basis by using the formula

$$a = \sum_{n=1}^{n=\infty} \frac{\alpha_n}{(\mu r)^n}$$

where the coefficients α_n for $\theta = 90°$ are all taken as zero except $\alpha_1 = 0{\cdot}311$ and $\alpha_2 = 0{\cdot}014$. Absolute values of a for other values of θ were derived from the values for $\theta = 90°$ as calculated above and the relative values as tabulated in the *International Tables*. The final absorption factor A for spherical crystals was then expressed relative to $A = 100$ for $\theta = 90°$ as in the cylindrical case.

To use the tables, calculate the value of μr and plot a graph of the corresponding values of A in the tables against the angle θ. The value of A for any angle can be read with sufficient accuracy from this graph. The table gives values of $100A$; for instance, when $r = 0{\cdot}05$ cm., $\mu = 20{\cdot}0$ cm.$^{-1}$, $\mu r = 1{\cdot}0$, a diffracted beam for which $\theta = 22\frac{1}{2}°$ is reduced by absorption to 25·2% of what it would have been had no absorption taken place.

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The Diffraction of X-rays by a Random Assemblage of Molecules Having Partial Alignment

BY HERBERT D. DEAS†
Queen's University, Belfast, Northern Ireland

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The medium considered consists of molecules or other like particles (e.g. micelles) of which one direction, called the molecular axis, has a probability distribution $D(\alpha)$ as in a fibre, i.e. depending only on the angle α between the molecular axis and a direction fixed in space, the fibre axis. Random orientation of the molecules about their molecular axes and random distribution of their centres is assumed. The intensity distribution for X-ray diffraction by this medium is expressed in Fourier space in terms of the intensity distribution (Patterson transform) of the single molecule. Two examples are given, one of which contains as a special case the previously determined effect of finite linear gratings in random orientation.

1. Introduction

The amplitude of coherent X-ray radiation scattered in the direction of a vector $\mathbf{k}$ from a molecule with density distribution $\varrho(\mathbf{x})$ referred to the origin $\mathbf{x}=0$ is given, if the usual constants are omitted, by the Fourier transform of the density,

$$F(\boldsymbol{\eta}) = \int \varrho(\mathbf{x}) \exp\left[-2\pi i(\boldsymbol{\eta}\mathbf{x})\right] dV_x\,,$$

where $\boldsymbol{\eta} = \mathbf{k}-\mathbf{k}_0$ is a vector of reciprocal space, $\mathbf{k}_0$ a vector in the direction of the incident plane wave and $\mathbf{k}$, $\mathbf{k}_0$ are such that $|\mathbf{k}| = |\mathbf{k}_0| = \lambda^{-1}$, λ being the wave-length of the radiation.

The intensity of the scattered radiation is given by

$$G(\boldsymbol{\eta}) = F(\boldsymbol{\eta})F^*(\boldsymbol{\eta})\,,$$

which, being a function defined in reciprocal space, is called the *intensity function* of the molecule. It is the Fourier transform of the Patterson-folded density of the molecule,

$$P(\mathbf{x}) = \int \varrho^*(\mathbf{s})\varrho(\mathbf{s}+\mathbf{x})dV_s\,. \tag{1}$$

If the molecule were to take up another orientation in space, the intensity function would have a similar change of orientation in reciprocal space. Hence the resultant amplitude from an assemblage of N variously orientated similar molecules which are shifted from the origin by random vectors $\mathbf{x}_j$ is

$$\mathfrak{F}(\boldsymbol{\eta}) = \sum_{j=1}^{N} F_j(\boldsymbol{\eta}) \exp\left[-2\pi i(\boldsymbol{\eta}\mathbf{x}_j)\right],$$

where $F_j(\boldsymbol{\eta})$ denotes the amplitude function $F(\boldsymbol{\eta})$ orientated in reciprocal space to correspond to the orientation of the jth molecule. The intensity of the radiation is

$$\mathfrak{G}(\boldsymbol{\eta}) = \sum_{j=1}^{N} F_j(\boldsymbol{\eta})F_j^*(\boldsymbol{\eta}) + \sum_{j \neq k}\sum F_j(\boldsymbol{\eta})F_k^*(\boldsymbol{\eta}) \exp\left[-2\pi i(\boldsymbol{\eta}\,.\,\mathbf{x}_j-\mathbf{x}_k)\right].$$

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† Now at Services Electronic Research Laboratory, Baldock, England.

