1052. *The Structure of Chimonanthine: X-Ray Analysis of Chimonanthine Dihydrobromide* [1]

By I. J. Grant, T. A. Hamor, J. Monteath Robertson, and G. A. Sim

Chimonanthine, $C_{22}H_{26}N_4$, an alkaloid from *Chimonanthus fragrans*, has been shown to have structure (III; R = R′ = H) by *X*-ray analysis of the dihydrobromide. Crystals of the dihydrobromide belong to the tetragonal system, space group $P4_12_12$ (or the enantiomorphous $P4_32_12$), with eight molecules of $C_{22}H_{28}Br_2N_4$ in the unit cell of dimensions $a = b = 13{\cdot}95$, $c = 26{\cdot}67$ Å. Several three-dimensional electron-density distributions were evaluated and followed by least-squares refinement of the atomic co-ordinates. The final discrepancy R over 2093 independent reflexions is 14·9%.

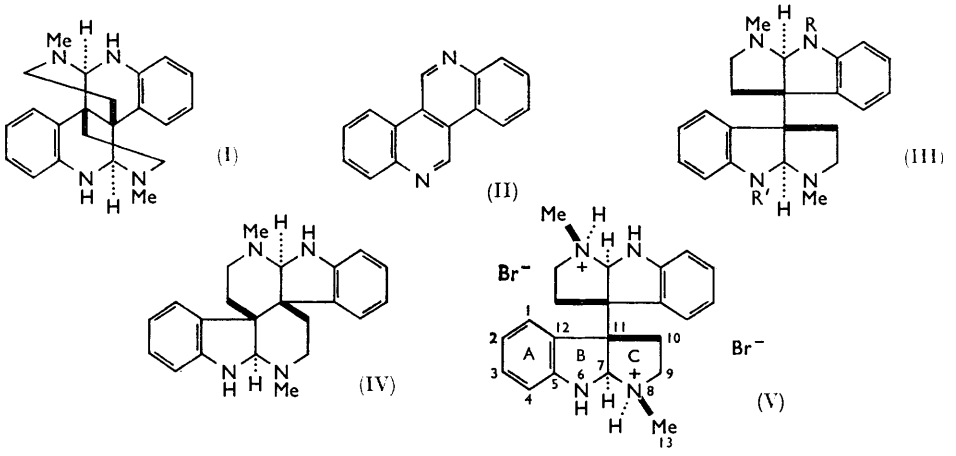
From *Chimonanthus fragrans*, the deciduous shrub commonly known as Winter Sweet, Hodson, Robinson, and Smith [2] isolated an alkaloid chimonanthine, $C_{22}H_{26}N_4$, isomeric with calycanthine (I).[3] The ultraviolet spectrum of the alkaloid indicated the presence of the grouping Ph·N·C·N, and reduction with zinc and hydrochloric acid yielded 3-2′-methylaminoethylindoline showing that, like calcyanthine, the alkaloid contains two tryptamine units. In contrast to calycanthine, chimonanthine on zinc dehydrogenation

[1] For a preliminary report see I. J. Grant, T. A. Hamor, J. M. Robertson, and G. A. Sim, *Proc. Chem. Soc.*, 1962, 148.

[2] H. F. Hodson, B. Robinson, and G. F. Smith, *Proc. Chem. Soc.*, 1961, 465.

[3] Sir R. Robinson and H. J. Teuber, *Chem. and Ind.*, 1954, 783; T. A. Hamor, J. M. Robertson, H. N. Shrivastava, and J. V. Silverton, *Proc. Chem. Soc.*, 1960, 78; R. B. Woodward, N. C. Yang, T. J. Katz, V. M. Clark, J. Harley-Mason, R. F. J. Ingleby, and N. Sheppard, *ibid.*, p. 76.

gave only traces of calycanine (II). Chimonanthine has aromatic NH groups and aliphatic tertiary *N*-methyl groups. The structural possibilities were narrowed to two formulæ (III; R = R′ = H) and (IV) which were not readily distinguished chemically.



At the suggestion of Dr. G. F. Smith we undertook an *X*-ray crystal-structure analysis of chimonanthine dihydrobromide in order to provide an unambiguous determination of the molecular structure. Our results establish structure (V) for the dihydrobromide so that chimonanthine has therefore to be assigned structure (III; R = R′ = H). Saxton, Bardsley, and Smith [4] have shown that two other naturally occurring alkaloids, calycanthidine and folicanthine, represent successive further stages of methylation of chimonanthine; it follows that calycanthidine must be formulated as (III; R = H, R′ = Me) and folicanthine as (III; R = R′ = Me).

The crystal structure was solved by means of the usual phase-determining heavy-atom method.[5] Four three-dimensional electron-density distributions were calculated and the positional and thermal atomic parameters were then further improved by the method of

TABLE 1

Atomic co-ordinates (origin of co-ordinates as in " International Tables for *X*-Ray Crystallography," The Kynoch Press, Birmingham, 1952, vol. I)

Atom	*x/a*	*y/b*	*z/c*	Atom	*x/a*	*y/b*	*z/c*
C(1)	0·7967	0·4854	0·4351	C(4′)	0·8641	0·4812	0·5988
C(2)	0·7670	0·5813	0·4280	C(5′)	0·8582	0·4132	0·5578
C(3)	0·6668	0·6053	0·4330	C(7′)	0·9096	0·3051	0·5048
C(4)	0·6007	0·5361	0·4435	C(9′)	0·8899	0·1697	0·5449
C(5)	0·6302	0·4449	0·4527	C(10′)	0·7932	0·1830	0·5187
C(7)	0·6303	0·2788	0·4689	C(11′)	0·8022	0·2895	0·5057
C(9)	0·6774	0·2363	0·3850	C(12′)	0·7815	0·3584	0·5487
C(10)	0·7690	0·2581	0·4115	C(13′)	0·0587	0·2324	0·5380
C(11)	0·7340	0·3136	0·4600	N(6)	0·5710	0·3692	0·4647
C(12)	0·7232	0·4192	0·4479	N(8)	0·6039	0·2065	0·4268
C(13)	0·5073	0·1977	0·4127	N(6′)	0·9423	0·3873	0·5262
C(1′)	0·7016	0·3649	0·5779	N(8′)	0·9607	0·2134	0·5122
C(2′)	0·6986	0·4311	0·6161	Br(I)	0·4868	0·1069	0·5537
C(3′)	0·7823	0·4912	0·6248	Br(II)	0·9715	0·0758	0·4173

least-squares. The average discrepancy between measured and calculated structure amplitudes, *R*, decreased to a final value of 14·9% over 2093 independent reflexions.

[4] J. E. Saxton, W. G. Bardsley, and G. F. Smith, *Proc. Chem. Soc.*, 1962, 148.
[5] J. M. Robertson and I. Woodward, *J.*, 1937, 219; 1940, 36; G. A. Sim, in " Computing Methods and the Phase Problem in *X*-ray Crystal Analysis," ed. R. Pepinsky, J. M. Robertson, and J. C. Speakman, Pergamon Press, Oxford, 1961, p. 227.

The third electron-density distribution is shown in Figure 1 as superimposed contour sections drawn parallel to (001) and covering the region of one molecule. The atomic arrangement corresponding to this electron-density distribution is explained in Figure 2. It will be noted that, in the crystal, the molecule is much closer to the *cis*- than to the

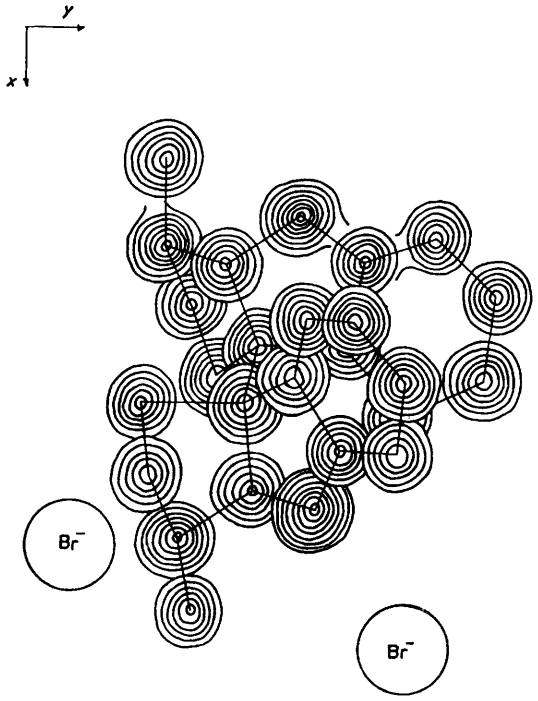


FIGURE 1. The third three-dimensional electron-density distribution for chimonanthine dihydrobromide shown by means of superimposed contour sections drawn parallel to (001). Contour interval 1eÅ^{-3}, starting at the 2-electron contour

trans-conformation indicated in (V). The final atomic co-ordinates are listed in Table 1 and the interatomic distances and valency angles calculated from the co-ordinates 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

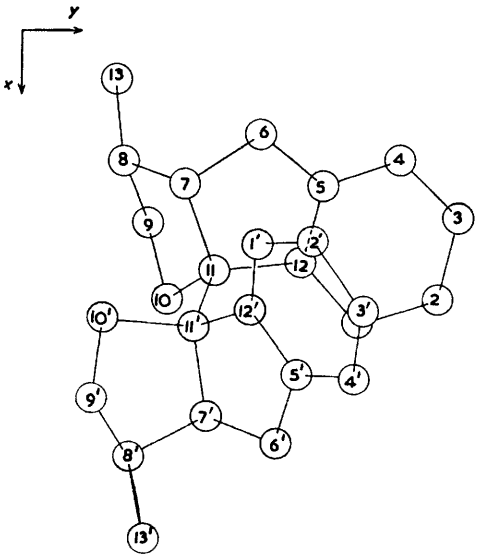


FIGURE 2. Atomic arrangement corresponding to Figure 1

Table 3; from the results the average estimated standard deviation (e.s.d.) of a carbon–carbon bond length is about 0·08 Å and the average e.s.d. of a valency angle about 4°.

