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The Crystal and Molecular Structure of Perchloro-(3, 4, 7, 8-tetramethylene-tricyclo[4.2.0.$0^{2,5}$]octane), $C_{12}Cl_{12}$

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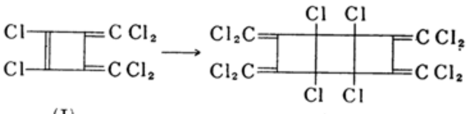
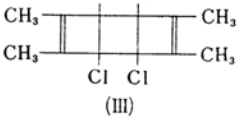
The stereochemistry of perchloro-(3, 4, 7, 8-tetramethylene-tricyclo[4.2.0.$0^{2,5}$]octane) has been studied by three-dimensional X-ray crystal analysis. The crystal of this compound is triclinic, with one molecule in a unit cell with the dimensions; $a=9.35$, $b=7.45$, $c=8.44$ Å, $\alpha=111.8°$, $\beta=117.6°$, and $\gamma=96.0°$. The space group is $P1$ or $P\bar{1}$, the latter being assumed throughout the present study. The crystal structure was elucidated by the minimum function method. The atomic parameters thus obtained were refined by the least-squares method, using the diagonal-matrix approximation. Each conjugated system in a molecule is nearly planar in spite of very close contact between the two adjacent dichloromethylene groups of the same system, the nearest approach occurring between the chlorine atoms with a distance of 3.28 Å. The whole molecule has a rather simple chair-like form, with an approximate symmetry of C_{2h}.

It has recently been found that the pyrolytic reaction of perchloro-(3, 4-dimethylenecyclobutene) (I) gives, depending on the heating temperature, at least four different isomeric compounds of $C_{12}Cl_{12}$.[1] One of these compounds, perchloro-(3, 4, 7, 8-tetramethylene-tricyclo[4.2.0.$0^{2,5}$]octane) (II), mp 266°C, is obtained from I upon pyrolysis at about 160°C.[1] The stereochemical configuration of II was speculated to be the anti-form with respect to the two junctures with the central ring, since the observed dipole moment for II was small enough to be judged zero.[1] If this structure is true, the whole molecule may show a fairly complicated appearance, since a part of the conjugated system may be distorted to a considerable extent as a result of the expected close contact between the two bulky dichloromethylene groups. In order to obtain more detailed information about the stereochemistry of this molecule, an X-ray investigation has been carried out.



(I) (II)



(III)

Prior to the structure determination of II, the two-dimensional X-ray analysis of a reduction derivative (III), with only four chlorine atoms per molecule, was carried out in order to obtain, in a short time, some information about the conformation of the three adjoining four-membered rings, which may closely resemble that of II.

Single crystals of II and III suitable for the structure determination were kindly supplied by Dr. Akira Fujino, Osaka City University.

The Structure of a Reduction Derivative

The crystals of III used for the present measurement were needles elongated along the *b* or *c* axis. The crystal data obtained are summarized in Table 1. The *h*0*l* and *hk*0 intensity data were collected from multiple-film integrating Weissenberg photographs, taken with Cu$K\alpha$ radiation about the *b* and *c* axes respectively. The intensities were estimated visually and were corrected for the Lorentz and polarization factors. The number of measured reflections was 87 for *h*0*l* and 89 for *hk*0.

TABLE 1. CRYSTAL DATA OF III

$a=8.68$ Å	$\alpha=63.0°$
$b=7.54$	$\beta=115.9°$
$c=7.42$	$\gamma=127.4°$
Space group	$P1$ or $P\bar{1}$
Z	1
ρ_{calcd}	$1.48\ \text{g}\cdot\text{cm}^{-3}$

The coordinates of the chlorine atoms were obtained from the Patterson functions, $P(u, w)$ and $P(u, v)$. On the other hand, the positions of the carbon atoms were elucidated by the Fourier syntheses, with signs based on the heavy atoms

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[1] K. Mano, K. Kusuda, A. Fujino and T. Sakan, *Tetrahedron Letters*, **1966**, 489.

TABLE 2. THE FINAL ATOMIC COORDINATES

Atom	x/a	y/b	z/c
Cl_1	0.166	0.390	−0.282
Cl_2	−0.327	−0.001	−0.247
C_1	0.102	0.143	−0.050
C_2	0.121	0.245	0.146
C_3	−0.075	0.103	0.144
C_4	−0.131	−0.018	−0.061
C_5	0.295	0.449	0.220
C_6	−0.205	0.074	0.263

alone, as well as by a trial method on the assumption that $P\bar{1}$ was the corresponding space group. The parameters thus obtained were refined by the diagonal-matrix least-squares method on HITAC 5020 using a program written by the present author. In the present stage, the discrepancy factor, R, including zero intensity data, is 0.153 for $h0l$ and 0.138 for $hk0$. The final coordinates thus determined are listed in Table 2.

