A General, Weighted Least-Squares Method for the Evaluation of Small-Angle X-ray Data Without Desmearing

BY BO SjöBERG

Department of Medical Biochemistry, University of Göteborg, Fack, S-400 33 Göteborg, Sweden

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In order to avoid some of the disadvantages associated with the desmearing methods, a procedure has been developed where the smeared, primary, intensity data can be evaluated directly without desmearing. The procedure consists of the following: first, a model depending on a vector of unknowns, \( x = (x_1, \ldots, x_n) \), is constructed; then, an iterative search is made for the vector \( x \) and a scale factor \( s \), which corresponds to a local minimum in the error square sum based on the primary, slit-smeared, intensity data. The main advantages with the present method are that the comparison between theory and experiment is made directly with the experimental quantity; thus the experimental errors can be considered in this comparison. Furthermore, some of the disadvantages associated with the desmearing methods are avoided; the method is numerically stable and no extrapolations outside the measured angular range are necessary. Several data sets measured at different concentrations and with different, completely arbitrary, primary-beam weighting functions can be considered in the same refinement. The interparticle scattering effect may also be included in the least-squares refinement. The method is general, so that different models can be tested simply by changing only one subroutine of the computer program. It may also be used to evaluate data impaired by other types of resolution errors; for example, effects due to polychromatic radiation or resolution errors in neutron scattering. Two constructed examples of the application of the method are given: (1) the calculation of the dimensions and the molecular weight of particles with a shape which can be approximated with an ellipsoid of revolution; (2) the calculation of the dimensions and electron-density distribution for spherical particles.

1. Introduction

The average X-ray intensity, \( I(h) \), scattered at small angles from a dilute solution containing identical particles, which take all orientations with equal probability, can generally be written as [Beeman, Kaesberg, Anderegg & Webb (1957), equation (6.1)]:

\[
I(h) = sc \cdot i(h, x),
\]

where \( h = (4\pi \sin \theta)/\lambda \) and where \( \theta \) is the scattering angle and \( \lambda \) the X-ray wavelength. The average concentration of the solute, in g cm\(^{-3}\), is denoted by \( c \), and the scattering power of the sample is determined by the scale factor, \( s \). If the small-angle X-ray measurements are on an absolute scale, then

\[
s = 0.0476 M d (\Delta z)^2 a^{-2},
\]

where \( M \) is the molecular weight of the solute substance, \( d \) the thickness of the sample in cm, \( \Delta z \) the number of excess moles of electrons per gram of the solute substance, and \( a \) the distance from the sample to the plane of registration in cm [Kratky (1963), equations (23)-(30)]. The scattering function of the particle, \( i(h, x) \), is normalized to be equal to unity at \( h = 0 \); in addition to \( h \), it also depends on a vector of parameters \( x = (x_1, \ldots, x_n) \), which are determined by the size and shape of the particles. For example, for an ellipsoid, \( x_1, x_2 \) and \( x_3 \) are equal to the semiaxes.

In order to admit sufficient scattered intensity into the detector, while still maintaining a beam fine enough to permit measurements at very small angles, one normally uses slit-shaped apertures (Hosemann, 1939). Thus, the observed, or slit-smeared, intensity curve \( \tilde{I}(h) \), is the true intensity curve, \( I(h) \), averaged over the dimensions of the primary beam (Beeman et al., 1957):

\[
\tilde{I}(h) = \int \int W(y) W(z) [I([h-z]^2 + y^2)^{1/2}] dz dy.
\]

\( W(y) \) and \( W(z) \) are the normalized (Kratky, Porod & Skala, 1960; Hendricks, 1972), instrumental weighting functions, for the slit length and slit width, that would be measured with the actual detecting slit; \( y \) and \( z \) are variables of integration with the same dimension as \( h \). The weighting functions are determined by the construction of the small-angle X-ray camera. They are known either from previous measurements or calculated from the geometry of the camera (Hendricks & Schmidt, 1973). In (3) it is assumed that the experimental setup is designed so that \( W(y) \) is independent of \( z \) and that \( W_z(z) \) is independent of \( y \). A combination of equations (1) and (3) gives

\[
\tilde{I}(h) = sc \cdot \tilde{i}(h, x),
\]

where \( \tilde{i}(h, x) \) is the scattering function of the particle smeared by an equation identical with (3).