The average bond length in the benzene ring, 1·39 Å, and the average carbon–carbon single bond length, 1·54 Å, agree well with the accepted values of 1·397 and 1·545 Å [6] for such bonds. The average C(sp^3)–N^+ bond length of 1·50 Å is in reasonable agreement with the lengths of such bonds in other alkaloids, *e.g.*, 1·49 Å in macusine-A iodide,[7] 1·54 Å in echitamine bromide.[8]

In the five-membered rings B and B′ the average valency angle is 108° whereas in the five-membered rings C and C′ the corresponding value is only 104°. A similar difference exists in the echitamine molecule.[8] In saturated five-membered rings the average valency

TABLE 2

Interatomic distances (Å) and angles

Intramolecular bonded distances

C(1)–C(2)	1·41	C(7)–C(11)	1·54	C(1′)–C(2′)	1·38	C(7′)–C(11′)	1·51
C(2)–C(3)	1·44	C(11)–C(12)	1·52	C(2′)–C(3′)	1·44	C(11′)–C(12′)	1·52
C(3)–C(4)	1·36	C(7)–N(8)	1·55	C(3′)–C(4′)	1·34	C(7′)–N(8′)	1·48
C(4)–C(5)	1·35	N(8)–C(9)	1·57	C(4′)–C(5′)	1·45	N(8′)–C(9′)	1·45
C(5)–C(12)	1·35	C(9)–C(10)	1·49	C(5′)–C(12′)	1·34	C(9′)–C(10′)	1·53
C(12)–C(1)	1·42	C(10)–C(11)	1·58	C(12′)–C(1′)	1·36	C(10′)–C(11′)	1·53
C(5)–N(6)	1·38	N(8)–C(13)	1·41	C(5′)–N(6′)	1·49	N(8′)–C(13′)	1·55
N(6)–C(7)	1·51			N(6′)–C(7′)	1·36	C(11)–C(11′)	1·58

Intramolecular non-bonded distances <4·0 Å

C(1) · · · N(6)	3·62	C(11) · · · C(13)	3·77	C(1′) · · · N(6′)	3·64	C(11′) · · · C(13′)	3·77
C(1) · · · C(7)	3·81	C(1) · · · C(5′)	3·53	C(1′) · · · C(7′)	3·59	C(9) · · · C(11′)	3·74
C(1) · · · C(9)	4·07	C(1) · · · N(6′)	3·45	C(1′) · · · C(9′)	3·89	C(10) · · · N(8′)	3·84
C(1) · · · C(10)	3·26	C(1) · · · C(7′)	3·50	C(1′) · · · C(10′)	3·25	C(10) · · · C(7′)	3·24
C(2) · · · C(11)	3·85	C(1) · · · C(11′)	3·32	C(2′) · · · C(11′)	3·83	C(10) · · · C(10′)	3·06
C(3) · · · N(6)	3·65	C(1) · · · C(12′)	3·51	C(3′) · · · N(6′)	3·74	C(10) · · · C(12′)	3·92
C(4) · · · C(7)	3·68	C(5) · · · C(1′)	3·66	C(4′) · · · C(7′)	3·57	C(11) · · · C(1′)	3·26
C(4) · · · C(11)	3·64	C(5) · · · C(11′)	3·53	C(4′) · · · C(11′)	3·75	C(11) · · · C(5′)	3·42
C(5) · · · N(8)	3·42	C(5) · · · C(12′)	3·53	C(5′) · · · N(8′)	3·36	C(11) · · · N(6′)	3·55
C(5) · · · C(9)	3·49	N(6) · · · C(1′)	3·53	C(5′) · · · C(9′)	3·44	C(11) · · · N(8′)	3·73
C(5) · · · C(10)	3·43	N(6) · · · C(11′)	3·58	C(5′) · · · C(10′)	3·49	C(11) · · · C(9′)	3·73
C(5) · · · C(13)	3·99	N(6) · · · C(12′)	3·70	C(5′) · · · C(13′)	3·80	C(12) · · · C(1′)	3·56
N(6) · · · C(9)	3·19	C(7) · · · C(1′)	3·30	N(6′) · · · C(9′)	3·16	C(12) · · · C(5′)	3·48
N(6) · · · C(10)	3·47	C(7) · · · C(10′)	2·95	N(6′) · · · C(10′)	3·53	C(12) · · · N(6′)	3·73
N(6) · · · C(13)	2·91	C(7) · · · C(12′)	3·19	N(6′) · · · C(13′)	2·72	C(12) · · · C(7′)	3·41
N(8) · · · C(12)	3·45	N(8) · · · C(10′)	3·62	N(8′) · · · C(12′)	3·36	C(12) · · · C(10′)	3·92
C(9) · · · C(12)	3·12	N(8) · · · C(11′)	3·66	C(9′) · · · C(12′)	3·04	C(12) · · · C(12′)	2·93
C(10) · · · C(13)	3·75	C(9) · · · C(10′)	3·99	C(10′) · · · C(13′)	3·80		

Intermolecular distances <4·0 Å

C(7) · · · Br(I)	3·86	C(2) · · · C(9′) (i)	3·82	C(4) · · · C(2′) (iii)	3·64
N(8) · · · Br(I)	4·00	C(3) · · · C(9′) (i)	3·68	N(6′) · · · Br(I) (iv)	3·43
C(10) · · · Br(II)	3·80	C(9) · · · C(13′) (i)	3·93	Br(II) · · · C(13′) (v)	3·84
C(13) · · · Br(I)	3·98	C(9) · · · Br(I) (ii)	3·92	Br(I) · · · C(4′) (vi)	3·76
N(8′) · · · Br(II)	3·18	C(3) · · · C(3) (iii)	3·77	C(10) · · · C(13) (vii)	3·92
C(9′) · · · Br(II)	3·82	C(3) · · · C(4) (iii)	3·77	Br(II) · · · C(4) (vii)	3·80
C(10′) · · · Br(II)	3·97	C(3) · · · C(2′) (iii)	3·77	Br(II) · · · C(5) (vii)	3·90
C(2) · · · C(3′) (i)	3·93	C(3) · · · C(3′) (iii)	3·80	Br(II) · · · N(6) (vii)	3·86
C(2) · · · C(4′) (i)	3·74	C(4) · · · C(4) (iii)	3·27	Br(II) · · · C(13) (vii)	3·85
C(2) · · · C(5′) (i)	3·89	C(4) · · · C(5) (iii)	3·76		

The figures in parentheses refer to the following equivalent positions.

(i)	$\frac{1}{2}+y, \frac{3}{2}-x, -\frac{1}{4}+z$;	(v)	$1+y, -1+x, 1-z$;
(ii)	$\frac{1}{2}+y, \frac{1}{2}-x, -\frac{1}{4}+z$;	(vi)	$\frac{3}{2}-x, -\frac{1}{2}+y, \frac{5}{4}-z$;
(iii)	$y, x, 1-z$;	(vii)	$\frac{1}{2}+x, \frac{1}{2}-y, \frac{3}{4}-z$.
(iv)	$1+y, x, 1-z$;		

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

[7] A. T. McPhail, J. M. Robertson, and G. A. Sim, *J.*, 1963, 1832.

[8] J. A. Hamilton, T. A. Hamor, J. M. Robertson, and G. A. Sim, *J.*, 1962, 5061.

TABLE 2 (*Continued*)

Valency angles

C(12)–C(1)–C(2)	116°	C(12′)–C(1′)–C(2′)	120°
C(1)–C(2)–C(3)	119	C(1′)–C(2′)–C(3′)	119
C(2)–C(3)–C(4)	121	C(2′)–C(3′)–C(4′)	123
C(3)–C(4)–C(5)	120	C(3′)–C(4′)–C(5′)	114
C(4)–C(5)–C(12)	121	C(4′)–C(5′)–C(12′)	124
C(5)–C(12)–C(1)	123	C(5′)–C(12′)–C(1′)	121
C(12)–C(11)–C(7)	104	C(12′)–C(11′)–C(7′)	96
C(11)–C(7)–N(6)	104	C(11′)–C(7′)–N(6′)	117
C(7)–N(6)–C(5)	109	C(7′)–N(6′)–C(5′)	100
N(6)–C(5)–C(12)	113	N(6′)–C(5′)–C(12′)	113
C(5)–C(12)–C(11)	109	C(5′)–C(12′)–C(11′)	110
C(11)–C(10)–C(9)	103	C(11′)–C(10′)–C(9′)	99
C(10)–C(9)–N(8)	106	C(10′)–C(9′)–N(8′)	106
C(9)–N(8)–C(7)	101	C(9′)–N(8′)–C(7′)	97
N(8)–C(7)–C(11)	108	N(8′)–C(7′)–C(11′)	111
C(7)–C(11)–C(10)	105	C(7′)–C(11′)–C(10′)	103
C(9)–N(8)–C(13)	117	C(9′)–N(8′)–C(13′)	114
C(7)–N(8)–C(13)	119	C(7′)–N(8′)–C(13′)	110
C(1)–C(12)–C(11)	128	C(1′)–C(12′)–C(11′)	129
C(4)–C(5)–N(6)	125	C(4′)–C(5′)–N(6′)	123
N(6)–C(7)–N(8)	111	N(6′)–C(7′)–N(8′)	121
C(12)–C(11)–C(11′)	116	C(12′)–C(11′)–C(11)	109
C(10)–C(11)–C(11′)	110	C(10′)–C(11′)–C(11)	109
C(7)–C(11)–C(11′)	112	C(7′)–C(11′)–C(11)	124
C(12)–C(11)–C(10)	109	C(12′)–C(11′)–C(10′)	115

TABLE 3

Standard deviations of the final atomic co-ordinates (Å)

Atom	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$	Atom	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$
C(1)	0·053	0·057	0·067	C(4′)	0·056	0·064	0·065
C(2)	0·060	0·059	0·061	C(5′)	0·044	0·041	0·053
C(3)	0·053	0·052	0·057	C(7′)	0·049	0·047	0·060
C(4)	0·058	0·053	0·059	C(9′)	0·059	0·058	0·060
C(5)	0·052	0·056	0·067	C(10′)	0·053	0·054	0·061
C(7)	0·054	0·053	0·062	C(11′)	0·050	0·043	0·057
C(9)	0·056	0·061	0·066	C(12′)	0·052	0·051	0·057
C(10)	0·052	0·052	0·054	C(13′)	0·061	0·063	0·077
C(11)	0·049	0·046	0·056	N(6)	0·039	0·040	0·049
C(12)	0·043	0·042	0·059	N(8)	0·047	0·044	0·052
C(13)	0·053	0·056	0·070	N(6′)	0·040	0·044	0·055
C(1′)	0·048	0·050	0·064	N(8′)	0·041	0·041	0·051
C(2′)	0·055	0·056	0·066	Br(I)	0·006	0·006	0·007
C(3′)	0·059	0·057	0·071	Br(II)	0·006	0·006	0·007

angles are consistently smaller than tetrahedral, *e.g.*, 105° in isoclovene hydrochloride [9] and bromodihydroisophotosantonic lactone acetate; [10] such values are consistent with the non-planarity and consequent angle deformations in cyclopentane.[11] Rings c and c′ in chimonanthine adopt the envelope conformation with C(9) and C(9′) constituting the flaps of the envelopes (see Figure 3); the angle between the mean plane through C(7), N(8), C(10), C(11) and that through C(13), N(8), C(9), C(10) is 72°, while in the other half of the molecule the corresponding angle is 64°.

