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 Editor (P. P. Ewald, Polytechnic Institute of Brooklyn, 333 Jay Street, Brooklyn 1, N.Y., U.S.A.) or to the Technical Editor (R. W. Asmussen, Chemical Laboratory B of the Technical University of Denmark, Sølvgade 83, Copenhagen K, Denmark)

The Use of the IBM 650 and 704 for Crystal Structure Analysis Computations

A Conference was held at the Mellon Institute, Pittsburgh, on November 4, 1958, for the purpose of exchanging information on the development and use of programs for crystal structure analysis. It was the second Conference on this topic for both computers; the previous meetings had been held separately, on 6 February 1957 for the 650 (*Acta Cryst.* (1957), **10**, 384); on 4 and 5 November 1957 for the 704 (*Acta Cryst.* (1958), **11**, 311).

The Conference was opened by Mr William B. Kehl of the University of Pittsburgh Computation and Data Processing Center. There were eight principal speakers and about sixty attended the Conference.

The following is a summary of the information, which was presented by the author indicated *.

An IBM *Code for Fourier Analysis of Line Shapes*

E. R. Boyko* and G. J. Mohn, (Westinghouse Atomic Power Division).

This program is designed to perform a Stokes analysis to determine the pure diffraction profile. Special tests which are performed on the Fourier coefficients of the pure diffraction profile are contained in the program, and these tests allow the series to be automatically broken off at the point where it is no longer converging to the right answer. It is also possible to by-pass these tests so that the final series will be computed using the number of coefficients specified in the input information. The 650 operating time depends upon the amount of input data and the number of Fourier coefficients which must be calculated. The operating time required to run the problem given in Stokes' original paper was 15 minutes.

A Fast Three Dimensional Fourier Program for the Basic IBM 650

D. R. Fitzwater and D. E. Williams*, (Iowa State College).

This program (TDF-2) calculates two- or three-dimensional Fourier synthesis in the general expanded form. The summation is carried out one dimension at a time on either 1/40 or 1/80 intervals in each direction. Provision is made to eliminate sorting of intermediate sums for two-dimensional series and to drastically reduce sorting for three-dimensional series. The series is divided into subseries having the same trigonometric form and evenness of indices so that only the basic $\frac{1}{4}\times\frac{1}{4}\times\frac{1}{4}$ of the unit cell is calculated by the 650. The remainder of the unit cell is obtained by trigonometric expansion on the tabulator while printing the results. Two-dimensional series generally require less than 0·25 hr. on the 650. The time required for three-dimensional series is variable and is given approximately by the formula

$$t \text{ (minutes)} = 0{\cdot}0005 \sum_s [H_s K_s L_s X + K_s L_s X Y + L_s X Y Z] + 0{\cdot}00125 \sum_s [K_s L_s X + L_s X Y + X Y Z] ,$$

where H_s, K_s, and L_s are the number of h, k, and l index values in subseries S, and X, Y, and Z are the number of points X_i, Y_i, Z_i on which the series is evaluated in the x, y, and z directions. An example with 2000 coefficients uniformly distributed among 16 subseries evaluated on $1/40\times1/40\times1/80$ intervals requires approximately 3·4 hours on the 650.

Fourier Synthesis, Structure Factor and Auxiliary Programs on the IBM 650

B. W. Brown, F. C. Lingafelter, J. M. Stewart and L. H. Jensen*, (The University of Washington, Washington).

The following set of programs in a self-consistent input-output form have been written and are in use: (1) *Scattering Factor Interpolation.* The program evaluates scattering factors at intervals of 0·005 in $\sin\varphi/\lambda$ by a four-point interpolation formula. Input are literature values for the scattering factor and output is in a form used by program (2). About two minutes are required per element to cover the range to the limit of Mo radiation. (2) *Reduction of Data.* The program may be used to reduce equi-inclination Weissenberg and zero level precession data. Input are the necessary scattering factors and a hand-punched intensity deck containing h, k, l, I_{rel} and $\sin^2\mu$. Output is a reflection deck, one reflection per card, in a form used by program (3). Calculation time is about 1·2 seconds per reflection. (3) *General Structure Factor.* The program is used in conjunction with a parameter load program and will handle up to 100 atoms of up to 8 atom types in a single pass. Any number of atoms of any number of kinds can be handled by using multiple passes. Output is in the form used by programs (4). Calculation time is at the rate of 12 atoms per second for a centrosymmetric structure with an overall temperature factor, and is slightly slower for non-centrosymmetric structures or with individual temperature factors. (4) *General Two- and Three-Dimensional Fourier Series.* Centrosymmetric structures up to 7·5 × 30 Å or equivalent can be handled in a single pass. In general larger structures, non-centrosymmetric projections and sections of three-dimensional Fourier series require more than one pass. Projections and sections may be evaluated at intervals of $n/200$ along either axis. The three-dimensional programs can be used to evaluate any section $n/1000$ of the axis corresponding to the index summed over first. Calculation time for a centrosymmetric oblique axis projection with 200 reflections evaluated at 676 points is about 10 minutes. The following auxiliary programs have also been written: *Sharpened Patterson. Patterson Superposition. Least Squares Temperature and Scale Factor. Linear and Least*

Squares Rescale Factor. Wilson Plot. Least Squares Plane. Bond Length-Bond Angle. Conversion of Fractional Coordinates (any Symmetry) to Orthogonal Coordinates in Ångströms. Calculation of Hydrogen Atomic Coordinates.

