steepest-descents method to R is equivalent to a method based on a Fourier difference synthesis.

$$D=\sum_{hkl}(F_o-F_c)\cos 2\pi(hx+ky+lz). \qquad (2)$$

In this series, x, y, z are the fractional co-ordinates, taken over one unit cell.

The method consists of drawing a map of the function D and marking the atomic positions x_i, y_i, z_i ($i=1, 2, \ldots, N$). The atomic shifts Δx_i, Δy_i, Δz_i, which would improve the structure according to the method of steepest descents, can be obtained by moving the atomic positions in the directions of the steepest ascent of D and by making the movements proportional to the gradient of D at the points x_i, y_i, z_i. Good use of this method in practical application has been made by Cochran (private communication).

As Booth (1949) has already pointed out, considerable simplifications in the steepest-descents calculations can be achieved if one takes

$$R=\sum_{hkl}|F_o-F_c|. \qquad (3)$$

This function can be obtained from (1a) by taking for the weight

$$W=\frac{1}{|F_o-F_c|}.$$

This form of weighting is not quite correct, as it gives too little weight to large discrepancies between the observed and calculated values. However, the function (3) is often used as a basis for the calculation of the figure of merit.

As the use of the difference synthesis is very convenient, it is of interest to investigate whether an analogous simpler function exists, which would be based on (3). For this purpose we can write R in the following form:

$$R=\Sigma(\alpha\,|F_o|-\beta F_c)=\Sigma\alpha\,|F_o|-\Sigma\beta F_c, \qquad (4)$$

where the coefficients $\alpha(hkl)$ and $\beta(hkl)$ have the values

$\alpha=+1$ for $|F_c|<|F_o|$, $\alpha=-1$ for $|F_c|>|F_o|$,

$\beta=+1$ for $|F_o|>F_c>0$ and $F_c<-|F_o|$,

$\beta=-1$ for $0>F_c>-|F_o|$ and $F_c>|F_o|$,

i.e. $\beta=+1$ for $(F_o-F_c)>0$,

$\beta=-1$ for $(F_o-F_c)<0$.

Limiting ourselves to a centrosymmetrical structure, we can substitute for F_c in (4):

$$F_c=2\sum_{i}^{N}f_i\cos 2\pi(hx_i+ky_i+lz_i), \qquad (5)$$

where N is the number of atoms per half unit cell. We obtain

$$R=\sum_{hkl}\alpha\,|F_o|-2\sum_{hkl}\beta\sum_{i}f_i\cos 2\pi(hx_i+ky_i+lz_i).$$

On reversing the order of summation, we can write

$$R=R_0-\sum_i R_i, \qquad (6)$$

where
$$\left.\begin{aligned} R_0&=\sum_{hkl}\alpha\,|F_o|,\\ R_i&=2\sum_{hkl}\beta f_i\cos 2\pi(hx_i+ky_i+lz_i).\end{aligned}\right\} \qquad (7)$$

We have achieved separation of R into R_0, which depends on F_o only, and into N functions R_i, each of which depends on the co-ordinates of the ith atom only. In addition, R_i have the form of a Fourier synthesis analogous to the difference synthesis (2), i.e. if we replace in (7) the discrete co-ordinates x_i, y_i, z_i, by continuous x, y, z, a single function is obtained, defined over the whole unit cell, which has the values R_i at the atomic positions. The synthesis (7) differs from (2) in that its coefficients have absolute values independent of F_o and F_c; only their signs depend on the inequalities for β and are incidentally the same as in (2). It should be noted, however, that although R is a continuous function of the atomic co-ordinates x_i, y_i, z_i, the functions R_0 and R_i are discontinuous, the discontinuities occurring every time the coefficient β changes sign. One can visualize this by imagining R as a function of the co-ordinates x_i, y_i, z_i, in $3N$-dimensional space, which is subdivided into a number of small cells, the boundaries of which are given by the changes of sign of β. Within each of the cells, R_0 and R_i are continuous functions of the co-ordinates. The number of such cells depends on the number of F terms included in the summations.

As formula (7) is based on incorrect weighting, it is to be expected that the above method would converge more slowly than a method based on (2), and therefore more steps would be required to attain a given degree of accuracy. However, the use of the series (7) may in some cases have the advantage that its coefficients are fixed quantities, and only their signs change during calculation. The series (7) might lend itself therefore better to calculations on automatic machines, analogue or digital, as it is easier in a calculation to change the sign of a term than its value. The inequalities for α and β lend themselves also admirably for automatic evaluation on both digital and analogue machines. One can therefore conclude that the calculations based on formula (3) might be more suitable for a fully or partly automatic cycle, especially where the simplicity of setting or programming is of more importance than the speed of convergence per cycle.

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Booth, A. D. (1949). *Proc. Roy. Soc.* A, **197**, 336.

Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. Copy should be sent direct to the British Co-editor (R. C. Evans, Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England).

X-ray Identification and Crystal Structures of Clay Minerals

The Mineralogical Society of Great Britain announces the publication of a new and original monograph of 345 pages. The preparation of this book results from the efforts and discussions of the Clay Minerals Group which was formed in 1947 for the express purpose of furthering the study of clay minerals.

The book provides an authoritative account of the X-ray identification and crystal structures of clays and

allied substances. The fourteen chapters are contributed by a number of different authors who are experts in their respective fields, the co-ordinating editor being Dr G. W. Brindley. The kaolin, montmorillonite, mica and chlorite minerals, vermiculite, sepiolite, attapulgite and oxides of iron and aluminium are all included in the survey. A great deal of information is presented in the form of tables, valuable, for reference purposes, not only to those concerned with the study and applications of clays, but also to X-ray crystallographers generally.

Copies (price 35*s.*; post free 36*s.*) are obtainable only from the General Secretary, Mineralogical Society, British Museum (Natural History), Cromwell Road, London S.W. 7, England or in the U.S.A. (price $6), from Dr R. E. Grim, Illinois Geological Survey, Urbana, Illinois, U.S.A.

International Union of Crystallography

Notification of adhesion from 1 January 1951 has been given by Sweden through the Swedish National Committee for Crystallography and by Italy through the National Research Council. The Adhering Bodies are now:

Australia	Group I
Belgium	Group III
Canada	Group IV
Czechoslovakia	Group I
Denmark	Group I
France	Group VII
India	Group I
Italy	Group III
Japan	Group I
Netherlands	Group IV
Norway	Group I
South Africa	Group I
Spain	Group IV
Sweden	Group I
Switzerland	Group I
United Kingdom	Group VIII
United States of America	Group VIII

Books Received

The undermentioned works have been received by the Editors. Mention here does not preclude review at a later date.

X-ray Identification and Crystal Structures of Clay Minerals. Edited by G. W. Brindley. Obtainable only from the General Secretary, Mineralogical Society, British Museum (Natural History), London S.W. 7, England; or Dr R. E. Grim, Illinois Geological Survey, Urbana, Illinois, U.S.A. Pp. 345 with many figures and tables. London: Mineralogical Society (Clay Minerals Group). 1951. Price 35*s.*; $6.

Geometrische Kristallographie und Kristalloptik. By F. Raaz and H. Tertsch. Pp. x+215, with 260 figs. Vienna: Springer. 2nd ed. 1951. Price 32*s.* 6*d.*

Acta Cryst. (1951). **4**, 287

International Union of Crystallography

The audited accounts of the Union for the calendar year 1950 are printed below.

Acta Crystallographica Account for the year ended 31 December 1950

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