The molecular arrangement in the crystal as seen in projection along the *b* axis is shown in Figure 3. Each of the crystallographically independent bromide ions has two contacts of less than 4 Å with nitrogen atoms. The distances involved, N(8) · · · Br(1) 4·00 Å, N(6′) · · · Br(1) 3·43 Å, N(8′) · · · Br(2) 3·18 Å, N(6) · · · Br(2) 3·86 Å, suggest that only the contacts N(6′) · · · Br(1) and N(8′) · · · Br(2) represent true hydrogen bonds. The closest approach between two chimonanthine molecules is 3·27 Å and involves C(4) of the reference molecule at (x,y,z) and C(4) of the molecule at position $(y,x,1-z)$. A list of the intermolecular contacts of less than 4 Å is given in Table 2.

[9] J. S. Clunie and J. M. Robertson, *J.*, 1961, 4382.
[10] J. D. M. Asher and G. A. Sim, *Proc. Chem. Soc.*, 1962, 111; *J.*, 1965, 1584.
[11] K. S. Pitzer and W. E. Donath, *J. Amer. Chem. Soc.*, 1959, **81**, 3213; F. V. Brutcher, T. Roberts, S. J. Barr, and N. Pearson, *ibid.*, p. 4915.

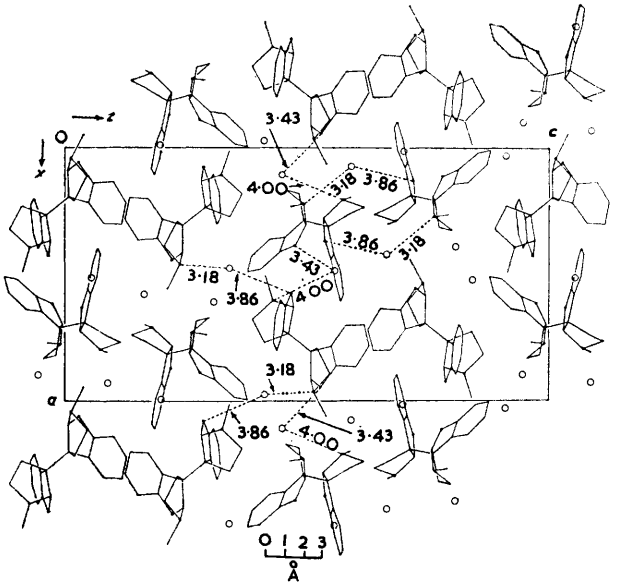


FIGURE 3. The crystal structure of chimonanthine dihydrobromide as viewed in projection along the *b*-axis

EXPERIMENTAL

Crystal Data.—Chimonanthine dihydrobromide, $C_{22}H_{28}N_4Br_2$; M, 508·3; m. p. 188—189°. Tetragonal, $a = b = 13{\cdot}95$, $c = 26{\cdot}67$ Å, $U = 5190$ Å^3, $D_m = 1{\cdot}35$ g. cm.$^{-3}$, $Z = 8$, $D_c = 1{\cdot}31$ g. cm.$^{-3}$. Space group $P4_12_12 - D_4^4$ (or the enantiomorphous $P4_32_12 - D_4^8$). Absorption coefficient for X-rays ($\lambda = 1{\cdot}542$ Å) $\mu = 42$ cm.$^{-1}$. Total number of electrons in the unit cell = F(000) = 2064. Σf^2 (heavy atoms)/Σf^2 (light atoms) = 2·4 at sin $\theta = 0$.

Crystallographic Measurements.—Rotation, oscillation, and Weissenberg photographs were taken with Cu-K_α ($\lambda = 1{\cdot}542$ Å) radiation. The unit-cell dimensions were obtained from rotation and equatorial-layer line Weissenberg photographs. The space group was determined from the systematic absences in the X-ray spectra. A small crystal, completely bathed in a uniform X-ray beam, was employed for the intensity measurements and no corrections for absorption were made. The $0kl$—$9kl$ spectra were recorded photographically by means of an equi-inclination Weissenberg camera and the intensities were estimated visually. The usual correction factors (Lorentz, polarization, and rotation [12]) were applied to the intensities. The various sets of structure amplitudes were placed on the same relative scale by comparison of equivalent reflexions hkl and khl; the absolute scale was obtained at a later stage by correlation with the final calculated structure amplitudes. A total of 2093 independent $|F_o|$ values was derived (Table 5).

Analysis of the Structure.—Three-dimensional methods were used throughout for the elucidation of the structure and the refinement of the atomic parameters.

In order to determine the positions of the two bromide ions in the asymmetric crystal unit we calculated a three-dimensional Patterson function P(UVW). Sections through this function at $W = \frac{1}{4}$, $W = \frac{1}{2}$, and $V = \frac{1}{2}$, which contain peaks representing vectors between symmetry-related bromide ions, are shown in Figure 4. We were able to assign initial co-ordinates to the bromide ions by consideration of these sections and of the general Patterson peaks corresponding to vectors between non-related bromide ions.[13]

The Fourier programme [14] for the DEUCE computer cannot be used conveniently for crystals belonging to the space group $P4_12_12$. To overcome this difficulty we treated the unit cell in the subsequent structure-factor and Fourier calculations as if it belonged to the

[12] G. Tunell, *Amer. Min.*, 1939, **24**, 448.
[13] I. J. Grant, Ph.D. Thesis, University of Glasgow, 1962.
[14] J. S. Rollett, in "Computing Methods and the Phase Problem in X-ray Crystal Analysis," ed. R. Pepinsky, J. M. Robertson, and J. C. Speakman, Pergamon Press, Oxford, 1961, p. 87.

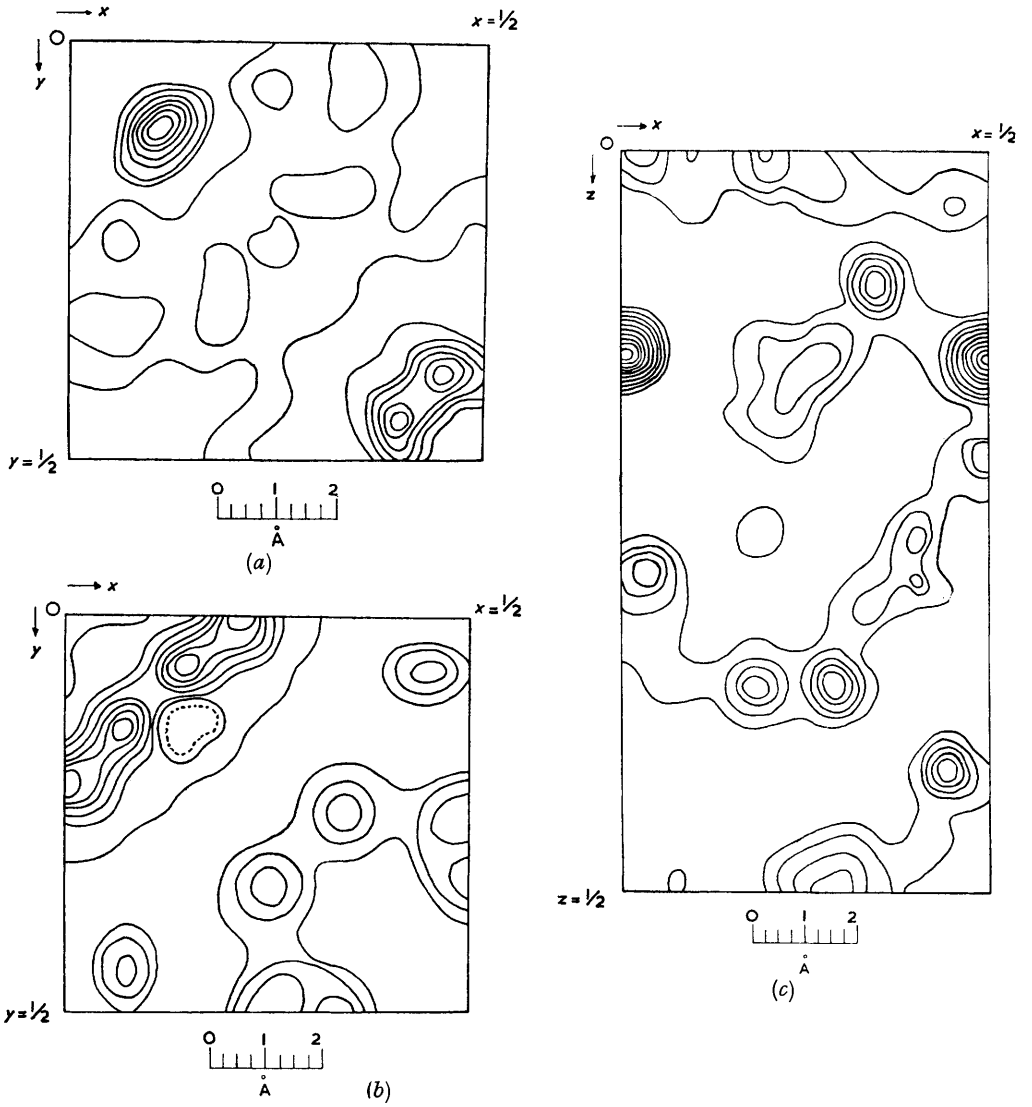


FIGURE 4. Sections through the three-dimensional Patterson function P(UVW), (a) at $W = \frac{1}{4}$, (b) at $W = \frac{1}{2}$, (c) at $V = \frac{1}{2}$. Contour scale arbitrary