The molecular structure projected along the c axis is given in Fig. 1. As this projection shows, the three four-membered rings in the molecule have the anti-configuration. The result thus obtained is very halpful in accomplishing the structure analysis of II.

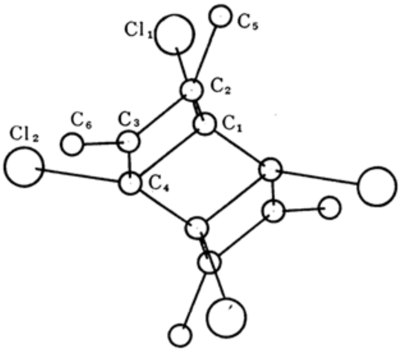

Fig. 1. The molecular structure of (III), projected along the c axis.

Experimental

From oscillation and Weissenberg photographs taken with CuKα radiation, the crystal data of II were found to be as shown in Table 3. The space group has been taken to be $P\bar{1}$ throughout the present work. This assumption is reasonable, for no contradiction has yet been encountered.

TABLE 3. CRYSTAL DATA OF (II)

$a=9.35$ Å	$\alpha=111.8°$
$b=7.45$	$\beta=117.6°$
$c=8.44$	$\gamma=96.0°$
Space group	$P1$ or $P\bar{1}$
Z	1
ρ_{calcd}	2.07 g·cm^{-3}
μ (for CuKα)	162.1 cm^{-1}

Equi-inclination Weissenberg photographs around the a and c axes were taken with CuKα radiation from the zeroth to the sixth layer. The intensities were estimated visually with the multiple-film technique. Lorentz and polarization corrections were made in the usual way. The crystals used for the intensity measurement were colorless and of the shape of non-cubic parallelepipeds, with nearly equal edges. Though the crystals were not very small, the maximum diameter being about 0.4 mm, no absorption correction was applied. Thus, the structure factors of 1643 unique reflections were obtained out of 2087 possible reflections. The relative values of these observed structure factors were converted into an absolute scale by Wilson's method.²⁾ The average temperature factor at this stage was 2.2 Å^2.

All the calculations necessary to derive the absolute values of the structure factors from the intensity data were carried out on a Bendix G-20 computer at the C. Itoh Electronic Computing Service Co., Ltd., using a program written by Yoshihisa Utsumi and Yujiro Tomiie of this university.

Structure Determination

A three-dimensional Patterson function, $P(u, v, w)$, was calculated for $u=0/30$—$30/30$, $v=0/30$—$15/30$, and $w=0/30$—$30/30$ on an IBM 7090 using an ERFR-2 programmed by Sly, Shoemaker and Van den Hende.³⁾ The minimum function method⁴⁾ was carried out by superposing two sets of three-dimensional Patterson maps with a markedly high peak situated at the position (4/30, 1/30, −10/30) and 3.5 Å apart from the point of origin. In the light of the molecular structure of III, previously determined, we could easily find not only the positions of chlorine atoms, but also those of all the carbon atoms. At this stage, it was concluded that the space group was preferably $P\bar{1}$, judging from the symmetry of the molecule obtained by the minimum function method.

The approximate atomic parameters of six independent chlorine and six carbon atoms were refined by the diagonal-matrix least-squares method on the IBM 7090 with an ERBR-1 programmed by Van den Hende.⁵⁾ The discrepancy factor, R, once rose from its initial value of 0.489 to 0.526 after the first cycle, but it began to drop rapidly after the second cycle. After six cycles of the least-squares refinement, with individual isotropic temperature factors, the R factor reached a value of 0.232.

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2) A. J. C. Wilson, *Nature*, **150**, 152 (1942).

3) W. G. Sly, D. P. Shoemaker and J. H. Van den Hende, ERFR-2: ESSO Research and Engineering Co. (1962).

4) M. J. Buerger, *Acta Cryst.*, **4**, 531 (1951).

5) J. H. Van den Hende, ERBR-1: ESSO Research and Engineering Co. (1961).

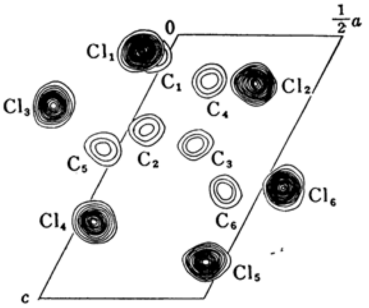

Fig. 2. The electron density distribution. Composite diagram of the (010) sections taken as through the atomic centers in the molecule. Contours are drawn at intervals of 2 e.Å^{-3}.