Since the vectors $\mathbf{x}_j$ are random, in general the cross terms of this summation may be neglected (James, 1948, p. 465), so that the resultant effect is given by the superposition of the suitably orientated molecular intensity functions $G_j(\boldsymbol{\eta}) = F_j(\boldsymbol{\eta}).F_j^*(\boldsymbol{\eta})$. It is true, however, that the impenetrability of the molecules produces certain restrictions on their positions and that the resulting diffraction halo may be observable. This refinement will not be considered here, since the main aim at present is to use the Patterson-folded density of a single molecule to express the intensity, at every point of reciprocal space, of the radiation scattered from a random assemblage such as this in which the molecules possess a partial alignment along a fixed direction. The diffraction effects of this assemblage (halos and part-halos) can then be found by constructing the sphere of reflexion appropriate to the wave length and the direction of the incident beam.

2. The co-ordinate systems and alignment

In order to describe the orientation of a molecule of the assemblage it is necessary to define a fixed direction in space, called the *fibre axis*, which is taken as the polar axis of a co-ordinate system (r, θ, φ). Each molecule of the system has a *molecular axis* defined by drawing a straight line through the same points in each molecule; the orientation of such an axis in space is given by the angles (α, β) referred to the fibre-axis co-ordinate system.

The molecular axis is next considered as the pole of a co-ordinate system $(r_1, \theta_1, \varphi_1)$ in which $\varphi_1 = 0$ is the plane common to the fibre axis and the molecular axis.

In each of the molecules there is defined a *molecular plane* $\varphi_1 = \gamma_1$ passing through the same point in each molecule and containing the molecular axis. The angle γ_1 defines the orientation of the molecule about its own axis.

Finally, the molecular plane is taken as the plane $\varphi_2 = 0$ of a co-ordinate system $(r_2, \theta_2, \varphi_2)$ fixed in the molecule, the molecular axis being the polar axis, and the origin being similarly placed in each molecule. Since the molecules are similar, the electron density $\varrho(r_2, \theta_2, \varphi_2)$ is the same function for each molecule.

The origins of these three systems are coincident and thus, for the same point, $r = r_1 = r_2$.

In the kind of partially aligned random assemblages under consideration, it is assumed that the molecules have random orientation about their own axis, and that these axes lie with a probability $D(\alpha)$ at an angle α to the fibre axis. $D(\alpha)$ is independent of φ, which means that the assemblage has a statistical axial symmetry about the fibre axis. The precise definition of $D(\alpha)$ is that the fractional number of molecules having the molecular axis lying at an angle between $\alpha, \alpha+d\alpha$ to the fibre axis is

$$dN(\alpha) = D(\alpha)\sin\alpha\, d\alpha\ ,$$

and the function is normalized so that

$$\int_0^\pi D(\alpha).\sin\alpha.d\alpha = 1\ .$$

For reasons which become apparent later, $D(\alpha)$ is expanded as

$$D(\alpha) = \sum_{\nu=0}^{\infty} D_\nu P_\nu(\cos\alpha)\ , \qquad (2)$$

where

$$D_\nu = \frac{2\nu+1}{2}\int_0^\pi D(\alpha)P_\nu(\cos\alpha)\sin\alpha.d\alpha\ .$$

The form of $D(\alpha)$, and therefore the values of D_ν's, are determined by the extent and the nature of the alignment present.

Partial alignment of this type occurs in fibres, in high-polymers, and in the cases of molecules having molecular dipoles if they are subjected to sufficiently strong homogeneous electric or magnetic fields.

3. The averaging process in reciprocal space

The actual position of each molecule does not occur in the expression for the mean intensity per molecule averaged over the whole assemblage. Hence it is possible and convenient to regard this average over all the molecules as equivalent to the time-average of the intensity from a single molecule, situated at the origin and rotating uniformly about its molecular axis: during this motion the molecular axis itself rotates uniformly about the fibre axis, the time spent by it at an angle between $\alpha, \alpha+d\alpha$ to the fibre axis being proportional to the probability function $dN(\alpha)$.