TABLE 4

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

	b_{11}	b_{22}	b_{33}	b_{12}	b_{23}	b_{13}		b_{11}	b_{22}	b_{33}	b_{12}	b_{23}	b_{13}
C(1)	661	663	182	−17	10	−700	C(4′)	468	422	196	−247	103	400
C(2)	899	627	182	−92	−2	−141	C(5′)	886	753	85	−9	−216	287
C(3)	638	553	174	−60	−63	−46	C(7′)	675	232	116	46	48	−195
C(4)	965	681	106	−243	−9	229	C(9′)	802	858	263	13	−475	434
C(5)	551	705	143	−51	−101	921	C(10′)	296	564	183	−199	82	256
C(7)	453	710	174	−58	44	−299	C(11′)	577	566	191	5	131	294
C(9)	619	324	104	85	179	−73	C(12′)	536	552	178	−152	18	429
C(10)	534	457	124	−39	−51	912	C(13′)	266	659	123	−26	−18	301
C(11)	421	1083	217	−305	−44	−636	N(6)	415	593	182	−151	−64	155
C(12)	592	745	175	175	115	703	N(8)	487	736	101	−332	−57	396
C(13)	892	607	197	2	−4	933	N(6′)	639	606	135	2	81	254
C(1′)	961	274	177	−11	63	82	N(8′)	541	505	128	180	−80	119
C(2′)	891	885	216	−79	−49	−507	Br(I)	681	735	209	−74	−6	−89
C(3′)	730	286	139	69	−172	−869	Br(II)	694	667	192	−131	−49	418

TABLE 5

Measured and calculated values of the structure factors

h	k	l	F_o	F_c	α	h	k	l	F_o	F_c	α	h	k	l	F_o	F_c	α
0	0	8	364	445	180			9	143	135	45			20	68	53	270
		12	15	2	180			10	106	129	0			21	51	35	45
		16	77	58	0			11	76	71	135			22	56	50	180
		24	93	78	0			12	117	105	270			24	18	14	270
		28	65	69	180			13	27	32	225			25	20	20	225
		32	28	29	180			14	14	15	0			26	25	19	0
0	1	5	68	73	225			15	55	72	135			27	46	33	135
		6	14	42	180			17	70	69	225			28	19	15	90
		7	54	65	315			18	142	127	180			29	15	13	225
		8	18	59	90			19	66	57	315			30	18	14	0
		9	69	111	45			21	38	31	45			31	13	13	315
		10	184	186	0			22	18	14	180			32	24	20	270
		11	23	41	315			23	68	46	315	0	6	0	79	82	180
		12	191	176	270			24	28	23	90			1	184	174	135
		13	33	20	225			26	74	70	0			2	48	53	90
		14	71	79	0			27	64	53	135			3	36	54	225
		15	57	67	135			28	12	11	90			4	22	11	180
		16	74	78	270			31	27	24	135			5	42	34	135
		18	154	127	180			32	31	25	270			6	115	136	270
		19	48	48	315	0	4	0	68	89	0			7	39	32	45
		20	35	40	90			1	61	54	135			8	20	35	0
		21	32	32	45			2	46	51	270			9	144	159	315
		22	37	36	0			3	59	107	225			10	71	53	270
		23	63	60	315			4	65	79	180			11	54	69	45
		24	59	53	90			5	9	8	135			12	28	23	180
		26	37	30	0			6	191	200	270			14	154	138	90
		27	13	9	135			7	54	86	45			16	15	24	0
		30	38	34	180			8	68	50	0			17	45	36	135
		31	10	9	135			10	62	57	270			19	37	33	45
0	2	3	75	54	45			11	37	21	225			22	112	87	270
		4	73	83	180			12	81	67	0			23	51	33	45
		5	49	35	315			13	38	36	135			24	20	20	180
		6	290	249	270			14	177	183	90			26	22	15	90
		7	290	343	45			15	95	88	225			27	23	26	225
		8	186	214	180			17	63	54	135	0	7	2	118	120	180
		9	119	92	315			19	28	21	45			3	76	93	135
		10	14	9	90			20	22	16	180			4	70	106	90
		11	59	66	45			21	68	53	315			5	130	145	225
		12	28	39	0			22	97	87	270			6	69	70	0
		13	44	59	135			23	23	16	45			7	29	3	315
		14	79	92	90			24	29	26	0			8	16	12	270
		15	130	154	225			27	35	25	225			9	65	46	45
		17	97	75	135			28	16	15	180			11	19	36	315
		18	14	5	90			30	21	23	90			12	24	25	270
		19	17	9	45			31	17	14	225			13	94	90	45
		20	12	12	0	0	5	1	89	74	225			14	38	31	180
		21	36	49	315			2	72	55	180			15	42	30	315
		22	41	65	270			3	182	208	135			16	26	17	90
		23	59	57	45			4	157	172	90			17	16	0	225
		24	16	14	0			5	107	83	225			18	32	27	0
		25	26	23	315			6	57	57	0			19	26	25	315
		27	15	2	225			8	48	40	270			20	25	18	270
		28	38	41	180			9	102	102	45			21	19	11	225
		29	30	23	135			10	82	84	0			28	22	22	90
		32	14	10	180			11	102	74	315			29	26	22	225
0	3	1	82	80	225			13	33	23	45			30	14	18	0
		2	18	54	180			14	11	19	0	0	8	0	29	34	0
		4	176	191	90			15	11	24	135			1	129	132	135
		5	95	97	45			16	42	54	90			2	106	82	90
		6	32	19	0			17	21	26	225			5	68	72	315
		7	101	76	135			18	106	90	180			6	50	37	90
		8	36	52	270			19	51	64	315			7	160	143	225

TABLE 5 (*Continued*)

h	*k*	*l*	F_o	F_c	α
		8	89	86	180
		9	48	47	315
		10	42	40	270
		11	16	13	45
		12	74	77	180
		13	21	22	135
		14	65	55	90
		15	40	28	45
		16	13	20	0
		17	28	30	315
		20	69	51	0
		22	55	41	270
		23	12	12	45
		24	15	18	180
		25	28	25	135
		26	28	22	90
		27	20	19	225
		29	25	19	315
0	9	1	27	42	45
		2	22	30	180
		3	33	38	135
		4	79	96	90
		5	84	76	225
		7	18	28	315
		10	15	12	180
		11	50	55	135
		12	36	46	270
		13	67	67	45
		15	13	13	315
		17	51	43	225
		18	48	37	0
		19	24	23	315
		20	26	19	90
		22	12	3	0
		23	25	28	135
		24	11	8	90
		25	13	12	45
		28	8	6	270
0	10	0	96	120	0
		1	62	81	135
		3	24	43	45
		5	114	115	315
		6	17	8	90
		7	29	24	225
		8	35	44	180
		10	18	22	90
		11	37	34	45
		13	87	75	135
		15	21	27	225
		16	45	56	0
		17	26	23	315
		19	52	41	225
		20	26	32	0
		21	23	18	315
		22	23	26	90
		23	49	40	45
0	11	3	43	40	315
		4	31	28	90
		5	49	46	225
		6	13	28	0
		7	29	31	315
		8	67	75	90
		9	41	44	45
		11	38	41	135
		12	34	29	270
		13	48	46	45
		14	23	16	180
		16	50	51	270
		17	37	36	225
		19	44	48	315
		20	34	36	90
		22	27	20	0
		23	10	15	135
		24	18	22	90
		25	33	34	45
0	12	2	21	30	270
		3	18	34	45
		4	39	39	180
		5	28	34	315
		10	56	56	90
		13	58	49	135
		14	18	18	270
		15	25	31	225
		21	21	17	315
		22	11	7	90
		23	31	31	45
0	13	1	26	29	225
		2	29	32	180
		4	59	60	270
		8	26	31	90
		9	41	50	45
		10	52	40	0
		11	46	42	135
		12	25	18	90
		13	17	22	45
		15	23	21	135
		17	29	33	225
		18	30	27	180
		19	20	19	315
		20	17	18	90
		21	13	16	225
0	14	1	20	16	135
		2	66	59	270
		5	25	26	315
		6	31	30	270
		9	19	20	315
		10	38	46	90
		11	17	20	225
		13	41	29	135
		15	19	18	225
0	15	1	17	23	225
		2	19	31	180
		3	20	30	135
		4	43	50	270
		5	16	26	225
		7	18	14	135
		8	16	19	90
		9	13	15	45
0	16	1	40	40	135
		2	19	20	270
		5	16	15	135
		6	14	16	270
		9	37	39	315
		10	21	26	90
		11	18	22	225
		12	14	21	180
		13	12	13	315
0	17	1	19	29	225
		3	26	28	135
		5	23	20	225
		7	27	34	135
1	1	3	73	110	270
		4	102	106	180
		5	9	60	270
		6	20	10	180
		7	77	130	90
		8	23	4	0
		9	108	121	270
		10	28	29	0
		11	15	30	90
		12	153	169	0
		13	61	51	270
		14	33	26	180
		15	18	13	270
		16	88	101	180
		17	15	2	90
		20	95	94	180
		22	35	25	0
		23	23	17	270
		24	89	78	0
		26	23	20	0
		27	21	22	270
		30	18	20	180
1	2	0	26	44	180
		1	58	61	303
		2	130	196	320
		3	179	274	155
		4	62	90	281
		5	105	155	241
		6	274	315	190
		7	42	15	121
		8	81	77	276
		9	75	104	175
		10	18	13	64
		11	145	149	288
		12	84	86	17
		13	59	47	302
		14	87	75	16
		15	68	67	62
		16	53	59	74
		17	79	83	25
		18	53	54	202
		19	28	28	111
		20	24	25	261
		21	49	36	45
		22	21	18	349
		23	25	20	228
		24	24	24	250
		25	46	45	229
		26	25	18	3
1	3	0	37	48	0
		1	118	131	111
		2	80	79	80
		3	162	186	229
		4	151	140	125
		5	194	206	105