In order to confirm this structure, a three-dimensional electron density distribution was calculated on the IBM 7090 with an ERFR-2. There were few significant ghost peaks in the Fourier map. Figure 2 shows the superimposed (010) sections of the map, taken as through the atomic centers of the molecule.

TABLE 4. THE FINAL ATOMIC PARAMETERS

Atom	x/a	y/b	z/c	B(Å^2)
Cl$_1$	−0.1604	0.2598	−0.0669	2.66
Cl$_2$	0.2425	0.2822	0.0649	2.63
Cl$_3$	−0.3095	0.1742	0.1964	3.77
Cl$_4$	−0.0283	0.2696	0.5852	4.12
Cl$_5$	0.3655	0.2978	0.7154	4.13
Cl$_6$	0.4976	0.2225	0.4613	3.02
C$_1$	−0.0644	0.1092	0.0387	2.29
C$_2$	−0.0054	0.1762	0.2564	2.32
C$_3$	0.1689	0.1816	0.3111	2.35
C$_4$	0.1280	0.1238	0.1014	2.20
C$_5$	−0.0992	0.2009	0.3378	2.79
C$_6$	0.3234	0.2254	0.4798	2.71

Six more cycles of the same least-squares refinement as before were carried out, but the R factor did not drop as much as had been expected, the final value being 0.200. This may be due to the absorption effect, since the samples used were not small enough, or it may be attributed to the incorrectness of the relative scale factors among the layers. As will be discussed in the following section, the bond lengths and angles thus obtained are all reasonable considering the accuracy of the present determination.

The final atomic coordinates and temperature factors are given in Table 4. The observed and calculated structure factors are listed in Table 5.

Discussion

The molecular framework thus obtained is shown in Fig. 3. This corresponds to the very

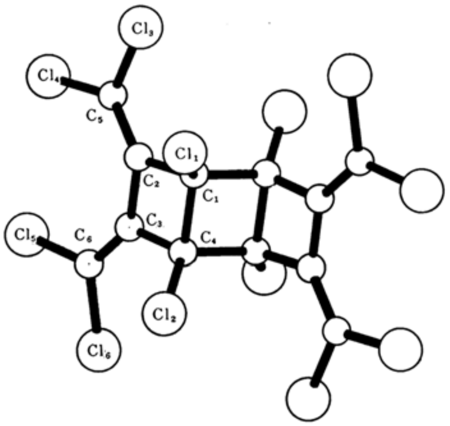

Fig. 3. The molecular structure of perchloro-(3, 4, 7, 8-tetramethylene-tricyclo[4.2.0.0^{2,5}]octane).

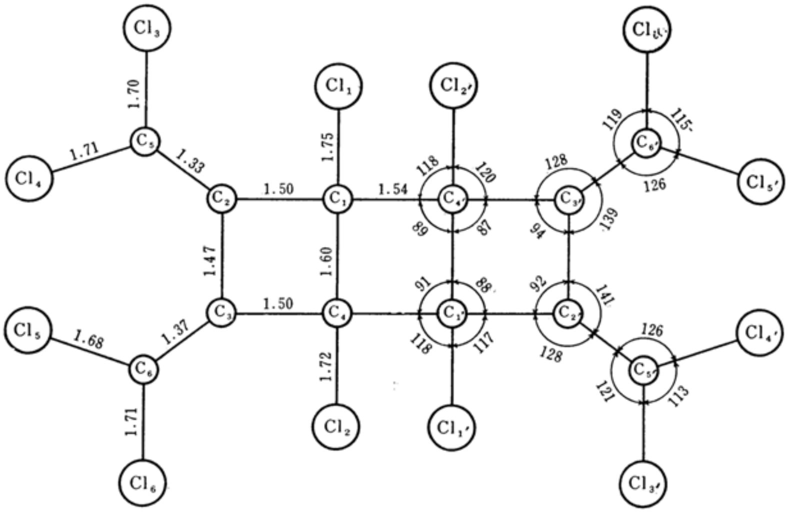

Fig. 4. The bond lengths (Å) and angles (°).

structure concluded by Mano *et al.*[1] The chair-like molecule has an unexpectedly simple form as a result of the fact that the two dichloromethylene groups in the same conjugated system are nearly coplanar. The conformation of the three four-membered rings is very similar to that of III. It may thus be said that the molecule has an approximate symmetry of C_{2h}.

