

The number of structural parameters measurable from a fiber diffraction pattern ultimately depends on the choice of  $\epsilon$ , the amount of noise amplification that can be tolerated in estimation of layer-line intensities from raw data. That number depends directly on the signal-to-noise ratio of the original data. In a previous analysis (Makowski, 1978), the intensities along layer lines were plotted as a function of distance from the meridian. Near the deconvolution limit, the noise in these estimated layer lines was greatly amplified. However, experience has indicated that this is not always the case and that systematic errors may be amplified and that this

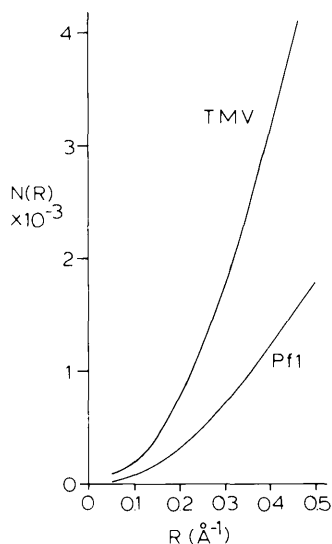


Fig. 4. The total number of structural parameters derivable from fiber diffraction patterns from tobacco mosaic virus (TMV) and filamentous bacteriophage Pf1 as a function of resolution. For this calculation,  $\sigma$  was set to  $1.4^\circ$  for both specimens. The larger number of parameters measurable for TMV is largely a result of its larger diameter (180 Å compared to 65 Å for Pf1).

amplification does not vary greatly with radius – it does not result in an apparent increase in noise levels along a layer line. In the analysis of most fiber diffraction patterns using angular deconvolution, we have found that using a value of  $\epsilon = 3$  results in acceptable results, but this may not always be the case. A comparable value is likely to be appropriate for estimates of structural parameters beyond the deconvolution limit.

The analysis presented here does not directly address the question of how to use the measurable structural parameters beyond the deconvolution limit. Equation (6) represents an indeterminate set of equations for the layer-line intensities beyond the deconvolution limit. The measurable structural parameters represent a partial set of data, from which intensities cannot be completely derived. However, they also represent a set of constraints on the structure of a helical assembly that with proper statistical tests can be used to constrain or refine (Tibbitts *et al.*, 1988) the structure of a diffracting unit. The rapidly increasing availability of computing power will provide the means for using these data. This paper provides a quantitative estimate of the amount of information contained in the observable data beyond the deconvolution limit.

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## An Atomicity-Constrained Least-Squares Phase-Refinement Method

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### Abstract

A phase-refinement method based on Sayre's squaring equation and on a suggestion made by Hoppe [*Z. Kristallogr.* (1963), **118**, 121–126] is presented. It takes

advantage of a lot of information initially known about a crystal structure such as all the measured structure-factor magnitudes and the atomicity constraint implicit in Sayre's equation. The method assumes that any squared structure factor  $|\mathbf{F}(\mathbf{H})|^2$  can

be approximately expressed in terms of the largest structure factors. This allows the quantity  $M = \sum_{\mathbf{H}} w(F_{\text{obs}}^2 - F_{\text{calc}}^2)^2$  to be expressed as a function of the phases of the largest  $F$ 's only, whereas the  $\mathbf{H}$  summation extends over all measured reflections. The refined phases of the largest  $F$ 's can then be found by least-squares minimization of  $M$ . The viability of the method is tested on a one-dimensional example. The physical meaning of minimizing  $M$  can be best illustrated by expressing  $M$  in Patterson space, *i.e.* in the form of the integral  $V_v \int (P_o - P_c)^2 dV$ , where  $P_o$  is the sharpened observed Patterson function and  $P_c$  is the calculated one expressed as a function of the phases of the largest  $F$ 's, taking into consideration the atomicity condition. The better the agreement between  $P_o$  and  $P_c$  over the whole unit cell, the smaller will be the integral and consequently  $M$ .