TABLE 5 (*Continued*)

h	*k*	*l*	F_o	F_c	α
		6	111	94	97
		7	71	49	332
		8	21	35	247
		9	140	150	306
		10	23	48	266
		11	52	60	347
		12	106	114	355
		13	37	38	290
		15	38	33	163
		16	27	22	126
		17	88	79	131
		18	27	23	192
		19	72	63	89
		20	38	30	172
		21	24	28	54
		22	17	4	243
		24	49	37	315
		27	31	32	260
1	4	0	21	44	0
		1	75	88	287
		2	162	180	344
		3	219	218	141
		4	113	100	92
		5	93	79	210
		6	122	98	199
		7	38	47	355
		8	93	73	264
		9	109	108	122
		10	102	95	184
		11	150	116	315
		12	37	43	358
		13	84	93	251
		14	28	16	341
		15	84	82	117
		16	44	36	96
		17	16	10	145
		18	66	63	354
		19	43	36	191
		20	38	34	259
		21	50	56	58
		22	29	32	5
		23	49	40	271
		24	31	24	26
		25	28	32	225
		26	28	30	162
		27	23	20	74
		28	40	30	78
		29	21	22	190
1	5	0	29	21	180
		1	62	59	37
		2	194	215	83
		3	98	127	246
		4	60	56	21
		5	20	43	118
		6	188	174	101
		7	60	50	5
		8	30	24	299
		9	117	97	240
		10	133	123	306
		11	87	68	35
		12	43	40	221
		13	66	65	203
		14	24	35	305
		15	44	56	200
		17	47	40	67
		18	34	30	195
		19	38	36	114
		21	51	45	307
		22	18	13	56
		23	27	19	31
		24	20	19	163
		25	19	19	191
		26	57	57	85
		27	23	19	246
		29	17	17	177
1	6	0	107	80	0
		1	18	14	56
		2	76	89	21
		3	60	86	285
		4	105	110	77
		5	107	119	128
		6	18	20	74
		7	113	96	327
		8	122	104	251
		9	105	86	52
		10	116	116	206
		11	73	65	130
		12	47	39	5
		13	51	45	299
		14	48	33	144
		15	59	61	140
		16	54	47	98
		17	68	58	245
		18	90	80	348
		19	45	42	299
		20	72	56	253
		21	51	51	54
		22	46	34	294
		23	28	30	299
		25	24	29	85
		26	21	26	183
		27	15	19	126
		28	37	34	124
		29	16	20	178
1	7	0	106	104	180
		1	46	54	35
		2	119	106	83
		3	51	58	212
		4	18	29	65
		5	88	102	30
		6	48	40	82
		7	37	37	321
		8	72	59	335
		9	66	53	108
		10	152	121	294
		11	89	75	32
		13	90	82	160
		14	28	22	26
		15	48	49	201
		16	34	32	287
		17	44	49	321
		18	25	19	165
		19	83	61	192
		20	18	16	239
		21	46	45	345
		22	18	15	201
		23	45	36	29
		24	19	16	112
		25	18	17	129
		26	23	21	64
		27	15	14	337
		28	15	20	26
1	8	0	49	51	0
		1	55	55	12
		2	30	36	125
		3	47	47	275
		4	42	39	303
		5	16	15	145
		6	23	29	32
		7	108	99	334
		8	90	79	240
		9	94	64	79
		10	42	37	249
		11	95	82	104
		12	76	57	91
		13	45	39	311
		14	24	24	141
		15	70	66	110
		16	82	66	87
		17	83	73	243
		19	43	37	294
		20	40	38	283
		21	17	18	0
		22	26	26	244
		23	19	19	251
		24	36	32	272
		25	47	45	56
1	9	0	142	132	180
		1	49	47	118
		2	15	28	186
		3	17	23	242
		4	56	63	78
		6	49	47	219
		7	45	45	269
		8	118	88	354
		9	25	26	144
		10	28	25	325
		11	104	98	28
		12	24	23	303
		13	50	45	145
		15	18	19	112
		16	51	42	189
		17	40	41	318
		18	40	39	179
		19	66	54	224
		20	39	36	239
		23	20	18	340
		24	15	12	100
		25	37	34	125
		27	21	15	34
		28	15	21	38
1	10	0	23	24	0
		1	92	89	42
		3	18	13	146
		4	76	72	258
		5	47	49	207

TABLE 5 (*Continued*)

h	*k*	*l*	F_o	F_c	α
		6	67	65	299
		7	78	74	328
		8	30	32	243
		9	54	52	200
		10	42	36	303
		11	27	34	144
		12	45	46	110
		13	31	26	41
		14	51	45	107
		16	40	42	77
		19	19	16	279
		20	19	18	320
		22	27	28	264
		23	30	26	153
		24	31	29	277
1	11	0	49	46	180
		1	54	63	114
		2	49	49	288
		3	19	30	215
		4	38	45	137
		7	77	86	250
		8	50	42	320
		9	22	24	357
		10	56	42	32
		11	46	48	53
		12	25	27	329
		14	25	27	329
		15	30	36	60
		16	27	24	145
		17	58	53	298
		18	25	21	165
		19	26	27	233
		20	22	18	193
1	12	0	35	33	0
		1	83	89	54
		2	30	32	5
		3	32	29	135
		4	64	66	293
		5	22	27	242
		6	49	48	178
		7	72	65	304
		8	33	40	122
		9	31	28	229
		10	25	28	179
		15	24	23	87
		16	29	32	265
1	13	0	28	27	0
		1	28	35	102
		2	18	27	196
		3	25	34	211
		4	31	31	72
		5	22	27	120
		6	39	40	103
		7	25	28	241
		10	52	45	55
		11	24	27	32
		14	59	64	270
1	14	0	17	24	0
		1	15	18	116
		2	17	18	330
		3	21	25	186
		4	15	19	275
		6	19	17	202
		7	37	37	324
		8	45	40	111
		10	18	18	191
		11	21	26	351
		13	17	18	219
		14	25	32	61
		15	22	28	99
		16	30	31	269
		18	17	21	18
1	15	1	18	23	343
		2	16	12	281
		3	18	27	221
		5	17	19	170
		7	26	32	24
		10	16	21	68
		11	20	23	82
		12	13	15	198
		14	17	29	290
		15	13	17	209
1	16	1	14	13	193
		2	12	12	260
		4	15	19	268
		5	13	22	26
1	17	0	10	18	180
		1	16	21	345
		2	11	9	299
		3	18	27	179
		7	15	24	52
2	2	0	23	81	0
		1	162	195	270
		2	24	53	0
		3	106	80	270
		4	11	12	180
		5	28	25	270
		6	32	45	180
		7	166	215	90
		8	43	74	180
		9	12	22	90
		10	12	27	180
		11	34	1	91
		12	58	70	0
		13	71	106	90
		14	39	41	180
		15	129	180	270
		16	49	50	180
		17	27	21	90
		18	44	35	180
		19	28	34	270
		21	131	135	270
		22	22	32	0
		24	41	35	0
		25	27	28	270
		26	25	22	0
		29	54	60	90
		30	27	27	180
		31	23	24	90
2	3	0	140	121	0
		1	158	181	246
		2	23	50	176
		3	136	198	56
		4	82	93	169
		5	67	98	4
		6	81	69	90
		7	47	39	314
		8	106	112	214
		9	100	124	51
		10	55	80	355
		11	104	119	225
		12	35	47	27
		13	91	91	233
		14	23	33	317
		15	46	44	117
		16	26	28	96
		17	54	55	184
		18	54	66	206
		19	49	51	24
		20	27	40	243
		21	66	62	59
		22	26	19	109
		23	47	47	318
		24	16	19	24
		25	29	36	300
		26	18	15	22
		27	31	34	123
		29	17	17	275
		30	12	19	253
2	4	0	111	85	180
		1	120	125	235
		2	29	54	13
		3	44	50	297
		4	20	32	266
		5	86	59	106
		6	105	103	212
		7	123	119	94
		8	27	28	313
		9	55	78	347
		10	46	38	286
		11	60	45	64
		12	39	50	49
		13	44	56	94
		14	125	131	73
		15	102	110	254
		16	26	27	86
		17	26	18	103
		18	20	21	112
		19	19	21	101
		20	42	43	202
		21	61	64	259
		22	60	55	305
		23	24	25	91
		24	36	36	277
		25	18	18	146
		26	25	21	342
		27	14	13	181
		28	28	26	334
		29	38	42	82
		30	19	24	128
2	5	0	25	9	180
		1	57	59	276
		2	60	84	148
		3	85	89	74
		4	93	81	161
		5	49	41	187

TABLE 5 (*Continued*)

h	*k*	*l*	F_o	F_c	α
		6	104	75	359
		7	68	47	11
		8	84	78	265
		9	81	77	2
		10	72	63	328
		11	154	136	251
		12	171	136	22
		13	29	44	254
		14	31	27	155
		15	54	64	193
		16	76	78	100
		17	63	59	146
		18	35	35	177
		19	39	30	65
		20	46	34	196
		21	18	14	131
		22	18	9	220
		23	26	23	356
		24	18	15	333
		25	51	47	313
		26	24	26	29
		28	27	25	96
		30	19	25	359
2	6	0	51	74	180
		1	99	104	191
		2	58	60	347
		3	134	123	238
		4	49	27	68
		5	70	57	128
		6	101	97	221
		7	141	111	178
		8	32	33	323
		9	155	126	336
		10	70	62	266
		12	17	15	97
		13	40	29	316
		14	99	101	77
		15	26	32	337
		16	40	37	92
		17	31	32	98
		18	33	28	164
		19	18	21	36
		20	26	24	288
		21	29	28	189
		22	68	54	270
		24	20	15	235
		25	15	18	171
		26	12	5	82
		27	22	28	190
		28	16	18	30
		29	19	20	25
		30	21	27	146
2	7	0	35	26	0
		1	74	68	62
		2	111	98	116
		3	125	128	110
		4	98	93	104
		5	91	90	224
		6	64	66	29
		7	70	53	276
		8	106	80	297
		9	84	65	263
		10	49	41	282
		11	68	58	266
		12	83	59	336
		14	37	32	148
		16	35	47	130
		17	40	41	165
		18	34	27	316
		19	50	41	48
		20	68	57	249
		21	20	12	305
		22	24	23	253
		23	28	26	127
		24	24	21	12
		25	20	22	280
		26	24	26	114
		28	19	14	78
2	8	0	29	15	0
		1	128	136	174
		2	53	67	47
		3	29	19	71
		4	76	73	14
		5	30	26	267
		6	22	34	188
		7	83	83	194
		8	44	49	269
		9	19	12	348
		10	36	39	272
		11	36	26	36
		12	100	83	165
		14	35	31	9
		15	45	33	329
		16	57	62	65
		19	22	11	182
		20	57	54	326
		21	49	46	146
		22	22	17	351
		23	17	14	31
		24	30	28	207
		25	19	18	172
		26	19	15	67
		27	14	20	216
2	9	1	77	71	37
		2	89	74	60
		3	32	30	14
		4	82	90	118
		5	64	70	240
		6	21	12	78
		7	44	40	339
		8	26	23	61
		9	50	48	279
		10	46	44	226
		12	82	63	318
		13	102	81	58
		14	27	21	60
		15	26	24	262
		16	27	21	203
		17	29	27	144
		18	29	27	335
		19	31	26	359
		20	30	27	164
		22	19	14	288
		23	29	28	113
		24	19	21	39
		25	20	21	358
		26	21	25	140
		27	12	10	199
2	10	0	34	40	0
		1	16	15	200
		2	34	43	13
		3	40	41	92
		4	40	34	79
		5	79	71	289
		6	63	68	108
		7	70	56	174
		8	82	79	244
		9	45	32	52
		10	23	22	181
		11	27	22	57
		12	46	41	219
		13	52	42	96
		14	50	45	290
		15	16	18	220
		16	29	37	78
		17	24	24	308
		19	45	35	214
		20	24	27	332
		22	25	23	70
		23	26	25	71
2	11	0	17	21	0
		1	36	35	139
		2	77	72	79
		3	48	49	313
		4	28	25	277
		5	23	17	212
		6	43	42	151
		7	49	38	255
		8	28	30	358
		10	41	36	249
		11	50	53	139
		12	29	24	329
		13	24	21	90
		14	22	16	101
		15	18	11	122
		16	32	37	242
		17	21	28	214
		19	30	38	335
		20	18	21	133
		21	13	9	240
		22	20	18	295
		23	15	19	79
2	12	0	22	17	180
		2	34	42	290
		3	13	11	198
		4	18	19	316
		5	34	36	295
		6	26	22	201
		7	13	8	320
		8	27	33	272
		9	20	19	115
		10	24	25	132
		11	18	18	66
		12	25	24	24
		13	54	58	114
		14	25	21	261

