378. *The Crystal and Molecular Structure of (+)-10-Bromo-2-chloro-2-nitrosocamphane.*

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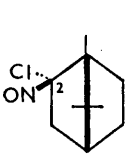
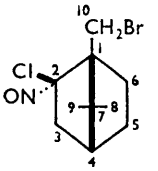
Crystals of (+)-10-bromo-2-chloro-2-nitrosocamphane have been subjected to quantitative *X*-ray analysis. They are orthorhombic, of space group $P2_12_12_1$-D_2^4, with eight molecules of $C_{10}H_{15}BrClNO$ in the unit cell. The asymmetric crystal unit consists of two chemical molecules. Successive three-dimensional Fourier syntheses served to locate all the atoms apart from hydrogen. The two crystallographically independent molecules appear to be identical chemically, differing only in orientation in the unit cell. The presence of the bulky chlorine atom *cis* to the CMe_2 bridge causes some distortion of the camphane molecular framework.

A number of rotatory dispersion studies of monomeric nitroso-compounds have been reported by Mitchell and his co-workers. In the case of (−)-2-chloro-2-nitrosocamphane[1,2] (I) it was found that irradiation of an alcoholic solution with red light caused a gradual inversion of the Cotton effect and this was attributed to inversion of configuration at position 2.

The behaviour of (+)-10-bromo-2-chloro-2-nitrosocamphane (II) on irradiation with red light is somewhat different,[3] for although the Cotton effect is altered its sign remains unchanged and there is a marked shift in the absorption maximum, suggesting that the



(I)



(II)

change in molecular structure on irradiation in this case may not be simply an inversion at position 2. An *X*-ray study of the starting material and of the irradiated material seemed an attractive way of establishing the details of the reaction in this case, and we have now completed the analysis of the starting material and find that its stereochemistry is represented by (II) (or its mirror image). It is hoped to be able to report the study of the irradiated material later.

Crystal Data.—(+)-10-Bromo-2-chloro-2-nitrosocamphane, $C_{10}H_{15}BrClNO$; $M = 280{\cdot}6$. Orthorhombic, $a = 23{\cdot}11$, $b = 11{\cdot}32$, $c = 9{\cdot}03$ Å, $U = 2362$ Å^3, $D_m = 1{\cdot}562$ (by flotation), $Z = 8$, $D_c = 1{\cdot}578$, $F(000) = 1136$, space group $P2_12_12_1$ (D_2^4). Absorption coefficient for *X*-rays ($\lambda = 1{\cdot}542$ Å), $\mu = 66{\cdot}7$ cm.$^{-1}$.

Structure Analysis.—The crystal data show that the asymmetric crystal unit consists of two crystallographically independent chemical molecules, necessitating the location of 28 atoms other than hydrogen. Because of the presence of the bromine and chlorine atoms, however, there was no need to postulate trial structures with assumptions as to the stereochemistry and relative orientation of the molecules, the analysis proceeding on the basis of the usual phase-determining heavy-atom method.

The positions of the bromine atoms were determined initially from two-dimensional Patterson syntheses along the *b* and *c* crystal axes and were confirmed by inspection of the three-dimensional Patterson function. The projections are shown in Fig. 1.

Attempts to elucidate the structure in projection proved fruitless because of the considerable overlap and in consequence recourse was made to three-dimensional methods for the location of the remaining atoms in the asymmetric crystal unit. The first three-dimensional Fourier synthesis was calculated with phase angles appropriate to the bromine atoms alone and served

[1] Mitchell, Watson, and Dunlop, *J.*, 1950, 3440.
[2] Hope and Mitchell, *J.*, 1953, 3483.
[3] Davidson, Ph.D. Thesis, University of Glasgow, 1958.

to locate the two chlorine atoms in the asymmetric unit. A number of other peaks corresponding to some of the lighter atoms were also well resolved in this synthesis, but as it was not possible at this stage to identify chemically many of these atoms with certainty, only the bromine and chlorine atoms were included in the next calculation of phase angles.

The improved phase angles were employed in the computation of a second three-dimensional Fourier synthesis in which it was possible to locate, in addition to the bromine and chlorine atoms, the nitroso-group and carbon atoms (1), (2), (3), (4), and (10) of both molecules in the asymmetric crystal unit. These atoms were then included in the calculation of a third set of phase angles which led, in turn, to a third three-dimensional Fourier synthesis in which all the atoms (apart from hydrogen) in the asymmetric crystal unit could be located.

FIG. 1*a*.

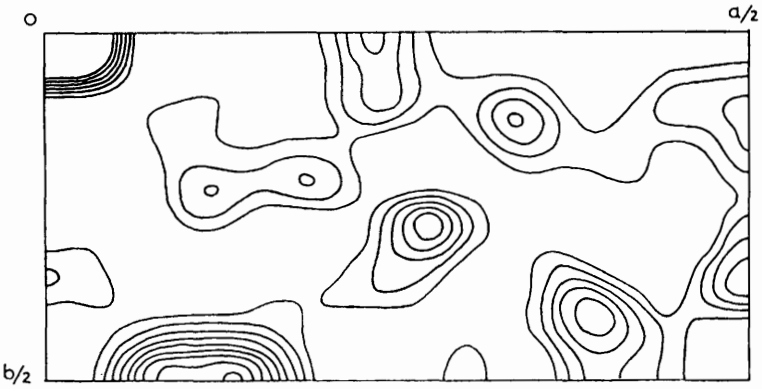


FIG. 1*b*.

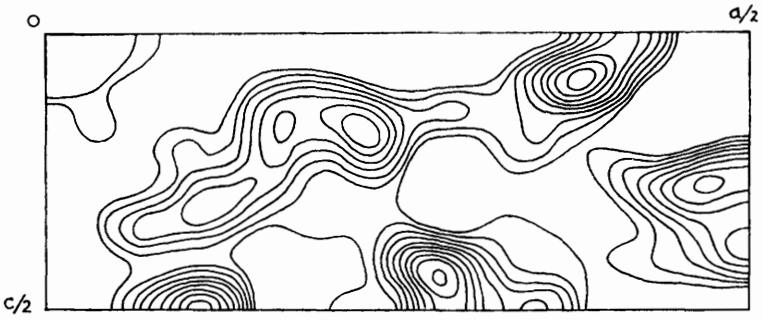


FIG. 1*a and b*. *Patterson projections along the c and b axes. Contour scale arbitrary.*

Refinement was continued by means of a further F_o synthesis, followed by a cycle of least-squares adjustment of the positional and thermal parameters of the bromine, chlorine, nitrogen, and oxygen atoms, and completed by calculation of a final F_o synthesis with correction for termination-of-series errors by means of an F_c synthesis. The final average discrepancy between observed and calculated structure amplitudes is 15·5%.

The final co-ordinates are listed in Table 1, details of the progress of the structure analysis are shown in Table 2, and the final set of calculated and observed structure amplitudes is given in Table 3.

Superimposed contour sections parallel to (001) illustrating the final electron-density distribution over the two molecules in the asymmetric crystal unit are shown in Fig. 2. The atomic arrangement corresponding to this electron-density distribution is illustrated in Fig. 3.

Discussion.—In the application of the heavy-atom method to a non-centrosymmetrical crystal structure such as the present, the final electron-density distribution is dependent to a considerable extent on the choice of the correct set of atomic sites for the lighter atoms. It is not too difficult to obtain reasonable electron-density distributions in which wrongly placed

or even completely spurious atoms are present. This is brought out clearly, for example, in the description by Hodgkin *et al.* of the analysis of the structure of B_{12} hexacarboxylic acid.[4] In the case of projections along the crystallographic axes in $P2_12_12_1$, however, centrosymmetrical electron-density distributions are involved and these are much less dependent on the assumed light-atom positions, the signs of the structure factors employed in the Fourier syntheses being largely determined by the heavy atoms, *i.e.*, by the bromine and chlorine atoms in the present

FIG. 2. *Final three-dimensional electron-density distribution for* (+)-10-*bromo*-2-*chloro*-2-*nitrosocamphane, shown by means of superimposed contour sections parallel to* (001). *Contour interval* 1e/Å^3 *except around the* Cl *and* Br *atoms where it is* 2e/Å^3 *and* 5e/Å^3, *respectively.*

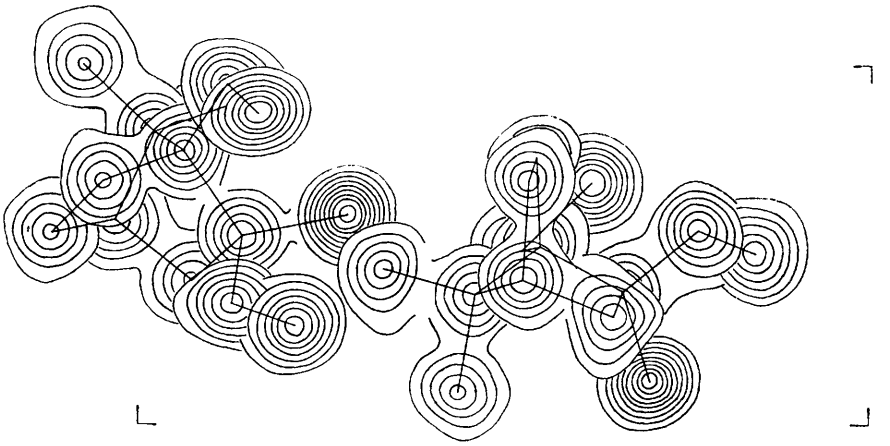
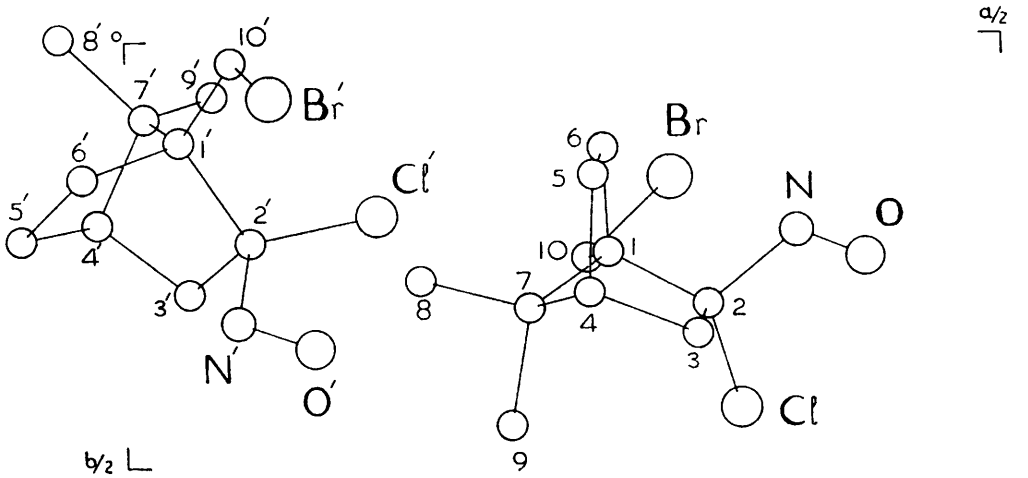


FIG. 3. *Atomic arrangement corresponding to* Fig. 2.



case. It is gratifying that the atomic positions deduced by the three-dimensional Fourier method conform extremely well with the electron-density projection along the *c* axis shown in Fig. 4.