For any particular position of the molecule, the intensity in any given point $\boldsymbol{\eta}$ of reciprocal space is given by the value of $G(\boldsymbol{\eta})$ at this point in reciprocal space. The intensity function $G(\boldsymbol{\eta})$ orientates itself in reciprocal space as though it were firmly attached to the molecule; hence as the molecule moves through the averaging positions in physical space, the function $G(\boldsymbol{\eta})$ moves similarly in reciprocal space and the time average of the values of $G(\boldsymbol{\eta})$ at the point $\boldsymbol{\eta}$ is the average intensity for the reflexion represented by that point. The determination of these averages in reciprocal space constitutes the core of the problem.

It is convenient to use similarly orientated co-ordinate systems in physical and reciprocal space respectively, e.g. $(r_1, \theta_1, \varphi_1)$ and $(r_1^*, \theta_1^*, \varphi_1^*)$ such that the directions $\theta_1 = 0$ and $\theta_1^* = 0$ are parallel, and the planes $\varphi_1 = 0$ and $\varphi_1^* = 0$ also.

4. The general solution

The intensity function $G(\boldsymbol{\eta})$ of the molecule, referred to the reciprocal-space co-ordinate system fixed in the molecule, may be expanded as

$$G(r_2^*, \theta_2^*, \varphi_2^*) = \sum_{n=0}^{\infty}\sum_{m=-n}^{+n} G_n^m(r_2^*)P_n^m(\cos\theta_2^*)\exp[im\varphi_2^*]\ , \qquad (3)$$

where, in this development,

$$G_n^m(r_2^*) = \frac{2n+1}{4\pi}\cdot\frac{(n-m)!}{(n+m)!}\times$$

$$\iint G(r_2^*,\theta_2^*,\varphi_2^*)P_n^m(\cos\theta_2^*)\exp\left[-im\varphi_2^*\right]\sin\theta_2^* d\theta_2^* d\varphi^*$$

and $P_n^m(\cos\theta_2^*)$ is an associated Legendre polynomial (Hobson, 1931, p. 146). $G(\boldsymbol{\eta})$ has a centre of symmetry, being the Fourier transform of the Patterson fold of the molecule, so that in this particular problem $G_{2n+1}^m = 0$ for all n, m.

(i) If the molecular plane makes an angle γ_1 with the plane $\varphi_1 = 0$, $G(\boldsymbol{\eta})$ may be expressed as a function of $r_1^*, \theta_1^*, \varphi_1^*$ by making in (3) the substitutions

$$\begin{aligned} r_2^* &= r_1^*\,, \\ \theta_2^* &= \theta_1^*\,, \\ \varphi_2^* &= \varphi_1^* - \gamma_1\,. \end{aligned}$$

Since the molecule rotates uniformly about its axis, the time average of $G(\boldsymbol{\eta})$ for this motion is obtained by integrating with respect to $d\gamma_1$, and dividing by 2π. This integration leaves only the terms with $m=0$ standing, so

$$\overline{G}(\boldsymbol{\eta}) = \sum_{n=0}^{\infty} G_n^0(r_1^*)P_n(\cos\theta_1^*)\,.$$

(ii) The uniform motion of the molecule about the fibre axis with the molecular axis inclined at an angle α to it is considered next by redeveloping $\overline{G}(\boldsymbol{\eta})$ in terms of the fibre axis (reciprocal space) co-ordinate system $(r^*, \theta^*, \varphi^*)$. This is achieved by noting that if $(\theta_1^*, \varphi_1^*)$ and (θ^*, φ^*) are the angular co-ordinates in the two systems of co-ordinates of the same general direction in reciprocal space and (α, β) the direction of the molecular axis, then

$$\cos\theta_1^* = \cos\alpha\cos\theta^* + \sin\alpha\sin\theta^*.\cos(\varphi^*-\beta) \quad (4)$$

from the spherical triangle formed by the fibre axis, the molecular axis and the general direction (see Fig. 1). Hence, by the addition theorem for Legendre polynomials,

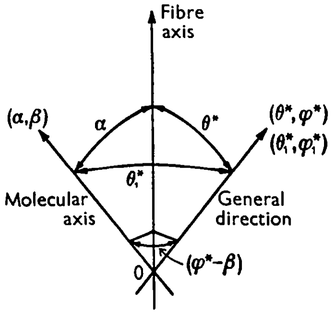

Fig. 1.

$$P_n(\cos\theta_1^*) =$$

$$\sum_{m=-n}^{n}\frac{(n-m)!}{(n+m)!}P_n^m(\cos\theta^*)\,P_n^m(\cos\alpha)\exp\left[im(\varphi^*-\beta)\right]\,, \quad (5)$$

and the redevelopment of $\overline{G}(\boldsymbol{\eta})$ is immediate. The required time average is now obtained by an integration with respect to $d\beta$ similar to the previous one. The terms for which $m \neq 0$ again disappear, giving

$$\overline{\overline{G}}(\boldsymbol{\eta}) = \sum_{n=0}^{\infty} G_n^0(r^*)P_n(\cos\alpha)\,P_n(\cos\theta^*)\,,$$

which is symmetrical about the fibre axis and depends on α.

