'SILLIAC' COMPUTER PROGRAMS FOR X-RAY CRYSTAL STRUCTURE ANALYSIS

by

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1. INTRODUCTION

The object of a crystal structure analysis is the determination of the positions of all the atoms in the 'unit cell', which is the basic unit by whose repetition the crystal is built up. The observables from which the structure is to be deduced are the intensities and directions of the X-rays diffracted by a small crystal bathed in a beam of monochromatic X-radiation. The square-roots of the intensities can be inserted in Fourier syntheses which, if the appropriate phase-constant for each term (or 'structure factor') can be found, reproduce the electron density function throughout the unit cell. On the other hand, the structure factors can be calculated from trial-values of the coordinates of the atoms, and can then be compared with the observed structure factors.

The required calculations are not particularly complicated but they are particularly voluminous. Hence both the limits of the range of complexity of the crystals amenable to structure determination, and the accuracy of the refinements, have increased remarkably in the last decade, largely due to the availability of computing aids.

Two of the SILLIAC programs for crystal structure analysis perform the two basic calculations mentioned above; a third carries out the automatic adjustment of the atomic coordinates so as to minimise the disagreement between the calculated and observed structure factors. A choice has to be made when such programs are being coded: complete generality enables a program to be used for any crystal structure, no matter what the symmetry of the crystal space group may be, but the coding of both programs and data is much simplified if the programs cover a more restricted range of symmetry conditions. The SILLIAC Fourier program is almost completely general; structure factor and refinement programs have so far been developed for only two of the most common classes of space-groups.

2. NOTATION

λ = wave-length of X-rays used in recording the diffraction pattern

V = volume of unit cell

a, b, c = lengths of unit cell edges parallel to (not necessarily orthogonal) x-, y-, z-directions

γ, α, β = angles between a and b, b and c, c and a, respectively

x/a, y/b, z/c = coordinates of a point in the unit cell

$\rho(x,y,z)$ = electron density at the point $(x/a, y/b, z/c)$

h, k, l = Miller indices of the crystal plane making intercepts a/h, b/k and c/l on the unit cell edges

θ_{hkl} = Bragg-(diffraction-)angle for X-ray reflection from the hkl-plane

I_{hkl} or $I(hkl)$ = intensity of the reflection from the hkl-plane

F_{hkl} or $F(hkl)$ = structure factor of the hkl-reflection

A_{hkl}, B_{hkl} = real and imaginary parts of F_{hkl}, respectively

α_{hkl} = phase constant

= $\tan^{-1}(B/A)$

F^2_{hkl} = $I_{hkl} = A^2_{hkl} + B^2_{hkl}$

x_j, y_j, z_j = coordinates of j^{th} atom expressed as fractions of a, b, and c

f_j = atomic scattering factor of the j^{th} atom = $f_j(\theta_{hkl})$

T_f = temperature factor which modifies f_j to take into account the thermal vibrations of the atoms

= $\exp(-B \sin^2\theta / \lambda^2)$

B = vibrational parameter

3. SUMMATION OF TWO - DIMENSIONAL FOURIER SERIES

The electron density function of a crystal can be described by means of a three-dimensional Fourier series, whose coefficients are the structure factors F_{hkl} :

$$\rho(x,y,z) = \frac{1}{V} \sum\sum\sum_{h,k,l=-\infty}^{+\infty} \left| F_{hkl} \right| \cos 2\pi(hx/a + ky/b + lz/c - \alpha_{hkl})$$

A program for evaluating such series has been described for SWAC by Sparks, Prosen, Kruse and Trueblood (1956; cf. also Mayer and Trueblood, 1953). For practical purposes it is, however, often adequate to make a projection of the electron density parallel to one of the unit cell axes. The expression for the electron density projected on the point (x/a, y/b, 0) —

$$\rho(x,y) = \frac{1}{A_c} \sum\sum_{h,k=-\infty}^{+\infty} \left| F_{hko} \right| \cos 2\pi\,(hx/a + ky/b - \alpha_{hko}) \text{ —}$$

may be simplified for computation by expressing the trigonometrical function in the product-form and by making use of the symmetry-relations (if any) among the structure factors. The Fourier series is then conveniently calculated in two stages by a method suggested by Lipson and Beevers (1936), which is also most suitable for automatic computation (Bennett and Kendrew, 1952; Fowweather, 1955).

