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A Generalized Polynomial For the Extraction of the Periodic Vector Set From the Patterson Function

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(*Received* 23 *February* 1970 *and in revised form* 18 *June* 1970)

Crystal-structure analysis *via* the Patterson function may be considered as consisting of two distinct steps. In the first step, the weighted periodic vector set is determined by establishing the location of each peak in the Patterson function. In the second step, the weighted periodic vector set is analysed to determine the crystal structure. The second step apparently offers little difficulty, since existing procedures for the analysis of periodic vector sets appear to be capable of dealing with complex structures, provided of course that the vector set is accurately determined. Unfortunately, a general and powerful method for the location of peaks in the Patterson function has not yet been developed and therefore it is the first step in the solution process which now prevents the formulation of a general method of structure analysis *via* the Patterson function. Such a method would be extremely useful, since the Patterson function is not restricted to centrosymmetric structures. In the present paper a way of representing the Patterson function as a linear generalized polynomial in a system of independent interatomic functions is developed. The coefficients of this polynomial determine the weighted periodic vector set. This approach, therefore, reduces the problem of extracting the periodic vector set from the Patterson function to a relatively simple problem in linear approximation, namely the determination of the coefficients of a generalized polynomial.

Introduction

During the past fifty years many methods for the solution of crystal structures have been proposed. These existing methods are all limited to crystals with special characteristics, and a general method, capable of dealing with virtually any sort of crystal in a routine manner, remains to be discovered.

In order to formulate a general and practical method of structure analysis, one would naturally think of working in terms of the Patterson function, since this function is not restricted to centrosymmetric structures. It is now well known that a weighted periodic vector set (Buerger, 1959) can be associated with the Patterson function of an arbitrary crystal. In the following discussion, weighted vector sets will often be referred to simply as periodic vector sets, since unweighted sets will never be considered. For a crystal containing N atoms per unit cell, the periodic vector set consists of N periodic images of the crystal structure. The essence of the phase problem lies in the separation of the various points of the periodic vector set into these images. This separation can be accomplished for periodic vector sets by the image-seeking method of Buerger (1950), even though this method was originally devised in terms of non-periodic vector sets. Tokonami & Hosoya (1965) have developed a different procedure for unravelling periodic vector sets. Their method depends explicitly on certain periodic characteristics of the periodic vector sets. It also offers certain computational advantages over the image-seeking methods.

These considerations indicate that crystal-structure analysis *via* the Patterson function may be viewed as consisting of two distinct steps. In the first step, the peaks in the Patterson function are located; this determines the periodic vector set. In the second step, the periodic vector set is solved to yield the crystal structure. Unfortunately we do not have, at the present time, a general and practical method for the location of peaks in the Patterson function. Consequently, it is the first step in the solution process, that of locating the peaks in the Patterson function, which now prevents the development of a general method of structure analysis in terms of the Patterson function. It would seem that if the periodic vector set could be determined from the Patterson function in some way, the crystal structure could be obtained by means of existing vector-set methods. Of course, the image-seeking method and the Tokonami–Hosoya procedure have not been widely used in practice, and it may therefore turn out that their power is restricted in some ways which are not now recognized. At present, however, it appears that these procedures could be successfully applied to extremely complex crystals, provided the vector set could be accurately determined.

The problem of recovering the periodic vector set from the Patterson function has, in the past, been approached mainly *via* Patterson sharpening procedures (Patterson, 1934; Wunderlich, 1965). The power of these methods depends to a large extent on the resolution of the Patterson function, and therefore they do not appear to the capable of yielding the vector set except for comparatively simple structures. Other methods, which in effect locate individual peaks in the Patterson function, have also been proposed. These methods, like the symmetry minimum function (Simpson, Dobrott & Lipscomb, 1965), can only be applied to crystals of sufficiently high symmetry, and are therefore non-general.