The interatomic distances and interbond angles calculated from the atomic co-ordinates listed in Table 1 are given in Table 4. The two crystallographically independent molecules in the asymmetric crystal unit appear to be identical chemically. Even the bromine and oxygen atoms, which because of easy rotation about the C–C and C–N single bonds might have been expected to have rather different orientations in the two molecules, appear in fact to occupy positions with respect to the carbon framework of each molecule which are very similar.

[4] Hodgkin, Pickworth, Robertson, Prosen, Sparks, and Trueblood, *Proc. Roy. Soc.*, 1959, *A*, **251**, 306.

This is brought out clearly by examining the distances (Table 4) between bromine and oxygen atoms and carbon atoms. In each case $d(\mathrm{Br}\cdots\mathrm{C}(n)) \approx d(\mathrm{Br}'\cdots\mathrm{C}(n'))$ and $d(\mathrm{O}\cdots\mathrm{C}(n)) \approx d(\mathrm{O}'\cdots\mathrm{C}(n'))$. In view of this identity of the two molecules averaged dimensions for the molecule of (+)-10-bromo-2-chloro-2-nitrosocamphane are also listed in Table 4.

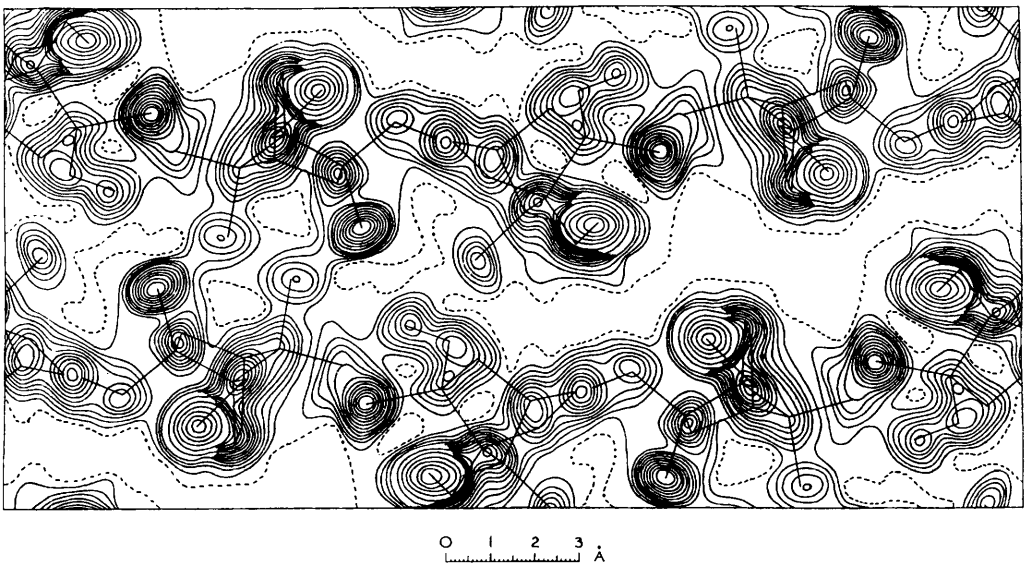
TABLE 1. *Co-ordinates of the atoms in the asymmetric crystal unit. (Origin of co-ordinates as in International Tables.)*

Atom	*x/a*	*y/b*	*z/c*	*B* *	Atom	*x/a*	*y/b*	*z/c*	*B* *
C(1)	0·2741	0·2545	0·0246	5·4	C(1′)	0·0317	0·1241	0·4058	5·4
C(2)	0·3311	0·3163	−0·0216	5·4	C(2′)	0·0703	0·2348	0·4350	5·4
C(3)	0·3232	0·3574	−0·1848	5·4	C(3′)	0·0373	0·2962	0·5685	5·4
C(4)	0·2643	0·2998	−0·2209	5·4	C(4′)	−0·0154	0·2191	0·5938	5·4
C(5)	0·2662	0·1599	−0·2217	5·4	C(5′)	−0·0607	0·2319	0·4679	5·4
C(6)	0·2723	0·1296	−0·0549	5·4	C(6′)	−0·0272	0·1662	0·3450	5·4
C(7)	0·2296	0·3198	−0·0800	5·4	C(7′)	0·0102	0·0897	0·5691	5·4
C(8)	0·1653	0·2850	−0·0766	5·4	C(8′)	−0·0366	−0·0026	0·5710	5·4
C(9)	0·2182	0·4556	−0·0368	5·4	C(9′)	0·0591	0·0582	0·6787	5·4
C(10)	0·2616	0·2578	0·1905	5·4	C(10′) ...	0·0607	0·0243	0·3240	5·4
O	0·4239	0·2620	0·0355	7·1	O′	0·1060	0·3646	0·2634	6·8
N	0·3807	0·2288	−0·0153	5·7	N′	0·0638	0·3307	0·3314	7·1
Br	0·3095	0·1662	0·3075	6·2	Br′	0·0817	0·0664	0·1290	6·5
Cl	0·3503	0·4429	0·0899	6·0	Cl′	0·1437	0·2090	0·4727	6·0

* The values of *B* for the C atoms are the isotropic values used in the analysis. The values of *B* for the O, N, Br, and Cl atoms are average values derived from the anisotropic parameters of the least-squares analysis.

The estimated standard deviation in bond length calculated from the differences between the two molecules is 0·044 Å. The corresponding value deduced from the least-squares calculation at an earlier stage is 0·080 Å. For the averaged dimensions in Table 4 we may take $0{\cdot}064/\sqrt{2}$, *i.e.*, 0·045 Å, as a reasonable estimate of the standard deviation in bond length.

FIG. 4. *Electron-density projection on* (001). *Contour interval* 1e/Å², *the* 1e/Å² *line being broken, except around the* Cl *atoms above* 6e/Å² *where the interval becomes* 2e/Å², *and around the* Br *atoms above* 5e/Å² *where the interval becomes* 5e/Å². *The positions deduced for the atoms by the three-dimensional refinement procedure are indicated.*



The average carbon–carbon single bond length is 1·554 Å, not significantly different from the value of 1·545 Å in diamond.

For the nitroso-grouping the C–N separation of 1·48 Å is in agreement with the accepted value of 1·48 Å for a C–N single bond. The N–O separation of 1·19 Å is slightly shorter than

the value of about 1·21 Å appropriate to a nitro-group, but in view of the fairly large standard deviation too much significance should not be attributed to the difference. The separation is very significantly shorter than the value of 1·36 Å appropriate to a single bond, suggesting that the N–O bond has a large amount of double-bond character and may in fact be a pure double bond. The angle CNO is 118°.

Two *X*-ray studies of dimeric nitroso-compounds have been reported,[5] but only one previous structure analysis of a monomeric organic nitroso-compound has been described.[6] *p*-Iodonitrosobenzene is a planar molecule with d(C–N) = 1·28, d(N–O) = 1·24 Å, ∠(C–N–O) = 125°. The short C–N bond may be indicative of conjugation across the benzene ring, but as relatively few intensity data were obtained and the analysis was confined to projections the light-atom positions may be subject to considerable error.

Various metallic nitrosyls have been described,[7] but the electronic structures of these must be different, for the metal–nitroso-grouping is invariably approximately linear. In the nitrosyl halides,[8] however, the angle at the nitrogen atom is 116° in good agreement with our value of 118°, though the N–O separation of 1·14 Å is somewhat shorter than our value of 1·19 Å.

TABLE 2. *Progress of the structure analysis.*

Patterson syntheses
↓
Br (2 atoms)
↓
1st F_c calculation
1st three-dimensional F_o synthesis
↓
Br, Cl (4 atoms)
↓
2nd F_c calculation (R = 36·4%)
2nd three-dimensional F_o synthesis
↓
Br, Cl, N, O, C(1), C(2), C(3), C(4), C(10) (18 atoms)
↓
3rd F_c calculation (R = 29·6%)
3rd three-dimensional F_o synthesis
↓
Br, Cl, N, O, C(1) · · · C(10) (28 atoms)
↓
4th F_c calculation (R = 24·6%)
4th three-dimensional F_o synthesis
↓
5th F_c calculation (R = 21·8%)
Least-squares refinement
↓
6th F_c calculation (R = 16·4%)
5th three-dimensional F_o synthesis
1st three-dimensional F_c synthesis
↓
7th F_c calculation (R = 15·5%)

So far as the stereochemistry of (+)-10-bromo-2-chloro-2-nitrosocamphane is concerned, the chlorine atom is *cis* to the CMe_2 bridge. This is the opposite of the configuration attributed [2] to (−)-2-chloro-2-nitrosocamphane, and in this connection it is perhaps significant that the two compounds have Cotton effects of opposite sign.

Our measurements provide evidence that the camphane molecular framework is distorted slightly by the bulky chlorine atom *cis* to the CMe_2 bridge, the two groups bending away from one another out of their ideal positions. Thus the angle C(2)C(1)C(7) at 102° is rather greater than the angle C(6)C(1)C(7) which is only 97°. In addition the distances from C(2) to C(7) and C(9) are 2·44 Å and 3·02 Å, respectively, rather greater than the distances from C(6) to C(7) and C(8) which are 2·37 Å and 2·92 Å, respectively.

