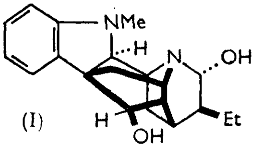
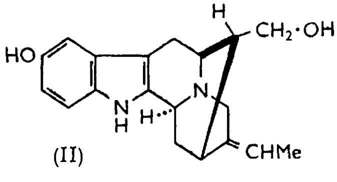
341. *The Structure of Macusine-A: X-Ray Analysis of Macusine-A Iodide.*

By A. T. McPhail, J. Monteath Robertson, and G. A. Sim.

In order to determine the molecular structure of macusine-A, a quaternary alkaloid isolated from *Strychnos toxifera*, the iodide has been subjected to *X*-ray analysis. The crystals are orthorhombic, space group $P2_12_12_1$ (D_2^4), with four molecules of $C_{22}H_{27}N_2O_3I$ in the unit cell of dimensions $a = 13{\cdot}82$, $b = 9{\cdot}06$, $c = 17{\cdot}43$ Å. Phase determination based initially on the iodine atom with subsequent Fourier and least-squares refinement methods led to the constitution and stereochemistry (apart from absolute configuration) given in formula (IV).

Among the quaternary alkaloids isolated[1] from *Strychnos toxifera* are macusine-A and macusine-B. By detailed chemical study involving correlation with ajmaline[2] (I) and sarpagine[3] (II), macusine-B has been shown[4] to have structure (III), the only uncertain point being the configuration of the ethylidene system. Scarcity of material precluded an unambiguous chemical derivation of the structure of macusine-A


(I)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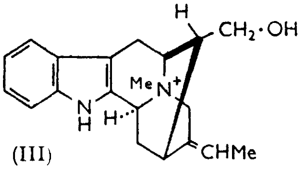
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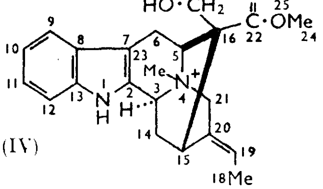
(IV)

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[1] Battersby, Binks, Hodson, and Yeowell, *J.*, 1960, 1848.

[2] Bartlett, Sklar, Taylor, Schlittler, Amai, Beak, Bringi, and Wenkert, *J. Amer. Chem. Soc.*, 1962, **84**, 622.

[3] Bartlett, Sklar, and Taylor, *J. Amer. Chem. Soc.*, 1960, **82**, 3790.

[4] Battersby and Yeowell, *Proc. Chem. Soc.*, 1961, 17.

and at the suggestion of Dr. A. R. Battersby we undertook an *X*-ray investigation of macusine-A iodide. After a number of cycles of three-dimensional Fourier syntheses and least-squares refinement of positional and thermal atomic parameters our final results establish the constitution and stereochemistry (apart from absolute configuration) of the alkaloid to be as in (IV); chemical studies at Bristol[5] are consistent with this structure. The absolute stereochemistry shown in (IV) has been defined[5] by a chemical correlation with macusine-B (III).

The final electron-density distribution for macusine-A iodide is shown in Fig. 1 as superimposed contour sections drawn parallel to (010) and covering the region of one molecule; the corresponding atomic arrangement is explained in Fig. 2. The inter-atomic distances and valency angles calculated from the final atomic co-ordinates (see Table 1) are listed in Table 2. The standard deviations of the final atomic co-ordinates were estimated in the usual manner from the least-squares residuals (see Experimental section) and are shown in Table 3; from the results the average estimated standard deviation (e.s.d) of a carbon–carbon bond length is about 0·07 Å and the average e.s.d. of a valency angle about 4°.

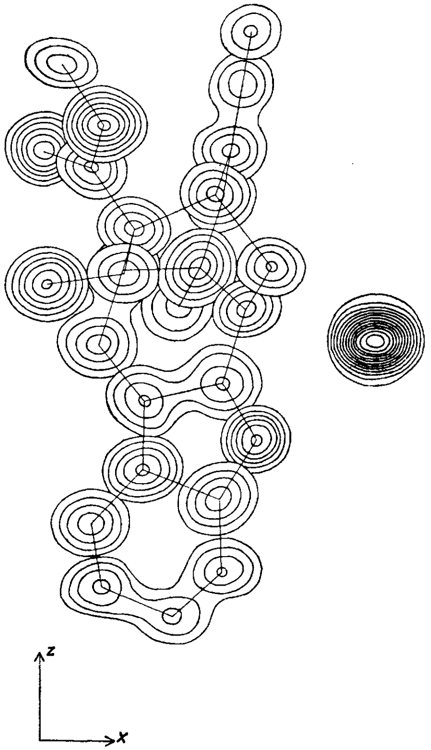

FIG. 1. Final three-dimensional electron-density distribution for macusine-A iodide shown by means of superimposed contour sections drawn parallel to (010). Contour interval 1e/Å^3 except around the iodide ion where it is 5e/Å^3.

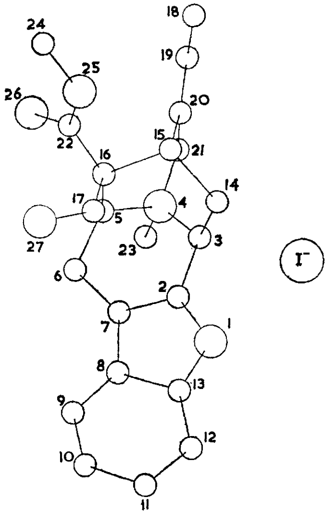

FIG. 2. Atomic arrangement corresponding to Fig. 1.

The average bond length in the benzene ring, 1·41 Å, and the average carbon–carbon single bond length, 1·57 Å, do not differ significantly from the accepted values of 1·397 Å

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[5] Battersby, personal communication; McPhail, Robertson, Sim, Battersby, Hodson, and Yeowell, *Proc. Chem. Soc.*, 1961, 223.

TABLE 1.

Atomic co-ordinates.

(Origin of co-ordinates as in " International Tables." *)

Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
N(1)	0·7927	0·2613	0·3229	C(11)	0·6782	0·1861	0·1342	C(20)	0·7490	0·3122	0·6269
C(2)	0·7402	0·2981	0·3830	C(12)	0·7558	0·2075	0·1824	C(21)	0·7405	0·4539	0·5774
C(3)	0·7777	0·3322	0·4615	C(13)	0·7394	0·2386	0·2594	C(22)	0·5622	0·1778	0·6138
N(4)	0·7120	0·4285	0·5038	C(14)	0·8075	0·1829	0·5081	C(23)	0·6873	0·5701	0·4638
C(5)	0·6077	0·3385	0·4993	C(15)	0·7321	0·1785	0·5779	C(24)	0·5208	0·0288	0·7220
C(6)	0·5674	0·3277	0·4224	C(16)	0·6190	0·1871	0·5464	O(25)	0·5808	0·0598	0·6571
C(7)	0·6399	0·3016	0·3646	C(17)	0·6080	0·0505	0·5001	O(26)	0·4999	0·2575	0·6303
C(8)	0·6364	0·2584	0·2852	C(18)	0·7759	0·1809	0·7551	O(27)	0·5096	0·0256	0·4856
C(9)	0·5600	0·2436	0·2323	C(19)	0·7633	0·3155	0·7011	I	0·9499	0·8024	0·4287
C(10)	0·5774	0·2139	0·1622								

* " International Tables for *X*-Ray Crystallography," The Kynoch Press, Birmingham, 1952, Vol. I.