Several different approaches have been used in considering the slit effect. One approach is to desmear the experimental \( I(h) \) functions; that is, one starts with the experimental functions \( \tilde{I}(h) \), \( W(y) \) and \( W_z(z) \) and then \( I(h) \) is calculated by solving (3). Several desmearing
methods have been developed; for a review see Schmidt (1975). There are, however, disadvantages associated with these methods: tests performed with theoretical models have shown that it is difficult to keep the experimental error under control (Sjöberg, unpublished results); furthermore, in order to be able to solve \( I(h) \) from (3), the experimental \( \tilde{I}(h) \) function must be known for a fairly wide \( h \) range. However, \( \tilde{I}(h) \) can be measured only in a limited angular range and, therefore, must be extrapolated outside the measured range. This loss of information increases the errors in the desmeared function \( I(h) \). The main disadvantage is, however, that the desmearing procedures involve an extensive mathematical manipulation of the data and that contact with the experimental data is lost after desmearing.

It should be noted that the \( I(h) \) curves can also be used directly to obtain some immediate information, provided that the primary beam shape fulfills certain requirements. For instance, it is possible to calculate the radius of gyration and the scattered intensity at zero angle (Luzzati, 1958), as well as the invariant (Porod, 1951).

Another approach is to start with theoretical \( I(h) \) functions calculated from (1), for various systems of particles. Next, the theoretical \( \tilde{I}(h) \) functions for the actual experimental setup are computed by using (3); and then the interpretation is based on a comparison between the experimental and theoretical \( \tilde{I}(h) \) functions (Beeman et al., 1957).

2. The present method

In this paper, a computerized modification of the approach involving a comparison between theoretical and experimental \( \tilde{I}(h) \) functions described above is presented. The best fit between the experimental and calculated intensity functions is defined with the least-squares criterion. Thus, for particles of specific shapes, say ellipsoids, elliptic cylinders, etc., a search is made for the vector of parameters, \( x = (x_1, ..., x_n) \), which gives a local minimum in the error-square sum:

\[
U^2(x) = \frac{1}{N} \sum_{k=1}^{N} w_k A_k^2
\]

where \( A_k = \tilde{I}_{ok} - s \cdot \tilde{I}(h_k, x) \), and \( I_{ok} \) is the observed intensity value obtained for \( h = h_k, k = 1, ..., N \). The proper weight, \( w_k \), to be assigned to the \( k \)th observed point is equal to \( 1/\sigma^2(I_{ok}) \), where \( \sigma^2(I_{ok}) \) is the estimated variance of that point. If \( I_{ok} \) is obtained by taking the difference between a 'sample' point and a 'background' point, with the estimated variances \( \sigma^2_S \) and \( \sigma^2_B \), then (Bevington, 1969)

\[
\sigma^2(I_{ok}) = \sigma^2_S + \sigma^2_B
\]

In this case the calculations are complicated by the fact that the functions \( \tilde{I}(h_k, x) \) are nonlinear, and the unknown vector \( x \) cannot be obtained simply by solving the Gauss normal equations. However, the vector \( x \) for which \( U^2(x) \) has a minimum, can also be obtained by one of the variational methods of optimization analysis. The minimization method used in this work has been devised by Powell (1973); it is an iterative method based on a combination of Newton-Raphson, steepest-descent and Marquardt methods.

The procedure starts with a guessed set of parameters, \( x_1, ..., x_n \), for which \( U^2(x) \) is calculated. The choice of new sets of parameters is guided by the values of \( U^2(x) \) already calculated, so that \( U^2(x) \) is steadily decreased. Finally, after a certain number of iterations, when a preset accuracy is obtained, the computation is terminated.

Before each calculation of \( U^2(x) \) the scale factor, \( s \), is calculated by the equation

\[
s = \frac{\sum_{k=1}^{N} w_k I_{ok} \cdot \tilde{I}(h_k, x)}{\sum_{k=1}^{N} w_k \tilde{I}^2(h_k, x)}
\]

Equation (7) is derived with the requirement that the value of \( s \) obtained will minimize the error-square sum of (5).