The bond lengths and angles calculated with the final coordinates are illustrated in Fig. 4. The average estimated standard deviations of the coordinates are 0.008 and 0.025 Å for chlorine and carbon atoms respectively. Therefore, the estimated standard deviations of the bond lengths are 0.026 Å for C-Cl and 0.035 Å for C-C.

The conjugated system (C_1, C_2, C_3, C_4, C_5, C_6, Cl_3, Cl_4, Cl_5, Cl_6) is almost planar. The best plane, determined by the least-squares method as through these ten atoms, is represented by the equation;

$$0.1296X + 0.9666Y + 0.2207Z - 0.7118 = 0$$

where X, Y, and Z are rectangular coordinates: $X = x\sin\gamma - z\sin\alpha\cos\beta^*$, $Y = x\cos\gamma + y + z\cos\alpha$, and

TABLE 5. THE OBSERVED AND CALCULATED STRUCTURE FACTORS

k	F_o	F_c
h=0, l=0		
1	27.63	28.40
2	98.53	-147.85
3	15.17	-17.43
4	33.11	41.43
5	5.90	-7.96
6	10.11	-10.37
7	10.09	10.04
8	3.42	1.44
h=0, l=1		
0	4.05	2.17
1	13.18	-14.06
2	33.53	-35.29
4	20.87	21.27
5	6.86	-4.18
6	9.68	-11.11
7	8.16	5.09
h=0, l=2		
0	27.83	25.31
1	23.65	-22.03
2	17.14	-16.50
3	8.08	6.66
h=0, l=3		
0	9.07	2.92
1	11.45	-8.04
2	4.91	4.74
3	9.20	10.44
4	7.59	-7.29
5	6.36	-9.17
6	4.65	2.35
h=0, l=4		
0	16.54	13.08
1	13.14	13.03
3	12.03	-11.09
4	7.48	-6.57
5	6.43	5.22
h=0, l=5		
0	18.12	-13.25
2	6.78	5.42
3	4.94	-4.17
4	3.96	-3.40
h=0, l=6		
0	24.65	-16.55
1	6.37	2.92
2	19.93	13.31
3	11.30	-9.89
h=0, l=7		
0	7.33	-9.05
1	16.76	-13.48
2	4.58	3.23
h=0, l=8		
[illegible]	15.32	-14.78
h=0, l=-1		
1	25.46	29.45
2	50.66	75.38
3	17.44	21.56
4	34.22	-53.05
5	29.42	-39.35
6	5.19	12.85
7	19.67	24.30
8	4.36	2.25
h=0, l=-2		
1	22.91	22.93
2	31.21	-32.37
3	15.50	14.00
4	46.48	54.33
5	18.43	-15.73
6	38.62	-52.20
8	17.19	25.43
h=0, l=-3		
1	10.37	-8.08
2	12.93	-9.84
3	29.81	32.57
4	18.87	19.35
5	21.32	-25.69
6	11.02	-9.90
7	8.34	11.81
9	7.20	-9.83
h=0, l=-4		
1	14.09	-11.19
2	15.08	-16.42
3	10.79	8.20
4	17.03	18.23
6	11.59	-9.58
7	6.21	-7.44
9	5.17	0.16
h=0, l=-5		
1	7.70	7.37
2	25.87	21.50
3	8.97	-8.98
4	21.17	-17.55
5	7.76	8.42
6	13.10	12.00
7	6.32	-1.99
9	3.84	-5.15
h=0, l=-6		
1	12.65	6.69
2	18.86	14.73
3	13.34	-10.22
5	13.79	9.87
6	6.38	-1.26
7	7.69	-6.02
8	5.54	2.64
9	3.69	1.81
h=0, l=-7		
1	15.65	15.04
2	11.32	14.25
3	8.06	-8.92
4	10.17	-13.26
6	10.85	10.11
8	5.75	-6.60
h=0, l=-8		
1	17.66	-13.31
2	19.50	16.19
3	17.65	11.38
4	17.80	-10.86
6	6.64	4.70
7	8.19	-8.00
h=0, l=-9		