All of these existing methods depend critically on the possibility of recognizing individual resolved peaks in the Patterson function. What is really needed is a method which can 'see through' the overlapping peaks regardless of any lack of resolution. This paper presents an attempt to formulate a practical method of that kind. This new method is based on the theory of approximation in generalized polynomials (Cheney, 1966). It provides an approach which can be applied to the problem of crystal-structure analysis in several different ways, for example as a phase test and as a way of solving the structure-factor equations. However, this paper will deal only with the most straightforward of these methods, which involves the Patterson function. A very brief account of one variant of these methods has already been published (Goldak, 1969). In the present paper, the formulation of a generalized polynomial representing the Patterson function is considered in detail. Following papers will present methods for the practical computation of these polynomials.

The Patterson function as a sum of interatomic functions

The Patterson function is defined as the convolution of the electron density function. A one-dimensional Patterson function $A(x)$, projected onto the a crystal axis, is then represented by the Fourier series

$$A(x) \simeq C \sum_{h=-\infty}^{+\infty} |F_h|^2 \exp\,[2\pi i h x] \tag{1}$$

where F_h is the structure factor of Miller index h. The constant $C=bc/v$ where b, c, and v are, as usual, unit-cell parameters. It is important to note that the sum of the series on the right-hand side does not necessarily equal $A(x)$, but only corresponds to $A(x)$. How well the series approximates $A(x)$ depends on its convergence properties. For the following work we will define a partial Patterson function of order M as the Mth partial sum of the series (1) so that

$$P_M(x) = C \sum_{h=-M}^{+M} |F_h|^2 \exp\,[2\pi i h x]\,. \tag{2}$$

All the following work will be done in terms of $P_M(x)$ rather than $A(x)$.

The one-dimensional partial Patterson function $P_M(x)$ can be written as

$$P_M(x) = C \sum_{h=-M}^{+M} \left\{ \sum_{n=1}^{N} \sum_{m=1}^{N} f_n f_m \exp\,[2\pi i h (x_n - x_m] \right\}_h \times \exp\,[2\pi i h x]\,. \tag{3}$$

In (3) N is the number of atoms per unit cell, and h is the Miller index; x_n is the fractional coordinate of the nth atom and f_n is its scattering factor. Following Kitaigorodskii (1961), we then refer to

$$P^{mn}_M(x) = C \sum_{h=-M}^{+M} \{f_n f_m \exp\,[2\pi i h (x_n - x_m)]\}_h \times \exp\,[2\pi i h x]\,. \tag{4}$$

as an interatomic function corresponding to the nth and mth atoms. We then call $(x_n - x_m)$ the interatomic function parameter. In order to obtain a simpler and more powerful notation for the interatomic functions, an arbitrary correspondence is established which uniquely defines an interatomic function kind index q and an interatomic function order index p in terms of the atom indices m and n. For example, in a given situation, $q=1$ may denote the several carbon–carbon interatomic functions associated with the crystal. Then the indices $q=1$ and $p=3$ would denote the third carbon–carbon interatomic function. Under this correspondence, the pth interatomic function of the qth kind may be written as

$$I_{Mq}(x - x^q_p) = C \sum_{h=-M}^{+M} \{f_n f_m \exp\,[2\pi i h (x_n - x_m)]\}_h \times \exp\,[2\pi i h x] \tag{5}$$

where $x^q_p = x_n - x_m$ is the interatomic function parameter. Let K denote the number of kinds of interatomic functions associated with crystal, and let N_j represent the number of interatomic functions of the jth kind. Then the partial Patterson function can be written exactly as

$$P_M(x) = \sum_{q=1}^{K} \sum_{p=1}^{N_q} I_{Mq}(x - x^q_p)\,. \tag{6}$$

The interatomic function $I_{Mq}(x-x^q_p)$ is periodic with a 'bell-shaped' maximum at $x=x^q_p$; the function is symmetric about the point $x=x^q_p$.