TABLE 2.

Interatomic distances (Å) and angles.

Intramolecular bonded distances

N(1)–C(2)	1·32	C(6)–C(7)	1·44	C(13)–C(8)	1·50	C(22)–O(26)	1·16
C(2)–C(3)	1·50	C(7)–C(8)	1·44	C(2)–C(7)	1·42	C(22)–O(25)	1·33
C(3)–C(14)	1·64	C(8)–C(9)	1·41	C(14)–C(15)	1·59	O(25)–C(24)	1·43
C(3)–N(4)	1·46	C(9)–C(10)	1·28	C(15)–C(16)	1·66	C(15)–C(20)	1·50
N(4)–C(23)	1·50	C(10)–C(11)	1·50	C(5)–C(16)	1·61	C(18)–C(19)	1·55
N(4)–C(21)	1·36	C(11)–C(12)	1·38	C(16)–C(17)	1·48	C(19)–C(20)	1·31
N(4)–C(5)	1·66	C(12)–C(13)	1·39	C(17)–O(27)	1·40	C(20)–C(21)	1·55
C(5)–C(6)	1·46	C(13)–N(1)	1·35	C(16)–C(22)	1·42		

Intramolecular non-bonded distances

N(1) · · · C(14)	3·33	N(4) · · · C(15)	2·62	C(7) · · · C(17)	3·31	C(17) · · · O(26)	3·30
N(1) · · · C(23)	4·00	N(4) · · · C(17)	3·71	C(7) · · · C(23)	3·06	C(18) · · · O(25)	3·38
C(2) · · · C(5)	2·76	N(4) · · · C(22)	3·62	C(14) · · · C(17)	3·01	C(19) · · · C(22)	3·40
C(2) · · · C(15)	3·57	C(5) · · · C(14)	3·10	C(14) · · · C(19)	3·61	C(19) · · · O(25)	3·51
C(2) · · · C(16)	3·45	C(5) · · · C(20)	2·97	C(14) · · · C(21)	2·88	C(20) · · · C(22)	2·86
C(2) · · · C(17)	3·54	C(5) · · · O(26)	2·82	C(14) · · · C(22)	3·85	C(20) · · · C(23)	3·78
C(2) · · · C(23)	2·93	C(5) · · · O(27)	3·15	C(15) · · · C(18)	3·15	C(20) · · · O(25)	3·30
C(3) · · · C(6)	2·99	C(6) · · · C(17)	2·91	C(15) · · · O(25)	2·73	C(20) · · · O(26)	3·48
C(3) · · · C(16)	2·95	C(6) · · · C(22)	3·60	C(15) · · · O(26)	3·41	C(22) · · · O(27)	2·72
C(3) · · · C(17)	3·53	C(6) · · · C(23)	2·85	C(16) · · · C(21)	2·99	C(24) · · · O(26)	2·63
C(3) · · · C(20)	2·92	C(6) · · · O(27)	3·06	C(16) · · · C(24)	3·64	O(25) · · · O(27)	3·16
N(4) · · · C(7)	2·86	C(7) · · · C(16)	3·35	C(17) · · · O(25)	2·76	O(26) · · · O(27)	3·28

Intermolecular distances (⩽4 Å)

N(1) · · · O(26)$_{\mathrm{I}}$	2·98	C(21) · · · C(11)$_{\mathrm{IV}}$	3·59	C(18) · · · C(13)$_{\mathrm{II}}$	3·81	C(15) · · · C(12)$_{\mathrm{II}}$	3·95
O(25) · · · C(12)$_{\mathrm{II}}$	3·34	C(2) · · · O(26)$_{\mathrm{I}}$	3·63	C(24) · · · C(12)$_{\mathrm{II}}$	3·82	I · · · C(23)$_{\mathrm{V}}$	3·95
I · · · O(27)$_{\mathrm{I}}$	3·43	C(14) · · · O(26)$_{\mathrm{I}}$	3·64	C(14) · · · O(27)$_{\mathrm{I}}$	3·85	C(18) · · · C(11)$_{\mathrm{II}}$	3·99
C(3) · · · O(26)$_{\mathrm{I}}$	3·56	C(15) · · · C(11)$_{\mathrm{II}}$	3·66	C(21) · · · O(27)$^{\mathrm{I}}$	3·88	C(18) · · · C(9)$_{\mathrm{I}}$	3·99
O(26) · · · C(24)$_{\mathrm{III}}$	3·57	N(1) · · · C(24)$_{\mathrm{I}}$	3·76	N(1) · · · C(22)$_{\mathrm{I}}$	3·92	C(14) · · · C(11)$_{\mathrm{II}}$	4·00
C(21) · · · C(12)$_{\mathrm{IV}}$	3·57	C(18) · · · C(12)$_{\mathrm{II}}$	3·77	C(24) · · · I$_{\mathrm{IV}}$	3·93	I · · · C(11)$_{\mathrm{IV}}$	4·00
C(3) · · · O(27)$_{\mathrm{I}}$	3·57	C(14) · · · C(6)$_{\mathrm{I}}$	3·79				

The subscripts refer to the following positions:

I $\frac{1}{2} + x, \frac{1}{2} - y, 1 - z.$
II $1\frac{1}{2} - x, -y, \frac{1}{2} + z.$
III $1 - x, \frac{1}{2} + y, 1\frac{1}{2} - z.$
IV $1\frac{1}{2} - x, 1 - y, \frac{1}{2} + z,$
V $\frac{1}{2} + x, 1\frac{1}{2} - y, 1 - z.$

Interbond angles

C(13)N(1)C(2)	113°	N(4)C(5)C(6)	114°	C(11)C(12)C(13)	119°	C(17)C(16)C(22)	110°
N(1)C(2)C(3)	126	N(4)C(5)C(16)	108	N(1)C(13)C(8)	105	C(16)C(17)O(27)	109
N(1)C(2)C(7)	111	C(6)C(5)C(16)	117	N(1)C(13)C(12)	137	C(18)C(19)C(20)	127
C(3)C(2)C(7)	123	C(5)C(6)C(7)	113	C(8)C(13)C(12)	118	C(15)C(20)C(19)	127
C(2)C(3)N(4)	112	C(2)C(7)C(6)	122	C(3)C(14)C(15)	104	C(15)C(20)C(21)	110
C(2)C(3)C(14)	112	C(2)C(7)C(8)	104	C(14)C(15)C(16)	112	C(19)C(20)C(21)	123
N(4)C(3)C(14)	113	C(6)C(7)C(8)	134	C(14)C(15)C(20)	108	N(4)C(21)C(20)	114
C(3)N(4)C(5)	103	C(7)C(8)C(9)	133	C(16)C(15)C(20)	107	C(16)C(22)O(25)	114
C(3)N(4)C(21)	113	C(7)C(8)C(13)	107	C(5)C(16)C(15)	107	C(16)C(22)O(26)	125
C(3)N(4)C(23)	115	C(9)C(8)C(13)	120	C(5)C(16)C(17)	115	O(25)C(22)O(26)	120
C(5)N(4)C(21)	112	C(8)C(9)C(10)	120	C(5)C(16)C(22)	115	IO(27)$_{\mathrm{I}}$C(17)$_{\mathrm{I}}$	107
C(5)N(4)C(23)	102	C(9)C(10)C(11)	122	C(15)C(16)C(17)	104	C(2)N(1)O(26)$_{\mathrm{I}}$	109
C(21)N(4)C(23)	111	C(10)C(11)C(12)	120	C(15)C(16)C(22)	104		

TABLE 3.