2	7.40	5.60
3	17.52	-15.27
5	18.18	19.73
6	4.73	5.30
7	9.76	-16.71
h=1, l=0		
0	18.77	24.44
1	2.40	2.18
2	17.73	19.98
3	4.15	3.91
4	17.78	-21.78
5	10.41	-11.76
6	6.86	4.89
7	4.63	5.92
h=1, l=1		
0	45.79	42.53
1	19.51	18.56
2	7.87	-7.47
3	21.40	-23.30
4	11.77	-12.68
5	13.33	14.17
6	7.51	8.99
7	8.52	-9.78
h=1, l=2		
0	10.95	-11.88
1	8.25	-7.14
4	9.51	-6.91
5	5.57	-3.27
6	4.45	4.50
h=1, l=3		
0	31.26	-24.50
1	35.77	31.37
2	11.62	9.68
3	36.37	-36.48
4	5.91	-5.57
5	22.74	25.90
6	4.34	4.23
h=1, l=4		
0	45.43	-44.96
1	37.80	-30.99
2	26.33	26.22
3	16.25	14.22
4	11.22	-9.71
5	3.52	-1.08
h=1, l=5		
0	5.64	-9.00
1	25.90	23.37
2	7.68	11.10
3	10.51	-9.07
4	4.35	-6.76
h=1, l=6		
0	20.79	-14.02
1	10.08	6.64
2	11.98	8.65
3	4.94	-5.04
h=1, l=7		
1	4.14	3.66
h=1, l=-1		
0	19.02	19.35
1	23.04	27.24
2	5.10	6.44
3	3.62	0.79
4	3.01	3.96
5	8.69	-8.51
6	8.80	-12.83
8	3.96	6.62
h=1, l=-2		
0	35.85	37.93
1	16.99	-14.30
2	35.10	-40.16
3	38.55	42.77
4	28.65	34.52
5	27.41	-30.65
6	17.65	-21.04
7	9.82	10.78
8	4.51	4.17
h=1, l=-3		
0	80.72	95.10
1	42.48	-61.43
2	50.07	-69.85
3	34.69	39.83
4	27.45	30.38
5	14.02	-14.70
6	10.15	-6.18
9	3.96	-1.57
h=1, l=-4		
0	5.04	7.96
1	38.40	40.35
2	17.46	20.84
3	16.61	-20.10
4	14.56	-18.68
5	9.07	-2.41
6	6.42	6.97
7	15.18	11.43
8	6.88	-2.84
9	11.37	-13.62
h=1, l=-5		
0	35.58	28.30
2	29.00	-27.01
3	32.98	33.54
4	40.44	37.82
5	38.14	-38.85
6	30.77	-32.95
7	23.04	24.15
8	13.58	15.10
9	10.13	-12.18
h=1, l=-6		
0	12.58	-10.22
1	16.15	-8.06
2	12.78	11.74
3	27.42	25.26
4	5.35	-0.68
5	18.52	-15.79
7	7.73	4.07
8	8.15	-9.27
9	6.69	-3.87
h=1, l=-7		
0	7.63	-4.01
1	15.41	-15.16
2	11.13	-7.98
3	13.27	11.02
4	19.03	19.01
6	10.80	-12.79
7	7.02	-4.51
8	5.79	3.76
9	3.35	-2.71
h=1, l=-8		
0	8.61	-5.16
1	6.89	5.68
3	14.71	-12.27
4	7.49	-2.49
5	12.36	13.46
6	8.63	8.11
7	6.06	-3.43
8	4.64	-7.86
h=1, l=-9		
1	6.36	5.04
2	5.45	2.80
h=-1, l=0		
1	17.46	22.86
2	24.56	-30.77
3	5.54	-8.21
4	18.12	22.02
5	10.14	-9.43
6	14.33	-17.32
7	9.44	10.34
8	6.31	7.03
h=-1, l=1		
1	8.01	-8.03
2	20.66	-22.92
3	6.69	-5.81
4	21.55	20.01
6	20.07	-20.36
7	3.29	-6.51
8	8.02	10.96
h=-1, l=2		
1	22.30	-19.65
2	11.15	-9.02
3	35.57	37.03
4	6.61	-1.34
5	31.86	-37.89
6	7.53	-5.67
7	15.75	20.72
h=-1, l=3		
1	62.17	65.04
2	55.77	-59.38
3	35.65	-37.90
4	22.70	21.16
6	8.59	-8.42
h=-1, l=4		
1	20.08	-18.04
2	16.54	-16.75
3	7.13	-3.85
4	4.95	4.38
5	4.89	1.56
h=-1, l=5		
1	16.67	-11.90