We may later refer to (4) as a full-cell representation of the partial Patterson function, and to the interatomic functions of the kind defined by (5) as full-cell interatomic functions. However, the partial Patterson function is always centrosymmetric and we can also obtain a representation in $0 \le x \le \frac{1}{2}$. We define a half-cell interatomic function as

$$I^{H}_{Mq}(x-x^{q}_{p}) = \frac{I_{Mp}(x-x^{q}_{p}) + I_{Mq}(x+x^{q}_{p})}{1+\delta(0,x^{q}_{p})+\delta(\frac{1}{2},x^{q}_{p})} \qquad (7)$$

where $\delta(i,j)$ is, as usual, the Kronecker delta. The half-cell interatomic functions are not symmetric about $x=x^{q}_{p}$ unless $x^{q}_{p}=0$ or $x^{q}_{p}=\frac{1}{2}$. If N_j denotes the number of half-cell interatomic functions of the jth kind, the Patterson function can be written as

$$P_M(x) = \sum_{q=1}^{K} \sum_{p=1}^{N_q} I^{H}_{Mq}(x-x^{q}_{p}) \,. \qquad (8)$$

Equations (6) and (8) of course hold true only if the scattering factors used in the computation of the $I_{Mq}(x-x^{q}_{p})$ are the same as those which occur in $P_M(x)$. The most convenient way of ensuring this compatibility is to place the observed structure amplitudes initially onto an absolute scale, and to determine an average temperature factor, so that an appropriate scattering-factor adjustment can be made. A fairly accurate way of doing this *via* the Patterson function will be described in a following paper. Depending on the scattering factors used, equations (6) and (8) can be applied to moving-atom crystals, to stationary-atom crystals, or to point-atom crystals.

For later matrix operations, it will be desirable to have the interatomic functions as 'sharp' as possible. Therefore it will be necessary to correct the observed structure factors so that they correspond to a stationary-atom crystal, or to sharpen them so that they correspond (approximately) to a point-atom crystal. For the stationary-atom case, the functions $I_{Mq}(x-x^{q}_{p})$ in (6) and (7) are given by the Fourier series (5). However, the representations (6) and (8) for a sharpened Patterson can be formulated in several different ways.

To sharpen the Patterson function according to Patterson's method (Patterson, 1935), it is assumed that the scattering factors can be represented with sufficient accuracy by an expression of the form

$$f_j = Z_j \hat{f} \,. \qquad (9)$$

In (9), f_j is a stationary-atom scattering factor, Z_j is an atomic number, and $\hat{f}$ is an average unit scattering factor. The observed structure amplitudes are divided by $\hat{f}$ so that the sharpened Patterson function is

$$P_M(x) = C \sum_{h=-M}^{+M} \Bigg\{ \sum_{m=1}^{N} \sum_{n=1}^{N} \frac{f_m}{\hat{f}} \frac{f_n}{\hat{f}} \times \exp\,[2\pi ih(x_n - x_m)] \Bigg\} \exp\,[2\pi ihx] \,. \qquad (10)$$

Therefore, just as in (5), the expression

$$I_{Mq}(x-x^{q}_{p}) = C \sum_{h=-M}^{+M} \Bigg\{ \frac{f_m}{\hat{f}} \times \frac{f_n}{\hat{f}} \times \exp\,[2\pi ih(x_n - x_m)] \Bigg\} \exp\,[2\pi ihx] \,. \qquad (11)$$

gives the interatomic functions which exactly correspond to the sharpened Patterson function. It is important to note that (6) is exact (aside from round-off errors) and when used as a representation of a sharpened Patterson function, is not affected by inaccuracies in the sharpening assumption (9).

However, when dealing with crystals for which (9) is a good approximation, the sharpened Patterson function will be almost identical with the point-atom Patterson function. In this case, we can obtain a sufficiently accurate representation of the sharpened Patterson function as a sum of point-atom interatomic functions. If this is done, an extremely advantageous representation of the interatomic function can be obtained.