The SILLIAC program has already been described in detail elsewhere (Freeman, 1957). It sums the expression

$$\rho(x,y) = \sum_{h=0}^{h_{max}} \sum_{k=0}^{k_{max}} F_{hk} \left\{ \begin{matrix} \cos \\ \underline{\text{or}} \\ \sin \end{matrix} \right\} 2\pi hx/a. \left\{ \begin{matrix} \cos \\ \underline{\text{or}} \\ \sin \end{matrix} \right\} 2\pi ky/b$$

where $\rho(x,y)$ = the projected electron density at (x/a, y/b), and the summation occurs at intervals of 1/64 of the unit cell edges. The limits of the summation are determined by parameters input with the data. The maximum value of $\underline{h}_{max}$ is 29; $\underline{k}_{max}$ can have any value. The total number of F_{hk}'s which can be accommodated is 550, but sequences of zero-values are stored in one location and add only one to the count of F_{hk}'s. The F's may have any positive or negative integral value, but the scale must be such that $\rho(x,y)$ nowhere exceeds 9999.

There is provision at present for the inclusion in the summation of two complete tables of F_{hk}'s, using different combinations of the trigonometrical functions for each. For each table, the product of trigonometrical functions which is to be used depends on the even/odd nature of the indices of each F_{hk}. There are only four possible combinations - $\underline{h}$ even, $\underline{k}$ even; $\underline{h}$ even, $\underline{k}$ odd; $\underline{h}$ odd, $\underline{k}$ even; and both odd. For each of these a parameter is supplied, which determines the product to be formed. If there are two tables of F_{hk}'s, two sets of parameters must be supplied. Complete generality of the program requires a provision for four tables of F's, and the corresponding modification of the program can easily be made.

The indices $\underline{h}$ and $\underline{k}$ do not appear on the data-tape; the machine determines the indices of each F_{hk} by counting. The data-tape consists of the list of F_{hk}'s in groups of constant $\underline{h}$ and increasing $\underline{k}$. The end of each group, preceding an increase in $\underline{h}$, is signalled by the symbol L on the tape, and the end of the table by the symbol F.

In the SILLIAC store, the F's are held as $F \times 2^{-37}$. This leaves the two least significant bits of each location free for identification purposes. Terminal numbers are added to those F_{hk}'s whose inclusion in the summation precedes an increase in $\underline{h}$, to the last F_{hk} of the table, and to those numbers which do not represent single F_{hk}'s but a sequence of zero-terms. The terminal bits are removed and examined before each F_{hk} enters the summation, and cause the machine to take appropriate action.

From the number of orders and the known times required for their execution, the calculation time is given approximately by the expression

$$(y_{max} + 1) \left[8.5 \, (\text{no. of } F_{hk}\text{'s}) + 3.5 \, (h_{max} + 1)(x_{max} + 1) \right] \text{msec}$$

Much more time, however, is occupied by punching the results. In an actual calculation, where

$$\text{no. of } F_{hk}\text{'s} = 150,$$
$$\underline{h}_{max} = 11,$$
$$0 \leqslant y/b \leqslant 16/64,$$
$$-32/64 \leqslant x/a \leqslant 32/64,$$

the predicted calculation time would have been about 0.6 min. The time actually required was :

Input of program and data : 1 min.

Computation and output: 4.5 min.

