FUJIMOTO, F. (1959). *J. Phys. Soc. Japan*, **14**, 1958.
FUJIWARA, K. (1959). *J. Phys. Soc. Japan*, **14**, 1513.
GJØNNES, J. & MOODIE, A. F. (1965). *Acta Cryst.* **19**, 65.
GOODMAN, P. & LEHMPFUHL, G. (1964). *Z. Naturforsch.* **19a**, 818.
GOODMAN, P. & LEHMPFUHL, G. (1965). *Z. Naturforsch.* **20a**, 110.
GOODMAN, P. & LEHMPFUHL, G. (1967). *Acta Cryst.* **22**, 14.
IBERS, J. A. & HOERNI, J. A. (1954). *Acta Cryst.* **7**, 405.
International Tables for X-ray Crystallography (1952). Vol. I. Birmingham: Kynoch Press.
KAMBE, K. (1957*a*). *J. Phys. Soc. Japan*, **12**, 13.
KAMBE, K. (1957*b*). *J. Phys. Soc. Japan*, **12**, 25.
KOHRA, K. (1954). *J. Phys. Soc. Japan*, **9**, 690.
LAUE, M. VON (1948). *Materiewellen und Ihre Interferenzen*, p. 257. Leipzig: Akad. Verl.
MIYAKE, S. & UYEDA, R. (1950). *Acta Cryst.* **3**, 314.
MIYAKE, S. & UYEDA, R. (1955). *Acta Cryst.* **8**, 335.
MOODIE, A. F. (1968). To be published.
SHINOHARA, K. (1932). *Sci. Pap. Inst. phys. chem. Res. Tokyo*, **18**, 223.
TANAKA, M. & HONJO, G. (1964). *J. Phys. Soc. Japan*, **19**, 954.
THIESSEN, P. A. & MOLIÈRE, K. (1939). *Ann. Physik*, **34**, 449.

Acta Cryst. (1968). A**24**, 347

The Derivation of a Set of Scattering Factors from X-ray or Neutron-Diffraction Structure-Factor Measurements

BY C. WILKINSON AND P. J. BROWN
Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England

(*Received* 14 *June* 1967)

Scattering factors for the atoms in a structure may be evaluated as functions of the scattering vector **s** when a complete set of two- or three-dimensional structure factor measurements is available.

Introduction

Recently (*e.g.* Dawson, 1967*a*,*b*) there has been interest in the variation of the atomic scattering factor with the orientation of the scattering vector. A method for the determination of a set of spherically averaged form factors $f_j(|\mathbf{s}|)$ from a zone of structure factors has been described by Brown & Wilkinson (1965). The purpose of the present note is to show that a similar calculation may be used to determine from a zone or sphere of observed structure factors of known phase the scattering factors $f_j(\mathbf{s})$ as functions of the scattering vector $\mathbf{s}(=\mathbf{d}^*)$.

Method of calculation

The electron-density distribution which is obtained by Fourier inversion of a three-dimensional set of structure factors is given by

$$\varrho(r_j)=(1/V)\sum_{\mathbf{k}} F(\mathbf{k})\exp(2\pi i\mathbf{r}_j\,.\,\mathbf{k})\exp(2\pi i\mathbf{Q}_j\,.\,\mathbf{k})$$

where $\mathbf{r}_j$ is the radius vector from the centre of the jth atom which is vector distance $\mathbf{Q}_j$ from the origin of the structure factors $F(\mathbf{k})$, V is the unit-cell volume and $\mathbf{k}$ is the scattering vector.

The scattering factor for this atom is defined to be

$$f_j(\mathbf{s})=\int\varrho(\mathbf{r}_j)\exp(2\pi i\mathbf{r}_j\,.\,\mathbf{s})d\tau_j\,,$$

the integration being over the whole 'volume' of the atom. Thus

$$f_j(\mathbf{s})=\int(1/V)\sum_{\mathbf{k}}\{F'(\mathbf{k})\exp(2\pi i\mathbf{r}_j\,.\,\mathbf{k})\exp(2\pi i\mathbf{r}_j\,.\,\mathbf{s})\}d\tau_j$$
$$=(1/V)\sum_{\mathbf{k}}F'(\mathbf{k})\int\exp[2\pi i\mathbf{r}_j\,.\,(\mathbf{s}+\mathbf{k})]d\tau_j\,,$$

where $F'(\mathbf{k})$ has been written for $F(\mathbf{k})\exp(2\pi i\mathbf{Q}_j\,.\,\mathbf{k})$.

Let α be the angle between $(\mathbf{s}+\mathbf{k})$ and $\mathbf{r}$. Then

$$f_j(\mathbf{s})=(1/V)\sum_{\mathbf{k}}\left\{F'(\mathbf{k})\int_{r_j=0}^{R_0}\int_{\alpha=0}^{\pi}\exp(2\pi i r_j|\mathbf{s}+\mathbf{k}|\cos\alpha)2\pi r^2\sin\alpha d\alpha dr\right\}$$
$$=\frac{1}{2\pi^2V}\sum_{\mathbf{k}}\left\{\frac{F'(\mathbf{k})\{\sin(2\pi R_0|\mathbf{s}+\mathbf{k}|)-2\pi R_0|\mathbf{s}+\mathbf{k}|\cos(2\pi R_0|\mathbf{s}+\mathbf{k}|)\}}{|\mathbf{s}+\mathbf{k}|^3}\right\},$$

where R_0 is the atomic 'radius'.