To obtain this representation we note that the partial Patterson function corresponding to a point-atom crystal can be written as

$$P_M(x) = C \sum_{h=-M}^{+M} \Bigg\{ \sum_{j=1}^{N} \sum_{k=1}^{N} Z_j Z_k \times \exp\,[2\pi ih(x_j - x_k)] \Bigg\}_{h} \exp\,[2\pi ihx] \,. \qquad (12)$$

In this expression Z_j is the atomic number of the jth atom, and M is the highest-order Miller index associated with the available structure amplitudes. Then setting $x_{jk} = x_j - x_k$ (12) can be rewritten as

$$P_M(x) = \sum_{j=1}^{N} \sum_{k=1}^{N} \Bigg\{ CZ_jZ_k \Bigg(1 + \sum_{\substack{h=-M \\ h\neq 0}}^{+M} \exp\,[2\pi ih(x+x_{jk})] \Bigg) \Bigg\} \qquad (13)$$

or

$$P_M(x) = \sum_{j=1}^{N} \sum_{k=1}^{N} \Bigg\{ CZ_jZ_k \Bigg[1 + \sum_{h=1}^{M} (\exp\,[2\pi ih(x+x_{jk})] + \exp\,[-2\pi ih(x+x_{jk})]) \Bigg] \Bigg\} \,. \qquad (14)$$

The last expression is the same as

$$P_M(x) = \sum_{j=1}^{N} \sum_{k=1}^{N} 2CZ_jZ_k \Bigg[\frac{1}{2} + \sum_{h=1}^{M} \cos 2\pi h(x+x_{jk}) \Bigg] \,. \qquad (15)$$

The finite sum in the square brackets has the property

$$\frac{1}{2} + \sum_{h=1}^{M} \cos 2\pi h(x+x_{jk}) = \frac{\sin\,[2\pi(M+\frac{1}{2})\,(x+x_{jk})]}{2\sin\,[\pi(x+x_{jk})]} \,. \qquad (16)$$

This function, which according to usual terminology would be denoted by $D_M(x+x_{jk})$, is of fundamental importance in the study of the convergence of Fourier series, and is known as the Dirichlet kernel of order M. Thus (15) is

$$P_M(x)=\sum_{j=1}^{N}\sum_{k=1}^{N}2CZ_jZ_k\,\frac{\sin\,[2\pi(M+\frac{1}{2})\,(x-x_{kj})]}{2\sin\,[\pi(x-x_{kj})]}\,. \tag{17}$$

Under the previously described index correspondence, a pth modified Dirichlet kernel of order M and of the qth kind, can be written as

$$D_{Mq}(x-x_p^q)=CZ_jZ_k\,\frac{\sin\,[2\pi(M+\frac{1}{2})\,(x-x_{kj})]}{\sin\,[\pi(x-x_{kj})]}\,. \tag{18}$$

Then (14) can be written in the form

$$P_M(x)=\sum_{q=1}^{K}\sum_{p=1}^{N_q}D_{Mq}(x-x_p^q) \tag{19}$$

which is analogous to (6). $D_{Mq}(x-x_p^q)$ may be termed a full-cell Dirichlet kernel. A half-cell Dirichlet kernel may be defined by

$$D_{Mq}^H(x-x_p^q)=\frac{D_{Mq}(x-x_p^q)+D_{Mq}(x+x_p^q)}{1+\delta(0,x_p^q)+\delta(\frac{1}{2},x_p^q)}\,. \tag{20}$$

The Dirichlet kernels in (19) arose because (12) represents a direct partial summation of (1). Although direct summation of Fourier series is very commonly employed, in certain cases other summation methods may possess better convergence characteristics (Lanczos, 1966). For the present work, Cesaro summation (Tolstov, 1962) and Lanczos sigma-summation (Lanczos, 1966) can be applied with considerable advantage. In Cesaro summation, the Mth partial Cesaro sum is the arithmetic mean of the first M direct partial sums. Using (17) to obtain the direct partial sums, a Cesaro summed partial Patterson function of the Mth order can therefore be defined as

$$C_M(x)=1/M\{P_0(x)+P_1(x)+\ \ldots\ P_{M-1}(x)\}\,. \tag{21}$$

From (17) and (21), it can be shown that

$$C_M(x)=C\sum_{j=1}^{N}\sum_{k=1}^{N}2Z_jZ_k\,\frac{\sin^2\left[\frac{M\pi}{a}\,(x-x_{kj})\right]}{2M\sin^2\left[\frac{\pi}{a}\,(x-x_{kj})\right]}\,. \tag{22}$$