(iii) The final averaging, to allow for the various values of α, is obtained by integrating $\overline{\overline{G}}(\boldsymbol{\eta})$ with respect to $d\alpha$, using $D(\alpha)\sin\alpha$ as a weight function in its expanded form (2). Thus

$$I(r^*, \theta^*) = \sum_{\nu=0}^{\infty}\int \overline{\overline{G}}(r^*, \theta^*; \alpha)D_\nu.P_\nu(\cos\alpha)\sin\alpha\, d\alpha\,.$$

Now, since

$$\int_0^\pi P_n(\cos\alpha)\,P_\nu(\cos\alpha)\sin\alpha d\alpha = \frac{2}{2n+1}\,\delta_{n,\nu},$$

the final result for the average intensity per molecule is

$$I(r^*, \theta^*) = \sum_{n=0}^{\infty}\frac{2}{4n+1}\cdot D_{2n}G_{2n}^0(r^*)P_{2n}(\cos\theta^*)\,, \quad (6)$$

since $G_{2n+1}^0 = 0$ for all n. This expression must be multiplied by the number of scattering molecules, but this does not alter its form.

5. Discussion of the result

It is worth noting that of all the coefficients G_n^m of the expansion (3) of the molecular intensity function, only those with $m = 0$ and n even are required in the final result. If the Patterson-folded density (1) of the molecule is expanded in spherical harmonics with coefficients $H_{2n}^m(r)$, then, since $G(\boldsymbol{\eta})$ is the Fourier transform of $P(\mathbf{x})$,

$$r^{*\frac{1}{2}}G_{2n}^m(r^*) = 2\pi(-)^n\int_0^\infty r^{\frac{3}{2}}H_{2n}^m(r)J_{2n+\frac{1}{2}}(2rr^*)dr\,, \quad (7)$$

where J_n denotes the Bessel function. This result is obtained by the evaluation of the Fourier transform with the aid of the expansions (5) and (8).† This means that the diffraction pattern from the assemblage of molecules is affected only by those terms in the expansion of the folded density which have cylindrical symmetry about the molecular axis, and, therefore, in this problem the molecular Patterson-folded density can be replaced by the 'smeared out' density obtained by rotating the folded density uniformly about the molecular axis. Conversely, the most general

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† The derivation of (7) and other relevant theorems is discussed in detail by Stratton (1941, chap. 7). Hobson (1893) gives (7) in a more general form.

result may be obtained by considering a flat molecule whose plane contains the molecular axis.

Given an experimental determination of the resultant intensity function $I(\boldsymbol{\eta})$, it can be expanded in spherical harmonics with coefficients

$$I^0_{2n}(r^*) = \frac{2}{4n+1} D_{2n} . G^0_{2n}(r^*) \, .$$

Thus, if the probability function $D(\alpha)$, equation (2), is known or assumed, the averaged Patterson-folded density $\overline{G}(\boldsymbol{\eta})$ can be determined; or alternatively $D(\alpha)$ can be found if the molecular intensity function $G(\boldsymbol{\eta})$ is known (strictly only $\overline{G}(\boldsymbol{\eta})$ is required).

6. Linear gratings

In this section and the next the general method is applied to the cases of certain simple molecules, considered to consist of 'point' atoms of known scattering power.