The arrangement of the molecules in the crystal as viewed in projection along the *c*-axis is shown in Fig. 4. The shorter intermolecular contacts are given in Table 4. None of these appears to be abnormal.

[5] Darwin and Hodgkin, *Nature*, 1950, **166**, 827; Fenimore, *J. Amer. Chem. Soc.*, 1950, **72**, 3226.
[6] Webster, *J.*, 1956, 2841.
[7] Johansson and Lipscomb, *Acta Cryst.*, 1958, **11**, 594; Thomas, Robertson, and Cox, *ibid.*, p. 599; Brockway and Anderson, *Trans. Faraday Soc.*, 1937, **33**, 1233.
[8] Ketelaar and Palmer, *J. Amer. Chem. Soc.*, 1937, **59**, 2629.

TABLE 3. *Measured and calculated values of the structure factors.*

h	*k*	*l*	*F* (meas)	*F* (calc)	α	*h*	*k*	*l*	*F* (meas)	*F* (calc)	α	*h*	*k*	*l*	*F* (meas)	*F* (calc)	α
2	0	0	14·8	16·8	180°	4	5	0	19·9	22·9	0°	9	13	0	7·7	8·0	270°
4	0	0	19·6	12·0	180	5	5	0	124·1	112·3	270						
6	0	0	42·4	56·4	180	6	5	0	71·3	79·8	180	4	14	0	6·9	7·5	180
8	0	0	107·1	116·1	180	7	5	0	4·7	4·0	270						
10	0	0	24·5	23·4	180	8	5	0	44·5	43·0	0						
12	0	0	43·0	49·1	0	9	5	0	9·6	5·8	270	2	0	1	68·7	86·3	270
14	0	0	28·4	29·5	0	10	5	0	60·6	68·2	0	3	0	1	94·1	100·5	90
18	0	0	32·7	31·2	180	11	5	0	18·0	16·2	90	4	0	1	35·8	35·6	90
20	0	0	10·4	11·4	180	12	5	0	38·7	35·9	180	5	0	1	131·0	197·0	270
22	0	0	11·5	6·6	0	13	5	0	34·6	28·3	270	6	0	1	83·6	83·6	90
24	0	0	27·0	19·3	180	14	5	0	11·5	8·1	0	7	0	1	53·0	59·8	270
						16	5	0	12·1	18·9	180	8	0	1	73·8	89·3	270
1	1	0	47·5	45·3	90	17	5	0	15·4	12·3	90	9	0	1	24·9	22·5	90
2	1	0	14·5	16·5	0	18	5	0	16·3	14·7	180	10	0	1	49·5	59·4	270
3	1	0	90·4	84·2	90	19	5	0	22·3	16·4	270	11	0	1	8·8	8·7	270
4	1	0	157·1	193·9	180	20	5	0	12·3	18·6	0	12	0	1	64·1	70·1	90
5	1	0	92·8	95·7	90	21	5	0	8·5	10·0	90	13	0	1	39·9	62·1	90
6	1	0	100·2	105·3	0	23	5	0	13·5	9·3	90	15	0	1	22·1	27·4	270
7	1	0	10·4	13·8	270												
8	1	0	43·8	31·4	180	0	6	0	10·7	4·8	180	1	1	1	125·1	101·4	286
9	1	0	105·2	122·9	270	1	6	0	74·8	74·9	90	2	1	1	125·2	126·3	252
10	1	0	6·3	8·6	0	2	6	0	74·2	75·9	180	3	1	1	119·2	104·3	218
11	1	0	8·4	12·7	270	3	6	0	48·8	37·8	270	4	1	1	104·4	98·6	193
12	1	0	66·1	55·7	0	4	6	0	40·4	44·0	0	5	1	1	81·3	82·1	165
14	1	0	16·1	23·6	180	5	6	0	47·0	52·4	270	6	1	1	83·6	92·1	288
15	1	0	8·3	2·3	90	6	6	0	67·0	75·1	0	7	1	1	28·6	38·8	237
16	1	0	26·6	23·8	180	8	6	0	29·7	34·6	180	8	1	1	26·0	30·4	51
17	1	0	38·3	46·4	90	9	6	0	11·5	10·4	270	9	1	1	92·4	102·4	115
18	1	0	33·7	34·2	0	10	6	0	19·6	21·5	0	10	1	1	13·7	11·8	69
19	1	0	10·2	3·5	270	12	6	0	28·3	35·9	180	11	1	1	43·2	59·4	343
23	1	0	9·1	3·1	90	13	6	0	46·1	51·4	90	12	1	1	61·1	68·5	35
						14	6	0	37·8	48·4	180	13	1	1	18·1	25·7	357
0	2	0	141·2	173·8	180	15	6	0	9·8	12·1	90	14	1	1	37·0	47·9	185
1	2	0	122·3	120·4	90	16	6	0	11·7	14·4	0	15	1	1	15·4	14·4	37
2	2	0	132·3	117·0	0	21	6	0	12·7	12·0	90	16	1	1	17·3	25·3	223
3	2	0	107·0	96·7	90							17	1	1	28·7	38·4	242
4	2	0	43·3	43·6	180	2	7	0	14·5	9·4	0	18	1	1	28·7	28·5	66
5	2	0	118·0	107·3	270	3	7	0	82·7	88·2	270	19	1	1	16·4	20·6	112
6	2	0	50·7	47·4	180	4	7	0	50·4	61·4	180	20	1	1	18 2	20·6	283
7	2	0	90·2	69·9	90	5	7	0	14·3	11·1	270						
8	2	0	20·0	16·8	180	6	7	0	12·2	9·9	0	0	2	1	154·0	131·7	180
9	2	0	61·4	58·0	270	7	7	0	38·6	38·9	90	1	2	1	99·1	81·6	25
10	2	0	12·3	11·5	0	8	7	0	35·7	31·3	0	2	2	1	130·0	108·5	65
11	2	0	4·1	6·9	270	9	7	0	24·7	23·4	90	3	2	1	76·9	67·9	201
12	2	0	14·7	22·6	0	10	7	0	19·0	15·0	180	4	2	1	91·1	73·2	98
13	2	0	77·2	86·1	90	12	7	0	32·2	38·5	0	5	2	1	115·9	97·1	175
14	2	0	9·4	26·7	0							6	2	1	45·6	37·2	195
16	2	0	36·4	32·7	180	0	8	0	70·3	68·4	180	7	2	1	76·0	94·3	317
17	2	0	34·4	34·3	270	1	8	0	37·0	32·8	270	8	2	1	109·5	120·0	332
20	2	0	14·0	7·5	0	3	8	0	18·6	26·0	90	9	2	1	39·2	38·7	4
24	2	0	10·4	10·5	0	4	8	0	36·3	31·0	0	10	2	1	47·6	52·8	174
						5	8	0	18·7	22·8	270	11	2	1	53·0	60·3	87
1	3	0	83·2	71·8	270	7	8	0	21·1	26·7	90	12	2	1	38·1	29·9	246
2	3	0	71·9	76·3	180	8	8	0	19·2	24·0	0	13	2	1	16·3	11·7	228
3	3	0	133·8	113·5	90	9	8	0	10·6	8·8	270	14	2	1	23·7	22·5	34
4	3	0	181·1	169·5	180	11	8	0	10·9	6·5	270	16	2	1	15·7	17·7	151
5	3	0	113·9	100·7	90	12	8	0	18·4	22·2	180	18	2	1	21·8	35·5	3
6	3	0	89·5	72·9	180	14	8	0	19·1	18·9	180	19	2	1	17·9	17·4	242
7	3	0	63·0	58·7	270	15	8	0	19·0	19·3	270						
8	3	0	113·3	127·8	0	18	8	0	13·1	15·0	0	0	3	1	121·4	95·5	90
9	3	0	9·1	2·2	90	19	8	0	11·1	11·8	90	1	3	1	49·2	47·2	302
10	3	0	24·1	27·2	0	20	8	0	9·7	5·5	180	2	3	1	162·4	131·0	169
11	3	0	42·0	46·0	270	21	8	0	11·0	10·7	270	3	3	1	106·4	87·0	264
12	3	0	30·5	23·0	180							4	3	1	94·9	76·7	308
13	3	0	29·7	26·5	90	2	9	0	19·0	24·2	0	5	3	1	51·2	44·9	176
14	3	0	24·3	19·8	180	5	9	0	30·9	30·1	270	6	3	1	60·6	62·3	196
16	3	0	9·6	4·2	180	9	9	0	45·2	50·7	90	7	3	1	66·9	55·9	25
17	3	0	19·9	22·9	270	10	9	0	11·0	5·8	180	8	3	1	33·5	32·9	299
18	3	0	21·2	28·9	180	11	9	0	11·0	6·0	270	9	3	1	41·6	42·3	57
19	3	0	32·2	30·2	90	12	9	0	10·5	11·8	180	10	3	1	63·5	64·6	335
20	3	0	10·2	5·4	180	13	9	0	16·4	17·2	270	11	3	1	37·9	33·9	149
25	3	0	11·3	12·3	90	14	9	0	10·5	9·4	0	12	3	1	55·8	58·7	159
26	3	0	9·3	7·9	180	15	9	0	10·7	10·8	90	13	3	1	42·9	49·2	346
												14	3	1	47·4	53·3	58
0	4	0	28·2	21·5	0							17	3	1	16·0	13·9	178
1	4	0	137·3	135·7	90	0	10	0	32·7	33·9	180	18	3	1	18·5	25·7	255
2	4	0	33·8	39·6	0	1	10	0	10·7	6·8	270						
3	4	0	52·5	57·4	270	2	10	0	13·2	10·0	0	0	4	1	53·0	46·6	0
4	4	0	24·5	19·1	180	5	10	0	24·7	29·2	90	1	4	1	84·0	68·4	204
5	4	0	27·9	19·4	270	6	10	0	12·2	15·8	0	2	4	1	132·5	103·3	206
6	4	0	45·0	36·8	180	8	10	0	11·9	17·3	0	3	4	1	40·5	31·5	235
7	4	0	105·8	97·1	270	12	10	0	10·8	8·7	180	4	4	1	27·6	24·9	7
8	4	0	24·1	27·0	0	13	10	0	10·7	13·3	270	5	4	1	25·4	28·7	59
9	4	0	29·6	29·1	270							6	4	1	152·4	125·3	13
10	4	0	59·2	62·2	180	4	11	0	25·7	33·7	0	7	4	1	24·9	18·6	336
11	4	0	45·8	60·6	90	8	11	0	22·1	22·3	180	8	4	1	27·3	29·0	132
14	4	0	31·9	30·1	0	10	11	0	16·1	12·0	180	9	4	1	66·0	70·7	347
15	4	0	17·2	19·6	90							10	4	1	14·7	13·1	109
21	4	0	11·6	10·8	90	1	12	0	14·2	17·2	270	11	4	1	34·6	35·1	32
						5	12	0	11·3	9·8	90	12	4	1	36·8	36·8	150
1	5	0	8·2	3·6	90	8	12	0	10·7	13·9	180	13	4	1	14·9	23·5	229
2	5	0	73·5	68·4	180	13	12	0	8·2	9·8	270	14	4	1	16·8	26·4	155
3	5	0	24·3	30·5	270	17	12	0	3·7	5·4	90	15	4	1	18·0	31·5	107