The trignometric term on the right side is called the Fejer kernel of order M and is denoted by $F_M(x-x_{kj})$. Under the usual index correspondence, the partial Patterson function can be written as a sum of modified Fejer kernels: that is,

$$C_M(x)=\sum_{q=1}^{K}\sum_{p=1}^{N_q}F_{Mq}(x-x_p^q) \tag{23}$$

which is analogous to (19). Half-cell kernels can be defined just as in (20). For the practical computation of the Cesaro-summed Patterson function, the cumbersome form (21) is replaced by the more convenient expression

$$C_M(x)=C\sum_{h=0}^{M-1}\frac{M-h}{M}\times|F_h|^2\times\cos 2\pi hx\,. \tag{24}$$

One of the advantages of using Cesaro summation in the present work is that the 'background ripples' characteristic of directly summed sharpened Patterson functions can be avoided. The direct partial sum of a Fourier series corresponding to a given function oscillates about the function, and these Gibbs oscillations* can be very important in neighbourhoods where the function changes rapidly. The Gibbs oscillations arise essentially because of the properties of the Dirichlet kernel. On the other hand, the Fejer kernel has much better characteristics, and the Gibbs oscillations do not occur in Cesaro-summed series. Furthermore, series which diverge everywhere under direct summation may converge under Cesaro summation. This is the case with the point-atom Patterson function, which diverges for every value of x under direct summation, but which converges everywhere under Cesaro summation.

Lanczos sigma-summation (Lanczos, 1966) can also be employed in the evaluation of the sharpened Patterson function, which is then given as a sum of modified Lanczos kernels. To obtain the Lanczos sum of a sharpened partial Patterson function $L_M(x)$, we simply compute

$$L_M(x)=C\sum_{h=0}^{M}M/h\pi\sin\,(h\pi/M)|F_h|^2\cos 2\pi hx\,. \tag{25}$$

The sigma factors, $M/h\pi\sin\,(h\pi/M)$, are specifically designed to smooth out the Gibbs oscillations. In dealing with point-atom interatomic functions, Lanczos summation has the advantage that it yields a sharper interatomic function than does Cesaro summation. The Gibbs oscillations, while not completely eliminated, as in the Cesaro procedure, are very greatly reduced. The only disadvantage of Lanczos summation is that the computation of the Lanczos kernel, since it involves the sine integral, is more difficult than the evaluation of the Fejer kernel.

For an excellent discussion of the application of summation methods to the practical evaluation of Fourier series, the reader is referred to Lanczos (1966).

To summarize the previous results, the Patterson function for a stationary-atom crystal may be computed by direct summation from (2) while (5) yields the interatomic functions. Sharpened Patterson functions corresponding to crystals for which the approximation (9) is inaccurate should be computed from (10), while the interatomic functions should be obtained from (11). However, the direct summation implied in the expres-

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* The term 'Gibbs oscillations' has traditionally been used to describe the behaviour of Fourier series in the neighbourhood of a jump discontinuity. However, essentially similar oscillations occur where a function remains continuous but changes very rapidly and it is in this sense that the term is used here.

sions will lead to severe Gibbs oscillations; to reduce these the best course would be to employ Lanczos summation to evaluate the series. When dealing with crystals for which the sharpening approximation (9) is sufficiently accurate, the most convenient approach is to Cesaro sum the sharpened Patterson, and to express the interatomic functions in terms of the Fejer kernel. In the following work, expressions like (6) and (8) will be used in a general sense, with the understanding that the $P_M(x)$ and $I_{Mq}(x-x_p^q)$ may represent direct, Cesaro, or Lanczos sums, depending on the particular crystal being studied.