Standard deviations of the final atomic co-ordinates (A).

Atom	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$	Atom	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$	Atom	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$
N(1)	0·042	0·032	0·034	C(11)	0·055	0·050	0·047	C(20)	0·053	0·051	0·043
C(2)	0·047	0·048	0·040	C(12)	0·061	0·045	0·045	C(21)	0·058	0·049	0·051
C(3)	0·057	0·053	0·053	C(13)	0·053	0·038	0·043	C(22)	0·054	0·044	0·042
N(4)	0·046	0·037	0·037	C(14)	0·056	0·053	0·048	C(23)	0·069	0·048	0·056
C(5)	0·061	0·054	0·052	C(15)	0·049	0·047	0·048	C(24)	0·070	0·051	0·043
C(6)	0·045	0·040	0·041	C(16)	0·059	0·045	0·046	O(25)	0·032	0·032	0·030
C(7)	0·058	0·052	0·044	C(17)	0·053	0·052	0·054	O(26)	0·033	0·031	0·034
C(8)	0·058	0·040	0·043	C(18)	0·057	0·048	0·048	O(27)	0·035	0·033	0·036
C(9)	0·053	0·037	0·045	C(19)	0·055	0·054	0·050	I	0·004	0·004	0·003
(C10)	0·049	0·040	0·037								

and 1·545 Å,[6] respectively. The average sp^3-carbon–nitrogen(4) bond length of 1·49 Å is in reasonable agreement with the lengths of such bonds in other alkaloids (for a fuller discussion see Hamilton *et al.*[7]). The average sp^2-carbon–nitrogen(1) bond length is considerably shorter (1·33 Å) and as the radius of an sp^2-hybridized carbon atom is only 0·02—0·03 Å smaller than that of an sp^3-hybridized carbon atom it follows that there is a difference in the covalent radii of the two types of nitrogen atom and/or a degree of

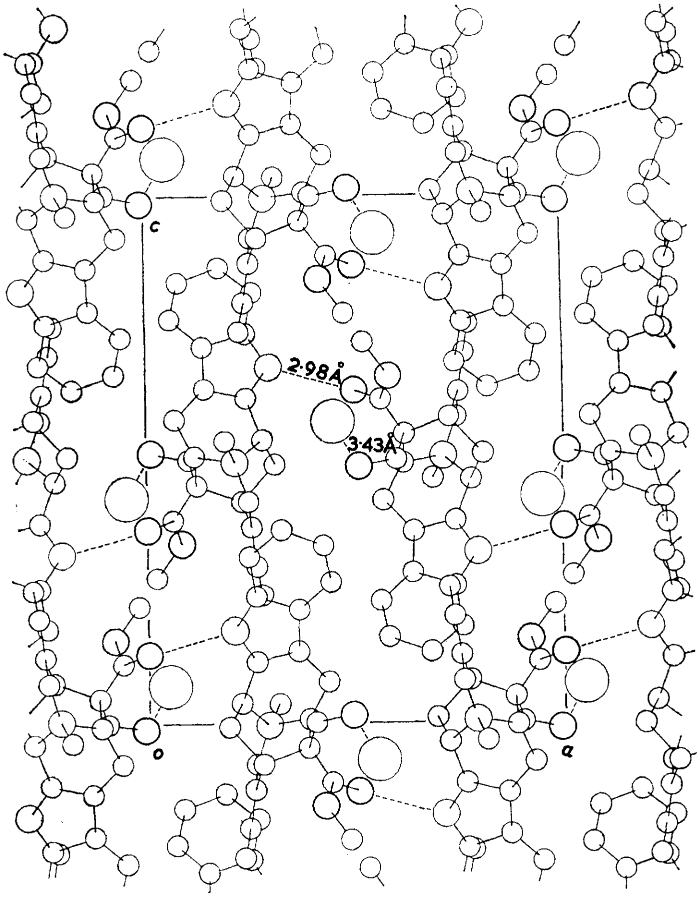

FIG. 3. The crystal structure as viewed in projection on (010).

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[6] Sutton *et al.*, "Tables of Interatomic Distances and Configuration in Molecules and Ions," *Chem. Soc. Special Publ.*, No. 11, 1958.

[7] Hamilton, Hamor, Robertson, and Sim, *J.*, 1962, 5061.

double-bond character associated with the sp^2-carbon–nitrogen(1) bonds. The carbon–oxygen bond lengths in the ester and alcohol groups show no significant deviations from the usual values. The length of the carbon–carbon double bond in the ethylidene group, 1·31 Å. does not differ significantly from the value of 1·334 Å in ethylene.[8]

The molecular arrangement in the crystal as seen in projection along the *b* axis is illustrated in Fig. 3. The positively charged macusine-A molecules and the negatively charged iodide ions are held together by the normal ionic forces, by van der Waals forces, and by hydrogen bonds which involve the indole nitrogen atom, the ketonic oxygen atom of the ester group, the hydroxyl oxygen atom O(27), and the iodide ion. The N(1)H • • • O(26) distance of 2·98 Å is comparable with N • • • O hydrogen-bonded distances in other crystals (*e.g.*, 2·79, 2·83, 2·96 Å in L-serine phosphate,[9] 2·68, 2·75, 2·86, 2·89 Å in glycyl-L-tryptophan dihydrate,[10] 2·86, 2·92, 2·94 Å in L-glutamic acid [11]). The C(2)N(1)O(26) angle is 109°. The O(27)H • • • I hydrogen-bonded distance of 3·43 Å is similar to O • • • I distances in muscarine iodide (3·57 Å),[12] (+)-de(oxymethylene)-lycoctonine hydriodide monohydrate (3·65 Å),[13] and (+)-demethanolaconinone hydriodide trihydrate (3·52—3·62 Å).[14] The C(17)O(27)I angle is 107°.

The closest contacts between an iodide ion and carbon atoms, 3·93 and 3·95 Å, are similar to the minimum C • • • I^- distances in the crystal structures of muscarine iodide (3·87 Å),[12] (+)-de(oxymethylene)lycoctonine hydriodide monohydrate (3·81 Å),[13] and isocryptopleurine methiodide (3·96 Å).[15]

A full list of the intermolecular contacts of less that 4 Å is given in Table 2.

EXPERIMENTAL

Crystal Data.—Macusine-A iodide, $C_{22}H_{27}IN_2O_3$; *M*, 494·4; m. p. 274° (decomp.). Orthorhombic, $a = 13{\cdot}82$, $b = 9{\cdot}06$, $c = 17{\cdot}43$ Å, $U = 2182$ Å^3, $D_m = 1{\cdot}50$ g. cm.$^{-3}$ (by flotation), $Z = 4$, $D_c = 1{\cdot}50$ g. cm.$^{-3}$, space group $P2_12_12_1 - D_2^4$. Absorption coefficient for *X*-rays ($\lambda = 1{\cdot}542$ Å) $\mu = 127$ cm.$^{-1}$.