4. CALCULATION OF STRUCTURE FACTORS

The general expression for the structure factor corresponding to the $\underline{hkl}$-reflection is

$$F_{hkl} = \sum_{j=1}^{N} f_j T_f \exp\left(-2\pi i \left[hx_j + ky_j + lz_j\right]\right)$$

where there are N atoms in the unit cell. The SWAC structure factor program (Sparks, Prosen, Kruse and Trueblood, 1956) is the only one so far reported which uses this form of the structure factor expression, symmetry-related atoms being indicated by code-words supplied with the data for each calculation. A similar calculation is implicit in the general refinement program developed by Friedlander, Lane and Sayre (1955) for the IBM 701 computer. Many substances crystallize in the monoclinic space-groups derived from the crystal class $2/m - C_{2h}$. The structure factor in these cases

is $$F_{hkl} = 4 \sum_{j=1}^{N/4} f_j T_f \cos 2\pi(hx_j + lz_j) . \cos 2\pi ky_j$$

or $$-4 \sum_{j=1}^{N/4} f_j T_f \sin 2\pi(hx_j + lz_j) . \sin 2\pi ky_j$$

and the choice between the two expressions is made on the basis of the even- or odd-ness of some combination of the indices *h*, *k* and *l*. The first SILLIAC structure factor program has been developed to cope only with structures for which the above expressions are appropriate; the same restriction applied to the first programs reported for the Manchester University (Mark II) computer (Ahmed and Cruickshank, 1953) and for the Electro Data Datatron (Lavine and Rollett, 1956).

For each value of *h*, *k*, *l*, the following quantities must be computed:

$$\sin\theta/\lambda = \tfrac{1}{2}\left[\frac{h^2/a^2 + l^2/c^2 - 2hl\cos\beta/ac}{\sin^2\beta} - k^2/b^2\right]^{\frac{1}{2}}$$

$$f_j = f(\sin\theta/\lambda)$$

$$T_f = \exp(-B\sin^2\theta/\lambda^2)$$

$$hx_j,\ ky_j,\ lz_j \quad \text{for } j = 1, 2, \ldots, N/4$$

$\cos 2\pi(hx_j + lz_j)\,.\,\cos 2\pi ky_j$ *or*

$-\sin 2\pi(hx_j + lz_j)\,.\,\sin 2\pi ky_j$

$$F_j = f_jT_f\,.\,\cos 2\pi(hx_j + lz_j)\,.\,\cos 2\pi ky_j) \text{ or}$$

$$- f_jT_f\,.\,\sin 2\pi(hx_j + lz_j)\,.\,\sin 2\pi ky_j)$$

$$F_{calc} = 4\sum_j F_j$$

In addition, there is an over-riding condition that $\sin\theta \leq 1$
i.e. $\sin\theta/\lambda \leq 1/\lambda$.

The SILLIAC program systematically computes all F_{hkl} for which $\sin\theta_{hkl} \leq 1$. All F_{hkl} for a constant value of *h*,*k* are computed before *h* is increased; and when all values of *h* have been traversed, *k* is increased and *h* and *l* are reset to zero. At the end of the calculation a program alteration is read into the store and calculation of the $F_{hk\bar{l}}$ occurs. The F_{hkl}'s are computed for at most 30 atoms of not more than 6 different kinds in the asymmetric unit. The only data which are supplied to the machine represent

the unit cell constants

the limiting value of $1/\lambda$

the number of atoms in the asymmetric unit ($N/4$)

the number of kinds of atoms

the x_j, y_j, z_j

the temperature parameter (B)

coefficients for the evaluation of the f_j and T_f.

The basic program contains a sub-routine which tests *h*, *k* and *l* for each reflection and causes the formation of the cosine-cosine product for even (*h* + *k* + *l*), and of the sine-sine product for odd (*h* + *k* + *l*).

This is correct for space-group $P2_1/n$. For each of the remaining space groups derived from C_{2h}, the conditions for the choice of the product are slightly different. The required modifications to the h,k,l-test are supplied as one or two order-pairs following the data.