TABLE 3. (*Continued.*)

h	k	l	F (meas)	F (calc)	α
16	4	1	15·9	21·7	327°
18	4	1	16·6	7·8	216
0	5	1	111·7	96·4	90
1	5	1	53·6	44·4	182
2	5	1	28·0	26·1	346
3	5	1	48·0	44·9	303
4	5	1	37·4	39·1	248
5	5	1	72·0	57·0	324
6	5	1	28·7	30·9	319
7	5	1	64·1	55·2	106
8	5	1	21·1	28·2	224
9	5	1	22·5	31·2	285
10	5	1	23·6	30·6	145
11	5	1	48·8	51·3	68
12	5	1	15·2	16·1	52
13	5	1	24·3	28·6	202
15	5	1	31·7	42·3	256
16	5	1	17·8	17·5	307
0	6	1	42·0	35·4	180
1	6	1	64·6	52·5	338
3	6	1	57·9	51·5	128
4	6	1	44·7	41·4	285
5	6	1	48·0	50·8	196
6	6	1	56·0	48·4	12
7	6	1	48·3	43·2	84
9	6	1	23·5	30·2	19
10	6	1	36·0	37·0	111
11	6	1	72·7	55·8	240
13	6	1	43·0	30·9	133
15	6	1	15·7	23·6	310
1	7	1	36·4	33·4	238
2	7	1	74·1	69·8	7
3	7	1	15·0	22·0	201
5	7	1	27·7	35·2	50
7	7	1	39·9	45·8	318
9	7	1	29·4	37·9	83
10	7	1	24·5	33·1	191
11	7	1	15·9	5·9	226
12	7	1	16·2	20·9	39
2	8	1	17·0	20·9	321
3	8	1	16·4	22·8	264
4	8	1	25·0	23·0	241
5	8	1	29·3	32·0	69
6	8	1	35·8	36·1	219
7	8	1	15·8	20·1	63
8	8	1	51·4	54·3	68
9	8	1	15·5	18·0	203
10	8	1	21·0	25·1	158
1	9	1	44·6	43·4	181
2	9	1	17·5	12·7	248
3	9	1	20·1	26·9	20
4	9	1	17·0	24·7	16
6	9	1	28·6	31·6	154
8	9	1	20·7	20·4	134
0	10	1	16·0	23·7	0
3	10	1	20·9	25·9	324
5	10	1	16·0	18·7	54
0	11	1	21·8	22·9	270
1	11	1	18·0	21·0	80
1	0	2	51·7	62·0	0
2	0	2	74·5	72·6	0
3	0	2	126·7	153·6	180
4	0	2	57·8	42·4	180
5	0	2	52·7	37·7	180
6	0	2	26·7	25·1	0
7	0	2	91·9	87·9	0
8	0	2	78·8	67·8	0
10	0	2	90·6	80·1	180
11	0	2	58·3	61·1	0
12	0	2	7·3	7·2	180
13	0	2	10·3	8·7	180
14	0	2	72·8	60·2	0
15	0	2	48·6	58·2	180
16	0	2	34·9	40·3	180
19	0	2	12·2	9·7	0
20	0	0	9·1	9·8	180
21	0	2	8·3	2·1	0
0	1	2	64·5	48·3	90
1	1	2	74·7	62·1	259
2	1	2	101·7	95·1	108
3	1	2	24·4	30·5	37
4	1	2	141·3	124·7	356
5	1	2	56·3	49·3	187
6	1	2	126·2	130·3	244
7	1	2	55·8	60·9	308°
8	1	2	56·7	48·2	217
9	1	2	38·7	30·9	120
10	1	2	36·1	36·3	91
11	1	2	61·3	68·3	176
12	1	2	41·7	50·6	102
13	1	2	39·6	33·8	13
14	1	2	12·0	15·9	70
15	1	2	15·3	14·9	160
16	1	2	22·9	15·3	201
17	1	2	7·7	3·1	218
18	1	2	8·8	4·4	181
19	1	2	8·6	15·2	30
20	1	2	30·2	34·1	331
22	1	2	15·5	13·3	161
27	1	2	7·0	1·6	262
0	2	2	53·1	56·2	180
1	2	2	125·7	130·0	149
2	2	2	147·5	154·4	243
3	2	2	111·5	96·0	230
4	2	2	87·0	72·8	355
5	2	2	69·6	53·0	33
6	2	2	56·6	54·3	298
7	2	2	18·1	14·6	110
8	2	2	58·0	61·3	94
9	2	2	56·1	52·4	339
10	2	2	44·8	58·0	55
11	2	2	41·8	47·6	46
12	2	2	7·3	5·4	109
13	2	2	15·3	22·2	239
14	2	2	27·2	29·3	203
15	2	2	32·9	35·9	143
16	2	2	22·4	26·5	275
17	2	2	13·6	22·9	194
18	2	2	8·9	12·5	220
19	2	2	8·2	6·8	323
20	2	2	10·0	11·5	61
21	2	2	11·0	12·9	98
22	2	2	9·8	7·3	289
23	2	2	9·1	11·0	251
0	3	2	83·1	85·6	90
1	3	2	77·0	78·3	169
2	3	2	32·8	25·3	0
3	3	2	85·9	73·6	262
4	3	2	28·6	25·3	126
5	3	2	83·5	70·7	350
6	3	2	42·3	33·8	184
7	3	2	107·0	114·3	30
8	3	2	43·3	47·6	297
9	3	2	74·2	61·6	276
10	3	2	37·9	40·4	88
11	3	2	44·1	46·1	159
12	3	2	31·4	32·3	221
13	3	2	43·5	47·9	157
14	3	2	14·9	18·8	304
15	3	2	23·5	27·0	248
16	3	2	8·6	5·2	52
17	3	2	15·3	18·0	104
18	3	2	32·9	32·6	246
19	3	2	11·7	16·2	350
20	3	2	12·1	11·3	185
22	3	2	9·7	11·0	28
0	4	2	141·1	123·3	0
1	4	2	59·4	58·8	229
2	4	2	86·0	70·1	263
3	4	2	72·3	70·7	57
4	4	2	94·1	97·3	243
5	4	2	19·3	22·0	270
6	4	2	45·4	49·1	80
7	4	2	33·5	34·6	96
8	4	2	32·3	28·3	170
9	4	2	31·1	27·2	50
10	4	2	21·4	25·3	60
11	4	2	15·4	20·9	258
12	4	2	36·2	38·7	104
13	4	2	15·5	12·7	114
14	4	2	43·5	45·3	267
15	4	2	23·7	24·7	301
16	4	2	22·7	29·8	286
17	4	2	9·0	3·2	40
18	4	2	15·0	11·8	112
21	4	2	8·5	9·8	289
0	5	2	59·6	54·3	270
1	5	2	36·4	37·4	207
2	5	2	47·4	50·0	341
3	5	2	75·4	89·0	174
4	5	2	38·2	37·5	141
5	5	2	76·3	82·1	339
6	5	2	40·0	43·7	28
7	5	2	41·8	48·3	308°
8	5	2	39·0	37·0	87
9	5	2	38·5	34·8	117
10	5	2	24·0	29·7	227
11	5	2	21·0	24·5	217
12	5	2	19·8	20·5	325
13	5	2	21·1	24·1	229
14	5	2	10·4	18·2	215
15	5	2	11·0	13·7	62
16	5	2	11·8	13·6	281
17	5	2	11·7	11·2	18
18	5	2	9·2	16·3	58
19	5	2	10·3	10·2	314
20	5	2	9·4	8·5	184
21	5	2	8·7	10·8	12
0	6	2	90·5	85·0	180
1	6	2	85·8	88·7	1
2	6	2	44·9	51·3	291
3	6	2	39·5	37·6	326
4	6	2	8·2	11·2	290
5	6	2	26·6	24·2	3
6	6	2	7·7	9·6	176
7	6	2	27·3	32·0	69
8	6	2	30·3	31·2	18
9	6	2	41·6	53·0	207
10	6	2	24·5	33·5	126
11	6	2	22·8	22·8	199
12	6	2	8·6	6·3	56
13	6	2	23·9	19·5	90
14	6	2	13·8	13·5	259
15	6	2	16·6	13·2	64
16	6	2	18·5	21·0	194
17	6	2	14·1	19·8	328
18	6	2	9·1	8·0	43
24	6	2	6·9	7·5	14
25	6	2	6·2	5·7	225
0	7	2	41·3	44·8	270
1	7	2	20·4	18·5	244
2	7	2	25·2	29·4	222
3	7	2	22·8	22·8	47
4	7	2	35·4	31·2	339
5	7	2	12·9	16·0	116
6	7	2	43·3	43·3	122
7	7	2	25·3	29·0	352
8	7	2	27·5	33·4	54
10	7	2	31·1	32·6	254
11	7	2	21·7	24·3	190
12	7	2	24·8	23·6	249
13	7	2	18·8	18·7	25
17	7	2	14·2	13·9	269
19	7	2	8·5	11·3	35
20	7	2	9·9	11·3	48
0	8	2	9·0	8·1	0
1	8	2	15·8	12·6	336
2	8	2	10·7	13·3	293
3	8	2	68·1	61·6	340
4	8	2	27·4	26·6	53
5	8	2	18·4	22·8	49
6	8	2	22·7	21·8	219
7	8	2	8·7	13·8	241
8	8	2	10·0	15·4	198
9	8	2	8·5	5·8	157
10	8	2	9·4	13·2	320
11	8	2	19·4	22·0	134
12	8	2	8·7	10·0	239
13	8	2	15·2	19·9	287
14	8	2	8·7	4·6	133
15	8	2	14·7	21·3	345
0	9	2	12·6	4·5	270
1	9	2	44·2	44·9	59
2	9	2	20·9	27·9	295
3	9	2	14·9	16·6	323
4	9	2	14·0	10·4	46
5	9	2	15·7	20·2	244
6	9	2	43·2	48·9	95
7	9	2	18·0	20·1	172
8	9	2	8·7	5·8	105
9	9	2	8·7	4·8	221
10	9	2	11·4	7·8	3
11	9	2	10·3	9·1	18
12	9	2	11·0	14·3	229
0	10	2	14·6	18·7	0
1	10	2	11·4	11·8	356
2	10	2	33·9	31·5	92
3	10	2	14·9	21·6	39
4	10	2	17·9	12·2	108
5	10	2	9·6	15·7	266
6	10	2	15·4	18·8	52