### 1. Introduction

Nowadays, multiresolution direct methods (Germain & Woolfson, 1968) based on the refinement of initially random sets of phases constitute the most widespread way of solving small-crystal structures. One attraction of these methods is that the refinement is done in reciprocal space and, therefore, no interpretation of Fourier maps is in general necessary during the refinement process.

Historically, the first method of refining phases was proposed by Hoppe (1963). In this method, the refined phases are found through least-squares minimization of the quantity

$$\sum_{\mathbf{H}} w(\mathbf{H}) [F(\mathbf{H}) - |\theta(\mathbf{H}) \sum_{\mathbf{H}'} \mathbf{F}_c(\mathbf{H}') \mathbf{F}_c(\mathbf{H} - \mathbf{H}')|]^2 \quad (1)$$

with

$$\theta(\mathbf{H}) = f(\mathbf{H}) / \sum_{\mathbf{H}'} f(\mathbf{H}') f(\mathbf{H} - \mathbf{H}'), \quad (2)$$

where  $F(\mathbf{H})$  is the observed structure-factor magnitude of the  $\mathbf{H}$  reflection,  $\mathbf{F}_c(\mathbf{H}') = F(\mathbf{H}') \exp i\varphi(\mathbf{H}')$  the calculated structure factor of  $\mathbf{H}'$  and  $f(\mathbf{H})$  the atomic scattering factor. As stated by the author, one of the drawbacks of the method is that the number of unknowns is of the same order as the number of observations. Consequently, the system is only slightly overdetermined and, in fact, there have been no practical applications of the method.

Later, Karle & Karle (1966) developed a phase-refinement method based on the tangent formula (Karle & Hauptman, 1956) that circumvents this difficulty. The tangent formula can be improved by including additional information, for example, negative quartets (Schenk, 1973), weak  $E$ 's (Debaerdemaeker, Tate & Woolfson, 1985) or minimum interatomic separation (Rius & Miravittles, 1989).

Following an alternative method, Krabbendam & Kroon (1971) and Sayre (1972) elaborated phase-refinement procedures based on expressions exploiting the complete information of Sayre's equation. Sayre proposed the least-squares solution of the equations

$$\mathbf{F}_c(\mathbf{H}) = \theta(\mathbf{H}) \sum_{\mathbf{H}'} \mathbf{F}_c(\mathbf{H}') \mathbf{F}_c(\mathbf{H} - \mathbf{H}') \quad (3)$$

by minimizing the expression

$$\sum_{\mathbf{H}} w(\mathbf{H}) |F(\mathbf{H}) \exp i\varphi_c(\mathbf{H}) - \theta(\mathbf{H}) \sum_{\mathbf{H}'} \mathbf{F}_c(\mathbf{H}') \mathbf{F}_c(\mathbf{H} - \mathbf{H}')|^2 \quad (4)$$

as a function of the phases. One argument adduced by the author for preferring minimization of (4) instead of (1) is that (4) really expresses two equations relating the real and imaginary parts of the two sides of (3), which is useful in producing a considerable degree of overdetermination of  $\varphi(\mathbf{H})$ . The utility of this method was shown by extending the phases of the small protein rubredoxin from 2.5 to 1.5 Å resolution (Sayre, 1974). It should be noted, however, that  $\varphi_c(\mathbf{H})$  in (4) is derived from  $\theta(\mathbf{H}) \sum_{\mathbf{H}'} \mathbf{F}_c(\mathbf{H}') \mathbf{F}_c(\mathbf{H} - \mathbf{H}')$ , *i.e.* it is not a measured quantity.

The present work explores a suggestion made by Hoppe (1963) that the overdetermination problem present in (1) may be solved by assuming that any structure factor  $\mathbf{H}$  can be approximately expressed as a function of the large structure factors alone. The refinement of phases can then be done by minimizing the quantity

$$\sum_{\mathbf{H}} w(\mathbf{H}) \left[ F(\mathbf{H})^2 - |\theta(\mathbf{H}) \sum_{\mathbf{h}'} \mathbf{F}_c(\mathbf{h}') \mathbf{F}_c(\mathbf{H} - \mathbf{h}')|^2 \right]^2, \quad (5)$$

where  $\mathbf{F}_c(\mathbf{h}')$  and  $\mathbf{F}_c(\mathbf{H} - \mathbf{h}')$  belong to the set of large  $F$ 's. In this way, only the phases of the large  $F$ 's need be refined, so that the resulting system is greatly overdetermined. This method is valid as long as Sayre's equation holds.