2	29.38	-26.74
3	5.88	0.29
4	12.84	11.76
h=-1, l=6		
1	9.61	-10.14
2	6.22	-0.87
3	9.85	9.35
4	4.27	3.45
h=-1, l=7		
1	9.89	7.83
2	5.73	5.30
h=-1, l=-1		
1	9.72	10.65
2	26.28	-28.35
3	4.52	-4.66
4	9.62	11.51
5	5.92	-3.06
6	7.43	-7.03
7	4.62	0.59
8	4.53	1.78
h=-1, l=-2		
1	19.04	17.36
2	37.57	37.73
4	27.04	-30.59
5	5.78	-5.26
6	8.09	12.35
7	5.34	2.57
9	5.30	-2.04
h=-1, l=-3		
1	18.12	-14.18
2	42.57	38.06
3	7.20	4.48
4	22.56	-21.61
5	5.61	2.91
7	8.03	-8.58
9	5.04	5.87
h=-1, l=-4		
1	41.60	36.44
2	44.17	48.44
3	23.17	-22.58
4	28.59	-27.37
5	12.76	11.69
6	15.06	9.76
7	8.84	-6.58
8	10.06	-5.88
9	4.84	3.77
h=-1, l=-5		
1	44.50	-36.40
2	4.55	1.38
3	39.46	33.32
4	6.17	4.12
5	14.71	-12.30
6	5.86	-0.85
7	9.09	-5.13
8	6.90	-3.94
9	8.71	8.03
h=-1, l=-6		
1	5.92	3.83
2	31.51	23.16
3	25.32	-21.03
4	37.75	-31.32
5	33.64	29.71
6	32.51	30.23
7	23.89	-24.24
8	18.93	-20.35
9	9.81	12.47
h=-1, l=-7		
1	5.97	2.88
2	6.30	4.12
3	9.10	-5.91
5	6.34	2.21
7	5.43	0.52
h=-1, l=-8		
1	4.08	6.56
2	4.86	4.31
4	6.82	-9.55
6	4.91	8.69
7	4.18	1.53
8	2.56	-6.98
h=2, l=0		
1	38.73	44.86
2	15.61	-19.90
3	30.24	-34.50
4	13.28	19.52
5	20.12	24.67
7	11.74	-14.86
h=2, l=1		
0	98.07	-110.59
1	9.91	10.18
2	57.10	65.05
3	11.03	-10.96
4	19.57	-22.79
5	11.30	11.43
7	6.40	-9.40
h=2, l=2		
0	3.88	-1.96
1	17.68	17.67
2	18.38	18.24
3	9.91	-8.17
4	14.26	-14.35
5	7.23	4.45
6	4.96	5.48
h=2, l=3		
0	10.36	-7.71
1	27.98	25.26
3	11.89	-12.62
4	5.19	-2.03
5	3.95	2.96
h=2, l=4		
0	12.89	-7.53
1	13.18	10.27
2	7.06	3.78
3	14.03	-10.73
4	3.52	-2.16
h=2, l=5		
1	14.13	-10.94
2	6.69	-1.80
3	6.15	6.78
h=2, l=6		
0	5.56	0.60
1	4.89	1.72
2	3.49	2.46
h=2, l=7		
0	12.21	11.93
h=2, l=-1		
0	16.78	-15.91
1	18.44	-18.33
2	19.74	20.82
3	3.63	2.84
4	20.06	-22.57
5	2.89	2.23
6	10.10	15.42
7	5.18	-3.63
8	3.08	-6.31
h=2, l=-2		
0	36.58	41.04
1	27.44	31.83
2	2.99	-3.40
3	30.01	-35.44
4	10.01	-7.54
5	18.17	24.73
6	4.86	0.86
7	13.36	-16.96
8	4.29	2.77
h=2, l=-3		
0	4.82	-3.32
1	13.93	20.82
2	31.25	34.08
3	4.19	-0.12
4	20.28	-22.57
5	10.21	-10.07
6	5.91	4.76
h=2, l=-4		
0	17.14	19.48
1	15.83	9.17
2	7.91	-9.38
3	14.01	16.61
4	15.45	17.74
5	14.09	-15.19
6	14.44	-17.23
7	5.66	1.27
8	5.23	5.72
9	2.66	2.41
h=2, l=-5		
0	31.24	24.85
1	25.35	-24.50
2	10.08	-10.31
3	40.12	46.09
4	13.02	10.90
5	28.30	-29.52
6	5.77	-3.99
7	11.82	9.37
8	5.06	-5.24
9	5.21	-4.38
h=2, l=-6		
0	10.92	-1.57
1	34.08	-34.16
2	4.35	-2.02
3	23.91	30.82