The greatest problem in designing this program consisted of the large amount of storage space which is required for the tables of the atomic scattering factors, f_j. In the programs for the Manchester, SWAC and Datatron computers, the f_j^j (hkl) could be found by interpolation or table-searching in complete tables of f_j versus $\sin\theta$, even though each table consisted of 100-150 values.

In order to overcome the difficulty occasioned by SILLIAC's small store, it has been found possible to represent the f_j as polynomials. At the time when the method was being tested it was not realised that it had already been tried on SWAC, and rejected as "not significantly faster than table-searching and appreciably less convenient unless the problem of storage is critical" (Sparks et al., 1956).

The coefficients a_n required to represent the f_j as

$$f_j = \sum_n a_n (\sin\theta/\lambda)^n$$

can be found from the published values of f_j versus $\sin\theta$ by means of standard routines in the SILLIAC library. Trial and error have shown that atomic scattering factors for C, N, O, H, Cu^+, K^+, Cl^- can be represented to 1% accuracy by sixth-degree polynomials. The evaluation of f_j by this method turns out to be rather faster than interpolation would be. On the other hand, the above statement regarding accuracy is true only within the range of $\sin\theta/\lambda$ observed with CuK_α radiation; higher polynomials appear to be needed outside this range. It is also rather inconvenient that the use of any new or modified scattering curve at present requires the evaluation of a new set of polynomial coefficients. The temperature factor T_f is similarly evaluated as a short polynomial in $B\sin^2\theta/\lambda^2$.

The results of the calculation are stated to one decimal place and are output in groups of constant, h,k. The signal value of l is followed by the signed value of F_{hkl}.

In an actual calculation for an asymmetric unit of 8 atoms of 4 different kinds, 1 200 structure factors took 11 min to evaluate plus 1 min for program and data input.

5. AUTOMATIC REFINEMENT BY METHOD OF LEAST SQUARES

A structure may be "refined" - the correct atomic coordinates may be found - by the repetition of a cycle consisting of the calculation of structure factors from an approximately correct model, the computation and plotting of a Fourier synthesis using the magnitudes of the observed structure factors and the phases of the calculated ones, and the deduction of an improved model from this Fourier synthesis. From a computational point of view this method has the disadvantage that it requires a relatively large output. Even when (Sparks et al., 1956) the results of the structure factor calculation are fed directly into the Fourier program without prior printing, the output from even a two-dimensional Fourier synthesis over a quarter of a unit cell, computed at 1/64's of the unit cell edges, still consists of 33 x 33 = 1 089 signed terms of 3-4 digits plus spaces, each.

Alternatively, structure refinement may be achieved by fitting the atomic coordinates and other parameters to be observed structure factors via the method of least squares (Hughes, 1941) or by means of 'differential Fourier summations' (Booth, 1946).

In both these methods, the structure factors calculated from an approximate structure are compared with the observed values; at the end of a refinement cycle, the parameters are adjusted and the process is repeated. The only output required is such as to tell the operator whether and how fast the refinement is converging. Programs for automatic least-squares refinement have been described by Friedlander, Lane and Sayre (1955), by Lavine and Rollett (1956), and by Sparks, Prosen, Kruse and Trueblood (1956); and for differential syntheses by Ahmed and Cruickshank (1953) and also by Sparks et al. (q.v.). The SILLIAC program for the least squares refinement of structures of the crystal class $2/m\text{-}C_{2h}$ involves the simultaneous adjustment of the coordinates of up to 20 atoms of not more than 6 kinds, and of an anisotropic temperature factor containing two vibrational parameters. Interactions between atomic coordinates other than the x- and z- coordinates of each atom are ignored. Under these conditions, the terms to be evaluated are :

Structure factor : $F_{hkl} = 4 \sum_j F_j$

Contribution of j^{th} atom : $F_j = f_j T_f \cos 2\pi(hx_j + lz_j) . \cos 2\pi k y_j$ or