The crystals were obtained from aqueous solution in the form of fine needles elongated along *a*.

Experimental Measurements.—Rotation, oscillation, and Weissenberg photographs were taken with copper-K_α ($\lambda = 1{\cdot}542$ Å) radiation; precession photographs were taken with molybdenum-K_α ($\lambda = 0{\cdot}7107$ Å) radiation. The cell dimensions were obtained from the precession and rotation photographs. The space group was determined uniquely from the systematic halvings in the reflexions. For the intensity survey a small crystal was employed, completely bathed in a uniform *X*-ray beam, and no corrections for absorption were applied. The intensities were estimated visually from equi-inclination Weissenberg photographs of the 0*kl*—8*kl* layers; the multiple-film technique was employed. The usual correction factors (Lorentz, polarization, and rotation [16]) were applied and 1145 independent structure amplitudes were derived. The exposures were such that the various layers were approximately on the same relative scale; the absolute scale of each layer was obtained at a later stage by correlation with the calculated structure amplitudes, $|F_c|$.

Analysis of the Structure.—The analysis proceeded directly on the basis of the usual phase-determining heavy-atom method.[17] The initial co-ordinates of the iodide ion were determined

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[8] Bartell and Bonham, *J. Chem. Phys.*, 1957, **27**, 1414.
[9] McCallum, Robertson, and Sim, *Nature*, 1959, **184**, 1863.
[10] Pasternak, *Acta Cryst.*, 1956, **9**, 341.
[11] Hirokawa, *Acta Cryst.*, 1955, **8**, 637.
[12] Jellinek, *Acta Cryst.*, 1957, **10**, 277.
[13] Przybylska, *Acta Cryst.*, 1961, **14**, 424.
[14] Przybylska, *Acta Cryst.*, 1961, **14**, 429.
[15] Fridrichsons and Mathieson, *Acta Cryst.*, 1955, **8**, 761.
[16] Tunell, *Amer. Min.*, 1939, **24**, 448.
[17] Robertson and Woodward, *J.*, 1937, 219; 1940, 36; Sim, in " Computing Methods and the Phase Problem in X-ray Crystal Analysis," ed. Pepinsky, Robertson, and Speakman, Pergamon Press, Oxford, 1961, p. 227.

by calculating the two-dimensional Patterson synthesis along the *a*-axis (Fig. 4) and the section at $z = \frac{1}{2}$ through the three-dimensional Patterson synthesis (Fig. 5).

The first three-dimensional Fourier synthesis was evaluated with the measured values of the structure amplitudes and the phase constants appropriate to the iodine atom alone. When the resulting electron-density distribution was displayed as contoured sections drawn on sheets of glass and stacked in a frame various significant peaks were apparent. These could be attributed to carbon atoms (2), (3), (5), (6), (7), (8), (9), (10), (11), (12), (13), (14), (15), (16), (19), (20), (21), (22), (23), nitrogen atoms (1) and (4), and oxygen atom (25). Co-ordinates were assigned to these atoms and they were included in the calculation of a second set of structure amplitudes and phase constants. The value of R, the average discrepancy between the calculated and measured structure amplitudes, was 27·4%.

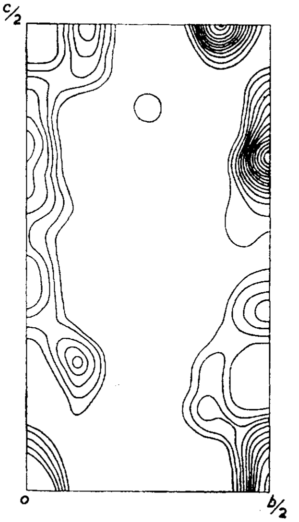

FIG. 4. Patterson projection along the *a*-axis.

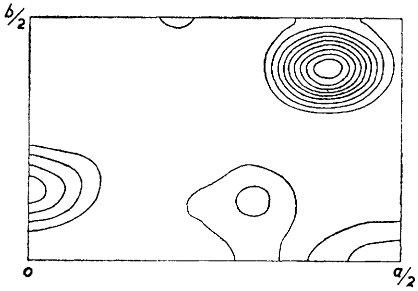

FIG. 5. Section through the three-dimensional Patterson synthesis at $z = \frac{1}{2}$.

The improved phase constants were employed in the computation of a second three-dimensional Fourier synthesis in which it was possible to locate without ambiguity the remaining atoms C(17), C(18), C(24), O(26), and O(27). When structure factors were recalculated with the inclusion of these additional atoms the value of R fell to 21·3%.

Three further rounds of structure-factor and Fourier calculations were carried out. Back-shift corrections for terminations of series were derived at each stage from a three-dimensional F_c synthesis and individual isotropic temperature factors were assigned. The value of R was reduced to 16·7%.

The refinement was concluded by performing two cycles of least-squares adjustment of the positional and anisotropic thermal parameters of the atoms; the programme employed was that devised by Dr. J. S. Rollett.[18] The value of the discrepancy factor R fell to 14·5%.

The theoretical atomic scattering factors employed in the structure-factor calculations were those of Berghuis *et al.*[19] for carbon, nitrogen, and oxygen, and the Thomas–Fermi values [20] for iodine. The final atomic co-ordinates are listed in Table 1, details of the progress of the analysis are summarized in Table 4 and the final values of $|F_o|$, $|F_c|$, and α are shown in Table 5. The parameters defining the anisotropic thermal vibrations are in Table 6; they are values of b_{ij} in the equation

$$\exp(-B\sin^2\theta/\lambda^2) = 2^{-(b_{11}h^2 + b_{22}k^2 + b_{34}l^2 + b_{12}hk + b_{23}kl + b_{13}hl}$$

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[18] Rollett, in " Computing Methods and the Phase Problem in X-ray Crystal Analysis," ed. Pepinsky, Robertson, and Speakman, Pergamon Press, Oxford, 1961, p. 87.

[19] Berghuis, Haanappel, Potters, Loopstra, MacGillavry, and Veenendaal, *Acta Cryst.*, 1955, **8**, 478.

[20] " Internationale Tabellen zur Bestimmung von Kristallstrukturen," Borntraeger, Berlin, 1935, Vol. II, p. 572.

TABLE 4.

Progress of the structure analysis.

Patterson syntheses

↓

I atom

↓

1st F calculation ($R = 31{\cdot}6\%$)
1st three-dimensional F_o synthesis

↓

I + 22 light atoms

↓

2nd F calculation ($R = 27{\cdot}4\%$)
2nd three-dimensional F_o synthesis

↓

I + 27 light atoms

↓

3rd F calculation ($R = 21{\cdot}3\%$)
3rd three-dimensional F_o synthesis
1st three-dimensional F_c synthesis

↓

4th F calculation ($R = 18{\cdot}7\%$)
4th three-dimensional F_o synthesis
2nd three-dimensional F_c synthesis

↓

5th F calculation ($R = 17{\cdot}3\%$)
5th three-dimensional F_o synthesis
3rd three-dimensional F_c synthesis

↓

6th F calculation ($R = 16{\cdot}7\%$)

↓

Two rounds of least-squares refinement of co-ordinates and anisotropic
temperature factors ($R = 14{\cdot}5\%$)

↓

Final three-dimensional F_o synthesis.