TABLE 3. (*Continued.*)

h	*k*	*l*	*F* (meas)	*F* (calc)	α
7	10	2	10·3	7·3	144°
16	10	2	8·6	12·5	77
17	10	2	10·2	5·8	245
0	11	2	9·4	2·9	90
1	11	2	10·5	16·1	336
6	11	2	9·9	11·6	348
8	11	2	13·4	8·4	142
11	11	2	12·9	14·4	343
12	11	2	11·1	11·5	0
13	11	2	8·0	2·0	291
2	12	2	15·2	18·4	60
4	12	2	8·7	9·6	77
7	12	2	8·0	5·9	25
8	13	2	9·0	4·2	323
3	14	2	6·0	5·5	181
2	0	3	108·7	139·1	270
3	0	3	12·2	12·6	270
4	0	3	58·0	47·9	90
5	0	3	66·8	42·7	270
6	0	3	8·0	10·2	90
7	0	3	88·5	74·0	270
8	0	3	30·4	29·4	90
9	0	3	48·4	38·3	270
10	0	3	21·6	35·3	90
11	0	3	38·9	48·3	90
12	0	3	47·4	52·3	270
13	0	3	31·8	14·3	270
15	0	3	38·6	38·2	90
16	0	3	45·5	44·1	270
19	0	3	16·8	24·1	270
20	0	3	22·8	25·9	90
0	1	3	51·7	58·9	90
1	1	3	61·3	69·9	168
2	1	3	147·0	139·2	192
3	1	3	107·0	86·7	323
4	1	3	37·2	28·3	116
5	1	3	23·0	22·6	287
6	1	3	57·0	42·9	121
7	1	3	52·9	57·2	30
8	1	3	68·1	60·5	277
9	1	3	29·5	23·4	238
10	1	3	69·9	61·3	70
11	1	3	60·8	59·6	140
12	1	3	28·2	32·1	297
13	1	3	23·0	17·8	130
14	1	3	27·8	33·0	238
15	1	3	43·4	37·2	259
16	1	3	18·9	25·0	124
17	1	3	15·1	20·3	326
18	1	3	9·9	7·7	25
19	1	3	12·5	15·4	15
20	1	3	16·7	13·0	338
21	1	3	10·0	7·7	179
22	1	3	8·9	4·7	292
26	1	3	7·8	6·3	41
0	2	3	35·6	28·4	180
1	2	3	31·4	27·6	177
2	2	3	109·6	82·4	134
3	2	3	111·4	99·3	27
4	2	3	79·0	68·8	285
5	2	3	44·2	41·8	322
6	2	3	90·3	84·1	12
7	2	3	78·0	80·1	220
8	2	3	37·0	39·3	89
9	2	3	37·9	31·4	45
10	2	3	27·8	23·1	66
11	2	3	34·6	41·5	146
13	2	3	12·9	17·1	65
14	2	3	29·0	30·8	264
15	2	3	41·5	48·9	342
16	2	3	21·6	18·8	17
17	2	3	16·1	12·3	150
19	2	3	10·5	9·0	287
20	2	3	10·1	10·6	11
21	2	3	9·5	8·5	235
0	3	3	39·5	36·2	270
1	3	3	46·1	41·8	324
2	3	3	50·2	46·5	321
3	3	3	102·9	95·9	212
4	3	3	42·9	52·1	138
5	3	3	47·7	49·9	9
6	3	3	40·5	41·9	55
7	3	3	32·9	25·1	205
8	3	3	22·9	20·0	107
9	3	3	29·5	27·5	161°
10	3	3	48·3	44·5	275
11	3	3	32·4	38·2	72
12	3	3	44·3	39·6	306
13	3	3	26·7	28·5	185
14	3	3	13·0	11·4	176
15	3	3	49·9	34·9	344
16	3	3	10·5	10·4	131
17	3	3	12·3	14·1	8
18	3	3	10·9	13·1	36
19	3	3	9·1	11·1	115
20	3	3	14·8	13·4	119
21	3	3	16·0	16·0	17
23	3	3	9·9	14·1	141
0	4	3	7·5	7·3	180
1	4	3	54·9	58·0	338
2	4	3	22·4	17·1	212
3	4	3	9·2	6·9	174
4	4	3	18·4	21·8	233
5	4	3	57·0	47·1	291
6	4	3	95·1	71·4	39
7	4	3	21·2	15·2	107
8	4	3	45·0	51·9	356
9	4	3	79·7	86·2	169
10	4	3	49·8	54·0	191
11	4	3	32·8	25·8	356
12	4	3	16·1	16·7	139
13	4	3	28·4	24·7	19
14	4	3	13·2	11·4	297
15	4	3	15·9	10·2	129
16	4	3	17·2	18·2	182
17	4	3	10·0	19·8	24
18	4	3	9·1	11·2	14
19	4	3	10·0	11·1	144
20	4	3	10·4	12·3	349
0	5	3	79·0	82·3	270
1	5	3	88·9	65·8	270
3	5	3	58·6	61·5	312
4	5	3	28·9	29·1	33
5	5	3	23·9	28·3	160
6	5	3	10·0	12·8	172
7	5	3	8·8	15·2	192
8	5	3	33·1	45·1	121
9	5	3	27·3	34·2	84
10	5	3	26·4	32·2	234
11	5	3	27·2	22·4	50
12	5	3	14·7	18·5	252
13	5	3	14·5	17·0	353
15	5	3	20·0	21·6	231
17	5	3	10·5	12·9	265
18	5	3	18·2	27·7	93
21	5	3	9·3	9·4	179
0	6	3	17·3	19·4	180
1	6	3	28·5	29·6	333
2	6	3	15·0	9·9	61
3	6	3	38·5	33·4	297
4	6	3	70·2	71·8	91
5	6	3	40·4	46·0	107
6	6	3	23·6	30·9	297
7	6	3	37·8	37·5	96
8	6	3	35·3	34·6	312
10	6	3	9·2	5·0	218
11	6	3	12·7	12·3	133
12	6	3	26·2	28·4	261
13	6	3	12·6	16·0	290
14	6	3	13·8	23·6	107
15	6	3	17·7	22·7	16
0	7	3	26·7	30·9	90
1	7	3	31·0	30·1	5
2	7	3	31·4	38·5	336
4	7	3	30·1	26·5	36
5	7	3	41·4	42·4	164
6	7	3	21·8	27·3	124
7	7	3	12·8	17·3	85
8	7	3	30·0	35·1	272
9	7	3	8·6	16·2	289
10	7	3	8·8	12·1	148
11	7	3	9·8	14·5	125
12	7	3	30·1	31·2	194
13	7	3	18·0	25·2	359
14	7	3	10·1	19·7	341
15	7	3	10·5	8·3	277
16	7	3	20·6	23·7	48
17	7	3	11·0	11·4	162
0	8	3	18·4	19·8	0
1	8	3	17·7	28·8	207
2	8	3	29·1	33·8	107
4	8	3	16·0	17·7	178
5	8	3	25·7	27·9	50°
7	8	3	19·9	27·6	138
8	8	3	24·3	25·3	190
9	8	3	11·3	16·7	16
10	8	3	15·5	22·5	254
11	8	3	19·1	22·9	274
12	8	3	13·3	15·2	82
0	9	3	19·2	19·8	90
1	9	3	19·4	18·2	46
2	9	3	15·9	19·0	23
3	9	3	12·8	15·6	146
4	9	3	10·4	11·2	217
6	9	3	11·1	12·7	268
7	9	3	23·6	28·7	199
10	9	3	10·5	16·7	182
11	9	3	18·5	26·3	350
15	9	3	8·7	5·5	25
3	10	3	20·8	21·9	211
5	10	3	16·3	18·4	198
6	10	3	16·0	19·5	162
7	10	3	15·3	18·1	52
8	10	3	15·4	13·2	263
11	10	3	11·7	13·7	315
12	10	3	10·0	12·3	53
3	11	3	10·4	13·6	102
4	11	3	5·5	3·1	235
7	11	3	10·4	7·3	304
7	12	3	11·3	6·4	323
8	12	3	8·7	6·0	134
1	13	3	7·7	9·2	130
1	0	4	32·1	55·7	180
2	0	4	79·8	93·2	180
3	0	4	7·7	15·0	0
5	0	1	32·4	22·4	0
6	0	4	39·7	32·8	0
7	0	4	86·9	62·1	180
8	0	4	48·9	42·8	0
9	0	4	84·1	69·2	0
10	0	4	14·3	8·5	180
12	0	4	34·5	35·4	180
13	0	4	12·1	2·6	0
14	0	4	12·2	19·0	180
15	0	4	30·4	28·9	0
16	0	4	19·5	16·0	0
17	0	4	21·9	25·3	180
18	0	4	13·7	21·8	0
1	1	4	33·8	46·6	338
2	1	4	37·6	38·6	333
3	1	4	149·3	129·1	212
4	1	4	75·1	57·8	59
5	1	4	87·7	71·3	307
6	1	4	62·9	47·1	24
7	1	4	66·2	49·9	135
8	1	4	50·8	52·4	210
9	1	4	70·5	67·6	116
10	1	4	44·5	43·3	133
11	1	4	19·5	22·4	28
12	1	4	10·3	15·5	243
13	1	4	12·2	13·8	251
14	1	4	14·1	13·8	306
15	1	4	19·9	23·9	322
16	1	4	28·2	23·9	127
18	1	4	19·3	18·1	352
19	1	4	12·7	11·2	194
21	1	4	12·9	15·6	30
0	2	4	118·8	115·5	180
1	2	4	74·7	73·1	279
2	2	4	52·1	44·9	101
3	2	4	11·5	9·4	188
4	2	4	68·4	61·8	346
5	2	4	53·0	55·6	35
6	2	4	60·6	58·0	45
7	2	4	38·1	40·8	60
8	2	4	8·5	9·1	346
9	2	4	61·6	54·3	188
10	2	4	27·6	26·4	304
11	2	4	39·4	39·0	317
12	2	4	46·6	50·9	120
14	2	4	33·0	35·3	232
15	2	4	19·4	21·9	173
16	2	4	11·1	9·9	68
20	2	4	11·4	15·0	277
0	3	4	30·9	35·6	270
1	3	4	22·7	25·5	260