TABLE 5 (*Continued*)

h	*k*	*l*	F_o	F_c	α
		15	21	22	272
		16	38	40	106
		17	23	22	276
		19	23	28	270
		20	16	16	276
		21	21	19	297
2	13	0	37	41	0
		1	22	19	168
		2	33	38	81
		3	29	26	5
		4	68	60	254
		5	41	38	343
		8	28	38	123
		10	36	37	318
		11	27	28	103
		12	17	20	69
		13	27	29	138
		16	26	29	230
		17	22	23	233
		18	14	17	192
		19	23	25	303
2	14	1	18	18	37
		2	48	62	288
		4	17	16	234
		5	15	19	222
		6	19	27	248
		7	17	14	358
		8	17	23	315
		10	28	28	105
		12	17	23	24
2	15	0	16	12	180
		1	18	15	175
		2	20	19	97
		3	24	32	143
		4	36	33	242
		5	18	24	273
		8	17	19	40
		9	15	15	326
		10	16	22	324
		11	23	29	346
		12	21	27	40
2	16	0	14	18	180
		2	17	23	300
		3	14	15	189
		4	15	23	299
		5	12	24	159
		6	13	19	193
		10	18	9	132
3	3	0	171	188	0
		1	88	92	90
		2	73	53	0
		3	85	99	270
		4	17	44	180
		5	245	230	90
		6	76	80	180
		7	22	0	270
		8	97	109	180
		9	114	152	270
		10	46	66	0
		13	97	99	270
		16	24	5	0
		17	63	73	90
		18	100	103	180
		19	73	89	90
		20	20	5	180
		21	16	13	270
		23	71	73	270
		26	27	30	0
		27	48	55	270
		29	22	16	90
3	4	0	126	125	0
		1	51	104	293
		2	67	48	328
		3	102	118	156
		4	152	153	107
		5	93	87	165
		6	76	54	268
		7	32	38	98
		8	45	53	136
		9	43	66	86
		10	90	106	210
		11	85	88	331
		12	115	120	304
		13	43	45	298
		14	40	50	139
		15	60	58	83
		16	37	36	235
		17	35	36	355
		18	54	47	4
		19	41	31	88
		20	42	33	142
		21	27	21	130
		22	27	25	306
		23	49	40	239
		24	52	48	58
		25	29	32	216
		27	19	20	131
3	5	0	95	82	0
		1	75	80	42
		2	83	86	71
		3	57	31	242
		4	79	89	65
		5	89	79	57
		6	64	68	189
		7	41	36	49
		8	48	44	208
		9	84	86	252
		10	36	41	356
		11	80	67	308
		12	103	93	197
		13	42	50	210
		14	60	60	62
		15	45	55	198
		16	49	51	2
		17	58	52	77
		18	74	67	183
		19	53	50	118
		20	67	65	15
		22	43	28	262
		23	27	27	10
		24	34	29	125
		25	26	23	254
		26	39	35	42
		27	22	23	290
3	6	0	107	122	0
		1	84	88	268
		2	85	66	173
		3	86	99	280
		4	124	137	98
		5	98	109	97
		6	83	77	305
		7	56	37	4
		8	96	88	204
		9	68	80	88
		10	56	50	182
		11	24	24	128
		12	84	82	277
		13	82	81	285
		14	46	51	81
		15	19	33	41
		17	58	69	249
		18	48	48	35
		20	17	12	124
		21	16	15	77
		22	15	11	211
		23	34	26	258
		24	29	31	35
		25	22	19	33
		26	35	24	130
3	7	0	10	15	180
		1	51	52	251
		2	40	50	73
		3	31	32	39
		4	122	126	85
		5	86	89	354
		6	99	89	207
		7	21	29	40
		8	44	24	253
		9	38	31	170
		10	65	55	321
		11	95	71	326
		12	115	95	206
		13	64	70	181
		14	51	46	45
		15	46	55	202
		16	24	18	48
		17	28	30	45
		18	65	52	195
		19	64	43	178
		20	30	28	292
		21	34	37	7
		22	31	36	298
		23	41	36	356
		24	28	26	134
		25	17	12	245
		26	24	23	19
		27	20	16	19
		28	18	17	107
3	8	0	137	139	0
		1	43	43	328
		2	113	104	137
		3	88	75	271
		4	37	34	110
		5	64	71	143
		6	83	81	358
		7	44	43	73

TABLE 5 (*Continued*)

h	*k*	*l*	F_o	F_c	α
		8	82	78	191
		10	69	59	309
		11	82	63	114
		13	32	27	10
		14	50	55	105
		15	45	46	230
		16	30	30	72
		17	28	35	249
		19	49	45	279
		20	23	22	281
		21	26	27	256
		22	50	48	234
		23	20	28	200
		24	17	18	338
		25	25	25	57
		26	22	23	88
		27	17	14	85
3	9	0	23	21	180
		1	16	18	83
		2	29	26	198
		3	33	36	13
		4	78	88	88
		5	74	83	332
		6	49	50	274
		7	38	42	289
		8	87	85	299
		10	25	32	16
		11	27	24	195
		12	20	18	294
		13	23	21	164
		14	70	60	93
		15	46	47	132
		16	49	42	84
		18	27	27	130
		19	28	29	195
		21	18	13	53
		22	27	32	275
		23	24	24	344
3	10	0	30	27	0
		2	72	54	162
		3	45	35	220
		4	56	61	265
		5	73	59	191
		6	52	42	337
		8	33	26	157
		9	41	42	188
		10	61	52	341
		11	59	46	53
		12	39	35	51
		13	55	54	51
		14	71	79	91
		15	25	29	330
		16	19	16	0
		18	28	27	164
		19	20	18	263
		21	21	19	229
		22	42	48	271
		23	19	21	139
3	11	0	16	19	0
		1	50	59	83
		2	30	32	231
		3	41	44	353
		4	76	73	102
		5	56	60	354
		6	28	28	232
		7	62	61	262
		8	25	21	284
		9	21	22	213
		10	49	45	12
		11	23	17	226
		12	21	24	340
		13	33	35	213
		15	38	42	69
		16	29	23	104
		17	18	17	210
		18	25	29	179
		19	27	12	353
3	12	0	19	33	0
		1	16	25	79
		2	27	32	67
		3	71	66	187
		5	60	56	217
		6	25	30	265
		7	55	49	176
		8	43	49	142
		9	30	27	239
		10	39	39	303
		11	42	47	34
		12	23	20	260
		13	30	29	39
		14	44	46	86
		15	18	23	332
		16	26	24	263
		17	19	17	1
		18	16	14	111
		19	13	14	219
		20	15	17	87
3	13	0	55	69	0
		1	49	47	81
		2	42	44	213
		3	25	19	122
		4	62	58	93
		5	33	28	229
		7	42	40	285
		8	38	37	183
		9	29	27	261
		10	50	45	29
		11	22	21	173
		14	21	29	289
		15	22	22	78
		18	17	23	185
		19	12	10	22
		20	15	19	293
3	14	0	22	36	0
		1	20	19	221
		2	26	29	348
		6	18	26	221
		7	20	17	196
		8	25	28	122
		11	28	35	47
		16	20	29	285
		17	17	24	319
3	15	0	14	24	0
		1	20	26	35
		4	16	21	62
		5	23	26	215
		6	16	17	177
		7	32	36	1
		9	13	17	254
		10	16	21	28
		11	14	13	202
3	16	0	22	37	0
		1	23	32	211
		3	17	18	278
		5	14	15	38
		7	15	11	172
		8	16	23	164
		9	20	30	36
4	4	0	181	215	180
		1	125	150	270
		2	61	72	0
		3	77	85	270
		4	27	20	180
		5	100	105	90
		6	143	131	180
		7	167	188	90
		8	156	153	0
		9	104	99	90
		10	9	9	0
		11	25	34	270
		12	32	37	0
		13	13	7	90
		14	64	61	0
		15	60	63	270
		16	20	25	180
		17	30	32	90
		18	66	67	180
		19	22	22	90
		20	38	47	180
		21	63	62	270
		22	13	12	0
		23	19	15	90
		25	27	32	270
		26	15	13	0
		27	12	9	270
		28	23	26	0
		29	38	34	90
4	5	0	84	113	0
		1	56	50	285
		2	8	3	125
		3	43	44	72
		4	102	112	235
		5	24	20	87
		6	58	59	349
		7	88	76	31
		8	99	87	240
		9	33	33	108
		10	10	7	254
		11	90	91	264
		12	81	84	55
		13	35	35	205
		14	24	28	84
		15	43	48	138
		16	71	77	106
		17	53	55	101
		18	33	26	26