The standard deviations of the final atomic co-ordinates were derived from the least-squares residuals by application of the equation

$$\sigma^2(x_i) = \sum w_j(\Delta F_j)^2/[(n - s)\sum w_j(\partial F_j/\partial x_i)^2].$$

The results are listed in Table 3.

The final three-dimensional electron-density distribution was evaluated on the basis of the phase constants in Table 5 and is shown in Fig. 1 by means of superimposed contour sections drawn parallel to (010). The corresponding atomic arrangement is illustrated in Fig. 2.

TABLE 5.

Measured and calculated values of the structure factors.

h	*k*	*l*	F_o	F_c	α°
0	0	2	130	164	0
		4	12	1	0
		6	70	78	180
		8	29	46	180
		10	12	18	180
		12	67	59	0
		14	74	68	0
		16	37	35	0
		20	24	21	180
		22	9	9	180
0	1	1	46	34	270
		2	29	21	90
		3	31	38	90
		4	58	69	270
		5	80	91	270
		6	16	20	270
		7	106	142	270
		8	28	30	90
		9	92	101	270
		10	31	32	90
		11	26	17	90
		12	8	7	90
		13	61	53	90
		15	28	24	90
		16	20	16	270
		17	9	3	90
		18	15	13	270
		19	25	13	270
		20	12	2	270
		21	15	12	270
0	2	0	343	325	180
		1	75	72	0
		2	32	18	0
		3	129	130	0
		4	101	91	0
		5	88	94	0
		6	110	119	0
		7	20	15	180
		8	50	68	0
		9	42	46	180
		10	28	29	0
		11	55	56	180
		12	23	19	180
		13	17	16	180
		14	31	29	180
		15	15	11	0
		16	29	28	180
		17	15	15	0
		18	14	7	0
		19	13	11	0
		20	22	16	0
0	3	1	84	80	270
		2	23	20	90
		3	52	51	270
		4	55	56	90
		5	20	11	90
		6	43	46	90
		7	43	45	90
		8	48	51	270
		9	26	33	90
		10	54	58	270
		11	29	29	270
		12	45	50	270
		13	52	50	270
		15	18	19	270
		16	23	18	90
		18	18	15	90
0	4	0	115	117	0
		1	52	46	180
		2	42	35	180
		3	178	177	180
		4	12	3	180
		5	166	151	180
		6	25	17	180
		9	52	55	0
		11	37	49	0
		14	13	11	0
		15	15	13	180
		17	34	29	180
		19	16	14	180
0	5	1	26	17	270
		2	48	39	270
		3	24	22	90
		4	93	91	270
		5	23	18	270
		6	36	38	270
		7	11	12	270
		8	33	33	90
		10	49	54	90
		12	31	36	90
		13	15	14	270
		16	29	21	270
		18	18	16	270
0	6	0	38	38	0
		1	41	34	0
		2	52	49	0
		3	79	73	0
		4	16	14	180
		5	56	53	0
		6	34	36	180
		8	24	20	180
		9	35	36	180
		11	31	35	180
		13	9	16	180
		14	12	12	0
		17	15	13	0
0	7	1	12	7	90
		2	22	17	90
		3	12	12	270
		4	53	55	90
		5	24	23	270
		6	15	14	90
		7	31	32	270
		8	24	29	270
		9	20	28	270
		10	22	26	270
		12	17	20	270
		13	11	12	90
		15	10	9	90
		16	14	13	90
0	8	0	76	74	180
		2	45	51	180
		3	24	25	180
		4	18	17	0
		5	13	11	180
		6	20	24	0
		8	19	25	0
		9	12	15	0
		12	13	12	180
		14	20	17	180
0	9	1	29	32	270
		4	12	18	270
		7	21	29	90
		9	11	16	90
		13	15	16	270
0	10	0	19	22	0
		2	13	19	0
		6	12	17	180
		8	14	18	180
0	11	1	13	18	90
1	0	2	8	8	0
		3	143	198	90
		4	47	57	180
		5	58	81	90
		6	33	34	180
		7	8	5	270
		8	15	17	0
		9	77	79	270
		10	13	12	0
		11	67	76	270
		12	16	16	0
		13	29	34	270
		15	13	11	90
		17	27	24	90
		18	10	7	180
		19	16	17	90
		20	8	0	180
1	1	0	23	10	90
		1	56	42	119
		2	104	79	152
		3	73	80	259
		4	157	169	176
		5	92	100	310
		6	56	78	174
		7	43	53	11
		8	65	66	7
		9	36	41	43
		10	77	93	7
		11	23	23	112
		12	48	47	347
		13	14	15	139
		15	21	21	214
		16	38	36	179
		17	10	13	260
		18	20	24	181
		19	9	7	338
1	2	0	174	142	270
		1	64	66	357
		2	80	66	306
		3	224	180	260
1	2	4	46	39	46
		5	83	85	263
		6	56	57	77
		7	14	15	212
		8	49	64	112
		9	52	52	88
		10	29	32	134
		11	37	39	86
		12	25	25	227
		13	12	17	67
		14	22	25	288
		17	29	28	279
		19	11	11	245
1	3	0	63	49	90
		1	221	170	338
		2	65	54	26
		3	51	41	45
		4	71	65	6
		5	51	39	143
		6	66	63	310
		7	61	66	191
		8	38	40	227
		9	27	35	205
		10	41	48	197
		11	15	17	339
		12	40	39	136
		13	56	56	350
		14	13	10	75
		15	30	33	6
		16	16	18	19
		21	11	11	175
1	4	0	102	86	90
		1	75	62	169
		2	66	63	106
		3	79	67	40
		4	45	42	280
		5	15	11	30
		6	106	100	270
		7	18	12	330
		8	76	82	277
		9	26	23	312
		10	13	20	280
		11	10	17	304
		12	18	22	81
		13	10	8	265
		14	26	27	90
		16	14	18	88
		17	9	8	102
		18	9	5	225
		20	12	11	266
1	5	0	58	50	270
		1	99	91	162
		2	45	41	314
		3	23	29	272
		4	26	22	251
		5	72	61	2
		6	20	21	98
		7	64	66	352
		8	21	19	84
		9	38	45	354
		11	10	12	186
		12	20	25	240
		13	33	40	176
		15	22	29	189
		19	10	9	10
1	6	0	113	102	270
		1	36	34	24
		2	51	49	282
		3	29	29	150
		4	13	17	161
		5	42	43	112
		6	45	42	86
		7	14	14	184
		8	37	43	90
		9	10	17	251
		10	10	14	55
		11	11	13	295
		12	17	25	282
		13	10	10	307
		14	25	25	267
1	7	0	19	11	90
		1	51	53	328
		2	32	31	180
		3	10	6	338
		4	39	39	182
		5	32	34	224
		6	18	15	227
		7	33	34	177
		8	17	17	302
		9	13	18	147
		10	18	25	344
		12	12	17	36
		13	12	17	4
		14	9	2	100
		15	11	12	352
		16	11	11	172
1	8	0	13	17	90
		1	22	23	242
		3	33	34	287
		4	17	22	342
		5	33	35	270
		6	18	18	274
		7	10	3	324
		8	16	19	257
		9	12	21	84
		11	16	22	103
		13	8	8	109
1	9	1	13	14	126
		2	24	27	351
		4	27	27	349
		5	14	20	80
		10	13	19	179
		11	11	6	281
		13	7	3	196
1	10	3	17	20	97
		4	11	13	209
		5	16	26	86
		10	11	5	325
1	11	1	8	7	200
		2	9	14	191
		4	10	15	171
2	0	2	70	94	0
		3	22	16	270
		4	42	50	180
		5	66	70	270
		6	83	94	180
		7	76	85	270
		8	54	70	180
		9	49	56	270
		10	22	26	180
		11	13	13	90
		12	39	31	0
		13	27	24	90
		14	53	52	0
		15	19	15	90
		16	11	5	0
		19	14	13	270
		20	13	13	180
2	1	0	272	237	180
		1	224	174	75
		2	76	64	195
		3	62	64	31
		4	82	82	302
		5	42	45	292
		6	66	77	341
		7	93	115	274
		8	38	41	342
		9	37	47	253
		10	24	22	46
		11	28	24	138
		12	22	22	177
		13	46	46	100
		14	39	43	173
		15	29	29	79
		16	13	12	214
		19	13	11	285
2	2	0	31	17	180
		1	146	115	303
		2	125	110	186
		3	95	86	352
		4	111	85	48
		5	47	35	6
		6	109	104	22
		7	21	27	81
		8	49	67	345
		9	48	57	141
		10	26	32	301