3. Estimation of standard deviations

Suppose that we have observed a set of \( N \) data points, \( I_{o1}, ..., I_{oN} \), and that there are \( n + 1 \) parameters \( x_0, ..., x_n \) to fit to the set of observations. The 'observational' equations then are (to simplify notations the scale factor, \( s \), will be denoted by \( x_0 \) in this paragraph)

\[
I_{o1} = x_0 \cdot \tilde{I}(h_1, x_1, ..., x_n)
\]

Thus, we have a set of \( N \) nonlinear equations and \( n + 1 \) unknowns; it is necessary that at least \( n + 1 \) of the \( N \) equations are independent. In the over-determined situation, where \( N > n + 1 \), we cannot normally satisfy all the \( N \) equations exactly owing to experimental error; therefore, an averaging is necessary. If \( N \) is much larger than \( n + 1 \), and the only errors are random, it is possible to obtain information regarding the accuracy of the \( I_{ok} \) and the fully refined parameters \( x_0, ..., x_n \) derived from them.

The general equation for estimating the variance \( \sigma^2(x_j) \) of the fully refined parameter \( x_j \) is (Cruickshank, 1965):

\[
\sigma^2(x_j) = \frac{c_{jj} \sum_{k=1}^{N} w_k \Delta_k^2}{N - n - 1}
\]

where \( \Delta_k = I_{ok} - x_0 \cdot \tilde{I}(h_k, x) \), and \( N - n - 1 \) is the num-
number of degrees of freedom left after determining the $n+1$ parameters from the experimental data. The quantity $c_{ij}$ is a diagonal element of the matrix $C^{-1}$, which is inverse to the matrix $C$ with the elements $c_{ij}$ defined by

$$c_{ij} = \sum_{k=1}^{N} w_k \frac{\delta \tilde{T}(h_k)}{\delta x_i} \frac{\delta \tilde{T}(h_k)}{\delta x_j}. \tag{10}$$

The covariance of two parameters, $x_i, x_j$, can be estimated as (Cruickshank, 1965)

$$\text{cov}(i,j) = \frac{c_{ij}}{N-n-1}. \tag{11}$$

Equations (9) and (11) hold for relative weights, that is for weights, $w_k$, which are only proportional to $1/\sigma^2(I_{ok})$. If absolute weights $w_k = 1/\sigma(I_{ok})$ have been chosen, and if the model exactly represents the physical basis for the data, it can be shown that (Cruickshank, 1965; Bevington, 1969)

$$\chi^2 = \sum_{k=1}^{N} w_k A_k^2 \approx N-n-1. \tag{12}$$

4. Programming of the method

The method has been programmed in Fortran IV for an IBM 360/65 computer. The program is built up around the subroutine VAO5A written by Powell (1973). This subroutine performs the minimization of $U^2(x)$ described earlier (§ 2). The program is provided with subroutines which for specific models calculate $i$ and $I$ [cf. equations (1) and (4)], and it is written generally so that different models can be tested by changing only the subroutine which calculates the scattering function of the particle, $i$. The evaluation of equation (3) is made numerically using the subroutines provided with the computer. The program is written so that several small-angle X-ray data sets, measured at different concentrations, $c$, and different weighting functions, $W_t(y)$ and $W_w(z)$, can be considered simultaneously. Sometimes it is advantageous to measure different parts of the scattering curves with different settings of the camera and consequently also different weighting functions. With the present computer program it is possible to consider all these data sets in the same refinement.

The program also calculates the $\sigma^2(x_j)$ and $\text{cov}(i,j)$ defined by (9) and (11). The derivatives $\delta I/\delta x_j$, which are used for the evaluation of the error matrix $C^{-1}$, are approximated as being equal to the corresponding ratio of differences $\Delta I/\Delta x_j$.

The execution time is, of course, dependent on the number of experimental points, the number of parameters to be refined and on the type of equation used for calculating the scattering function; on the IBM 360/65 computer, the computing is normally completed within a few minutes.

5. Testing the method

5.1. Determination of the dimensions of ellipsoids of revolution

This example was constructed in order to test the present least-squares method during a small-angle X-ray investigation of the protein elongation factor Tu from E. coli in the presence of guanosine diphosphate (Sjöberg & Elias, to be published). The data were recorded with a Kratky camera (Kratky & Skala, 1958), and the present least-squares method was applied in order to evaluate the data. The model which gave the best fit to the experimental data, recorded for this protein, is an ellipsoid of revolution with the semiaxes $A = B = 4.08$ nm and $C = 1.18$ nm.