TABLE 3. (*Continued.*)

h	k	l	F (meas)	F (calc)	α	h	k	l	F (meas)	F (calc)	α	h	k	l	F (meas)	F (calc)	α
2	3	4	92·6	70·7	66°	8	9	4	12·0	16·2	53°	3	4	5	43·5	40·0	3°
3	3	4	17·7	15·0	240	9	9	4	13·1	12·3	250	4	4	5	45·4	39·7	147
4	3	4	50·7	49·4	355	10	9	4	12·4	15·7	304	5	4	5	65·7	59·7	356
5	3	4	10·4	14·7	296							6	4	5	31·8	28·7	219
6	3	4	46·4	48·5	280	1	10	4	13·7	19·1	44	7	4	5	44·6	46·1	162
7	3	4	24·8	16·9	359	4	10	4	14·1	16·3	140	8	4	5	9·3	7·2	251
8	3	4	35·9	37·3	121	5	10	4	17·6	20·2	217	9	4	5	16·4	18·3	213
9	3	4	12·0	8·0	78	7	10	4	12·2	13·3	327	10	4	5	16·7	18·7	218
10	3	4	54·6	55·5	233							11	4	5	17·8	19·6	168
12	3	4	12·4	9·4	309	1	11	4	15·5	7·8	207	12	4	5	28·1	31·3	337
13	3	4	15·4	13·1	170	3	11	4	11·7	8·4	18	13	4	5	12·8	7·0	160
14	3	4	14·7	20·0	48	9	11	4	11·5	3·8	300	14	4	5	12·1	16·8	21
15	3	4	18·7	15·2	214							15	4	5	12·7	14·3	54
16	3	4	26·3	31·0	330	1	12	4	10·7	15·8	131	16	4	5	11·7	10·7	198
17	3	4	16·2	13·9	226							19	4	5	13·5	16·0	347
20	3	4	13·0	13·3	207	3	0	5	31·3	41·2	270						
						4	0	5	63·6	82·1	270	1	5	5	19·2	12·7	4
0	4	4	7·3	19·5	0	5	0	5	28·4	23·8	90	2	5	5	46·5	51·5	222
1	4	4	78·7	81·2	299	6	0	5	13·4	22·9	90	3	5	5	33·5	35·5	115
2	4	4	70·9	59·1	281	7	0	5	36·4	32·2	90	4	5	5	27·8	29·8	107
3	4	4	37·4	32·5	106	8	0	5	40·7	33·0	90	5	5	5	17·1	16·3	33
4	4	4	48·0	52·1	93	9	0	5	8·5	8·6	90	6	5	5	10·4	12·9	116
5	4	4	48·1	48·2	118	10	0	5	9·4	2·1	270	7	5	5	32·7	26·4	205
6	4	4	40·0	34·3	247	11	0	5	43·1	26·4	270	9	5	5	16·5	16·7	246
7	4	4	31·6	36·1	57	12	0	5	59·3	46·7	90	10	5	5	37·7	35·8	86
8	4	4	39·6	32·2	276	13	0	5	17·1	21·6	270	11	5	5	12·7	17·6	15
9	4	4	25·7	26·3	126	14	0	5	30·6	35·9	270	12	5	5	12·9	16·8	257
10	4	4	20·6	14·1	161	15	0	5	18·3	12·3	90	13	5	5	18·9	16·2	76
12	4	4	13·8	12·0	248	16	0	5	13·0	8·7	90	14	5	5	14·6	18·9	260
13	4	4	44·1	47·0	282	17	0	5	11·7	15·7	90	16	5	5	18·3	19·6	128
14	4	4	20·1	21·3	49	18	0	5	17·0	13·8	270						
15	4	4	11·2	11·7	217							1	6	5	13·4	15·0	71
16	4	4	23·5	20·0	266	0	1	5	28·1	49·3	270	2	6	5	21·9	31·2	65
17	4	4	19·2	22·9	52	1	1	5	23·8	32·4	138	3	6	5	18·7	23·1	310
22	4	4	10·6	10·2	268	2	1	5	24·0	31·9	59	4	6	5	12·6	14·4	229
						3	1	5	25·6	20·5	250	5	6	5	22·8	24·3	345
0	5	4	15·4	28·0	90	4	1	5	60·1	61·6	40	6	6	5	24·0	24·9	118
1	5	4	25·6	25·5	49	5	1	5	65·3	65·8	25	7	6	5	11·4	13·4	251
2	5	4	42·1	40·5	317	6	1	5	33·7	35·1	233	8	6	5	25·5	24·8	237
3	5	4	46·6	46·7	64	7	1	5	9·9	5·2	17	9	6	5	12·3	9·8	89
4	5	4	65·9	69·2	10	8	1	5	78·6	62·5	123	10	6	5	22·3	27·2	312
5	5	4	48·2	55·5	174	9	1	5	37·1	25·4	304	11	6	5	11·6	18·4	90
6	5	4	9·2	15·0	91	10	1	5	40·3	34·9	202	12	6	5	15·0	22·0	60
7	5	4	10·9	9·8	328	11	1	5	26·6	18·7	2						
8	5	4	47·1	49·9	205	12	1	5	16·2	12·6	7	0	7	5	36·7	42·9	270
10	5	4	24·9	28·7	145	13	1	5	48·7	42·7	171	1	7	5	37·0	40·5	26
11	5	4	21·2	25·8	188	14	1	5	17·2	16·9	319	2	7	5	10·5	11·3	94
13	5	4	26·4	36·2	3	15	1	5	17·7	11·6	221	3	7	5	19·0	25·4	177
14	5	4	16·4	18·8	295	16	1	5	16·0	14·9	306	4	7	5	20·3	19·1	180
15	5	4	12·1	14·1	117	17	1	5	11·7	10·2	355	5	7	5	18·0	14·2	118
17	5	4	14·8	12·7	151	18	1	5	15·4	16·9	78	6	7	5	11·4	15·7	220
						19	1	5	11·6	5·0	149	8	7	5	20·7	25·7	38
0	6	4	36·2	34·4	0	20	1	5	11·4	10·9	261	9	7	5	23·4	25·2	228
1	6	4	37·1	39·3	194							14	7	5	12·9	11·3	179
2	6	4	10·0	5·2	353	0	2	5	46·0	47·3	0						
3	6	4	17·9	21·3	325	1	2	5	63·0	67·3	320	1	8	5	17·1	18·5	58
4	6	4	22·5	20·4	166	2	2	5	12·5	11·8	13	3	8	5	13·1	12·6	141
5	6	4	24·5	22·5	80	3	2	5	34·4	28·8	95	4	8	5	22·0	24·6	100
6	6	4	11·1	12·9	182	4	2	5	39·4	36·9	258	5	8	5	24·2	22·0	249
7	6	4	21·0	23·4	142	5	2	5	21·6	18·5	90	7	8	5	15·0	21·0	324
8	6	4	17·1	14·4	172	6	2	5	68·1	47·6	239	9	8	5	15·4	21·4	164
9	6	4	36·7	40·2	357	7	2	5	42·5	36·1	19	11	8	5	11·0	12·3	24
11	6	4	15·2	16·8	240	8	2	5	22·5	21·4	105						
12	6	4	19·5	25·8	14	9	2	5	59·4	60·0	181	13	9	5	10·6	18·7	337
13	6	4	12·6	12·1	249	10	2	5	50·1	52·4	52						
15	6	4	16·7	21·5	351	12	2	5	29·6	29·7	301	3	10	5	13·1	12·9	239
17	6	4	11·9	16·2	159	13	2	5	14·1	14·5	287						
						14	2	5	26·2	26·9	90	0	11	5	11·5	15·4	90
0	7	4	36·9	39·0	90	15	2	5	19·0	16·1	215						
1	7	4	18·2	13·6	56	17	2	5	20·0	24·5	22	1	0	6	64·4	90·5	0
3	7	4	37·4	44·4	162							2	0	6	15·4	19·0	180
4	7	4	18·2	15·9	285	0	3	5	59·6	63·6	270	3	0	6	22·0	20·2	0
5	7	4	40·7	50·6	52	1	3	5	43·4	47·3	154	4	0	6	16·0	13·6	180
8	7	4	14·3	13·8	233	2	3	5	34·0	36·9	339	5	0	6	8·4	15·0	180
9	7	4	38·5	43·3	285	3	3	5	69·5	65·5	35	6	0	6	12·6	8·7	180
10	7	4	11·9	12·7	221	4	3	5	13·3	14·3	75	7	0	6	15·3	8·4	0
11	7	4	11·4	14·4	308	5	3	5	65·7	54·2	152	8	0	6	29·5	34·5	180
						6	3	5	50·3	43·4	67	9	0	6	47·0	42·9	180
0	8	4	39·6	41·5	0	7	3	5	45·2	42·3	322	10	0	6	31·0	24·4	0
1	8	4	13·3	13·2	335	8	3	5	17·3	13·8	115	11	0	6	14·5	9·5	180
2	8	4	11·7	17·7	38	9	3	5	26·7	31·9	304	16	0	6	16·9	16·8	0
3	8	4	15·3	19·1	119	10	3	5	10·3	5·7	146	17	0	6	12·9	16·4	0
4	8	4	18·3	21·9	217	11	3	5	32·8	36·3	199						
6	8	4	26·5	32·6	148	12	3	5	16·1	19·0	256	0	1	6	23·0	50·8	270
7	8	4	13·7	14·1	341	13	3	5	11·0	10·3	13	1	1	6	22·5	36·2	58
8	8	4	13·2	15·4	216	14	3	5	14·9	14·0	281	2	1	6	22·5	22·0	348
10	8	4	13·8	14·5	306	15	3	5	29·9	30·2	104	3	1	6	28·6	28·4	37
12	8	4	15·7	20·8	52	16	3	5	12·2	11·0	355	4	1	6	20·9	25·1	133
14	8	4	12·8	13·6	322	17	3	5	13·2	11·3	124	5	1	6	61·2	58·9	193
												6	1	6	65·0	43·5	44
2	9	4	14·3	19·6	101	0	4	5	42·7	49·8	0	7	1	6	11·7	5·8	163
3	9	4	14·8	20·9	64	1	4	5	39·8	38·5	182	8	1	6	41·2	31·7	103
4	9	4	17·2	16·2	211	2	4	5	33·0	34·4	319	9	1	6	9·1	3·8	260

