

Using equation (1) re-written in the index notation

$$X_i^{(q)} = \sum_k Q_{ik} h_k^{(q)} \quad (1a)$$

we introduce the required elements Q_{ij} into equation (2)

$$S = \sum_q \sum_i W^{(q)} [\sum_k Q_{ik} h_k^{(q)} - X_i^{(q)}(\text{obs})]^2 \quad (2a)$$

and from the conditions

$$\frac{\partial S}{\partial Q_{ml}} = 0, \quad m, l = 1, 2, 3, \quad (3)$$

we obtain three systems of three linear normal equations for the nine matrix elements Q_{ml}

$$\sum_q W^{(q)} \sum_k \{Q_{mk} h_k^{(q)}\} h_l^{(q)} = \sum_q W^{(q)} X_m^{(q)}(\text{obs}) h_l^{(q)}, \quad (4)$$

$l = 1, 2, 3 \quad \text{for } m = 1, 2, 3.$

The estimated standard deviations can be calculated in the usual way (*International Tables for X-ray Crystallography*, 1959)

$$s^2(Q_{ml}) = a^{ll} \sum_q W^{(q)} (\Delta_m^{(q)})^2 / (N_q - N) \quad (5)$$

where

$s(Q_{ml})$ is the estimated standard deviation of the matrix element Q_{ml} ,

a^{ll} is the diagonal matrix element of the matrix \mathbf{a} inverse to the matrix of the normal equations in (4),

$$\Delta_m^{(q)} = X_m^{(q)}(\text{calc}) - X_m^{(q)}(\text{obs}) = \sum_k Q_{mk} h_k^{(q)} - X_m^{(q)}(\text{obs})$$

is the difference between the observed and the calculated value of the m th component of the vector $\mathbf{X}^{(q)}$ of the q th setting reflexion,

N_q is the number of setting reflexions used,

$N = 3$ is the number of parameters determined (N is not equal to 9 as there are three systems of three normal equations, each of them for the determination of three parameters Q_{ml} , $l = 1, 2, 3$).

The whole problem of accuracy and in particular the assignment of correct weights clearly requires further attention.

My thanks to Dr J. P. G. Richards for valuable discussion.

References

- BUSING, W. R. & LEVY, H. A. (1967). *Acta Cryst.* **22**, 457.
International Tables for X-ray Crystallography (1959). Vol. II, p. 330. Birmingham: Kynoch Press.
 SHOEMAKER, D. P. (1969). *Acta Cryst.* **A25**, 575.

International Union of Crystallography

Opening of new Union office

The President of the Union, Professor A. Guinier, together with the Chairman of the Commission on Journals, the General Secretary, the Treasurer, employees of the Union and guests, attended a luncheon in Chester on 7 January to mark the opening of the new Union office. This office,

incorporating the office of the Technical Editor and the office of the Executive Secretary, is at 13 White Friars, Chester CH1 1NZ, England. All correspondence for the Technical Editor, Mr S. A. Bryant, and the Executive Secretary, Dr J. N. King, should be sent to this address. Dr King has now taken over the day-to-day business of the Union from the General Secretary and the Treasurer.

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, 13 White Friars, Chester CH1 1NZ, England). Publication of an item in a particular issue cannot be guaranteed unless the draft is received 8 weeks before the date of publication.

Third International Conference of Crystal Growth (I.C.C.G.-3) Marseille, France, 5-9 July 1971

The programme planned for the Conference includes the theory of crystal growth; the characterization of crystals in relation to their way of growing; fundamental experimental work dealing with growth from the vapour phase, from the melt and from aqueous solution, growth at high pressures or temperatures, transformations in the solid phase and recrystallization, crystallization of big polymers and biological crystals. Sessions will also be held on new techniques for the production of single crystals and on crystallization on an industrial basis.

Parallel sessions are planned and a film show and an exhibition will be held.

For further information apply to:

General Secretary of the I. C. C. G.-3
B. Mutaftschiev

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Second International Conference on Small-Angle X-ray Scattering Graz, Austria, 26-29 August 1970

The Second International Conference on Small-Angle X-ray Scattering will be held on 26-29 August, 1970 at Graz, Austria. Further information may be obtained from:

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