

space, only non-zero derivatives are saved, and these are stored in array *DT*. The indices which identify them are stored in arrays *IT* and *JT*, and the integer *N* serves to count them. The program also avoids storing the derivative if $I=J$, since the derivative of a parameter with respect to itself necessarily has the value one. After the derivatives associated with a particular $P(J)$ are stored, the parameters are reset to their original values and the process is repeated for another $P(J)$. In practice, we have used the value 2^{-10} for all increments $DP(J)$.

The program then begins the loop through the observations, calculating F or F^2 and its derivatives in the usual way for each reflection. Derivatives of F with respect to extra parameters are set to zero. If N is non-zero, indicating that there are some constraints, then these derivatives are modified appropriately in steps 20 to 24. Original derivatives DF are saved in array *DS*. The program then loops through the N constraints, picking up the indices and coefficients from tables *IT*, *JT*, and *DT* and adding terms to the derivatives as indicated in step 23.

The remainder of the program proceeds as for an unconstrained refinement, except that after the variable parameters are adjusted, *SETP* is called once more to modify the dependent ones.

A general constraint routine of this type has been added as an option to *ORXFLS*, a revision of *ORFLS* (Busing,

Martin & Levy, 1962). The revision, including many other new features, is available from the authors on request.

References

- BUSING, W. R., MARTIN, K. O. & LEVY H. A. (1962). *ORFLS, A Fortran Crystallographic Least-Squares Program*. ORNL-TM-305, Oak Ridge National Laboratory, Oak Ridge, Tennessee.
- CRUICKSHANK, D. W. J. (1970). *Crystallographic Computing*, pp. 187–197. Copenhagen: Munksgaard.
- DOEDENS, R. J. (1970). *Crystallographic Computing*, pp. 198–200. Copenhagen: Munksgaard.
- FINGER, L. W. (1969a). *Mineral. Soc. Amer. Spec. Pap.* **2**, 95.
- FINGER, L. W. (1969b). Paper H7, Amer. Cryst. Assn. Meeting, Seattle, Washington.
- LA PLACA, S. J. & IBERS, J. A. (1963). *J. Amer. Chem. Soc.* **85**, 3501.
- LA PLACA, S. J. & IBERS, J. A. (1965). *Acta Cryst.* **18**, 511.
- PAWLEY, G. S. (1964). *Acta Cryst.* **17**, 457.
- PAWLEY, G. S. (1968). *Acta Cryst.* **B24**, 485.
- PAWLEY, G. S. (1969). *Acta Cryst.* **A25**, 531.
- PAWLEY, G. S. (1971). *Advances in Structure Research by Diffraction Methods*, Vol. 4. New York: Pergamon Press.
- SCHERINGER, C. (1963). *Acta Cryst.* **16**, 546.
- STROUSE, C. E. (1970). *Acta Cryst.* **A26**, 604.

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 Union of Crystallography

Ninth General Assembly and International Congress of Crystallography

The *First Circular* for this meeting was despatched during September by air-mail to those persons who completed and returned a Pre-Registration Card. Requests for further copies of the *First Circular* should be sent to Professor Y. Saito, General Secretary, Organizing Committee Crystallography, Science Council of Japan, 22-34 Roppongi 7-chome, Minato-ku, Tokyo 106, Japan, or to Dr J. N. King, Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

The American Crystallographic Association is organizing a charter flight from the U.S.A. to Japan. European members of the A.C.A. might also seriously consider this method of travel to Japan. Further information may be obtained from ACA Charter Flight, c/o Dr E. C. Wang, Department of Crystallography, University of Pittsburgh, Pittsburgh, Pa. 15213, U.S.A. The European Crystallographic Committee is not organizing a charter flight from Europe but is considering several proposals for group flights from various cities in Europe. Further information may be obtained from: Professor A. Authier, Association

Française de Cristallographie, 9 Quai Saint Bernard, Tour 26, Paris 5e, France.

J. D. Bernal

1901-1971

We regret to record the death in September of Professor J. D. Bernal, F.R.S., who was Professor of Physics at Birkbeck College, London from 1937 onwards and became its first Professor of Crystallography in 1963. He was a pioneer in the application of crystallographic methods to biological materials and carried out some of the early work on hormones and vitamins. His X-ray photographs of pepsin in 1933 were the first ever taken of single crystals of a protein. Professor Bernal was for many years closely associated with the work of the International Union of Crystallography, having been a member of the Commission on *Structure Reports* from 1948 to 1951, a member of the Executive Committee from 1951 to 1957, and Chairman of the Commission on Crystallographic Data from 1957 to 1963. In 1963 he was elected President of the Union, but owing to ill health he was subsequently unable to take a very active part in Union affairs and resigned in 1966 a short time before the opening of the Seventh General Assembly in Moscow.