		11	35	38	209
		12	29	26	198
		13	35	38	240
		14	34	38	178
		15	16	16	307
		16	15	15	138
		17	15	16	342
		19	11	10	28
2	3	0	68	59	0
		1	85	77	248
		2	109	95	86
		3	103	96	178
		4	100	92	99
		5	61	61	175
		6	79	74	150
		7	53	57	80
		8	38	40	222
		9	43	51	32
		10	50	59	256
		11	25	28	4
		12	35	37	265
		13	29	29	303
		14	11	14	2
		15	11	7	216
		16	15	16	87
		17	15	16	197
		18	17	16	102
2	4	0	55	47	0
		1	53	39	141
		2	38	40	329
		3	85	81	179
		4	41	42	276
		5	50	46	195
		6	28	27	248
		8	17	20	74
		9	51	53	347
		10	37	46	94
		11	29	35	16
		12	15	20	86
		13	15	22	22
		14	16	16	338
		16	10	12	269
		17	23	22	169
2	5	0	12	10	180
		1	43	32	324
		2	79	75	286
		3	72	68	355
		4	92	80	258
		5	52	48	1
		6	29	30	246
		7	10	9	230
		8	12	17	134
		9	31	35	176
		10	39	48	92
		11	24	24	161
		12	11	22	98
		13	13	17	160
		16	16	18	290
		18	17	17	261
2	6	0	27	19	0
		1	38	38	21
		2	32	29	26
		3	56	52	6
		4	57	50	72
		5	37	41	1
		6	30	24	124
		7	10	7	274
		8	20	29	220
		9	33	36	189
		10	19	28	275
		11	21	32	181
2	7	0	47	41	180
		1	35	35	113
		2	47	46	131
		3	31	31	162
		4	35	37	61
		5	37	37	240
		6	13	18	53
		7	24	23	263
		8	16	20	318
		9	19	20	306
		10	17	21	280
		15	10	17	104
2	8	0	17	12	180
		2	13	17	216
		3	13	14	187
		4	13	18	292
		5	16	23	147
		6	23	26	349
		7	15	22	101
		8	20	31	12
2	9	0	20	23	0
		1	27	32	264
		2	15	20	327
		4	13	16	181
		5	10	17	82
		6	14	13	179
2	10	0	9	14	0
		1	15	16	104
		6	13	18	195
3	0	1	75	109	90
		2	94	100	180
		3	71	86	90
		4	146	161	180
		5	32	36	90
		6	42	51	180
		7	49	40	270
		8	95	74	0
		9	24	22	270
		10	90	87	0
		11	31	33	270
		12	36	35	0
		13	38	39	270
		15	12	12	90
		16	48	48	180
		17	18	16	90
		18	24	27	180
		19	10	11	90
3	1	0	151	137	270
		1	35	51	306
		2	85	82	229
		3	138	134	278
		4	110	115	174
		5	60	80	308
		6	46	60	180
		7	43	46	340
		8	14	21	68
		9	62	62	58
		10	74	68	3
		11	52	49	95
		12	27	25	336
		14	18	17	267
		15	12	6	150
		16	14	13	193
		17	14	18	270
		18	11	14	193
		19	12	12	285
3	2	0	71	67	270
		1	86	63	301
		2	99	89	338
		3	116	101	298
		4	78	73	351
		5	61	58	205
		6	37	41	39
		7	73	73	165
		8	21	32	158
		9	26	36	162
		10	56	57	184
		11	23	23	49
		12	37	38	213
		13	41	41	29
		14	20	23	256
		15	22	22	327
		16	29	33	339
		17	23	20	269
		18	13	12	346
3	3	0	80	71	90
		1	103	75	10
		2	48	43	79
		3	86	79	66
		4	78	61	301
		5	75	62	109
		6	72	68	286
		7	77	74	180
		8	49	59	255
		9	43	51	225
		10	39	46	201
		11	21	22	279
		12	11	14	198
		13	20	23	0
		14	14	15	93
		15	12	10	342
		16	11	11	74
		17	13	18	80
3	4	0	64	55	90
		1	113	107	167
		2	42	39	102
		3	51	48	155
		4	45	37	199
		5	45	37	11
		6	53	47	262
		7	64	60	344
		8	31	35	281
		9	33	39	350
		10	11	16	325
		11	24	29	189
		12	16	17	78
		13	57	66	193
		14	17	20	73
		15	26	28	166
3	5	0	96	83	270
		1	52	48	195
		2	53	48	291
		3	29	25	142
		4	37	35	97
		5	34	33	31
		6	54	56	95
		7	54	54	1
		8	42	48	106
		9	31	36	2
		10	11	12	49
		12	14	15	206
		13	17	18	202
		14	21	22	269
3	6	0	54	50	270
		1	32	32	15
		2	42	42	217
		3	25	19	13
		4	15	11	175
		5	34	38	174
		6	31	29	106
		7	48	50	184
		8	18	20	69
		9	25	31	201
		10	17	21	2
		11	12	14	284
		12	14	19	315
		13	18	25	358
		14	19	19	254
		15	19	12	350
3	7	0	57	56	90
		1	26	21	332
		2	39	41	131
		3	33	31	277
		4	32	31	201
		5	23	22	238
		6	23	20	236
		7	25	22	193
		8	12	17	285
		12	15	21	50
		13	10	14	45
		14	17	17	85
3	8	1	19	22	218
		2	26	29	14
		3	22	22	267
		4	29	27	340
		5	17	17	308
		6	18	19	318
		7	11	15	354
		8	16	20	216
		10	18	22	185
3	9	1	11	12	125
		2	16	19	356
		3	26	28	91
		4	17	18	10
		5	17	18	86
		6	15	12	30
		9	13	16	276
3	10	0	12	2	270
		2	15	18	180
4	0	1	70	92	90
		2	9	9	0
		3	34	47	90
		4	12	9	180
		5	83	86	270
		6	73	67	180
		7	119	132	270
		9	46	53	270
		10	12	3	180
		12	14	12	0
		13	54	51	90
		15	33	29	90
		16	18	19	0
		19	15	14	270
4	1	0	268	235	180
		1	66	55	0
		2	106	97	205
		3	69	67	40
		4	25	21	283
		5	20	23	22
		6	73	83	356
		7	37	40	266
		8	89	91	353
		9	31	34	236
		10	16	19	21
		11	33	27	165
		12	56	50	176
		13	17	19	116
		14	33	35	181
		15	13	15	42
		16	15	18	205
		20	11	15	353
4	2	0	88	70	180
		1	84	75	267
		2	59	40	60
		3	27	21	28
		4	94	76	55
		5	89	66	55
		6	39	33	30
		7	73	85	97
		8	32	41	286
		9	34	41	106
		10	39	43	283
		11	18	17	177
		12	30	32	254
		13	45	47	269
		15	18	19	277
		16	25	24	138
		18	14	14	73
4	3	0	90	80	0
		1	69	52	195
		2	53	41	41
		3	141	126	198
		4	13	4	100
		5	93	89	185
		6	44	47	172
		7	35	39	81
		8	39	45	198
		9	37	39	13
		11	33	42	353
		12	36	38	320
		14	20	20	332
		15	12	11	222
		16	12	13	13
		17	26	25	175
4	4	0	50	44	0
		1	35	29	106
		2	103	85	272
		3	48	46	176
		4	89	79	267
		5	41	41	213
		6	30	33	263
		7	27	25	272
		8	26	29	70
		9	11	14	336
		10	41	50	93
		11	17	25	350
		12	36	43	82
		16	23	24	289
		18	15	14	266
4	5	1	48	44	338
		2	37	39	312
		3	95	89	357
		4	31	27	289
		5	68	69	3
		6	19	20	216
		9	29	38	188
		11	25	36	177
		13	12	14	198
		14	12	7	43
		17	20	21	346
4	6	0	11	11	0
		2	41	39	89
		3	21	16	323
		4	56	62	87
		5	23	24	306
		6	19	21	118
		7	23	23	246
		8	28	30	244
		9	22	28	246
		10	22	32	275
		11	13	13	150
		12	15	23	267
		16	15	17	104
4	7	0	48	47	180
		1	19	17	148
		2	32	36	155
		3	35	36	176
		5	18	23	195
		6	22	28	12
		7	13	4	30
		8	13	21	359
		9	15	24	332
		11	15	22	0
		13	11	6	41
4	8	1	22	29	275
		2	15	17	257
		3	18	18	226
		4	15	23	272
		5	15	17	95
		6	12	15	331
		7	24	29	91
		8	12	17	45
		9	12	21	80
		13	13	12	270
4	9	0	25	28	0
		1	12	14	245
		2	12	21	2
		6	16	24	182
		7	11	8	90
		8	15	21	178
4	10	1	19	21	94
5	0	1	11	19	90
		2	34	57	180
		3	5	4	90
		4	152	178	180
		5	20	16	270
		6	47	50	180
		8	27	30	0
		9	24	20	270