### 2. Theory

The method supposes that any structure factor  $\mathbf{F}(\mathbf{H})$  can be approximately expressed in terms of the  $n$  largest ones by means of Sayre's (1952) equation

$$\mathbf{F}(\mathbf{H}) \cong \theta(\mathbf{H}) \sum_{\mathbf{h}'} \mathbf{F}(\mathbf{h}') \mathbf{F}(\mathbf{H} - \mathbf{h}'). \quad (6)$$

If the atomic peaks are assumed spherical and Gaussian with width  $\sigma$ , then  $\theta(\mathbf{H})$  can be approximated by

$$\theta(\mathbf{H}) \cong K \exp(-\pi^2 \sigma^2 s_{\mathbf{H}}^2) = K v(\mathbf{H}) \quad (7)$$

$$s_{\mathbf{H}} = [2 \sin \vartheta_{\mathbf{H}}] / \lambda \quad (8)$$

with  $K$  a scaling factor sensitive to the resolution and to the number of selected large  $F$ 's. After substitution of (7) in (6), it follows that

$$\mathbf{F}(\mathbf{H}) \cong K v(\mathbf{H}) \sum_{\mathbf{h}'} \mathbf{F}(\mathbf{h}') \mathbf{F}(\mathbf{H} - \mathbf{h}'). \quad (9)$$

If the phases  $\varphi(\mathbf{h}_i)$  ( $i=1$  to  $n$ ) of the largest  $F$ 's (henceforth represented collectively by  $\Phi$ ) as well as  $K$  and  $\sigma$  are known, then (9) allows direct estimation of any structure factor  $\mathbf{H}$ .

Next, let the function  $M$  be defined as

$$M(\Phi, K, \sigma) = \sum_{\mathbf{H}} w(\mathbf{H}) j(\mathbf{H}) [F(\mathbf{H})^2 - F_c(\mathbf{H})^2]^2 \quad (10)$$

with  $\mathbf{H}$  representing the  $m$  measured reflections belonging to one asymmetric unit of the reciprocal space,  $j(\mathbf{H})$  the corresponding multiplicities and  $w(\mathbf{H})$  the associated weighting factors and where

$$F_c(\mathbf{H}) = A_c(\mathbf{H}) + i B_c(\mathbf{H}) \quad (11)$$

$$= K_c v_c(\mathbf{H}) \sum_{\mathbf{h}'} |F(\mathbf{h}') F(\mathbf{H} - \mathbf{h}')| \times \{ \cos [\varphi_c(\mathbf{h}') + \varphi_c(\mathbf{H} - \mathbf{h}')] + i \sin [\varphi_c(\mathbf{h}') + \varphi_c(\mathbf{H} - \mathbf{h}')] \}. \quad (12)$$

$M$  will be a minimum for the correct values of the parameters  $\Phi$ ,  $K$  and  $\sigma$  and, since  $m \gg n$ , it can be minimized by means of a least-squares procedure [see e.g. Rollet (1970) for a fairly complete description of the least-squares method]. The application of the least-squares method to the minimization of  $M$  requires, however, the functional form of  $F(\mathbf{H})^2$  to be linear in the parameters. Since this is not the case,  $F(\mathbf{H})^2$  must be first approximated by a truncated Taylor series. The value of  $F(\mathbf{H})^2$  at  $K_c + \Delta K$ ,  $\sigma_c + \Delta\sigma$  and  $\varphi_c(\mathbf{h}_i) + \Delta\varphi(\mathbf{h}_i)$  ( $i=1$  to  $n$ ) is then given by

$$F_c(\mathbf{H})_{\text{new}}^2 \cong F_c(\mathbf{H})^2 + [\partial F_c(\mathbf{H})^2 / \partial K] \Delta K + [\partial F_c(\mathbf{H})^2 / \partial \sigma] \Delta \sigma + \sum_j [\partial F_c(\mathbf{H})^2 / \partial \varphi(\mathbf{h}_j)] \Delta \varphi(\mathbf{h}_j). \quad (13)$$