Anisotropic Structure Refinement Using Differential Synthesis on the IBM 650

R. Shiono*, (University of Pittsburgh).

A set of programs for the anisotropic structure refinement using differential Fourier synthesis have been written and used. The anisotropic structure factors are calculated in general form with a $P1$ or $P\bar{1}$ program, and the differential synthesis programs compute electron density, slopes and curvatures at points assumed as atomic coordinates, and thence the shifts of coordinates. The shifts of temperature factors are calculated from the derivatives of the curvatures, and the difference of observed and calculated curvatures, using Cruickshank's approximation. The anisotropic structure factor of 28 atoms of 2 kinds in $P1$ took ca. 18 sec./reflexion. The differential synthesis of 672 reflexions in $P2_12_12_1$ took 28 min./atom, and the summation of derivatives of curvatures took 2·5 hours for isotropic to anisotropic cycle, 7·7 hours for anisotropic to anisotropic cycle on the basic 650. These computation times have been reduced 10–20% by minor modifications for the use of indexing accumulator and core storage.

'*Programs Using an* IBM 650 *Equipped with Tapes, Immediate Access Storage and Indexing Registers. I. Fourier Syntheses*'

Lynne L. Merritt, Jr.*, (Indiana University).

This Fourier program, written for an IBM 650 with core storage, indexing registers and four magnetic tapes computes two- or three-dimensional syntheses at intervals of n/100ths where n can be any integer. There is no limit on the number of reflections nor on the maximum index in any zone. The interval could be changed to 1/200th by a slight modification. Any space group can be handled. One control card at the start of each stage of the summation eliminates the computation of unnecessary terms. The speed is approximately 55 milliseconds per reflection × term × point in the first dimension, 44 milliseconds per sum × term × point in the second dimension and approximately the same time in the third dimension. In the above statement, the word 'reflection' refers to the number of pieces of data after grouping reflections so that only positive indices need be considered. The word 'term' refers to the number of terms to be computed in the general equation. The word 'point' means the number of values of x (or y or z) over which the summation is to be made, and the word 'sum' refers to the number of values of (klx) or (lxy) going into the second or third dimension.

'*II. Structure Factor and Least Squares*'

Dick Van der Helm*, (Indiana University).

The programs were written for an IBM 650 with core storage, indexing registers and magnetic tape. The first program calculates structure factors for the monoclinic space groups with either separate isotropic, or separate anisotropic or without temperature factors (and consecutive calculation of an overall temperature factor). The maximum number of atoms is 50, and there can be 6 different kinds of atoms, the scattering factors of which are in the data cards. The setting of the program is done by a control card, and no changes have to be made by the operator for the different calculation. Every zone is rescaled after computation with its own calculated scale factor. An R for every zone and an overall R are punched out. The output cards have also F_o-F_c, and in the non-centrosymmetric space groups, a second card which has the A and B parts and A_o-A_c and B_o-B_c is punched out for every reflection. The speed is 0·4–0·7 seconds per atom per reflection. It seems that the auxiliary units of the IBM 650 can speed up the calculation to an average of about 80% of the time for the basic unit. The second program calculates shifts of coordinates and temperature factors for each atom in floating decimal form for the centrosymmetric, monoclinic space groups. To use these two different programs one may set the least squares program to operate on only a part of the reflections. The speed is 0·9 seconds per atom per reflection.

Review of IBM 650 *Programs Available and Tested at the University of Pittsburgh Computation and Data Processing Center*

G. A. Jeffrey*, (University of Pittsburgh).

At the previous 650 conference it was agreed that the center would (1) accept and distribute copies of programs submitted in standard form, (2) record the testing of these programs either by the Crystallography Laboratory at the University of Pittsburgh or by the first re-user. The following programs are available: eight Fourier synthesis programs, of which we had used and tested five; four structure factor programs, of which we had used three; one least squares (isotropic, diagonal terms) which we had used; five miscellaneous auxiliary programs of which we had used three. Details of these programs were distributed in tabulated form to the conference.

A Versatile Least Squares Program for the IBM 704

W. R. Busing* and H. A. Levy, (Chemistry Division, Oak Ridge National Laboratory).

A least squares program for the IBM 704 computer has been written which makes use of the complete matrix of the normal equations. Some of its features are (1) choice of overall, symmetric, or anisotropic temperature factors, (2) refinement on F or F^2, (3) use of X-ray or neutron diffraction data, and (4) arbitrary selection of parameters to be varied. The program allows the symmetry and choice of origin to be specified easily and usually automatically so that any space group may be accommodated. The program will be distributed through SHARE.

E. R. Boyko	L. H. Jensen
W. R. Busing	Lynne L. Merritt
D. R. Fitzwater	R. Shiono
D. Van der Helm	D. E. Williams
G. A. Jeffrey (Conference Chairman)	