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Computer programming strategy for crystallographic Fourier synthesis: Program MIFR1.*

By DAVID P. SHOEMAKER and WILLIAM G. SLY.† *Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts, U.S.A.*

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A highly efficient program has been written for carrying out two- and three-dimensional crystallographic Fourier calculations on the IBM 704 electronic digital computer. This program, known as MIFR1, is described in detail elsewhere‡ (Sly & Shoemaker, 1960*a, b*); the present communication will be concerned only with the programming strategy. The program is limited to the 74 space groups of symmetry orthorhombic and lower; higher symmetries are handled through their subgroups in this set.

The method is based on the Beavers & Lipson (1934) factorization of the sums of trigonometric triple products obtained by expansion of the Fourier terms, and the omission of certain classes of triple products in accord with the requirements of symmetry (Ahmed & Barnes, 1958). We are here principally concerned with systematic application of symmetry criteria and with organization of the Fourier calculation for high computational efficiency.

The electron density expression may be written in the form

$$\rho(x, y, z) = K \sum_l \left\{ \sum_k \left[\sum_h (\alpha_{hkl}^{(1)} m_{hkl} A_{hkl}^{(1)} \cos 2\pi hx + \beta_{hkl}^{(2)} m_{hkl} B_{hkl}^{(2)} \sin 2\pi hx) \cos 2\pi ky + \sum_h (\alpha_{hkl}^{(4)} m_{hkl} A_{hkl}^{(4)} \sin 2\pi hx + \beta_{hkl}^{(3)} m_{hkl} B_{hkl}^{(3)} \cos 2\pi hx) \sin 2\pi ky \right] \cos 2\pi lz + \sum_k \left[\sum_h (\alpha_{hkl}^{(2)} m_{hkl} A_{hkl}^{(2)} \cos 2\pi hx + \beta_{hkl}^{(1)} m_{hkl} B_{hkl}^{(1)} \sin 2\pi hx) \sin 2\pi ky + \sum_h (\alpha_{hkl}^{(3)} m_{hkl} A_{hkl}^{(3)} \sin 2\pi hx + \beta_{hkl}^{(4)} m_{hkl} B_{hkl}^{(4)} \cos 2\pi hx) \cos 2\pi ky \right] \sin 2\pi lz \right\}, \quad (1)$$

where the summations are taken only over zero and positive values of the Miller indices and m_{hkl} is a multiplicity factor (calculated by the program). The $A_{hkl}^{(i)}$ and $B_{hkl}^{(i)}$ are sum and difference combinations of observed amplitudes for various combinations of signs of the indices. The quantities $\alpha_{hkl}^{(1)} \dots \beta_{hkl}^{(4)}$ are restricted to the binary integers 0 and 1. This set of eight integers (hereinafter referred to as an $\alpha\beta$ set) may be considered as the logical 'AND' of all $\alpha\beta$ sets corresponding to the individual requirements of the several symmetry elements that (together with the translation group) generate the space group. The needed elements are 2, 2_1 , m , a , b , c , and n in the three principal directions and with coordinates

possessing all possible combinations of 0 and $\frac{1}{4}$, plus d in the three directions with coordinates 0. These $48 + 3 = 51$ elements suffice for all triclinic, monoclinic, and orthorhombic space groups. Only for $Fdd2$ and $Fddd$ is there any material restriction on choice of origin, owing to the inadmissibility of coordinates equal to $\frac{1}{8}$. The $\alpha\beta$ sets for these 51 elements are easily derived and will not be given here. For $C_{2h}^2 - P2_1/c$, for example, we have

	$(k+l)$ even	$(l+l)$ odd
$2_1 \parallel \mathbf{b}$, at $(x, z) = (0, \frac{1}{4})$	10101010	01010101
$c \perp \mathbf{b}$, at $y = \frac{1}{4}$	10100101	01011010
2_1 AND c : $\alpha\beta$ for group	10100000	01010000

For MIFR1 a one-card subprogram was prepared for each of the 51 elements. Each such subprogram selects the appropriate $\alpha\beta$ set, after examining the Miller indices where necessary. In practice the space group is specified by including in the program deck the cards for the required elements, and observing the required lattice extinctions in preparing the input data.

The grouping of terms in equation (1) provides high efficiency operation when the Fourier sum is being developed inside high-speed memory while the coefficients (A 's and B 's) are stored outside the machine on tape and read in serially as needed. It implies that on tape the terms have been previously sorted h within k within l , with appropriate separation of cosine and sine terms within each index group, to minimize the number of l - and k -summation operations (during each of which the read-in and h -summation operations are suspended). The preparation and ordering of the coefficients, application of the $\alpha\beta$ procedure, and writing of the input tape are accomplished by an input program. The subsequent main Fourier program (which uses a very fast table look-up procedure closely related to the 'M-card' method of V. Schomaker (unpublished) is executed as many times as there are blocks of the unit cell (e.g., $\frac{1}{8} \times \frac{1}{8} \times \frac{1}{4}$, in 120ths) to be calculated. As many as 100,000 terms per second are calculated by this program.

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References

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† Present address: Department of Chemistry, Harvey Mudd College, Claremont, California.

‡ Program decks of binary punched cards, and copies of the manual of operation, may be obtained on request from D. P. Shoemaker, M.I.T., subject to limited supply.

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