By a linear grating is meant a molecule of N similar atoms, lying equally spaced along a straight line so that the atoms are located at the points $\mathbf{x}_0+k\mathbf{a}$, where $k = 0, 1, 2, \ldots, N-1$. For such a structure

$$F(\boldsymbol{\eta}) = m \exp\left[-2\pi i(\boldsymbol{\eta}.\mathbf{x}_0)\right] \sum_{k=0}^{N-1} \exp\left[-2\pi i k(\boldsymbol{\eta}.\mathbf{a})\right] ,$$

where m is the atomic structure factor for the atoms of the grating. Hence

$$G(\boldsymbol{\eta}) = mm^*N + 2mm^* \sum_{k=1}^{N-1} (N-k) \cos\left(kz^* \cos\theta^*_1\right) ,$$

where $z^* = 2\pi a r^*$, and θ^*_1 is the angle between the molecular axis and the vector $\boldsymbol{\eta} = (r^*_1, \theta^*_1, \varphi^*_1)$ of reciprocal space. $G(\boldsymbol{\eta})$ is, of course, the Fourier transform of the Patterson-fold of the grating. The parameters a, m, N give the dependence of $G(\boldsymbol{\eta})$ upon the kind and size of the grating, and its dependence upon the direction is given by the direction of $\mathbf{a}$, i.e. by $\cos\theta^*_1$. The first term in $G(\boldsymbol{\eta})$ is a constant background term which will be dropped out of the working to be reintroduced at the end.

The averaging process follows a pattern similar to the general case, but contracted because the cylindrical symmetry of the grating gives $\overline{G}(\boldsymbol{\eta}) = G(\boldsymbol{\eta})$ immediately. Using the expansion (Watson, 1948, p. 368)

$$\cos(z\cos\theta) = (\pi/2z)^{\frac{1}{2}} \sum_{n=0}^{\infty} (-)^n (4n+1) J_{2n+\frac{1}{2}}(z) P_{2n}(\cos\theta) ,$$

$\overline{G}(\boldsymbol{\eta})$ can be written as

$$\overline{G}(\boldsymbol{\eta}) = 2mm^* \sum_{n=0}^{\infty} \sum_{k=1}^{N-1} \{(-)^n (4n+1) \times (N-k)(\pi/2kz^*)^{\frac{1}{2}} J_{2n+\frac{1}{2}}(kz^*) . P_{2n}(\cos\theta^*_1)\} ,$$

which can be regarded as an expansion of $\overline{G}(\boldsymbol{\eta})$ in spherical harmonics with

$$G^0_{2n+1}(r^*) = 0 ,$$

$$G^0_{2n}(r^*) = 2mm^*(-)^n(4n+1) \times \sum_{k=1}^{N-1} (N-k)(\pi/2kz^*)^{\frac{1}{2}} J_{2n+\frac{1}{2}}(kz^*) .$$

Hence the final solution, on adding in the background term, is

$$I(r^*, \theta^*) = mm^*\left[N + 2\sum_{n=0}^{\infty}\sum_{k=1}^{N-1} \{(-)^n D_{2n} \times (N-k)(kar^*)^{-\frac{1}{2}} J_{2n+\frac{1}{2}}(2\pi kar^*) . P_{2n}(\cos\theta^*)\}\right] .$$

For the case of random orientations $D(\alpha) = \frac{1}{2}$ for all α, and

$$I(r^*, \theta^*) = mm^*\left[N + 2\sum_{k=1}^{N-1} (N-k) \frac{\sin 2\pi akr^*}{2\pi kar^*}\right] ,$$

using the trigonometrical form of $J_{\frac{1}{2}}$. This is the same expression as that found by Jones (1949, equation (1·4)) for this case.

7. Planar molecule

Another example is a planar molecule whose molecular axis is perpendicular to the plane of the molecule. Since the molecule is considered to consist of point atoms its Patterson-folded density is not only a flat molecule but consists of point atoms too. Each of these atoms will contribute to the intensity in a similar manner, so only one need be considered. Suppose, therefore, an atom of magnitude μ, of the Patterson-fold of the molecule, is situated at a distance d from the molecular axis. This is an adequate description of the position of the atom, but for convenience in the deduction, the complete description of the position is taken as $\mathbf{d} = (d, \frac{1}{2}\pi, \varphi_1)$ referred to the $(r_1, \theta_1, \varphi_1)$ system of co-ordinates.

