilson plots were

Table 1. *Results of first calculation of B and s*

$[(\sin\theta)/\lambda]_{\max}$	B	s
0·60	1·01	0·99
0·65	0·97	0·99
0·70	1·05	0·98

Table 2. *Results of second calculation of B and s*

$[(\sin\theta)/\lambda]_{\max}$	B	s	Points
0·60	0·85	1·18	7
0·65	0·71	1·19	8
0·70	0·89	1·12	9

calculated dividing the range of $(\sin^2\theta)/\lambda^2$ into seven, eight and nine equidistant zones respectively. A straight line was interpolated with the help of the method of least squares into each of the diagrams and the values for s and B in Table 2 were obtained.

If the temperature factors are so large that the effective interpenetration of the atoms is considerable, one should use (18) instead of (17). This is equivalent to replacing b in (17), (21), (22) and (23) by $b + B$. Hence, in (21) and (23) the errors resulting from thermal interpenetration of the atoms decrease, but the errors from series termination increase with b.

If one wants to find s and $\boldsymbol{\beta}_\mu$, $\mu = 1, 2, \ldots, p$, or s and $\boldsymbol{\beta}$ it seems appropriate first to determine s and B by (21) and (23) and then to refine this result by (15) or (16) and finally by (12).

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Extrapolative Filtering.
I. Maximization of Resolution for One-Dimensional Positive Density Functions

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A one-dimensional formalism based on extrapolative filtering can lead to electron-density maps at more than twice the resolution displayed by maps obtained by straightforward Fourier synthesis of structure factors. A worked example illustrates the computations for a hypothetical one-dimensional structure.

1. Introduction

Norbert Wiener's *Extrapolation, Interpolation, and Smoothing of Stationary Time Series* (1949) is of forbidding difficulty to most physical scientists. Originally published under military classification (Wiener, 1949, p. v), its importance was ironically acclaimed as those with access termed it 'The Yellow Peril' for the color of its binding (Bode & Shannon, 1950). Motivated by the need to simplify Wiener's work and relate it in a more obvious way to physical problems, Bode & Shannon (1950) presented a simplified development of Wiener's principal results in terms of electric-circuit theory. However helpful their work may have been, it does not appear to have provided an immediate impetus to scientific applications involving discrete time series, possibly because in the case of discrete time it is difficult to follow the mathematics intuitively. After some years, Enders Robinson (1967) put together an elementary account of discrete filters and included Bode & Shannon's presentation of Wiener's work in a still simpler form adapted to discrete time series. But