At the minimum, the derivatives of  $M$  with respect to the parameters have to be zero. After introduction of (13) in each derivative expression, one equation of the following type is found for each parameter to be refined:

$$\begin{aligned} \partial M / \partial \varphi(\mathbf{h}_i) = \sum_{\mathbf{H}} w(\mathbf{H}) j(\mathbf{H}) \left\{ F(\mathbf{H})^2 - F_c(\mathbf{H})^2 \right. \\ \left. - [\partial F_c(\mathbf{H})^2 / \partial K] \Delta K - [\partial F_c(\mathbf{H})^2 / \partial \sigma] \Delta \sigma \right. \\ \left. - \sum_j [\partial F_c(\mathbf{H})^2 / \partial \varphi(\mathbf{h}_j)] \Delta \varphi(\mathbf{h}_j) \right\} \\ \times \partial F_c(\mathbf{H})^2 / \partial \varphi(\mathbf{h}_i) = 0. \quad (14) \end{aligned}$$

By rearrangement of (14), the normal equation for

$\varphi(\mathbf{h}_i)$  is obtained:

$$\begin{aligned} \sum_{\mathbf{H}} w(\mathbf{H}) j(\mathbf{H}) [\partial F_c(\mathbf{H})^2 / \partial K] [\partial F_c(\mathbf{H})^2 / \partial \varphi(\mathbf{h}_i)] \Delta K \\ + \sum_{\mathbf{H}} w(\mathbf{H}) j(\mathbf{H}) [\partial F_c(\mathbf{H})^2 / \partial \sigma] \\ \times [\partial F_c(\mathbf{H})^2 / \partial \varphi(\mathbf{h}_i)] \Delta \sigma \\ + \sum_j \sum_{\mathbf{H}} w(\mathbf{H}) j(\mathbf{H}) [\partial F_c(\mathbf{H})^2 / \partial \varphi(\mathbf{h}_j)] \\ \times [\partial F_c(\mathbf{H})^2 / \partial \varphi(\mathbf{h}_i)] \Delta \varphi(\mathbf{h}_j) \\ = \sum_{\mathbf{H}} w(\mathbf{H}) j(\mathbf{H}) [F(\mathbf{H})^2 - F_c(\mathbf{H})^2] \\ \times [\partial F_c(\mathbf{H})^2 / \partial \varphi(\mathbf{h}_i)]. \quad (15) \end{aligned}$$

There is one normal equation of this type for each parameter, so that a system with an equal number of equations and unknowns results. The solution of this system for  $\Delta K$ ,  $\Delta\sigma$  and the  $\Delta\varphi(\mathbf{h}_i)$  [ $i=1$  to  $n$ ] yields the new estimates of the parameters. Since (13) is only an approximation, the refinement process must be repeated until successive cycles produce insignificant changes of the parameters.

The derivatives of  $F_c(\mathbf{H})^2$  with respect to the parameters are found to be:

(a) for the scaling factor  $K$

$$\partial F_c(\mathbf{H})^2 / \partial K = 2 F_c(\mathbf{H})^2 / K_c; \quad (16)$$

(b) for the width  $\sigma$  of the Gaussian atomic peaks

$$\partial F_c(\mathbf{H})^2 / \partial \sigma = -4 \pi^2 \sigma_c s_{\mathbf{H}}^2 F_c(\mathbf{H})^2; \quad (17)$$