$- f_j T_f \sin 2\pi(hx_j + lz_j) . \sin 2\pi k y_j$

Temperature factor : $T_f = \exp(-B\sin^2\theta/\lambda^2 - \alpha h^2)$

Derivatives of F_j -

with respect to the coordinates x_j, etc. : $\left(\frac{\partial F_{hkl}}{\partial x_j}\right) = -4 . 2\pi h f_j T_f \sin 2\pi(hx_j + lz_j) . \cos 2\pi k y_j$ or

$-4 . 2\pi h f_j T_f \cos 2\pi(hx_j + lz_j) . \sin 2\pi k y_j$

etc.

with respect to the $\left(\frac{\partial F_{hkl}}{\partial B}\right) = -(\sin^2\theta/\lambda^2) . F_{hkl}$

vibrational parameters : $\left(\frac{\partial F_{hkl}}{\partial \alpha}\right) = - h^2 . F_{hkl}$

Discrepancy in F_{hkl} : $\Delta F_{hkl} = (F_{obs} - F_{calc})_{hkl}$

It is obvious that the formation of the derivatives involves only a few products in addition to those which are required in any case for the structure factor. Appropriate weight factors, w_{hkl}, taking into account both the multiplicities and the accuracy of measurement of the F_{hkl}'s, are included (cf. Hughes, 1941; Lavine and Rollett, 1956).

The above quantities are appropriately cross-multiplied and the products are included in summations which give the following 'normal equations' :

$$\sum_{hkl} w\left(\frac{\partial F}{\partial x_j}\right)^2 \Delta x_j \quad + \sum_{hkl} w\left(\frac{\partial F}{\partial x_j}\right)\left(\frac{\partial F}{\partial z_j}\right) \Delta z_j = \sum_{hkl} w\left(\frac{\partial F}{\partial x_j}\right) \Delta F$$

$$\sum_{hkl} w\left(\frac{\partial F}{\partial y_j}\right)^2 \Delta y_j = \sum_{hkl} w\left(\frac{\partial F}{\partial y_j}\right) \Delta F$$

$$\sum_{hkl} w\left(\frac{\partial F}{\partial x_j}\right)\left(\frac{\partial F}{\partial z_j}\right) \Delta x_j + \sum_{hkl} w\left(\frac{\partial F}{\partial z_j}\right)^2 \Delta z_j = \sum_{hkl} w\left(\frac{\partial F}{\partial z_j}\right) \Delta F$$

$$\sum_{hkl} w\left(\frac{\partial F}{\partial \alpha}\right)^2 \Delta \alpha \quad + \sum_{hkl} w\left(\frac{\partial F}{\partial \alpha}\right)\left(\frac{\partial F}{\partial B}\right) \Delta B = \sum_{hkl} w\left(\frac{\partial F}{\partial \alpha}\right) \Delta F$$

$$\sum_{hkl} w\left(\frac{\partial F}{\partial \alpha}\right)\left(\frac{\partial F}{\partial B}\right) \Delta \alpha + \sum_{hkl} w\left(\frac{\partial F}{\partial B}\right)^2 \Delta B = \sum_{hkl} w\left(\frac{\partial F}{\partial B}\right) \Delta F$$

(For the sake of clarity, the sub-scripts hkl after F_{hkl} and w_{hkl} are omitted.)

At the end of each cycle, these equations are solved and the parameters are adjusted for the next cycle. The output at each stage consists (unless cancelled) of -

the coefficients of the normal equations

the changes in the parameters

the new values of the parameters

the totals $\Sigma\left|F_{obs}\right|$, $\Sigma\left|F_{calc}\right|$, $\Sigma\left|\Delta F\right|$, $\Sigma w(\Delta F)^2$, $\dfrac{\Sigma|\Delta F|}{\Sigma\left|F_{obs}\right|}$.

In addition, the complete list of h, k, l, F_{obs}, F_{calc}, ΔF may be punched during the refinement. This is generally done only in the final cycle.