A generalized polynomial for the extraction of the vector set from the Patterson function

Equations (6) and (8) show that the Patterson function is a non-linear function of the interatomic function parameters. On account of the great difficulties usually associated with non-linear mathematical methods, the formulation of a general method for the determination of the interatomic function parameters directly from these expressions would appear to be a hopelessly difficult task. In order to circumvent this difficulty, we seek expressions which approximate the non-linear forms (6), (8), (16) and (20), and in which the interatomic function parameters occur, indirectly or directly, in a linear way. Expressions of this kind can be formulated *via* constructive function theory. Given the one-dimensional partial Patterson function $P_M(x)$, we seek a generalized polynomial (Cheney, 1966)

$$G(x)=\sum_{i=1}^{S} c_i f_i(x)$$

where the $f_i(x)$ are a given set of S independent functions and the coefficients c_i are chosen so that, according to some selected norm, $G(x)$ is a 'good' or perhaps best approximation to $P_M(x)$.

In constructing the approximating polynomial, it is first of all necessary to make a choice of the functions $f_i(x)$ to be used, and to choose the norm or metric to be employed in the evaluation of the accuracy of the approximation. Rice (1964) has pointed out that neither of these questions allows a rigorous analysis, and the choice must be guided by computational experience and a consideration of any special requirements involved in a specific application. In practice, for the problem of computing approximations on some chosen interval, it is usually desirable to replace that interval by a finite set of points. One then seeks an approximation which is, in some desired sense, optimum on that set; in this way the problem is discretized.

In the present application, interatomic functions are used as approximating functions. D divisional points are allowed for each kind of interatomic function. For a Patterson function with K kinds of interatomic functions, there is a total of KD divisional points in $[0,\frac{1}{2}]$. Consequently there are $(KD-1)$ equal intervals in $[0,\frac{1}{2}]$, each interval being of fractional length $l/(2KD-2)$. Under this divisional scheme x_p^q is the pth divisional point for interatomic functions of the qth kind. Then the fractional coordinate associated with a given x_j^r is

$$x_j^r=\frac{(r-1)+K(j-1)}{2(KD-1)}\,. \tag{26}$$

Thus the sequence of divisional points is $x_1^1, x_1^2, x_1^3 \ldots x_1^K, x_2^1, x_2^2, x_2^3 \ldots x_2^K, x_3^1 \ldots x_D^K$ with $x_1^1=0$ and $x_D^K=\frac{1}{2}$. This divisional scheme may at first seem needlessly complicated, but it will be seen in later papers that it is required for reasons of accuracy.

We then consider the generalized polynomial in the half-cell interatomic functions

$$G(x)=\sum_{q=1}^{K}\sum_{p=1}^{D} N_p^q I_{Mq}^H(x-x_p^q)\,. \tag{27}$$

Alternatively, $[0,1]$ could be divided into an appropriate set of KD divisional points, and the generalized polynomial in the full-cell interatomic functions

$$G(x)=\sum_{q=1}^{K}\sum_{p=1}^{D} N_p^q I_{Mq}(x-x_p^q)$$

could be considered. However, it will be shown in the following papers that (27) is computationally preferable to (28).

The coefficients N_p^q in (27) are now to be evaluated in some way so that $G(x)$ will in some useful sense be a 'good' approximation to $P_M(x)$. Ideally, the N_p^q would be defined as the number of interatomic functions of the qth kind in $\frac{1}{2}(x_{p-1}^q+x_p^q)\leq x<\frac{1}{2}(x_p^q+x_{p+1}^q)$; these will be called the node-integral N_p^q and denoted $\bar{N}_p^q$. If they could be determined in some way, the $\bar{N}_p^q$ would give all the interatomic function parameters except for a translational error of maximum value $l/(4D-4)$. Then by choosing D sufficiently large, the translational error could be made negligible. However, in practice the N_p^q must be determined from $P_M(x)$, and thus only an approximation to the $\bar{N}_p^q$ can be obtained.

