

structure the E values, E_L , are defined by:

$$E_L = F_L (\varepsilon \sum_i f_i^2)^{-1/2} \exp(B_L \sin^2 \theta / \lambda^2) \quad (3)$$

where F_L is the light atom contribution to the structure factor and, for space group $P2_1/c$, $\varepsilon=2$ for $h0l$ and $0k0$ reflexions and $\varepsilon=1$ for all other reflexions (Hauptman & Karle, 1953).

The 'strong' reflexions have positive structure factors and we have $F_L = F_{\text{obs}} - F_H$; the magnitude and the sign of the E_L value is obtained by equation (3). This resulted in 365 signed E_L values, with $|E_L| > 1.3$. For the 'weak' reflexions we have $|F_L| = |F_{\text{obs}}|$ and only the magnitude of the E_L value is obtained. This resulted in 270 reflexions with $|E_L| > 1.3$.

The third step is the application of equation (1) to obtain the signs of the 'weak' reflexions. When several interactions of the type $(\mathbf{h} + \mathbf{h}') = (\mathbf{h}) + (\mathbf{h}')$ occur for $|E_L| > 1.3$, where both $S_{\mathbf{h}}$ and $S_{\mathbf{h}'}$ are known, several predictions of the sign $S_{\mathbf{h}+\mathbf{h}'}$ are obtained by application of (1). These predictions should be reasonably consistent before $S_{\mathbf{h}+\mathbf{h}'}$ is considered to be determined and singly occurring interactions should never be trusted. We have followed a procedure similar to the sign correlation procedure (Beurskens, 1963). The origin was partly fixed by the choice of the gold atom positions and further determined by assigning arbitrary signs to two 'weak' reflexions: 221 ($|E_L|=4.0$) and 348 ($|E_L|=2.9$). We define the following sets of reflexions, all with $|E_L| > 2.0$:

- \mathbf{h}_1 are 'strong' reflexions, hkl ($h=2n, k+l=2n$).
- \mathbf{h}_2 are the two origin determining choices.
- \mathbf{h}_3 are the reflexions $\mathbf{h}_1 + \mathbf{h}_2$ and $\mathbf{h}_2 + \mathbf{h}_1$.
- \mathbf{h}_4 are the reflexions $\mathbf{h}_1 + \mathbf{h}_3$, $\mathbf{h}_2 + \mathbf{h}_3$ and $\mathbf{h}_3 + \mathbf{h}_1$.

The application of equation (1) on only reflexions \mathbf{h}_1 cannot give new signs; together with the reflexions \mathbf{h}_2 probable signs for 36 reflexions \mathbf{h}_3 were calculated. Upon en-

tering \mathbf{h}_3 in equation (1), many reflexions take part in the calculations and consequently the sign of one reflexion \mathbf{h}_4 will often be found from several independent sign relations (1). Signs were calculated for 48 reflexions \mathbf{h}_4 ; of these the signs of 24 reflexions were determined by at least five consistent relations (1) and accepted to be correct. Although some of the signs for reflexions \mathbf{h}_3 may be incorrectly determined, it is highly improbable that all reflexions \mathbf{h}_3 used for the sign determination of one reflexion \mathbf{h}_4 are incorrect. The intermediate results for \mathbf{h}_3 and the rest of \mathbf{h}_4 were rejected.

Continued application of equation (1) on 365 'strong' reflexions, 2 reflexions \mathbf{h}_2 and 24 reflexions \mathbf{h}_4 resulted in the sign determination of 158 more 'weak' reflexions with $|E_L| > 1.3$. A Fourier synthesis revealed the positions of all of the light atoms, except the hydrogen atoms.

Calculations were performed using computer programs written by R. Dewar and A. Stone, modified by one of the authors (JHN).

The above described procedure may be generalized for heavy atoms on general positions. In this case there also exist reflexions with intermediate heavy atom contributions. For these reflexions $|F_L| = ||F_{\text{obs}}| \pm |F_H||$ and the lowest F_L value is taken to avoid incorrect sign indications. In our opinion this procedure is well suited to an automatic solution of structures containing heavy atoms.

References

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- HAUPTMAN, H. & KARLE, J. (1953). *Solution of the Phase Problem. I. The Centrosymmetric Crystal*. A.C.A. Monograph No. 3.
- PARTHASARATHY, S. (1966). *Z. Kristallogr.* **123**, 27.
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Acta Cryst. (1971). **A27**, 188

Resonance effects in low and high energy electron diffraction by crystals. Erratum. By SHIZUO MIYAKE and KAZUNOBU HAYAKAWA, *Institute for Solid State Physics, University of Tokyo, Roppongi-7, Minato-ku, Tokyo 106, Japan*

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Corrections to a previous paper [*Acta Cryst.* (1970). **A26**, 60] are given.