TABLE 3. (*Continued.*)

h	*k*	*l*	*F* (meas)	*F* (calc)	α	*h*	*k*	*l*	*F* (meas)	*F* (calc)	α	*h*	*k*	*l*	*F* (meas)	*F* (calc)	α
10	1	6	18·6	18·3	252°	18	5	6	10·2	8·2	14°	0	2	7	9·7	21·1	180°
11	1	6	18·8	12·9	197	19	5	6	9·2	14·4	185	1	2	7	21·0	31·6	202
12	1	6	28·7	29·8	319							2	2	7	37·8	44·1	45
13	1	6	36·3	35·3	354	0	6	6	18·2	16·5	0	3	2	7	19·3	20·1	218
14	1	6	10·6	11·6	224	1	6	6	14·9	21·7	11	4	2	7	10·7	10·5	313
15	1	6	11·8	6·9	22	2	6	6	27·0	25·7	95	5	2	7	25·5	17·1	95
16	1	6	11·9	9·9	219	3	6	6	36·2	33·3	162	6	2	7	50·6	38·9	197
17	1	6	12·4	11·2	194	5	6	6	12·7	8·0	230	7	2	7	14·4	12·3	205
18	1	6	12·7	16·5	67	6	6	6	20·2	23·4	351	9	2	7	27·9	20·9	11
19	1	6	11·5	11·8	292	7	6	6	20·7	24·4	350	10	2	7	18·0	17·4	239
						8	6	6	21·2	18·1	190	13	2	7	17·8	14·4	228
0	2	6	21·3	25·5	180	11	6	6	11·9	11·8	345	14	2	7	13·7	12·3	47
1	2	6	7·9	4·9	238	14	6	6	10·6	8·4	64						
2	2	6	26·2	22·4	28	15	6	6	13·1	15·9	191	0	3	7	21·2	23·3	90
3	2	6	26·8	35·9	11							1	3	7	39·3	38·2	63
4	2	6	49·2	50·1	76	0	7	6	16·2	20·5	90	2	3	7	12·6	11·6	133
5	2	6	51·7	48·8	335	1	7	6	12·6	15·9	246	3	3	7	20·7	18·3	112
6	2	6	45·2	39·1	228	2	7	6	26·2	29·7	101	4	3	7	23·7	23·0	345
7	2	6	24·2	20·1	186	4	7	6	28·1	27·2	224	5	3	7	8·6	7·1	62
9	2	6	24·8	18·9	159	5	7	6	16·0	17·3	143	6	3	7	47·1	37·7	208
10	2	6	16·1	13·9	296	6	7	6	20·6	24·5	292	7	3	7	12·6	10·5	201
11	2	6	10·8	13·4	200	9	7	6	10·3	12·9	302	8	3	7	9·5	8·0	289
12	2	6	28·5	22·9	289	12	7	6	10·6	18·0	38	10	3	7	21·8	15·9	54
13	2	6	11·0	6·4	76							11	3	7	26·1	22·8	311
14	2	6	18·9	19·1	99	1	8	6	18·3	21·8	172	12	3	7	23·2	25·5	145
15	2	6	22·8	24·4	311	2	8	6	16·9	15·7	253	13	3	7	15·6	15·7	197
16	2	6	10·3	11·4	103	3	8	6	17·6	19·8	133	15	3	7	10·9	13·3	80
17	2	6	10·3	5·8	122	4	8	6	11·4	14·5	95						
18	2	6	10·7	9·3	325	6	8	6	10·9	8·5	274	0	4	7	37·6	38·3	0
						8	8	6	10·2	12·1	19	1	4	7	16·2	13·4	107
0	3	6	25·9	36·3	90	9	8	6	10·6	12·9	28	3	4	7	30·0	29·8	189
1	3	6	15·0	17·8	307	10	8	6	11·5	12·4	161	4	4	7	14·6	11·4	245
2	3	6	40·2	42·3	231	11	8	6	10·2	10·2	4	7	4	7	14·1	14·5	20
3	3	6	28·4	25·2	69	14	8	6	8·8	7·9	34	8	4	7	32·6	25·4	189
4	3	6	7·5	6·2	62							10	4	7	19·9	17·4	312
5	3	6	38·3	33·6	154	6	9	6	9·8	7·3	216	15	4	7	14·8	20·6	156
6	3	6	29·4	26·5	91	10	9	6	10·1	13·8	78	16	4	7	9·4	10·3	6
7	3	6	29·8	26·7	179												
8	3	6	18·7	15·8	300	2	10	6	9·3	7·7	233	1	5	7	18·4	19·9	121
9	3	6	14·1	14·6	76	4	10	6	9·7	17·3	244	2	5	7	19·0	22·1	113
10	3	6	14·3	10·2	27							3	5	7	11·1	5·3	105
11	3	6	27·9	28·3	323							4	5	7	26·4	18·4	171
12	3	6	11·9	18·9	307	3	11	6	8·4	12·7	219	6	5	7	38·4	35·5	290
13	3	6	10·1	4·2	27	5	11	6	8·1	12·5	19	7	5	7	11·6	12·1	68
15	3	6	10·3	6·9	113							8	5	7	10·3	5·8	114
16	3	6	10·9	11·8	69	2	0	7	8·5	14·8	90	9	5	7	15·8	16·9	261
						4	0	7	38·2	46·7	90	12	5	7	16·6	18·7	29
0	4	6	14·5	5·5	0	5	0	7	7·7	10·1	270						
1	4	6	26·7	27·0	181	6	0	7	7·8	6·3	270	0	6	7	14·8	11·8	180
2	4	6	41·6	37·8	90	7	0	7	61·7	54·7	90	1	6	7	12·1	13·1	145
3	4	6	9·2	10·0	33	8	0	7	18·9	19·5	270	2	6	7	18·9	22·7	284
4	4	6	18·2	14·1	102	9	0	7	9·9	9·2	270	3	6	7	18·7	20·4	122
5	4	6	9·7	12·8	184	11	0	7	22·2	24·5	270	5	6	7	15·0	19·7	254
6	4	6	26·2	23·8	134	12	0	7	11·1	13·1	270	6	6	7	16·5	18·2	208
7	4	6	37·4	34·2	259	13	0	7	11·8	11·3	90	7	6	7	20·5	17·9	326
8	4	6	38·1	34·8	296	14	0	7	21·0	24·5	90	10	6	7	14·4	17·9	63
9	4	6	23·7	22·5	15	16	0	7	10·4	8·9	90	11	6	7	9·8	11·3	339
10	4	6	39·6	35·5	265							13	6	7	12·6	17·5	100
11	4	6	22·0	22·2	89	0	1	7	8·8	17·7	90						
12	4	6	13·1	13·3	99	1	1	7	23·7	32·2	304	1	7	7	14·5	14·3	215
13	4	6	17·8	19·9	253	2	1	7	26·6	32·2	26	4	7	7	16·6	17·5	197
15	4	6	10·3	13·0	61	3	1	7	29·2	29·8	47	7	7	7	14·8	17·3	325
						4	1	7	8·6	8·3	286	11	7	7	16·3	23·6	198
1	5	6	43·9	48·4	25	5	1	7	22·1	23·9	156						
2	5	6	27·1	29·1	169	6	1	7	24·9	13·7	5	2	8	7	13·5	14·0	303
3	5	6	23·9	23·7	189	7	1	7	24·7	21·5	195	7	8	7	14·9	19·7	237
4	5	6	11·3	15·6	18	8	1	7	30·8	22·2	277	11	8	7	9·6	10·9	119
5	5	6	12·2	8·8	18	9	1	7	20·3	14·1	46						
6	5	6	30·0	22·6	267	10	1	7	31·7	32·0	131	2	9	7	15·1	19·5	199
7	5	6	54·1	46·5	159	11	1	7	10·8	8·6	341	5	9	7	13·1	17·3	330
8	5	6	11·7	10·6	198	13	1	7	16·7	15·4	25						
11	5	6	18·7	20·7	21	14	1	7	11·5	6·1	273	2	10	7	10·2	11·7	204
12	5	6	14·2	14·2	134	16	1	7	10·4	11·9	33	6	10	7	9·8	10·3	26