The intensity due to this atom is

$$\begin{aligned} G(\boldsymbol{\eta}) &= \mu \exp\left[-2\pi i(\boldsymbol{\eta}\mathbf{d})\right] \\ &= \mu \exp\left[-iz^* \cos\varepsilon\right] , \end{aligned}$$

where $z^* = 2\pi d r^*$ and ε is the angle between $\mathbf{d}$ and $\boldsymbol{\eta}$. On expansion (Watson, 1948, p. 368) this gives

$$G(\boldsymbol{\eta}) = \mu(\pi/2z^*)^{\frac{1}{2}} \sum_{n=0}^{\infty} (2n+1)(-i)^n J_{n+\frac{1}{2}}(z^*) P_n(\cos\varepsilon) . \tag{8}$$

The molecular axis, the vector of the atomic position $\mathbf{d}$, and the reciprocal vector $\boldsymbol{\eta} = (r^*_1, \theta^*_1, \varphi^*_1)$ form a spherical triangle (Fig. 2) so that

$$\cos\varepsilon = \cos\theta^*_1 . \cos\tfrac{1}{2}\pi + \sin\theta^*_1 \sin\tfrac{1}{2}\pi . \cos(\varphi^*_1 - \varphi_1) ,$$

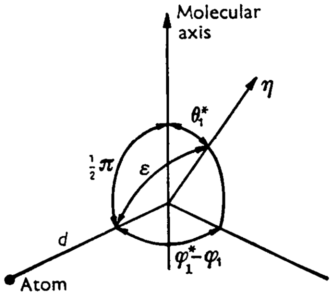

Fig. 2.

which, using (5), gives

$$G(\boldsymbol{\eta}) = \mu.(\pi/2z^*)^{\frac{1}{2}} \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \Big\{(2n+1)(-i)^n J_{n+\frac{1}{2}}(z^*) \times \frac{(n-m)!}{(n+m)!} P_n^m(\cos \tfrac{1}{2}\pi) P_n^m(\cos \theta_1^*) \exp[im(\varphi_1^*-\varphi_1)]\Big\} .$$

This is an expansion of $G(\boldsymbol{\eta})$ in spherical harmonics. Now

$$P_{2n+1}(0) = 0 ,$$

$$P_{2n}(0) = (-)^n.(2n)!/2^{2n}(n!)^2 .$$

Hence

$$G^0_{2n+1}(r^*) = 0,$$

$$G^0_{2n}(r^*) = \mu \cdot \frac{(4n+1)(2n)!}{2^{2n}.(n!)^2} \cdot (\pi/2z^*)^{\frac{1}{2}}.J_{2n+\frac{1}{2}}(z^*) .$$

Therefore, the contribution this atom makes to the average intensity per molecule from the whole assemblage is

$$I_i(r^*,\theta^*) = \sum_{n=0}^{\infty} \frac{(2n)!}{2^{2n}(n!)^2} D_{2n}\mu_i(d_i r^*)^{-\frac{1}{2}} J_{2n+\frac{1}{2}}(2\pi d_i r^*) P_{2n}(\cos\theta^*) .$$

Here subscripts i have been added to all quantities referring to the particular atom considered. The average intensity per molecule is therefore

$$I(r^*,\theta^*) = \sum_i I_i(r^*,\theta^*) ,$$

where the summation is taken over all atoms in the Patterson fold of the real molecule.

Two things about this summation should be noted. First, since d_i always occurs together with r^* as the product r^*d, a change in the value of d leaves the form of $I(r^*, \theta^*)$ unchanged and the effect can be regarded as a change in the scale of r^*. A similar remark is true of the previous example. Secondly, the contribution of the large atom at the origin of the Patterson fold is large, positive and constant, and will therefore prevent $I(r^*, \theta^*)$ from becoming negative, as it would do otherwise.

The method of this paper is to express $G(\boldsymbol{\eta})$ etc. as spherical harmonic expansions. This is the mathematical form most suited for averaging a function over various orientations about a fixed point. In this paper the function so averaged is $G(\boldsymbol{\eta})$. This choice is dictated by the physics of the problem. The averaging process can be applied equally well to $F(\boldsymbol{\eta})$, the Fourier transform of the molecular density, to give a mean structure factor (Zachariasen, 1945, p. 223) though in certain problems difficulties may arise from phase factors.

The author is indebted to Prof. P. P. Ewald, who suggested this problem, for advice and encouragement and to The Queen's University of Belfast for the award of a Senior Studentship.

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Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 500 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible; and proofs will not generally be submitted to authors. Publication will be quicker if the contributions are without illustrations.*

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A graphical method for applying Harker–Kasper inequalities to structure determination.

By Kiichi Sakurai, *Department of Physics, Faculty of Science, Osaka University, Nakanoshima, Osaka, Japan*

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For a centro-symmetrical structure, the inequalities of Harker & Kasper (1948) permit us to determine the signs of structure factors or to deduce relations among them. One important inequality generally applicable to a centro-