To give an example of the time taken for a single stage of refinement we may take the following calculation: For an asymmetric unit of 8 atoms of 4 different kinds, refinement with respect to 585 different values of F_{hkl} required for

program input : 1 min

data input : 1 min 5 sec

alteration input (for $F_{hk\bar{l}}$) : 30 sec

computation only : 6 min 5 sec

computation and punching F_{obs}, F_{calc} and ΔF : 10 min 45 sec

solution of normal equations and adjustment and punching of parameters : 1 min 45 sec

The total time taken for one cycle of refinement was therefore 10 min 25 sec if the list of structure factors was not punched, and 15 min 5 sec if it was.

The principal features and limitations of this program are the following:

(i) It is not possible to store the whole table of F_{obs}'s in SILLIAC. In fact, the tape carrying the F_{obs}'s is placed on the reader at the beginning of each cycle, and each F_{obs} is read and processed in turn. Provision is made for the identification of unobserved reflections, systematically missing reflections, and the last F_{hkl} in a row (of constant <u>h,k</u>) or in a group (of constant <u>k</u>) of the table.

(ii) The F's are not segregated into groups according to the even or odd nature of one or more of the indices. As in the structure factor program, the F_{hkl}'s are dealt with in increasing order of the indices, the form of each product being chosen by the machine following a test of the <u>h</u>, <u>k</u> and <u>l</u>. The values of the indices do not appear on the tape, but are determined by counting.

(iii) The atomic scattering factors f_j are stored as the coefficients of polynomials in $(\sin\theta / \lambda)$, as in the structure factor program.

(iv) The temperature factor has two parameters instead of the four required for a fully anisotropic temperature factor for a monoclinic crystal.

(v) Even so, considerable storage difficulties were encountered during the coding of this program. Its order scheme is more complicated than that of the structure factor program due to the necessity of packing more than one quantity into many of the storage locations.

6. OTHER PROGRAMS

Considerable use has already been made of the above programs, as well as of a simple but helpful one which merely disgorges a list of all the reciprocal lattice spacings, $d^*_{hkl} = 2\sin\theta_{hkl} / \lambda$, from a list of the unit cell dimensions.

A further program, which has been coded (April, 1957) but not yet used, computes structure factors for the orthorhombic space-groups of the classes $222\text{-}D_2$, $mm2\text{-}D_{2h}$ and $mmm\text{-}C_{2v}$ (with the exception of the space groups $Fddd\text{-}D^{24}_{2h}$ and $Fdd2\text{-}C^{19}_{2v}$). The expression which this program evaluates is

$$\left|F_{hkl}\right| = 4 \text{ (or 8 or 16) } \left[A^2_{hkl} + B^2_{hkl} \right]^{\frac{1}{2}}$$

where A_{hkl} and B_{hkl} have the form

$$\pm \sum_{j=1}^{N/4 \text{ (or } N/8 \text{ or } N/16)} f_j T_f \left\{ \begin{matrix} \cos \\ \underline{\text{or}} \\ \sin \end{matrix} \right\} 2\pi h x_j \left\{ \begin{matrix} \cos \\ \underline{\text{or}} \\ \sin \end{matrix} \right\} 2\pi k y_j \left\{ \begin{matrix} \cos \\ \underline{\text{or}} \\ \sin \end{matrix} \right\} 2\pi l z_j$$

For each of the eight possible cases -

h even, k even, l even

h even, k even, l odd *etc.* -

the program chooses for both A_{hkl} and B_{hkl} the correct combinations out of the possible sixteen,

$$\pm(\sin \text{ or } \cos).(\sin \text{ or } \cos).(\sin \text{ or } \cos),$$

according to parameters involving only four binary digits. For centro-symmetric space groups, $B_{hkl} = 0$ and the signed value of A_{hkl} corresponds to F_{hkl}. For non-centro-symmetric cases the potential output from this program consists of

$$h\ k\ l,\quad F_{hkl},\quad A_{hkl},\quad B_{hkl},\quad \cos\alpha_{hkl},\quad \sin\alpha_{hkl}$$

7. COMPARISON OF COMPUTING TIMES

The following tables summarise some of the reported computing times for various crystallographic calculations. The times include input of data and programs and output of results, but obviously not the time taken by data-preparation.