TABLE 5 (*Continued*)

h	*k*	*l*	F_o	F_c	α
		19	38	32	91
		20	51	41	237
		21	26	27	343
		22	16	16	182
		23	18	12	272
		24	53	52	310
		25	28	33	280
		26	17	19	135
		27	18	15	271
		28	11	2	225
		29	28	28	119
		30	14	10	34
4	6	0	126	160	180
		1	94	96	208
		2	83	59	62
		3	60	54	196
		4	39	40	39
		5	91	78	122
		6	102	81	178
		7	95	96	178
		8	124	129	347
		9	38	34	35
		10	56	56	335
		11	23	27	290
		12	83	54	138
		13	47	47	307
		14	44	33	1
		15	65	64	33
		16	79	81	105
		17	13	11	45
		18	41	32	159
		19	23	22	65
		20	31	31	211
		21	19	13	100
		22	18	18	317
		23	24	23	245
		24	22	20	212
		25	12	8	215
		26	18	19	40
		27	11	12	150
		28	26	33	4
4	7	0	14	3	0
		1	61	51	43
		2	52	53	129
		3	31	33	105
		4	71	67	240
		6	55	39	316
		7	50	48	32
		8	77	74	239
		9	74	76	250
		10	76	70	231
		11	87	76	249
		12	69	60	29
		13	32	26	331
		14	26	34	117
		15	33	27	282
		16	47	55	112
		17	70	78	88
		18	63	56	9
		19	71	60	94
		20	25	24	233
		21	18	18	26
		22	22	27	236
		24	35	39	325
		25	23	20	314
		26	24	26	154
		27	20	24	306
4	8	0	18	24	180
		1	57	56	196
		2	67	76	90
		3	37	36	127
		4	26	37	61
		5	64	51	174
		6	110	102	111
		7	66	75	195
		8	73	66	280
		10	31	30	240
		11	28	24	5
		12	43	32	137
		13	74	64	317
		14	47	52	253
		15	69	69	62
		16	28	30	96
		18	42	38	207
		19	23	17	201
		20	45	38	277
		21	37	36	128
		23	24	23	238
		25	15	20	207
		26	16	24	68
		28	16	14	88
4	9	0	18	23	180
		1	78	72	49
		2	83	91	57
		3	27	34	314
		4	48	44	139
		5	41	29	51
		6	41	40	106
		7	21	26	28
		9	48	46	231
		10	79	87	232
		11	28	26	191
		12	26	29	322
		13	30	26	275
		14	54	54	106
		15	26	27	296
		16	29	26	231
		17	38	37	153
		18	38	47	8
		20	40	34	171
		21	15	12	141
		22	31	29	292
		23	16	12	118
		24	18	20	93
		25	17	13	23
		26	23	26	143
4	10	0	26	25	0
		1	30	36	311
		2	51	53	52
		3	39	35	134
		4	48	51	84
		5	54	54	265
		6	49	61	122
		8	68	62	265
		9	62	70	134
		10	21	22	238
		11	42	41	15
		12	16	12	178
		14	34	38	285
		15	48	46	30
		16	45	50	81
		17	41	40	291
		18	16	16	34
		19	36	35	242
		20	21	15	279
		22	20	21	76
		23	18	14	213
4	11	0	22	21	180
		1	41	38	64
		2	69	72	63
		3	62	53	282
		5	48	50	19
		6	34	42	131
		7	45	43	245
		8	42	31	89
		9	34	28	303
		10	42	43	242
		11	23	28	138
		14	22	24	50
		16	22	18	227
		19	18	13	270
		22	18	14	292
4	12	1	45	48	317
		2	42	35	293
		3	42	34	22
		4	46	41	126
		5	28	26	263
		6	45	44	231
		7	49	45	14
		8	28	32	265
		9	26	30	120
		10	29	28	103
		11	20	25	119
		12	22	30	20
		13	18	14	83
		16	20	26	133
		17	20	27	263
		19	18	31	246
		20	18	36	242
		21	13	12	305
		22	13	12	86
4	13	0	16	16	0
		1	21	23	113
		2	18	17	89
		4	21	27	283
		5	34	41	5
		6	22	29	128
		7	24	29	257
		9	20	15	161
		10	40	33	295
		11	15	11	73
		13	25	33	179
		17	16	15	4
		18	28	31	188
		19	15	15	193
		20	13	10	43

TABLE 5 (*Continued*)

h	*k*	*l*	F_o	F_c	α
4	14	1	15	18	329
		2	23	30	323
		4	17	26	177
		5	32	37	181
		6	21	23	195
		7	25	26	0
		8	17	18	320
		10	16	16	41
		11	18	24	131
		12	23	29	8
		13	21	21	6
4	15	1	20	23	113
		4	21	23	245
		5	17	18	335
		7	15	17	275
		10	12	16	355
		11	20	27	326
		12	18	24	23
		13	20	27	164
4	16	1	12	8	72
		2	12	19	21
		3	15	23	197
		5	23	34	170
		7	15	15	316
5	5	0	12	7	0
		1	54	54	270
		2	15	13	180
		3	78	68	90
		4	105	112	0
		6	94	84	180
		7	97	90	90
		8	54	64	180
		9	14	14	90
		10	42	55	0
		11	71	66	270
		12	102	88	180
		13	49	54	270
		14	78	70	0
		15	22	22	270
		16	41	53	0
		17	34	31	90
		18	30	36	180
		19	44	44	90
		20	67	59	0
		24	42	41	180
		25	47	43	270
5	6	0	112	120	0
		1	95	87	240
		2	73	76	131
		3	70	63	299
		4	108	111	85
		5	68	81	85
		6	92	79	28
		7	94	88	106
		8	44	59	149
		9	65	73	3
		10	18	11	186
		11	37	34	179
		12	65	56	329
		13	45	46	348
		14	25	24	160
		15	38	35	299
		16	28	34	231
		17	47	49	175
		18	50	49	345
		19	40	36	28
		20	26	22	162
		22	29	27	167
		23	26	29	282
		24	44	41	54
		26	20	20	132
		27	17	20	193
5	7	0	21	10	180
		1	76	91	267
		2	62	53	328
		3	106	105	61
		4	63	71	59
		5	70	59	305
		6	43	31	177
		7	61	72	71
		8	37	39	256
		9	57	53	118
		10	21	18	200
		11	43	38	250
		12	61	58	210
		13	27	34	228
		14	78	65	77
		16	43	42	22
		18	19	18	16
		20	40	38	348
		21	23	21	51
		23	24	20	357
		24	19	18	176
		25	18	23	305
		26	20	17	301
		27	16	17	73
5	8	0	24	22	0
		1	25	26	289
		2	83	91	152
		3	74	65	293
		4	20	21	99
		5	41	41	58
		6	47	48	10
		7	93	86	95
		8	30	32	237
		9	33	28	298
		10	75	65	306
		11	53	49	144
		12	21	16	287
		13	28	26	26
		14	39	40	88
		15	44	39	282
		17	54	46	109
		21	34	33	245
		22	37	32	276
		25	20	21	352
5	9	0	36	47	180
		1	26	30	281
		2	60	52	305
		3	73	76	50
		4	60	55	81
		5	43	43	357
		6	50	50	256
		8	33	39	244
		9	45	33	78
		10	32	39	130
		11	31	26	250
		13	40	34	162
		14	48	57	89
		15	24	22	90
		16	19	16	93
		17	24	24	163
		20	24	26	288
		21	20	17	106
		22	31	39	273
5	10	0	42	35	180
		1	26	25	70
		2	84	78	139
		6	28	27	275
		7	53	53	117
		8	30	39	18
		9	40	31	232
		10	94	86	315
		12	27	25	36
		13	27	36	78
		14	44	44	102
		15	53	54	287
		17	25	25	72
		18	54	52	171
		21	28	34	235
		22	24	25	235
		23	16	17	68
5	11	0	18	14	0
		2	47	53	280
		3	44	51	37
		4	44	38	107
		5	35	35	243
		6	30	34	314
		7	33	36	237
		8	29	32	238
		9	27	26	7
		11	44	36	192
		13	29	33	341
		14	19	21	113
		16	41	44	100
		19	20	21	11
		20	25	29	293
		21	24	35	135
5	12	0	24	19	180
		1	34	33	188
		2	31	29	118
		3	19	16	22
		4	26	35	97
		5	24	31	270
		6	40	38	169
		7	47	47	176
		8	19	22	72
		9	33	32	219
		10	35	46	313
		12	18	18	303
		13	24	30	70
		14	20	15	25
		15	30	37	322
		17	37	34	19
		18	32	38	176
5	13	0	36	40	0