4	11.87	12.98
5	11.58	-8.01
6	9.47	-6.95
9	4.37	-1.68
h=2, l=-7		
0	18.27	17.91
1	12.95	4.04
2	31.47	-25.02
3	6.41	-2.24
4	24.14	22.84
6	6.36	-5.46
7	8.25	7.36
8	4.76	-5.36
9	6.49	-13.01
h=2, l=-8		
0	14.87	11.76
1	17.25	-12.10
2	12.63	-9.48
3	27.05	20.52
5	21.51	-22.03
6	5.86	5.44
7	16.34	20.93
8	5.00	-5.63
h=2, l=-9		
0	6.14	-3.25
2	8.93	5.11
4	5.47	-3.21
5	5.28	-3.08
7	5.06	3.76
h=2, l=-10		
3	4.73	7.65
4	8.86	7.03
6	3.95	-6.21
h=-2, l=0		
1	33.76	-39.59
2	26.19	32.25
3	23.34	27.94
4	18.89	-21.58
5	13.26	-13.68
h=-2, l=1		
1	27.54	34.95
2	28.02	32.43
3	8.93	-9.48
4	25.15	-29.29
5	8.87	-11.13
6	10.42	10.14
7	5.91	8.89
h=-2, l=2		
1	13.44	14.43
2	26.88	-30.06
3	20.13	-23.52
4	6.92	7.76
5	5.86	6.10
6	6.80	-3.52
h=-2, l=3		
2	15.38	-13.91
3	11.97	-10.54
4	12.53	9.99
6	8.33	-9.22
7	4.84	2.96
h=-2, l=4		
1	15.84	-11.61
2	18.72	-19.66
4	5.40	6.38
6	4.15	-0.69
h=-2, l=5		
1	4.52	0.02
2	40.41	-33.86
3	7.34	5.26
4	25.74	23.22
5	3.90	-5.94
h=-2, l=6		
1	27.37	22.63
3	15.17	-12.59
4	6.10	5.21
h=-2, l=7		
1	8.72	-4.66
2	10.80	-11.23
3	3.98	1.06
h=-2, l=8		
1	4.74	4.31
2	10.75	-11.04
h=-2, l=-1		
1	6.90	-4.96
2	81.55	102.21
3	2.90	-1.37
4	37.51	-48.68
5	4.96	8.38
6	14.19	16.20
7	8.75	-12.06
8	7.43	-7.24
9	4.75	7.23
h=-2, l=-2		
1	21.67	-19.26
2	23.81	-21.23
3	6.12	5.44
4	15.90	20.93
5	8.07	7.03
6	5.68	-6.48
7	11.44	-9.90
8	6.42	-3.80
9	6.15	5.95
h=-2, l=-3		
1	27.26	-22.65
2	30.86	26.25
3	6.43	6.42
4	47.16	-46.20
5	6.88	1.97
6	36.51	46.02
7	7.79	-3.53
8	19.54	-28.08
9	5.84	3.14
h=-2, l=-4		
1	6.29	4.37
2	25.01	19.63
3	19.84	-16.90
4	28.58	-25.68
5	14.58	13.83
6	16.80	13.71
7	10.94	-9.51
8	6.36	-1.24
9	8.87	7.78
h=-2, l=-5		
1	20.65	13.89
2	13.27	11.45
3	10.29	-5.41
4	16.63	-14.59
5	6.26	-7.32
6	11.58	7.02
8	7.00	-2.69
9	5.06	-0.41
h=-2, l=-6		
1	10.94	-7.18
3	17.06	13.36
4	8.34	5.32
5	14.72	-12.38
6	7.73	-8.16
7	6.64	0.99
8	5.03	4.11
9	5.47	6.31
h=-2, l=-7		
2	9.59	-11.62
3	7.34	-3.43
4	7.42	7.45
7	8.25	-6.53
h=3, l=0		
0	9.52	9.09
1	17.11	18.22
2	5.31	-4.07
3	9.32	-10.07
4	5.42	-2.39
5	5.51	4.91
h=3, l=1		
0	6.70	-7.19
1	17.28	15.06
2	14.52	-11.39
3	15.59	-13.80
4	11.29	12.47
5	11.50	12.61
6	3.23	-2.82
h=3, l=2		
0	34.46	-29.21
1	19.90	-17.55
2	10.76	10.60
3	19.12	19.73
4	9.29	6.62
5	9.10	-9.35
h=3, l=3		
1	11.91	10.20
2	15.02	12.55
3	5.00	4.83
4	6.44	-5.70
h=3, l=4		
0	~~29.85~~	~~-24.99~~
1	11.57	-7.86
2	9.03	-5.51
3	13.78	11.71
h=3, l=5		