Two-Dimensional Fourier Syntheses

Computers/Authors	No. of F-terms	No. of points of summation	Total time (min.)
Manchester Mk.II	145	1 089	36
(Fowweather, 1955)	63	561	22
EDSAC (Bennett &	260	561	30
Kendrew, 1952)	410	2145	97
SILLIAC (Present work)	150	561	5.5

Structure Factors

Computer/Authors	No. of atoms	No. of kinds of atoms	No. of F's	Total time (min)	Time per F (sec)
Manchester Mk.II	9	3			1.9*
(Fowweather, 1955)	16	2			2.6*
	18	1			2.9*
(* plus 2.4 sec for printing result)					
Manchester Mk.II	19	3	1199	35.5	1.8
(Ahmed & Cruickshank, 1953)	10	1	667	10.2	0.9

Computer/Authors	No. of atoms	No. of kinds of atoms	No. of F's	Total time (min)	Time per F (sec)
SWAC (Sparks, Prosen, Kruse, Trueblood, 1956)	3 - 100				2 - 7
Contract(Rollett, Deuce (1957	99	-	2 200	660	18
	7	-	700	55	4.8
SILLIAC (Present work)	8	4	1 200	12	0.6
	11	5	400	6	0.9

Least Squares Refinement

Computer/Authors	No. of atoms	No. of kinds of atoms	No. of F's	Time per iteration	Time per F (sec)
LEO (Thompson, Caminer, Fantl, Wright, King, 1954)	9	1	939	40 min	2.6*
		(*Method of 'steepest descents')			
IBM 701 (Friedlander, Love, Sayre, 1955)	N		F	NF/1 000 min	0.06N
SWAC (Sparks et al. 1956)	34*	3	2 800	7-8 hr	9
		(*15 included only in s.f. - calculation)			
Datatron (Lavine, Rollett, 1956)	13	3	1 200	6 hr	18
Contract(Rollett Deuce (1957	26	-	2 200	6 hr*	11
	4	-	700	1 hr*	5
SILLIAC (Present work)	8	4	585	10.5 min	1.1

*estimates only

REFERENCES

Ahmed, F. and Cruickshank, D.W.J. (1953). Acta Cryst., 6, 765.
Bennett, J.M. and Kendrew, J. (1952). Acta Cryst., 5, 109.
Booth, A.D. (1946). Trans. Faraday Soc., 42, 444.
Fowweather, F. (1955). Acta Cryst., 8, 633.
Freeman, H.C. (1957). Aust. J. Chem. (in the press).
Friedlander, P.H., Love, W. and Sayre, D. (1955). Acta Cryst., 6, 732.
Hughes, E.W. (1941). J. Amer. Chem. Soc., 63, 1737.
Lavine, L.R. and Rollett, J.S. (1956). Acta Cryst., 9, 269.
Mayer, S.W. and Trueblood, K.N. (1953). Acta Cryst., 6, 427.
Rollett, J.S. (1957). Private Communication.
Sparks, R.A., Prosen, R.J., Kruse, F.H. and Trueblood, K.N. (1956). Acta Cryst., 9, 350.
Thompson, T.R., Caminer, D.T., Fantl, L., Wright, W.B. and King, G.S.D. (1954). Acta Cryst., 7, 260.

DISCUSSION

Mr. I. Bassett, University of Melbourne.

How many numbers have to be stored simultaneously for a given number of atoms?

Mr. H.C. Freeman (In Reply)

We have to store three co-ordinates for each atom seven times as many polynomial coefficients as there are types of atoms and as many temperature parameters as we choose to include.

In addition we keep certain functions which are not changing e.g. $\cos 2\pi(h_x + l_z)$ if we are keeping h and l constant and varying k.