The following corrections should be made in our paper of the above title (Miyake & Hayakawa, 1970).

P. 64, col. 1, line 15 from bottom: For 'lowest Bragg reflexion 004.' read 'lowest Bragg reflexions 004 and 006.'

P. 64, col. 1, line 14 from bottom: For 'as an extra peak caused by' read 'as the 006 peak influenced by'.

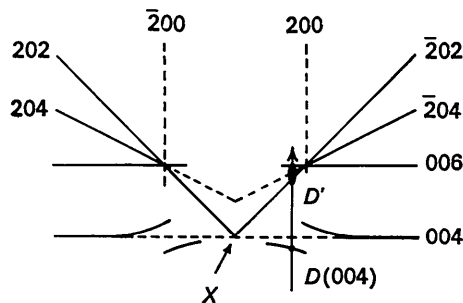
Fig. 10 (facing p. 64): The vertical dotted line (D) should be displaced by 5 mm to the right.

P. 65, Fig. 11(a): The reflexion indices should be corrected as follows:

- for 006 read 008
- for 008 read 0010
- for 0010 read 0012
- for 0012 read 0014.

P. 65, Fig. 11(b), lines 4-5 of the legend: For 'The peak D is the non-Bragg reflexion caused by' read 'The peak

D' is the 006 reflexion influenced by'.
P. 66, Fig. 12: This should be replaced by



Reference

- MIYAKE, S. & HAYAKAWA, K. (1970). *Acta Cryst.* **A26**, 60.

Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England).

International Symposium on Physics and Chemistry of Ice

Ottawa, Canada, 14-18 August 1972

This symposium, which is being sponsored by the Royal Society of Canada, will emphasize the fundamental physics and chemistry of ice in all its phases including the clathrate hydrates. The symposium follows earlier ones which were held at Erlenbach in 1962 and Munich in 1968. Copies of the *First Circular* and further details may be obtained from Mr M. K. Ward, Executive Secretary, International Symposium on the Physics and Chemistry of Ice, c/o National Research Council of Canada, Ottawa 7, Canada.

International Colloquium on the Study of Crystalline Transformations at High Temperatures

Odeillo, France. 27 September - 1 October 1971

This is one of several international colloquia of the Centre National de la Recherche Scientifique, which are devoted to well-defined topics and are attended by a limited number of specialists. This colloquium will deal with the different methods (X-ray and neutron diffraction, microscopy, thermal analysis and other physical or physico-chemical methods) available to give evidence of or to determine the nature of these crystalline transformations or to study phase changes and phase diagrams at high temperatures. The results obtained by these methods at temperatures above 1700°C will be considered for metals, oxides, carbides or other refractory elements or compounds.

Further details are obtainable from: Professor M. Foex, Laboratoire des Ultra Réfractaires, B.P.5, 66 Odeillo, France.

Third Thermal Expansion Symposium

Corning, New York, U.S.A., 27-29 October 1971

This meeting, which is sponsored jointly by the Department of Physics, University of Toronto, and the Corning

Glass Works, will provide the opportunity to exchange new ideas and techniques in fundamental and applied studies of thermal expansion. Contributed papers are solicited on basic experimental and theoretical studies of thermal expansion; on the relation of thermal expansion to other properties; on the technology of low expansion and of composite materials; on studies at extremely high or low temperatures; on thermal effects in diffraction studies and on thermal expansion standards. A number of invited papers will be presented by leading scientists and engineers and an exhibition by manufacturers of thermal expansion equipment is planned. The plans for publication of the proceedings are incomplete at present.

Abstracts should be submitted, by 30 June 1970, to Dr G. M. Graham, Department of Physics, University of Toronto, Toronto, Ontario, Canada. Further information may be obtained from Mr H. E. Hagy, Corning Glass Works, Sullivan Park, Corning, New York 14830, U.S.A.

Fedorov's *Symmetry of Crystals*

An English version of the 1890 Russian Classic, *Symmetry of Crystals* by E. S. Fedorov, has been prepared under the joint sponsorship of the American Crystallographic Association and the National Science Foundation. Translated by David and Katherine Harker, it encompasses the five monographs which together contain Fedorov's development of the principles of crystalline symmetry and his derivation of the 230 space groups. This work also embodies his complete theory of the division of three-dimensional periodic space into stereohedra, a subject not well known to scholars unable to read Russian. Many of Fedorov's analytical and mathematical methods are original and, the translators note, could be used profitably by modern workers and teachers. Published in 1971 as ACA Monograph 7, the ~325 page hard cover book is available at \$25 from the ACA, c/o Polycrystal Book Service, P.O. Box 11567, Pittsburgh, Pennsylvania 15238, U.S.A. Additional information may be obtained from the ACA secretary, Dr Walter Roth, General Electric Research and Development Center, P.O. Box 8, Schenectady, New York 12301.