A similar expression can be derived for the extraction of a scattering factor from a zone of reflexions. If **s** is any scattering vector in the zone then

$$f_j(\mathbf{s})=R_0/A\sum_{\mathbf{k}}\left\{\frac{F'(\mathbf{k})J_1(2\pi|\mathbf{s}+\mathbf{k}|R_0)}{|\mathbf{s}+\mathbf{k}|}\right\}.$$

J_1 is the first order Bessel function and A the area of the unit cell in projection.

Numerical calculation of form factors

The calculations have been programmed for the TITAN computer and have been tested with 'prepared' data generated for an imaginary structure having Mn^{3+} ions with one 3*d* electron placed on a primitive cubic lattice of cell side 3 Å. The single 3*d* electron was given

e_g orbital symmetry and defined to scatter in the way calculated by Watson & Freeman (1961).

Two-dimensional data

The formula for the two-dimensional summation was checked by using structure factors for the [001] zone of reflexions and evaluating $f(\mathbf{s})$ at values of $\mathbf{s}$ for which the structure factors had been generated. The atomic radius was defined to be 1·5 Å and the data were terminated at $|\mathbf{s}| = 1{\cdot}49$ Å^{-1}. Fig. 1 shows a plot of the resultant form factor and the data from which it was generated. The form factor was obtained by normalization of the computed scattering factors by $f(0)$, which in this case was 0·986. The smooth curve is the spherically symmetric Mn^{3+} form factor. The goodness of fit may be expressed in the form of a reliability index defined to be

$$R = \frac{\sum_{\mathbf{k}} |f_{\text{input}} - f_{\text{output}}|}{\sum_{\mathbf{k}} |f_{\text{input}}|} .$$

For the Mn^{3+} data the value of R was 0·014.

Three-dimensional data

A similar test was carried out on the three-dimensional data out to a limit of $|\mathbf{s}| = 1{\cdot}49$ Å^{-1} again defining the atomic radius to be 1·5 Å. The scattering factors were extracted at values of $\mathbf{s}$ for which the structure factors had been calculated. A value of $R = 0{\cdot}047$ was obtained.

Discussion

The principal limitations of the method are likely to arise from overlap of the electron density in projection and the difficulty of defining a 'radius' for an atom. These effects and also those due to series termination

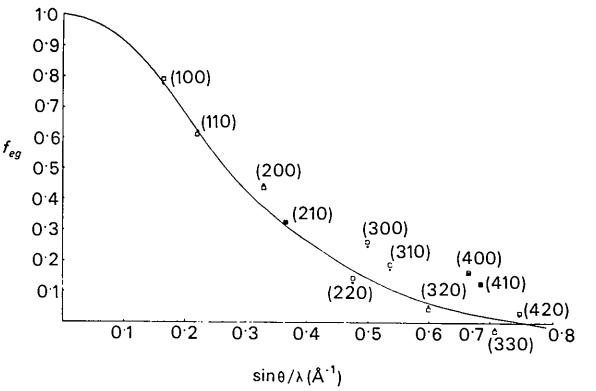

Fig. 1. Input (black dots) and output (squares) $Mn^{3+}e_g$ form-factor data for two-dimensional summation.

are discussed in the earlier paper (Brown & Wilkinson, 1965).

One of us (C.W.) wishes to thank the Science Research Council for the award of a Research Fellowship. We are indebted to Professor M.V.Wilkes, F.R.S., of the Mathematical Laboratory, for making available to us computational facilities on the TITAN and also to Mrs L. J. Billett, who wrote the programs. The project of which this research forms part is supported by generous grants from the Science Research Council and the United Kingdom Atomic Energy Authority Extra-Mural Research Board to which we express our thanks.

References

BROWN, P. J. & WILKINSON, C. (1965). *Acta Cryst.* **18**, 398.
DAWSON, B. (1967*a*). *Proc. Roy. Soc.* A**298**, 255.
DAWSON, B. (1967*b*). *Proc. Roy. Soc.* A**298**, 264.
WATSON, R. E. & FREEMAN, A. J. (1961). *Acta Cryst.* **14**, 27.

Acta Cryst. (1968). A**24**, 348

A Method of Absorption Correction by X-Ray Intensity Measurements

BY G. KOPFMANN AND R. HUBER

Abteilung für Röntgenstrukturforschung am Max-Planck-Institut für Eiweiss- und Lederforschung, München, und Physikalisch-Chemisches Institut der Technischen Hochschule München, Abteilung für Strukturforschung, München, Germany

(*Received* 6 *October* 1966 *and in revised form* 3 *July* 1967)

The theoretical and experimental principles of a method are described, which permits an approximate evaluation of the absorption correction by intensity measurements with the aid of a four-circle diffractometer.

The normal calculation of the absorption correction requires an exact knowledge of the crystal shape. With protein crystals, which are normally covered by liquid, the determination of the shape is extremely difficult, if not impossible. For this reason, an experimental method for absorption correction was developed by