The scattering function, $i(h,x)$ for an ellipsoid of revolution with the semiaxes $A$, $A$ and $C=\sqrt{A}$, can be calculated with the equation given by Guinier (1939)

$$i(h,x) = \pi^2 [hA \sin^2 x + \varphi \cos^2 x]^{1/2} \sin x \varphi, \tag{13}$$

where

$$\Phi(u) = \frac{\sin u - u \cos u}{u^2}. \tag{14}$$

Equations (13)–(14), together with equations (1) and (3), were used to calculate theoretical $I$ functions for an ellipsoid of revolution with the semiaxes $A = B =$...
The theoretical values, using the subroutine

\[ 4.300 \times 10^{-2} \]

with intermediate values of the unknowns and \( U_2(x) \)

\[ 4.200 \times 10^{-3} \] \( C = 1 \times 1000 \text{ nm} \), and the scale factor \( s = 4.300 \times 10^{-2} \).

The refinement procedure, with intermediate values of the unknowns and \( U_2(x) \) for data with a relative standard deviation equal to 1\% and 131 data points, is shown in Table 1. After 15 iterations the accuracy criterion of the subroutine V405A (Powell, 1973), with \( ACC = 2 \times 10^{-8} \), was satisfied; the final result is \( x = (4.1986, 1.1005) \), \( s = 4.304 \times 10^{-2} \), corresponding to \( U^2(x) = 0.0105 \) or \( U(x) = 0.0105 \). For this solution \( \chi^2 = 144 [\text{cf. equation (12)}] \), which is not very far from the number of degrees of freedom = 128. The standard deviations of \( A \) and \( C \) are given in Table 2. In Table 2 are also given the results obtained for different relative standard deviations in the input data.

In this case, dealing with ellipsoids of revolution, at least two local minima in \( U^2(x) \) should be expected: one for an oblate and another for a prolate particle. As a matter of fact, with the starting vector \( x = (2, 5) \), the computer reached the local minimum corresponding to a prolate particle with \( A = B = 1.5 \text{ and } C = 11.1 \text{ nm} \). However, for this minimum, \( U^2(x) \) is equal to \( 0.36 \times 10^{-1} \), which is 327 times larger than that for the oblate particle. In this case there is little doubt that the correct minimum is also the lowest one.

5.2. Calculation of the dimensions and excess electron density distribution of spherical particles

This example of the application of the present least-squares method was constructed in connection with a small-angle X-ray investigation of satellite tobacco necrosis virus (STNV), (Sjöberg, 1977). For this icosahedral virus (Strandberg et al., 1975), and for other such almost spherical particles, it is important to know the spherically averaged excess electron density distribution, \( q(r) \).

The usual method to calculate \( q(r) \) consists of performing a Fourier transform of \( hF(h) \), where the absolute value of the structure factor of the particle, \( F(h) \), is proportional to the square root of the intensity values. The sign of \( F(h) \) must be guessed or determined from other available information. Attempts to calculate \( q(r) \) by a Fourier transform of \( hF(h) \) with theoretical models and theoretically calculated intensity curves, were quite disappointing. Fourier methods require data with a precision which, because of low concentration, could not be obtained in the STNV investigation. Particularly at the tail end of the curve the precision must be very high, so that several of the side maxima can be resolved. Furthermore, we have the difficulty of determining the sign of \( F(h) \) in addition to the uncertainty induced by the desmearing procedure.

Instead of calculating \( q(r) \) with the help of a Fourier transform, the following approach was used: it was
first assumed that the electron density of the spherical particles can be described by concentric, spherical shells of equal thickness, and with a constant electron density \( \tilde{\rho}_j \) within each shell. Thus, the \( \tilde{\rho}_j \) value for each shell should be considered as a mean value of the real \( \rho \) distribution within the shell. For such a shell structure the scattering function of the particle, \( \ii(h, x) \), can be written as [Guinier & Fournet (1955), equation (13)]:

\[
\ii(h, x) = \left[ \sum_{j=1}^{n} \tilde{\rho}_j (\sin hr_j - hr_j \cos hr_j) \right]^2 
\]

where \( r_j = jr/n \) is the outer radius of the \( j \)th shell, \( r \) the radius of the particle and \( n \) the total number of shells. Consequently, the vector of unknowns in this case is \( x = (r, \tilde{\rho}_1, \tilde{\rho}_2, ..., \tilde{\rho}_{n-1}) \). The excess electron density of the outermost shell, \( \tilde{\rho}_n \), is used as a reference, arbitrarily given the value one, and it is kept constant during the refinement.

