Table 1

No.	Symmetry	1	2	3, 3a	4, 5	6	7	8a	8	9	10	11	12	13	En.	O.A.
33	R_∞	1	0	1	1	0	1	2	2	2	3	0	3	4	1	1
34	R^i_∞	1	0	1	1	0	0	2	2	2	3	0	3	4	0	0
35	C_∞	1	1	2	3	4	7	5	8	12	19	11	10	22	1	2
36	$C_{\infty v}$	1	1	2	2	3	4	5	6	7	10	8	9	16	0	0
37	C^h_∞	1	0	2	3	0	0	5	8	12	19	0	10	22	0	0
38	D_∞	1	0	2	2	1	3	5	6	7	10	3	9	16	1	2
39	D^h_∞	1	0	2	2	0	0	5	6	7	10	0	9	16	0	0

where the negative sign has to be taken with ψ in the case of optical activity and enantiomorphism.

Using $\chi(\varphi)$ and $\psi(\varphi)$ from Table 1 of Bhagavantam & Suryanarayana in the above formulae we get the integers shown in Table 1, which can be placed at the bottom of their Table 2.

These results are all in agreement with those of Jahn in the paper already mentioned.

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Three-dimensional Fourier summations on a high-speed digital computer.

By S. W. MAYER and K. N. TRUEBLOOD, *Department of Chemistry, University of California, Los Angeles* 24, *California, U.S.A.*

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The application of digital computers to crystal-structure investigation has been receiving increased attention concomitant with the further development and increased availability of such computers (Bennett & Kendrew, 1952; Ordway, 1950, 1952; Shoemaker, 1952). We have been using the National Bureau of Standards Western Automatic Computer (Huskey, 1950) in calculations for our studies of the structures of sulfamide (Mayer & Trueblood, 1953) and cyclopropylamine hydrochloride. Three-dimensional Fourier summations over one-sixteenth of the unit cell of sulfamide, including all of the 180 observed reflections from this crystal (space group $Fdd2$), have been carried out in less than 35 min. of computing time. Because the asymmetric unit for sulfamide is contained in one-sixteenth of the unit cell the time required for computing was less than can ordinarily be expected, but it is estimated that in most cases not more than 90 min. would be needed.

Data is fed into the computer on I.B.M. cards at the rate of 240 cards per minute. Each card holds the required data for ten spectra—the indices, observed structure factors and calculated phases. (The structure factors were also calculated on the computer.) These cards, containing information in the binary system, are prepared automatically from decimally punched cards. Several duplicate packs of the cards are prepared to expedite the necessary recycling operations. The Fourier summation is then carried out in the machine as a programmed sequence of basic operations. The memory of the computer at present holds 256 36-digit binary numbers; the machine performs such operations as addition and subtraction at the rate of more than nine hundred thousand per minute. Computed results are punched decimally on I.B.M. cards, at a maximum rate of fifty cards per minute. Each card contains fifteen values of the electron density; in sulfamide, this corresponds to one line (fifteen one-sixtieths) in the (x, y) grid at a constant value of z. Upon completion of the map for one z plane, an increment is automatically added to z, and the cycle of programmed calculations is repeated until the electron-density distribution has been calculated over the desired range of z.

Although the interval now employed for the grid of the electron-density map is 1/60 of the unit cell edge, it is feasible to change the interval to 1/120 or 1/30. The Fourier equations employed are of the type in which all the indices are positive (Lonsdale, 1936). Although we have to date programmed only for space groups $Fdd2$ and $Pbn2_1$, our programming may easily be extended to any space group for which the summation terms can conveniently be put into the form

$$\pm \sum_0^k \sum_0^h \sum_0^l |F_{hkl}| \begin{matrix}\cos\\ \sin\end{matrix} 2\pi(lz-\alpha) \cdot \begin{matrix}\cos\\ \sin\end{matrix} 2\pi hx \cdot \begin{matrix}\cos\\ \sin\end{matrix} 2\pi ky \, .$$

Three-dimensional Patterson functions can of course be rapidly computed in a similar fashion. We expect to present a fuller description of these computing procedures with an account of the structure of sulfamide when our investigation of this substance has been completed.

We wish to express our gratitude to the Institute for Numerical Analysis of the National Bureau of Standards on this campus for the use of the SWAC and other computing facilities.

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