TABLE 4. *Interatomic distances* (Å) *and angles.*

Intramolecular bonded distances

				Average				Average
C(1)–C(2)	1·55	C(1′)–C(2′)	1·56	1·56	C(7)–C(8)	1·54	C(7′)–C(8′)	1·50	1·52
C(2)–C(3)	1·56	C(2′)–C(3′)	1·59	1·57	C(7)–C(9)	1·61	C(7′)–C(9′)	1·55	1·58
C(3)–C(4)	1·54	C(3′)–C(4′)	1·52	1·53	C(7)–C(4)	1·52	C(7′)–C(4′)	1·59	1·56
C(4)–C(5)	1·58	C(4′)–C(5′)	1·55	1·57	C(10)–Br	1·85	C(10′)–Br′	1·89	1·87
C(5)–C(6)	1·55	C(5′)–C(6′)	1·54	1·55	C(2)–Cl	1·81	C(2′)–Cl′	1·75	1·78
C(6)–C(1)	1·59	C(6′)–C(1′)	1·54	1·56	C(2)–N	1·52	C(2′)–N′	1·44	1·48
C(1)–C(10)	1·53	C(1′)–C(10′)	1·51	1·52	N–O	1·16	N′–O′	1·21	1·19
C(1)–C(7)	1·58	C(1′)–C(7′)	1·60	1·59					

TABLE 4. (*Continued.*)

Intramolecular non-bonded distances

				Average				Average
C(1) · · · C(4)	2·29	C(1′) · · · C(4′)	2·28	2·29	C(4) · · · C(6)	2·45	C(4′) · · · C(6′)	2·34	2·40
C(1) · · · C(8)	2·70	C(1′) · · · C(8′)	2·60	2·65	C(4) · · · C(8)	2·64	C(4′) · · · C(8′)	2·57	2·60
C(1) · · · C(9)	2·68	C(1′) · · · C(9′)	2·65	2·66	C(4) · · · C(9)	2·65	C(4′) · · · C(9′)	2·62	2·64
C(1) · · · C(5)	2·48	C(1′) · · · C(5′)	2·52	2·50	C(5) · · · C(7)	2·37	C(5′) · · · C(7′)	2·47	2·42
C(1) · · · C(3)	2·49	C(1′) · · · C(3′)	2·44	2·47	C(5) · · · C(8)	3·03	C(5′) · · · C(8′)	2·87	2·95
C(1) · · · Br	2·86	C(1′) · · · Br′	2·83	2·85	C(6) · · · C(7)	2·38	C(6′) · · · C(7′)	2·36	2·37
C(1) · · · Cl	2·83	C(1′) · · · Cl′	2·83	2·83	C(6) · · · C(8)	3·04	C(6′) · · · C(8′)	2·80	2·92
C(1) · · · O	3·47	C(1′) · · · O′	3·47	3·47	C(6) · · · C(10)	2·66	C(6′) · · · C(10′)	2·60	2·63
C(2) · · · C(4)	2·38	C(2′) · · · C(4′)	2·45	2·42	C(7) · · · C(10)	2·65	C(7′) · · · C(10′)	2·61	2·63
C(2) · · · C(6)	2·53	C(2′) · · · C(6′)	2·52	2·53	C(8) · · · C(10)	3·30	C(8′) · · · C(10′)	3·18	3·24
C(2) · · · C(7)	2·41	C(2′) · · · C(7′)	2·47	2·44	C(9) · · · C(10)	3·20	C(9′) · · · C(10′)	3·22	3·21
C(2) · · · C(9)	3·05	C(2′) · · · C(9′)	2·99	3·02	N · · · Cl	2·70	N′ · · · Cl′	2·63	2·66
C(2) · · · C(10)	2·59	C(2′) · · · C(10′)	2·59	2·59	N · · · Br	3·42	N′ · · · Br′	3·53	3·48
C(2) · · · Br	3·46	C(2′) · · · Br′	3·37	3·41	O . . . Cl	2·71	O′ · · · Cl′	2·73	2·72
C(3) · · · C(5)	2·62	C(3′) · · · C(5′)	2·55	2·58	O · · · Br	3·77	O′ · · · Br′	3·63	3·70
C(3) · · · C(7)	2·40	C(3′) · · · C(7′)	2·42	2·41	Cl · · · Br	3·82	Cl′ · · · Br′	3·78	3·80
C(3) · · · C(9)	2·99	C(3′) · · · C(9′)	2·92	2·95	Cl · · · C(9)	3·26	Cl′ · · · C(9′)	3·19	3·23
C(3) · · · Cl	2·74	C(3′) · · · Cl′	2·79	2·76	Cl · · · C(7)	3·48	Cl′ · · · C(7′)	3·48	3·48
C(3) · · · O	3·25	C(3′) · · · O′	3·27	3·26					

Intermolecular distances ($\leqslant$4 Å)

C(8) · · · O′	3·48	C(10) · · · Cl′	3·77	C(9′) · · · O_I	3·87	C(8′) · · · O_I	3·94
C(10′) · · · N_I	3·49	C(10′) · · · O_I	3·78	C(10′) · · · N'_V	3·88	C(9′) · · · N_I	3·94
O′ · · · $C(3)_{II}$	3·58	C(5′) · · · Br_{III}	3·80	C(9) · · · O′	3·89	C(8′) · · · $C(3')_{VI}$	3·97
C(4′) · · · O_{III}	3·64	O′ · · · Cl_{II}	3·80	Cl · · · $C(9)_{II}$	3·90	C(6′) · · · O'_V	3·99
C(8) · · · Br′	3·65	C(8′) · · · $C(8)_V$	3·83	Br′ · · · $C(5')_V$	3·92	Cl′ · · · $C(5)_{VII}$	3·99
C(6′) · · · O_{IV}	3·71	C(5′) · · · $C(3)_{IV}$	3·84	C(9) · · · $C(3)_{II}$	3·94	N′ · · · Cl_{II}	4·00
C(8′) · · · O'_V	3·74	C(6′) · · · N_{IV}	3·85	C(3′) · · · Cl_{II}	3·94	C(9) · · · $C(4)_{II}$	4·00
C(6′) · · · $C(3)_{IV}$	3·76	C(10) · · · O′	3·85				

The subscripts refer to the following positions:

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

Interbond angles

								Average
C(1)	C(2)	C(3)	107°	C(1′)	C(2′)	C(3′)	102°	104°
C(2)	C(3)	C(4)	100	C(2′)	C(3′)	C(4′)	104	102
C(3)	C(4)	C(5)	114	C(3′)	C(4′)	C(5′)	112	113
C(4)	C(5)	C(6)	103	C(4′)	C(5′)	C(6′)	98	101
C(5)	C(6)	C(1)	104	C(5′)	C(6′)	C(1′)	110	107
C(6)	C(1)	C(2)	108	C(6′)	C(1′)	C(2′)	108	108
C(2)	C(1)	C(7)	100	C(2′)	C(1′)	C(7′)	103	102
C(6)	C(1)	C(7)	97	C(6′)	C(1′)	C(7′)	97	97
C(3)	C(4)	C(7)	103	C(3′)	C(4′)	C(7′)	102	103
C(5)	C(4)	C(7)	100	C(5′)	C(4′)	C(7′)	103	102
C(1)	C(7)	C(8)	120	C(1′)	C(7′)	C(8′)	114	117
C(1)	C(7)	C(9)	114	C(1′)	C(7′)	C(9′)	115	114
C(4)	C(7)	C(8)	119	C(4′)	C(7′)	C(8′)	112	116
C(4)	C(7)	C(9)	116	C(4′)	C(7′)	C(9′)	113	114
C(10)	C(1)	C(2)	115	C(10′)	C(1′)	C(2′)	115	115
C(10)	C(1)	C(6)	118	C(10′)	C(1′)	C(6′)	117	117
C(10)	C(1)	C(7)	117	C(10′)	C(1′)	C(7′)	114	115
C(1)	C(7)	C(4)	95	C(1′)	C(7′)	C(4′)	91	93
C(1)	C(10)	Br	116	C(1′)	C(10′)	Br′	113	114
C(1)	C(2)	N	110	C(1′)	C(2′)	N′	116	113
C(3)	C(2)	N	109	C(3′)	C(2′)	N′	97	103
C(1)	C(2)	Cl	115	C(1′)	C(2′)	Cl′	117	116
C(3)	C(2)	Cl	109	C(3′)	C(2′)	Cl′	113	111
Cl	C(2)	N	108	Cl′	C(2′)	N′	111	109
C(2)	N	O	117	C(2′)	N′	O′	119	118
C(8)	C(7)	C(9)	95	C(8′)	C(7′)	C(9′)	111	103

Experimental.—Copper-K_α radiation, $\lambda = 1{\cdot}542$ Å, was employed in all the measurements. As the crystals are somewhat sensitive to light all experimental work with them was carried out in subdued light. Rotation, oscillation, and moving-film photographs were taken from crystals rotated about the principal zone axes, and these were analysed in the usual way to determine the cell dimensions and systematic halvings, from which the space group was determined uniquely.

The density was determined by flotation in zinc chloride solution.

For the intensity measurements small crystals were employed, completely bathed in a uniform X-ray beam. No corrections for absorption were applied. The multiple-film technique [9] with visual estimation was applied to equatorial and equi-inclination upper-layer Weissenberg photographs taken from crystals rotated about the b and c crystal axes. The usual formulæ for mosaic-type crystals were used to derive values of $|F_o|$. The various layers were put on the same relative scale by comparison of common reflexions on different photographs. The absolute scale was obtained at a later stage by correlation with the final calculated values, $|F_c|$. A total of 1233 independent structure amplitudes was obtained and these are listed in Table 3.

In deriving the calculated $|F|$ values from the atomic co-ordinates theoretical atomic scattering factors were employed: those of Berghuis *et al.*[10] were chosen for carbon, nitrogen, and oxygen, those of Tomiie and Stam [11] for chlorine, and the Thomas–Fermi values [12] for bromine.

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GLASGOW, W.2, SCOTLAND. [*Received, October 20th*, 1960.]

[9] Robertson, *J. Sci. Instr.*, 1943, **20**, 175.
[10] Berghuis, Haanappel, Potter, Loopstra, MacGillavry, and Veenendaal, *Acta Cryst.*, 1955, **8**, 478.
[11] Tomiie and Stam, *Acta Cryst.*, 1958, **11**, 126.
[12] "Internationale Tabellen zur Bestimmung von Kristallstrukturen," Borntraeger, Berlin, 1935, Vol. II, p. 572.