(c) for the phases  $\varphi(\mathbf{h}_i)$  of the largest structure factors

$$\begin{aligned} \partial F_c(\mathbf{H})^2 / \partial \varphi(\mathbf{h}_i) = 2 \{ A_c(\mathbf{H}) [\partial A_c(\mathbf{H}) / \partial \varphi(\mathbf{h}_i)] \\ + B_c(\mathbf{H}) [\partial B_c(\mathbf{H}) / \partial \varphi(\mathbf{h}_i)] \} \quad (18) \end{aligned}$$

where, for acentric reflections,

$$\begin{aligned} \partial A_c(\mathbf{H}) / \partial \varphi(\mathbf{h}_i) \\ = 2 K_c v_c(\mathbf{H}) F(\mathbf{h}_i) \sum_s \{ -F(\mathbf{H} - \mathbf{h}_i R_s) \\ \times \sin [\varphi_c(\mathbf{h}_i) + \varphi_c(\mathbf{H} - \mathbf{h}_i R_s) - 2 \pi \mathbf{h}_i \mathbf{t}_s] \\ + F(\mathbf{H} + \mathbf{h}_i R_s) \\ \times \sin [\varphi_c(-\mathbf{h}_i) + \varphi_c(\mathbf{H} + \mathbf{h}_i R_s) + 2 \pi \mathbf{h}_i \mathbf{t}_s] \} \quad (19) \end{aligned}$$

and, similarly,

$$\begin{aligned} \partial B_c(\mathbf{H}) / \partial \varphi(\mathbf{h}_i) \\ = 2 K_c v_c(\mathbf{H}) F(\mathbf{h}_i) \sum_s \{ F(\mathbf{H} - \mathbf{h}_i R_s) \\ \times \cos [\varphi_c(\mathbf{h}_i) + \varphi_c(\mathbf{H} - \mathbf{h}_i R_s) - 2 \pi \mathbf{h}_i \mathbf{t}_s] \\ - F(\mathbf{H} + \mathbf{h}_i R_s) \\ \times \cos [\varphi_c(-\mathbf{h}_i) + \varphi_c(\mathbf{H} + \mathbf{h}_i R_s) + 2 \pi \mathbf{h}_i \mathbf{t}_s] \} \quad (20) \end{aligned}$$

with  $R_s$  being the rotation matrix and  $\mathbf{t}_s$  the translation vector of the symmetry operation  $s$ .

The physical meaning of minimizing (10) can be best understood by expressing  $M$  in Patterson space:

$$M = V_v \int [P_o(\mathbf{u}) - P_c(\mathbf{u}, \Phi, K, \sigma)]^2 d\mathbf{u}. \quad (21)$$

$P_o$  is the sharpened observed Patterson function (Patterson, 1935) computed with coefficients  $[w(\mathbf{H})]^{1/2}F_o(\mathbf{H})^2$  and  $P_c$  is the calculated one expressed as a function of the phases of the largest  $F$ 's, taking into consideration the atomicity condition. Obviously, the better the agreement between  $P_o$  and  $P_c$  over the unit cell, the smaller will be the integral in (21). Notice that the weights  $w(\mathbf{H})$  determine the degree of sharpening of the Patterson function. Jones, Marsh & Richards (1965) described a weighting function useful for obtaining rapid convergence of  $M$  in the initial least-squares refinements of atomic parameters consisting in giving each observation a weight  $w(\mathbf{H}) \propto 1/f(\mathbf{H})^2$ . The similar weighting function  $w(\mathbf{H}) \propto 1/f(\mathbf{H})^{3/2}$  was employed in the test calculations given in § 3.

Instead of (10), the function

$$P = \sum_{\mathbf{H}} w'(\mathbf{H}) [F(\mathbf{H}) - F_c(\mathbf{H})]^2 \quad (22)$$