TABLE 5 (*Continued*)

h	*k*	*l*	F_o	F_c	α
		1	30	29	79
		3	27	30	77
		4	23	24	227
		5	21	21	211
		7	26	24	272
		8	48	55	209
		9	22	28	311
		11	26	31	213
		13	31	41	21
		16	21	21	56
		17	21	25	154
		18	11	13	159
		19	15	17	52
5	14	1	33	42	174
		2	33	35	18
		5	25	21	303
		6	21	24	172
		7	36	42	168
5	15	0	24	36	0
		1	21	24	345
		5	22	26	243
		8	19	25	165
6	6	0	127	156	180
		3	43	39	90
		5	51	58	90
		6	21	2	180
		7	37	33	270
		8	67	60	0
		10	48	60	0
		11	88	83	270
		12	24	19	0
		13	82	93	270
		14	27	23	0
		15	57	81	90
		16	28	31	180
		18	36	34	180
		19	25	30	90
		20	19	18	180
		21	40	41	90
		22	31	23	180
		23	71	71	270
		24	23	16	180
		25	23	18	270
6	7	0	28	23	0
		1	42	56	332
		2	21	20	275
		3	45	54	212
		4	15	12	327
		5	62	49	129
		6	63	58	304
		7	85	76	69
		9	73	72	254
		10	43	46	172
		11	88	77	3
		12	22	18	73
		13	30	33	340
		14	52	55	121
		15	61	58	257
		17	57	54	48
		18	27	20	349
		19	44	44	133
		20	16	11	197
		21	19	13	279
		22	22	29	256
		23	23	22	171
		25	22	19	213
6	8	0	20	19	180
		1	38	27	347
		2	25	25	134
		3	44	42	125
		4	50	62	86
		5	24	25	91
		6	56	46	35
		7	49	49	233
		8	47	41	302
		9	50	50	162
		10	64	57	331
		11	72	58	294
		12	28	33	220
		13	66	66	268
		14	27	22	292
		15	44	45	23
		16	24	26	49
		17	29	22	25
		18	30	30	194
		20	18	17	320
		21	47	43	90
		22	21	22	147
		23	23	25	268
6	9	1	26	20	91
		2	62	57	13
		3	70	66	273
		4	25	18	48
		5	53	49	113
		6	38	41	263
		7	34	33	151
		9	80	68	257
		10	74	71	216
		11	56	51	49
		12	29	32	231
		14	30	36	120
		15	44	48	328
		16	36	38	358
		18	32	36	8
		19	24	31	125
		20	25	25	26
		21	25	25	190
		22	34	35	295
6	10	0	52	51	0
		1	65	69	342
		2	39	34	120
		3	49	51	67
		4	73	78	88
		6	50	48	37
		8	47	41	204
		9	48	47	128
		10	17	15	253
		11	19	22	218
		12	22	17	296
		13	23	18	299
		14	40	39	251
		15	28	29	85
		20	22	24	274
		21	22	19	124
		22	18	21	89
6	11	0	31	38	0
		1	47	50	119
		2	44	49	37
		3	54	55	326
		4	24	21	340
		5	57	56	66
		6	29	32	196
		7	17	24	238
		8	19	27	206
		11	27	23	93
		12	35	30	166
		13	23	18	280
		14	28	27	54
		16	21	34	10
		17	17	16	348
		22	18	15	307
		23	11	15	345
6	12	1	48	56	340
		2	19	17	157
		3	27	29	323
		4	47	40	100
		6	21	23	35
		7	40	41	351
		9	30	37	139
		11	24	23	155
		12	28	32	315
		13	25	27	34
		14	23	22	185
6	13	3	23	22	327
		4	23	37	247
		5	38	42	23
		6	24	24	185
		9	20	24	172
		10	17	19	352
		11	21	21	66
		12	18	20	131
		13	25	30	179
		14	20	21	25
6	14	1	27	31	12
		2	21	17	151
		5	21	21	137
		7	20	22	5
		8	16	24	30
		10	15	13	306
		11	21	21	157
		12	24	34	339
		13	22	24	7
6	15	0	15	16	0
		2	18	26	297
		5	16	17	340
		6	20	21	235
		7	14	12	191
		8	15	19	242
7	7	0	25	15	180
		1	97	129	270
		2	30	31	0
		3	99	89	90
		5	62	54	270
		6	30	27	180
		7	71	60	90
		9	80	68	90

TABLE 5 (*Continued*)

h	*k*	*l*	F_o	F_c	α
		10	56	59	180
		11	40	37	270
		12	48	59	180
		14	20	21	0
		16	22	33	0
		18	26	34	0
7	8	0	78	79	180
		2	58	52	86
		3	91	87	330
		4	24	17	245
		5	80	63	35
		6	49	46	50
		7	56	59	89
		8	27	34	337
		9	68	53	314
		12	22	24	136
		13	54	48	172
		14	20	22	244
		15	47	44	254
		17	57	46	134
		18	20	20	216
		19	45	40	63
		21	38	39	272
7	9	1	83	76	243
		3	48	35	56
		5	33	34	263
		6	52	51	286
		7	55	52	172
		8	46	47	326
		9	70	64	60
		10	65	64	174
		11	81	72	215
		12	47	43	10
		13	36	32	311
		14	25	33	136
		15	24	26	31
		16	29	29	118
		17	31	24	241
		18	47	51	19
		19	13	16	308
		20	37	39	222
7	10	0	79	87	180
		1	22	26	229
		2	30	33	123
		3	38	40	336
		4	34	28	281
		5	28	26	3
		6	22	26	66
		8	54	57	349
		10	50	40	311
		11	20	25	227
		13	22	25	104
		15	22	24	275
		17	16	18	92
		18	18	15	158
7	11	0	47	35	0
		5	32	32	160
		6	43	42	344
		8	32	34	286
		9	34	33	111
		11	41	39	194
		12	27	35	42
		13	44	52	359
		15	27	32	22
		16	44	43	99
		17	22	24	202
		18	24	22	343
		19	17	17	358
		20	20	24	219
		21	15	25	173
7	12	0	37	46	180
		1	20	20	86
		2	31	34	42
		3	26	23	69
		5	35	39	318
		6	26	21	166
		7	22	22	183
		8	39	37	351
		9	29	32	225
		11	26	25	309
		14	23	23	330
		15	20	24	346
		17	24	27	31
		19	30	31	134
7	13	0	44	47	0
		1	30	27	20
		2	19	16	68
		4	32	38	252
		5	25	26	206
		8	25	24	203
		9	18	20	203
		10	23	23	205
		12	22	24	53
		13	27	31	8
		15	20	24	355
7	14	0	19	26	180
		1	24	25	151
		2	21	23	345
		3	24	21	79
		4	27	30	103
		6	23	31	147
		7	24	33	195
		8	18	21	346
8	8	1	27	16	270
		2	57	49	180
		3	57	63	90
		6	28	30	0
		9	50	45	90
		10	39	42	180
		11	47	48	270
		12	23	15	0
		15	35	40	90
		18	31	28	0
		21	36	48	90
8	9	0	55	65	180
		1	31	31	132
		2	36	34	16
		3	41	45	267
		4	55	61	60
		5	47	45	108
		6	39	36	207
		7	35	36	169
		8	29	30	40
		12	48	45	194
		13	26	31	342
		14	35	34	73
		15	22	32	359
8	10	0	46	41	0
		2	29	27	162
		4	26	25	127
		5	30	21	257
		6	46	51	17
		7	23	27	313
		8	62	53	171
		9	30	36	192
		10	23	26	187
		11	37	37	253
		13	26	24	273
		14	22	27	230
		18	33	37	347
		19	21	21	72
8	11	1	37	30	260
		3	30	33	292
		4	29	33	19
		5	32	38	29
		6	29	27	139
		7	43	36	153
		11	22	23	111
		12	46	52	194
8	12	0	32	33	0
		1	29	37	354
		2	26	24	158
		4	28	27	84
		6	28	29	4
		7	25	30	18
		11	23	16	192
		12	25	25	299
8	13	0	21	8	180
		2	24	21	248
		4	24	17	17
		6	23	9	159
		8	19	26	250
		9	25	33	116
		10	19	24	7
9	9	0	60	75	180
		1	49	47	270
		3	39	32	270
		4	22	15	180
		5	68	66	90
		6	77	68	0
		7	39	30	90
		8	35	45	0
		9	50	45	90
		11	35	32	90
		12	43	37	0
		13	18	24	270
		14	15	16	180
		15	24	29	90
		16	29	41	180
		17	24	37	270
		18	46	47	0
		20	24	34	180
9	10	0	28	36	180
		1	20	29	38
		2	16	16	114
		4	53	49	322

TABLE 5 (*Continued*)

h	*k*	*l*	F_o	F_c	α	*h*	*k*	*l*	F_o	F_c	α	*h*	*k*	*l*	F_o	F_c	α
		5	46	37	36			4	25	27	266			8	35	23	5
		6	27	25	150			5	38	33	124			9	16	15	163
		7	22	21	344			6	42	48	26			11	20	27	309
		8	49	32	319			7	23	23	207			12	22	25	136
		9	22	24	222			11	18	20	99			14	12	12	16
		10	18	9	1			12	20	18	54			15	15	17	61
		11	15	17	23			13	25	27	331			17	14	19	27
		12	53	51	148			14	21	24	180	9	13	2	19	17	131
		13	22	18	225			15	21	21	353			3	17	17	274
		14	20	17	49			16	18	27	153			4	15	14	258
		15	16	15	229			18	19	19	10			5	26	26	150
		16	23	25	60	9	12	0	60	53	180			6	22	21	34
		18	20	12	125			2	41	37	314			7	15	14	122
		19	16	25	152			3	33	28	54			9	26	31	235
		20	20	21	314			5	14	18	328			10	21	19	277
9	11	2	49	49	172			6	32	30	200			11	14	12	91
		3	28	34	282			7	39	36	250						

orthorhombic space group $P2_12_12_1$, with two molecules in the asymmetric crystal unit. This change involves a shift of the origin to $(\frac{1}{4},0,\frac{3}{8})$.

The first set of structure amplitudes and phase angles was calculated on the basis of the bromide ions alone; the value of R, the average discrepancy between measured and calculated structure amplitudes, was 39·9%. With the measured $|F|$ values and the calculated phase angles we then evaluated a three-dimensional electron-density distribution and displayed it as contoured sections drawn on sheets of glass and stacked in a frame. From this electron-density distribution we were able to assign co-ordinates to all the carbon and nitrogen atoms in the molecule and to establish structure (V) for the dihydrobromide of chimonanthine.

Each atom was allotted an isotropic temperature factor B of 4·5 Å^2 and a second set of structure factors was calculated. The value of R decreased to 29·3%.

Three further rounds of Fourier and structure-factor calculations served to reduce the value of R to 19·1%.

The analysis was completed by means of two cycles of least-squares adjustment of positional and thermal atomic parameters. The programme devised by Rollett [14] was employed. The value of R fell to 14·9%. The final values of $|F_o|$, $|F_c|$, and α are shown in Table 5. The theoretical atomic scattering factors used in the structure-factor calculations were those of Berghuis *et al.*[15] for carbon and nitrogen and the Thomas–Fermi [16] values for bromine.

The final atomic co-ordinates, molecular dimensions and some non-bonded distances are given in Tables 1 and 2. The standard deviations of the final atomic co-ordinates were derived from the least-squares residuals by means of the equation:

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

The results are listed in Table 3. The parameters defining the anisotropic thermal vibrations are listed in Table 4; they are values of b_{ij} in the equation:

$$\exp(-B \sin^2\theta/\lambda^2) = 2^{-(b_{11}h^2 + b_{22}k^2 + b_{33}l^2 + b_{12}hk + b_{23}kl + b_{13}hl)}.$$

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