TABLE 5. (*Continued.*)

h	*k*	*l*	F_o	F_c	α°
		10	75	74	0
		12	39	40	0
		16	20	20	180
		18	18	25	180
5	1	0	49	57	270
		1	79	72	54
		2	31	32	343
		3	143	137	269
		4	19	8	65
		5	48	64	269
		6	20	24	118
		7	28	26	146
		8	20	24	105
		9	71	65	85
		10	11	12	86
		11	50	51	92
		12	12	12	274
		13	28	38	91
		14	16	13	264
		15	23	23	259
		17	25	28	267
5	2	1	120	98	341
		2	95	73	356
		3	42	35	322
		4	158	123	359
		5	56	44	139
		6	32	38	19
		7	65	77	202
		8	28	28	156
		9	30	34	188
		10	53	60	180
		12	33	37	165
		13	20	23	356
		15	21	21	355
		16	18	17	1
5	3	0	117	91	90
		1	14	8	144
		2	65	57	119
		3	76	71	83
		4	30	26	316
		5	39	40	95
		6	78	82	285
		7	10	7	359
		8	53	58	264
		9	32	34	287
		11	21	22	238
		12	34	39	91
		13	21	22	246
		14	26	29	87
		16	12	17	97
		17	12	14	79
5	4	0	18	12	90
		1	126	99	164
		2	25	13	138
		3	9	4	224
		4	39	32	192
		5	48	43	333
		6	15	14	81
		7	70	76	359
		9	42	46	359
		10	18	14	20
		13	23	29	189
		15	20	22	185
5	5	0	97	91	270
		1	25	21	41
		2	42	40	279
		4	17	9	107
		5	25	17	24
		6	62	61	90
		7	12	10	264
		8	46	52	94
		12	24	32	274
		14	25	30	258
5	6	1	72	65	347
		2	24	21	174
		3	21	15	2
		4	32	27	185
		5	37	32	166
		6	25	22	158
		7	48	50	179
		9	16	28	186
		11	13	15	334
		12	13	16	25
		13	15	20	3
5	7	0	44	47	90
		1	30	37	295
		2	13	15	118
		3	33	33	299
		4	13	11	300
		5	16	24	286
		6	23	28	269
		7	13	14	51
		8	26	33	252
		9	13	13	69
		11	12	21	94
5	8	1	21	25	147
		2	21	21	350
		4	32	34	357
		6	13	18	351
		9	12	8	32
5	9	1	12	20	69
		3	24	26	95
		5	12	21	76
5	10	4	12	23	194
6	0	1	85	127	90
		2	6	1	0
		3	18	20	90
		4	24	26	0
		5	20	25	270
		6	57	50	0
		7	74	81	270
		8	41	41	0
		9	49	54	270
		11	12	5	90
		12	32	32	180
		13	33	36	90
		15	30	31	90
		16	13	7	180
6	1	0	77	86	180
		1	21	19	343
		2	67	70	189
		3	38	34	6
		4	57	53	15
		5	24	21	0
		6	112	117	3
		7	19	17	108
		8	60	64	339
		9	31	33	152
		10	14	15	351
		11	17	19	201
		12	37	36	191
		13	16	20	238
		14	33	38	185
		15	13	7	331
		16	12	18	169
		20	10	12	348
6	2	0	80	70	0
		1	142	116	260
		2	61	52	81
		3	70	51	194
		4	97	80	69
		5	23	23	164
		6	55	56	135
		7	59	65	87
		8	22	19	176
		9	27	35	85
		10	29	32	274
		11	15	15	349
		12	23	25	299
		13	30	32	271
		15	20	24	259
6	3	0	44	38	0
		1	66	50	123
		2	46	38	348
		3	107	93	192
		4	21	14	181
		5	53	51	181
		6	65	58	182
		7	13	8	355
		8	24	23	182
		9	46	59	345
		10	12	14	169
		11	35	40	6
		12	20	17	23
		13	16	17	50
		14	16	14	5
		15	13	13	163
		17	13	19	187
6	4	0	11	8	0
		1	30	23	84
		2	72	60	286
		3	55	51	347
		4	80	70	268
		5	42	40	351
		6	43	41	288
		7	32	37	223
		8	17	15	46
		9	19	25	205
		10	34	44	86
		11	13	14	161
		12	24	34	106
		16	18	14	273
6	5	1	43	32	329
		2	13	11	101
		3	74	70	6
		4	21	21	154
		5	44	42	1
		9	36	51	192
		11	24	35	171
		15	11	11	347
6	6	0	25	21	180
		1	34	29	92
		2	48	44	108
		3	49	39	139
		4	54	56	74
		5	12	12	219
		6	30	30	63
		8	13	12	321
		10	22	33	265
		12	15	20	284
6	7	0	31	29	180
		1	13	14	140
		2	16	15	198
		3	34	38	205
		4	29	30	314
		5	20	23	197
		6	24	26	339
		8	18	29	12
6	8	0	22	28	0
		1	26	28	257
		2	16	20	296
		3	16	15	291
		4	18	19	224
		5	15	17	89
		6	12	10	235
		7	15	21	108
6	9	0	22	25	0
		2	12	17	7
6	10	1	11	20	63
7	0	1	16	24	270
		2	67	94	180
		3	73	86	270
		4	78	87	180
7	0	5	20	25	270
		6	43	51	180
		7	23	24	270
		8	16	13	0
		9	42	41	90
		10	68	71	0
		11	28	26	90
		12	20	28	0
		14	17	3	0
		15	17	13	270
		16	20	21	180
		17	15	12	270
7	1	0	28	37	270
		1	46	46	317
		2	32	34	332
		3	73	84	300
		4	78	74	9
		5	40	63	275
		6	26	28	76
		7	15	15	189
		8	23	29	153
		9	41	38	82
		10	32	34	185
		11	38	36	73
		12	20	17	182
		13	17	18	43
		16	16	20	343
		17	15	14	288
7	2	0	56	55	90
		1	45	33	4