could be alternatively minimized, *i.e.* the amplitudes rather than the intensities of the structure factors are used. This leads to a set of normal equations similar to (15) except that the product  $w(\mathbf{H})j(\mathbf{H})$  is replaced by  $w'(\mathbf{H})$ ,  $[F(\mathbf{H})^2 - F_c(\mathbf{H})^2]$  by  $[F(\mathbf{H}) - F_c(\mathbf{H})]$ ,  $\partial F_c(\mathbf{H})^2/\partial K$  by  $[2F_c(\mathbf{H})]^{-1}\partial F_c(\mathbf{H})^2/\partial K$ ,  $\partial F_c(\mathbf{H})^2/\partial \sigma$  by  $[2F_c(\mathbf{H})]^{-1}\partial F_c(\mathbf{H})^2/\partial \sigma$  and  $\partial F_c(\mathbf{H})^2/\partial \varphi(\mathbf{h}_i)$  by  $[2F_c(\mathbf{H})]^{-1}\partial F_c(\mathbf{H})^2/\partial \varphi(\mathbf{h}_i)$ . There are, however, good reasons (Rollet, McKinlay & Haigh, 1976) for preferring minimization of (10) instead of (22) when the errors in the initial estimates of the parameters are large.

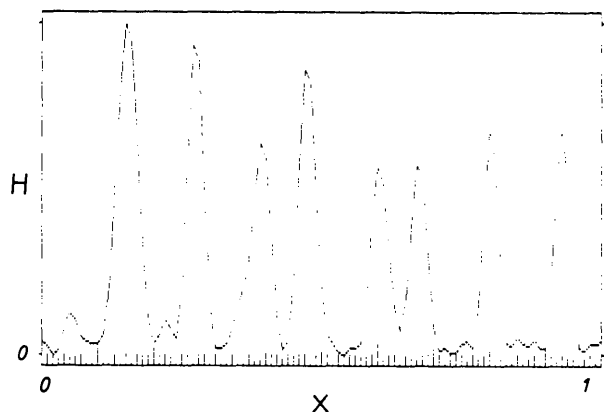


Fig. 1. Final Fourier map for trial 5 computed with the estimates of the structure factors obtained after introducing the refined phases of the large  $F$ 's in (9).  $H$  = height of the Fourier synthesis in arbitrary units;  $x$  = fractional coordinate.

Table 1. Results of the least-squares refinement of initially random phases for the one-dimensional example (MPHE = mean phase error with *e.s.d.*'s in parentheses;  $i$  = initial,  $f$  = final)

Trial no.	Number of cycles	$M_i$ (%)	$M_f$ (%)	$R_i$ (%)	$R_f$ (%)	MPHE (°)
1	4	47.1	5.8	53.3	22.6	30 (18)
2	5	54.0	5.0	44.7	21.0	29 (15)
3	2	45.1	14.0	48.1	42.2	48 (47)
4	4	53.2	5.6	40.6	29.0	28 (19)
5	5	62.1	4.0	48.6	26.4	28 (15)
6	5	66.2	3.7	42.1	25.2	23 (22)
7	5	88.8	4.7	45.4	21.2	26 (14)
8	5	66.3	4.9	37.8	21.8	19 (20)
9	5	107.2	5.8	55.3	21.8	29 (15)
10	2	44.5	17.4	46.0	36.2	55 (52)

$$M = \left\{ \sum_{\mathbf{H}} w(\mathbf{H}) [F(\mathbf{H})^2 - F_c(\mathbf{H})^2]^2 \right\} / \sum_{\mathbf{H}} w(\mathbf{H}) F(\mathbf{H})^2.$$

$$R = \left[ \sum_{\mathbf{H}} w(\mathbf{H}) |F(\mathbf{H}) - F_c(\mathbf{H})| \right] / \sum_{\mathbf{H}} w(\mathbf{H}) F(\mathbf{H}).$$

Table 2. Details of the least-squares phase refinement for trial 5; \* = after a shift of 0.54 Å to place the origin on an inversion centre of the structure

Initial and final refined values for  $K_c$ : 0.07506 and 0.07508; for  $\sigma_c$ : 0.28 and 0.20 Å.