In order to test the procedure, 203 \( \ii \) values were calculated for the arbitrary electron density distribution, shown in Fig. 2(a) as the dotted line, and the scale factor \( s = 0.4200 \). The \( h \) values, for which \( \ii \) was calculated \((0.1 \leq h \leq 2.4 \text{ nm}^{-1})\), and also \( W_y(y) \) and \( W_z(z) \), Fig. 1(b), were exactly the same as in the investigation of STNV (Sjöberg, 1977). Random errors, with 1% standard deviation, were generated into the theoretical \( \ii \) values (§ 5.1), and they were then used as input for the present least-squares method. The trial vector of unknowns in a refinement with the number of shells \( n = 7 \) was \( x = (10.0, 1.0, 1.0, 1.0, 1.0, 1.0) \), which corresponds to \( U^2(x) = 0.723 \times 10^{-3} \). After 87 iterations, including rescaling of the unknowns (Powell, 1973), the result together with the standard deviations obtained was \( x = (10.26 \pm 0.02, 1.62 \pm 0.2, 23.14 \pm 0.3, 19.34 \pm 0.2, 25.6 \pm 0.3, 19.4 \pm 0.2, 28.9 \pm 0.3) \), and \( s = 0.4210 \pm 0.0008 \). This solution corresponds to \( U^2(x) = 0.204 \times 10^{-3} \) or \( U(x) = 0.0143 \). Note that the values of \( \tilde{\rho}_1, ..., \tilde{\rho}_6 \) are only relative, with the value of the reference shell, \( \tilde{\rho}_7 = 1.0 \). This result, normalized to the same total number of electrons as in the original model, is shown in Fig. 2(a) as the solid line. From Table 3, it follows that the number of electrons obtained in each shell is, within the standard deviations, the same as in the original model.

Table 3. Result of the least-squares fit using the shell model described in the text

<table>
<thead>
<tr>
<th>Shell No.</th>
<th>( r_j ) (nm)</th>
<th>( Z \pm \sigma(Z) )</th>
<th>( Z_{\text{theor}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.47</td>
<td>900 \pm 160</td>
<td>870</td>
</tr>
<tr>
<td>2</td>
<td>2.93</td>
<td>9000 \pm 1200</td>
<td>9280</td>
</tr>
<tr>
<td>3</td>
<td>4.40</td>
<td>20500 \pm 2900</td>
<td>19240</td>
</tr>
<tr>
<td>4</td>
<td>5.87</td>
<td>53000 \pm 6400</td>
<td>53460</td>
</tr>
<tr>
<td>5</td>
<td>7.33</td>
<td>66000 \pm 8900</td>
<td>70040</td>
</tr>
<tr>
<td>6</td>
<td>8.80</td>
<td>147000 \pm 18000</td>
<td>131300</td>
</tr>
<tr>
<td>7</td>
<td>10.26</td>
<td>7039</td>
<td>19220</td>
</tr>
</tbody>
</table>

Also, in this case, a search for more than one local minimum in \( U^2(x) \) has been made simply by varying the starting vector \( x \). In fact, with the starting vector \( x = (10.0, 1.0, 0.5, 0.5, 0.5, 0.5, 0.5) \), the result was \( x = (8.92 \pm 0.04, 1.14 \pm 0.20, 0.76 \pm 0.20, 0.64 \pm 0.20, 1.01 \pm 0.20, 0.74 \pm 0.06, 0.85 \pm 0.13) \). This alternative solution, which corresponds to \( U(x) = 0.0203 \), is shown as absolute electron densities in Fig. 2(b).

As a result, we must consider at least the two solutions given above which, from the small-angle X-ray point of view, are almost equally probable. No systematic search of parameter space has been made in order to see whether or not there exist more than...
two local minima. On the other hand, many different combinations of starting vectors have been tested; but only the two solutions described above have appeared.

The approximation of the excess electron density \( \rho(r) \) with the shell model described above is of course an approximation of the real situation. Other alternatives are to approximate \( \rho(r) \) with continuous functions, say polynomials or spline functions.

