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 General Secretary of the International Union of Crystallography (D. W. Smits, Rekencentrum der Rijksuniversiteit, Grote Appelstraat 11, *Groningen, The Netherlands). Publication of an item in a particular issue cannot be guaranteed unless the draft is received* 8 *weeks before the date of publication.*

Colloque sur les Calculs Cristallographiques

Grenoble, 7–8 Octobre 1965

Les 7 et 8 Octobre 1965 s'est tenu au Centre d'Études Nucléaires de Grenoble, un colloque sur les Calculs Cristallographiques, sous les auspices de l'Association Française de Cristallographie.

Dans une première partie ont été présentés des exposés sur des méthodes éventuellement applicables aux machines à calculer électroniques, et susceptibles d'apporter une aide, tant au travail de corrections systématiques des mesures, qu'à la recherche des structures cristallines.

La seconde partie a été consacrée à une discussion générale, sous forme de 'table ronde', organisée afin de tenter de normaliser les publications des programmes et algorithmes en France, et, d'autre part, d'harmoniser les relations entre les chercheurs désireux de faire exécuter des calculs cristallographiques classiques et les centres de calculs non spécialisés.

Les voeux émis à la suite des discussions, et les textes des exposés ont été réunis dans un ouvrage maintenant disponible. Pour l'obtenir, il suffit d' écrire au secrétaire du Colloque: Mr. G. Bassi, Centre d'Études Nucléaires de Grenoble, Laboratoire de Diffraction Neutronique, B.P. 269, 38 Grenoble, France.

Book Reviews

Works intended for notice in this column should be sent direct to the Editor (A. J. C. Wilson, Department of Physics, The University, Birmingham 15, England). As far as practicable books will be reviewed in a country different from that of publication.

Optical transforms, their preparation and application to X-ray diffraction problems. By C. A. Taylor and H. Lipson. Pp. x + 182. London: G. Bell and Sons, 1964. 45*s*.

The utilization of Fourier synthesis in building up the electron density from diffraction data began a dozen years after the discovery of X-ray diffraction. Its routine use in crystal-structure analysis was initiated by Zachariasen, who used it in determining the structure of potassium chlorate in 1929. The trend in applying Fourier synthesis in crystal-structure analysis was reinforced by the discovery of the Patterson function in 1934 and the discovery of its Harker sections in 1936, both expressed in the form of Fourier syntheses. The trend was implemented by the invention of the Beevers–Lipson method of Fourier summation in 1934, and the Patterson–Tunell method in 1942.

Fourier synthesis was in the air in the late 1930's. While it had been appreciated by physicists that the production of a diffraction image at the back focal plane of a lens was a physical analog of Fourier synthesis, it appears that the first suggestion for using this method for producing a picture of the electron density by diffraction of visible light with a grating having the geometrical features of the reciprocal lattice of a crystal was made by H. Boersch in October, 1938. His inspiration came from observing the lattice-like diffraction patterns which were produced in the back focal plane of a microscope when its objective was focused on various regular patterns of holes in opaque sheets. Boersch was keenly aware of the requirement that to build up an electron-density map by such a method the phases must be controlled.

The April 22, 1939 issue of *Nature* contained the basic note by W. L. Bragg upon which subsequent technical developments were based. Bragg used as a diffraction grating a brass plate in which were drilled holes at points of a zero level of the reciprocal lattice of diopside, $CaMg(SiO_3)_2$, the hole areas being proportional to the $F(h0l)$'s of the reciprocal-lattice points. In this projection of this crystal structure, the superposed Ca and Mg atoms at the origin dominated the scattering, so that the phases of all $F(h0l)$'s were zero; consequently the phases required no special control. When the diffraction from this grating was focused by a lens at its back focal plane, a crude representation of a few cells of the electron-density projection $\varrho(xz)$ of diopside appeared. The tricky requirements for controlling phase had not been solved, so that the method unfortunately could not be extended to other structures.

This reviewer was entranced by Bragg's 'X-ray microscope', as it was called, and immediately (July, 1939) pointed out that (*a*) there were several ways of controlling phases (one of which later became the basis of the method used by the authors of this book), (*b*) that Patterson and some Harker syntheses could be performed without phase control, and (*c*) that by utilizing positive prints made by the Dawton process from de Jong–Bouman photographs, from which the Lorentz and polarization factors had been removed by an appropriate shutter, this print suspended in oil between plane-parallel glass flats could be substituted for a grating, and that this procedure was especially direct for Patterson projections. Equipment for doing all this in a well-engineered way was designed, built and operated before the war intervened. After the war the new developments in interpretation of Patterson functions at M.I.T. required numerical values of the function, so that photographic analog synthesis gradually fell into disuse.

Although the inverse Fourier synthesis (that is, the computation of the characteristics of the X-ray diffraction by