		2	69	48	13
		3	54	45	71
		4	69	63	324
		5	50	43	134
		6	34	39	327
		7	38	43	177
		8	30	34	237
		9	42	53	232
		10	45	48	193
		11	16	18	278
		12	21	22	171
		13	24	25	339
		16	16	14	0
7	3	0	107	81	90
		1	48	36	132
		2	78	58	125
		3	45	38	93
		4	60	51	207
		5	49	42	35
		6	27	28	279
		7	34	37	354
		8	18	18	268
		9	33	37	321
		11	17	26	245
		13	21	23	193
		14	21	24	85
		15	16	13	155
		16	22	21	122
7	4	0	89	69	270
		1	56	46	177
		2	48	38	252
		3	23	25	197
		4	20	18	159
		5	55	47	350
		6	37	29	101
		7	69	71	348
		8	20	22	102
		9	35	44	22
		10	17	17	342
		13	21	25	183
7	5	0	81	74	270
		1	39	37	349
		2	50	43	261
		3	24	16	23
		4	19	22	63
		5	19	23	187
		6	34	38	118
		7	31	31	173
		8	17	20	102
		9	17	20	186
		13	16	20	8
		14	19	24	252
7	6	0	43	37	90
		1	43	32	350
		3	29	29	311
		4	24	27	230
		5	17	19	206
		6	24	23	233
		7	27	31	163
		8	17	25	295
		9	21	22	187
7	7	0	17	19	90
		1	24	20	188
		3	24	24	235
		4	24	20	295
		6	27	34	304
		8	17	19	230
7	8	0	17	19	270
		1	17	15	135
		2	20	21	2
		3	17	23	104
		4	20	21	354
7	9	3	15	23	95
8	0	1	39	68	90
		2	34	43	180
		3	26	29	90
		4	23	25	0
		5	44	45	270
		6	51	53	0
		7	23	33	270
		8	64	63	0
		9	16	20	270
		12	35	38	180
		13	33	32	90
		14	23	24	180
		15	18	21	90
8	1	0	54	60	180
		1	103	98	272
		2	11	15	195
		3	10	12	36
		4	23	24	85
		5	48	52	63
		6	30	35	11
		7	54	54	93
		8	43	43	339
		9	17	15	120
		10	12	21	315
		11	18	17	110
		13	23	30	258
		15	23	21	272
8	2	0	58	47	0
		1	55	38	220
		2	73	66	32
		3	61	50	210
		4	32	27	70
		5	56	43	123
		6	41	39	167
		7	40	41	88
		8	33	40	196
		9	27	32	17
		10	22	24	278
		11	23	19	5
		12	38	38	336
		14	19	20	1
8	3	0	65	55	0
		1	63	43	119
		2	64	43	294
		3	39	41	222
		4	74	62	267
		5	43	44	228
		6	22	28	266
		7	23	26	252
		8	17	19	145
		10	29	37	96
		11	23	26	330
		12	27	25	59
8	4	1	36	24	0
		2	31	29	268
		3	54	49	11
		4	46	44	272
		5	47	44	339
		6	17	24	290
		8	29	32	49
		9	26	36	189
		12	13	19	118
8	5	1	30	26	335
		2	42	32	79
		3	30	25	353
		4	50	49	85
		5	18	23	356
		6	23	22	82
		10	23	32	262
8	6	0	19	12	180
		1	23	20	160
		2	23	22	111
		3	33	35	188
		4	27	27	62
		5	23	25	207
		6	19	22	32
8	7	1	27	27	244
		2	13	18	248
		3	19	19	216
		4	19	25	265
8	8	0	22	26	0

TABLE 6.

Anisotropic temperature-factor parameters ($b_{ij} \times 10^5$).

	b_{11}	b_{22}	b_{33}	b_{12}	b_{23}	b_{13}
N(1)	494	1540	544	−1	−9	114
C(2)	325	1770	586	95	37	314
C(3)	144	2676	935	−356	682	−688
N(4)	996	1549	601	−8	20	−304
C(5)	992	2397	737	84	791	271
C(6)	119	2068	602	228	379	−1019
C(7)	918	2049	699	735	−151	−460
C(8)	1033	1226	504	419	112	1026
C(9)	351	1496	726	3	−935	−709
C(10)	463	1625	524	−82	−68	−293
C(11)	1243	1489	818	60	−263	−678
C(12)	1647	1349	677	497	−559	132
C(13)	528	1243	607	188	113	322
C(14)	707	2673	724	617	−313	723
C(15)	244	2157	680	−230	−494	456
C(16)	1329	1122	744	−356	263	1411
C(17)	341	2307	808	−684	338	−506
C(18)	915	2044	787	−63	303	46
C(19)	406	2424	858	−249	92	−977
C(20)	667	2121	588	−358	63	114
C(21)	1129	2700	651	244	290	627
C(22)	491	1677	744	−65	165	−1689
C(23)	1654	1371	1033	1016	−88	74
C(24)	2465	2033	476	−111	−1226	−185
O(25)	336	2138	625	79	149	242
O(26)	298	1697	889	−22	107	−370
O(27)	398	2081	976	3	120	−407
I	814	1964	609	66	145	1

The extensive calculations were carried out on the Glasgow University DEUCE computer with programmes devised by Dr. J. S. Rollett and Dr. J. G. Sime. We are grateful to Dr. A. R. Battersby for suggesting the problem and for supplies of material. One of us (A. T. McP.) is indebted to the Department of Scientific and Industrial Research for financial support.

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[*Received, October 5th,* 1962.]