6. Discussion

The present least-squares method seems to be helpful as a complementary method for the evaluation of small-angle X-ray data, as the two examples presented in the previous section illustrate. For these examples the resolution effects can be described by (3), which includes effects due to the primary beam shape. The method is, however, quite general and can also be used to evaluate data impaired by other types of resolution errors; for example, effects due to polychromatic radiation or resolution errors in neutron scattering can be considered by simply changing (3). Furthermore, by changing (1), the method can also easily be used to analyse data recorded from other types of systems, not only dilute solutions of identical particles.

The main advantage with the least-squares method is that some of the drawbacks associated with the desmearing methods are avoided; the calculation of \( I_0 \) can be performed with the required accuracy and the calculations are numerically stable. Furthermore, \( I_0 \) can be calculated for any value of \( h \), and extrapolations are not necessary. Another advantage with this method is that the comparison between theory and experiment is made directly with the measured quantity, \( I_0 \) (after subtraction of background). Thus, the experimental errors can be estimated and considered in the comparison (Wilson, 1952). All information which can be obtained from a small-angle X-ray measurement is, of course, contained in the measured function \( I_0 \), together with the functions \( W(z,y) \) and \( W(y,z) \). Desmearing is only a mathematical manipulation of the data which does not add any additional information to the system.

In the two examples presented above (§ 5) the slit length weighting functions were even functions of \( y \). It should be noted that the present method, like the desmearing methods of for instance Lake (1967), Glatter (1974) and Mazur & Wims (1966), can be used with completely arbitrary weighting functions.

It must be emphasized that the present method, like the traditional method of data analysis described earlier (§ 1), is based on assumptions about the type of system which is present; then a search is made for the set of parameters describing the system so that \( U^2(x) \) is minimized. Consequently, the result will be dependent on the basic assumptions made. The present method is, however, rather fast and therefore it is easy to test several models in order to see which model gives the lowest value of \( U^2(x) \). Furthermore, the model describing the system under investigation can be quite generally defined (Stuhrmann, 1970).

In the investigations of the elongation factor \( T_u \) (Sjöberg & Elias, to be published) and STNV (Sjöberg, 1977) no interparticle interference could be detected. In a general case, however, we also have to consider the interparticle interference effect. There are two distinct ways to treat data with an interparticle scattering effect which cannot be neglected: (1) the \( I_0/c \) curves for the different concentrations, \( c \), are extrapolated at constant \( h \) to zero concentration before the least-squares fit (Ninio, Luzzati & Yaniv, 1972); (2) the effect of the interparticle interference is included in the calculation of \( I \) by modifying equation (1). For instance, one of the equations given by Fournet (1951) can be used for this purpose. One approach is to combine (1) with the hard-sphere model of interaction [Fournet (1951), equation (17)]. We thus obtain

\[
I(h) = \frac{sc \cdot I(h,x)}{1 + ck_1 \cdot \Phi(k_2h)} \quad (16)
\]

where \( \Phi \) is defined by (14); \( k_1 \) and \( k_2 \) are unknown parameters which can be refined together with the other unknowns, provided that the small-angle X-ray data have been recorded at several different concentrations. Equation (16) is, of course, an approximation of the real situation. In many cases it is, however, more accurate than the linear extrapolation procedure normally adopted in order to eliminate the interparticle scattering effect. Alternatively, we can also use the more general model of interaction [Fournet (1951), equation (19)], in order to correct for the interparticle effect.

A general property of the small-angle X-ray method is that completely different models can give almost identical scattering curves. It is therefore not surprising that the \( U^2(x) \) function has several local minima; therefore, we will also obtain several solutions when we are analysing the experimental data. If the \( U^2(x) \) values of these solutions are nearly identical, we cannot distinguish between them from the small-angle X-ray data alone; in order to accomplish this we need additional information. In the present program there is no systematic search for all local minima; the result obtained is dependent on the starting value of the vector \( x \). In simple cases it is rather easy to find all the local minima simply by varying the starting value of the vector \( x \) (§ 5.1). In more complicated cases a more systematic search of parameter space must be made. Such a search could, for instance, be based on the ravine search method (Tyapkin, 1960).

The definition of \( U^2(x) \) by (5) is chosen so that \( U^2(x) \) is independent of the number of points, \( N \), and of the scale used for the intensity data, provided that all the points have the same error. The quantity \( U(x) \) will therefore reflect only the precision of the intensity data and the success of refinement (cf. the \( R \) value of X-ray crystallography). Table 2 shows some values of
Such a weighting scheme will also account for the errors which result because our models are approximations of the real situation.

References