The simplest way of determining the N_p^q is to set

$$G(x_j^r)=P_M(x_j^r) \quad r=1,2,\ldots K;\quad j=1,2,\ldots D \tag{29}$$

or, more explicitly

$$\sum_{q=1}^{K}\sum_{p=1}^{D}[I_{Mq}^H(x_j^r-x_p^q)]N_p^q=P_M(x_j^r)$$
$$r=1,2,\ldots K;\quad j=1,2,\ldots D\,. \tag{30}$$

In (30), $I_{Mq}^H(x_j^r-x_p^q)$ gives the value of the pth interatomic function of the qth kind at the rth divisional point of the jth kind. Thus (30) represents a system of KD equations in the KD unknowns, which can be solved for the N_p^q. Under (29), $G(x)$ interpolates to $P_M(x)$ at KD points.

As a second method, we again divide $[0,\frac{1}{2}]$ into KD divisional points for the location of interatomic functions, but now consider another set $\{\bar{x}_1,\bar{x}_2,\ldots \bar{x}_Q\}$ of Q points, where $Q\lesseqgtr KD$, for the evaluation of the accuracy of the approximation. We then choose the N_p^q

so that the maximum error of the approximation on the set of points $\bar{x}_1, \bar{x}_2, \ldots \bar{x}_Q$

$$E_{\max} = \max_{1 \le i \le Q} \{ |P_M(\bar{x}_i) - G\bar{x}_i)| \} . \qquad (31)$$

is a minimum. Then $G(x)$ is said to be at best Tchebycheff or minimax approximation to $P_M(x)$ on the set $\{\bar{x}_1, \bar{x}_2, \ldots \bar{x}_Q\}$. The N_p^q can most conveniently be determined using the flexible and powerful methods of linear programming (Rice, 1964).

The above approach has reduced the problem of extracting the periodic vector set from the Patterson function to a problem in linear approximation. There are many mathematical questions of a theoretical nature involved in the determination of the interpolatory and Tchebycheff approximations, and these cannot be treated adequately in this paper; the interested reader is referred to the excellent book of Rice (1964) for a thorough treatment. In any case, the application of (30) and (31) is not limited by theoretical considerations; the limitations are imposed by problems of numerical computation. Numerical difficulties may arise when the approximation problem is formulated in such a way that an extremely large system of equations results. For example, a three-dimensional interpolatory solution of the Patterson function, in which 30 divisional points were used along the *a*, *b*, and *c* axes, would require the solution of 27,000 equations in 27,000 unknowns! While such systems can be solved in practice (provided the system is mathematically stable), there would appear to be little reason for doing so; in the present method two- and three-dimensional solutions appear to offer no significant advantages over the one-dimensional formulations dealt with in this paper. The details involved in the practical computation of the interpolatory approximations have been briefly described in a previous paper (Goldak, 1969). The more powerful Tchebycheff methods will be dealt with in a following paper.

This work was supported by a National Research Council grant. The author is also grateful to Dean A. D. Booth for discussion and for his general support of the author's crystallographic work.

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The Determination of Cyclicity, Hexagonality, and other Properties of Polytypes

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(*Received* 17 *August* 1970)

The cyclicity of a polytype, the percentage of hexagonality, and the distribution of figures '1' among even and odd places of the Zhdanov symbol may be deduced directly from measured intensities. These values are given for a 66*R* polytype whose sequence has been determined earlier and for a hypothetical 114*R* polytype. A discussion is given of the errors in these values originating from the errors of the $|S|^2$ values used and of the errors produced, if instead of the exact formula for the cyclicity an approximation advocated by Mardix and his coworkers is used.

Introduction

A method for the direct determination of periodic polytypes of ZnS, SiC or similar substances from measured intensities of X-ray diagrams has been published by two of us (Farkas-Jahnke; 1966, Dornberger-Schiff & Farkas-Jahnke 1970) and successfully applied (Gomes de Mesquita, 1968; Farkas-Jahnke & Dornberger-Schiff, 1970). The method is applicable if rather accurate values $|S(kl)|^2 = |F(hkl)|^2/|F_0(hkl)|^2$ are ob-