$H$	$[w(\mathbf{H})]^{1/2}$	$F_{\text{obs}}$	$F_{\text{calc}}$	$\varphi(h)_{\text{ini}}$ (°)	$\varphi(h)_{\text{ref}}$ (°)
0	1.00	5.66	5.66	0	fixed 0
1	1.00	1.00	1.08	149	-43
2	1.01	0.41	0.49	-	-
3	1.03	0.48	0.63	-	-
4	1.05	1.28	1.16	-118	163
5	1.08	0.35	0.04	-	-
6	1.11	1.78	1.83	-51	-159
7	1.15	0.54	0.15	-	-
8	1.20	1.41	1.27	145	-24
9	1.26	2.80	2.68	130	fixed 180
10	1.34	1.29	1.24	-145	134
11	1.42	0.48	0.29	-	-
12	1.52	0.64	0.19	-	-
13	1.63	0.52	0.53	-	-
14	1.77	0.38	0.11	-	-
15	1.92	1.81	1.66	6	-30
16	2.10	0.77	0.72	-142	46
17	2.31	0.72	0.74	43	-155
18	2.56	0.38	0.36	-	-
19	2.85	0.05	0.14	-	-
20	3.19	0.07	0.16	-	-
21	3.60	0.10	0.23	-	-
22	4.07	0.03	0.13	-	-
23	4.64	0.17	0.24	-	-
24	5.32	0.37	0.38	-	-
25	6.13	0.36	0.26	-	-
26	7.11	0.03	0.09	-	-

### 3. Test calculations

A one-dimensional equal-atom structure (Sayre, 1952) consisting of Gaussian atoms of width  $\sigma = 0.28$  Å at  $x = \pm 0.113, \pm 0.234, \pm 0.361$  and  $\pm 0.438$  has been selected for testing the present method (Fig. 1). Although the structure belongs to line group  $P1$ , the reflections are treated as acentric. By making  $F_{\text{min}} = 0.71$  ( $s_{\text{max}} = 1.30$  Å<sup>-1</sup>), ten large  $F$ 's were found

[including the  $F(0)$  term calculated from the known chemical composition]. This represents ten parameters to be refined (eight phases +  $K + \sigma$ ) from 27 observations. The initial estimate of  $K_c$  was derived from

$$K_c = F(0) / \sum_h F(h')^2. \quad (23)$$

Equation (23) assumes that the  $F(h')$  are on an absolute scale.

Table 1 summarizes the results of the refinement of random phases for ten consecutive trials. To obtain

an additional figure of merit, the  $R$  value was also computed at the end of each refinement cycle. The refinement process stopped when further minimization of  $M$  produced no decrease of  $R$ . Inspection of Table 1 indicates that most trials (eight out of ten) converged in four–five cycles. Trial 5 has been selected to show the refinement process in more detail. Table 2 lists the results of the refinement, Fig. 2 illustrates the evolution of  $M$  and  $R$  as functions of the number of cycles and Fig. 1 reproduces the final Fourier map computed with the estimates of the structure factors obtained from (9).

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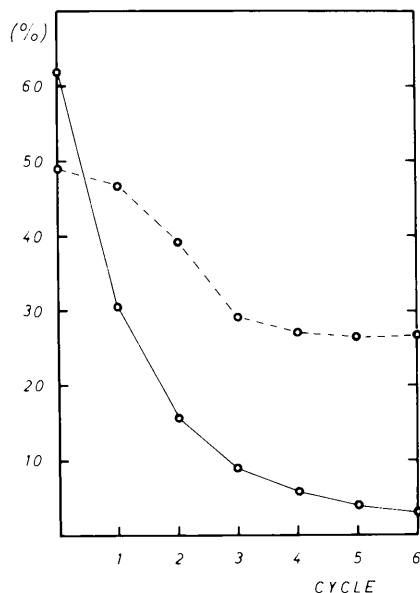


Fig. 2.  $M$  (solid line) and  $R$  (dashed line) as a function of the number of cycles of refinement for trial 5.

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## Resolution Functions of Powder Diffractometers at a Synchrotron-Radiation Source

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### Abstract

The resolution functions for various powder diffractometers using parallel-beam geometry are calculated. These diffractometers consist of monochromator, sample and eventually a post-specimen analyser. The theory is thus similar to that of two- or three-axis

diffractometers. Special attention has to be given to the different diffraction mechanisms occurring at perfect crystals, synthetic multilayers or mosaic crystals. Resolution functions for all three types of monochromators are presented. Experiments performed at HASYLAB and other laboratories show good agreement with theory.