0	20.45	20.16
1	7.47	3.25
2	11.91	-10.78
h=3, l=6		
0	4.89	3.36
1	11.39	-12.80
h=3, l=-1		
0	25.61	-31.45
1	17.92	17.97
2	28.70	33.42
3	23.65	-26.45
4	15.13	-20.28
5	16.47	19.95
6	3.67	6.94
7	8.77	-10.45
h=3, l=-2		
1	72.60	100.86
2	37.57	42.44
3	44.34	-54.82
4	11.59	-12.21
5	19.65	22.61
7	10.29	-8.79
8	4.50	6.54
h=3, l=-3		
0	8.80	-8.24
1	6.17	-4.52
2	2.43	-1.52
3	12.52	15.43
4	10.77	14.67
6	9.14	-13.34
7	11.93	-6.97
8	4.33	5.81
h=3, l=-4		
0	25.43	-28.51
1	3.08	3.23
2	24.85	26.65
3	18.77	-18.25
4	16.64	-15.19
5	27.15	29.40
6	7.78	8.79
7	22.07	-24.64
8	4.31	-5.08
h=3, l=-5		
0	17.64	15.81
1	8.71	8.47
2	9.48	-12.56
3	20.64	-19.07
4	12.06	12.12
5	21.25	19.05
6	7.45	-8.85
7	14.66	-10.95
8	4.60	5.37
h=3, l=-6		
0	4.95	-0.36
1	17.72	20.47
2	19.23	14.44
3	7.89	-7.59
4	16.32	-12.97
5	5.45	0.28
6	9.95	8.76
7	5.68	1.19
8	5.66	-4.96
h=3, l=-7		
0	15.51	6.62
1	18.77	-17.56
2	11.36	-5.99
3	32.72	28.07
4	17.72	11.97
5	23.70	-17.72
6	10.73	-9.36
7	5.63	4.94
8	4.45	3.67
h=3, l=-8		
1	21.35	-14.58
2	6.28	-0.08
3	24.39	14.39
4	6.27	-0.95
5	8.67	-3.44
6	14.15	6.94
7	5.05	-0.57
8	13.02	-8.79
h=3, l=-9		
0	12.06	-5.66
1	5.03	-10.47
3	9.74	13.09
4	11.21	6.30
5	7.61	-8.51
6	4.91	-3.21
7	11.45	8.27
h=3, l=-10		
2	20.69	-15.25
3	18.76	10.25
4	20.99	12.83
5	13.56	-5.92
h=-3, l=0		
1	20.13	-24.84
2	4.68	3.90
3	19.68	23.83
4	22.74	-22.18
5	17.78	-23.22
6	21.43	21.78
7	10.53	15.50
8	10.76	-11.87
h=-3, l=1		
1	14.99	17.88
2	14.66	18.62
3	31.99	-37.41
4	17.28	-16.02
5	22.83	27.73
6	15.71	13.53
7	9.95	-13.13
8	9.69	-8.48
h=-3, l=2		
4	~~67.21~~	~~-90.23~~
2	35.36	42.83
3	34.62	38.79
4	25.06	-27.61
5	7.97	-8.24
6	13.59	15.06
7	4.65	-3.04
h=-3, l=3		
1	11.96	-12.82
2	6.29	8.93
3	14.74	13.99
4	4.83	-5.50
5	7.17	-7.84
6	4.55	0.91
h=-3, l=4		
1	5.06	4.25
2	25.57	23.33
4	18.47	-15.35
5	10.50	-8.79
6	7.14	3.91
h=-3, l=5		
1	13.21	12.33
2	12.89	-10.01
3	19.93	-20.49
4	5.06	-1.05
5	8.32	10.01
h=-3, l=6		
1	18.70	-16.27
2	10.86	-11.44
4	8.36	8.17
h=-3, l=7		
2	13.94	-10.84
h=-3, l=8		
1	13.71	6.83
2	13.85	-13.32
h=-3, l=-1		
1	12.96	-13.06
2	30.93	33.79
4	33.70	-42.34
5	3.43	0.91
6	20.47	28.18
7	6.67	-6.39
8	10.74	-12.58
9	5.79	8.59
h=-3, l=-2		
1	9.48	5.41
2	32.60	30.22
4	19.32	-17.68
5	4.36	-5.93
6	6.75	3.57
h=-3, l=-3		
1	22.41	-20.00
2	25.26	-22.59
3	10.96	11.29
4	24.76	24.81
6	14.44	-13.37
7	8.37	-3.45
8	5.12	2.20
9	6.35	5.39
h=-3, l=-4		
1	16.61	13.98
2	31.12	-30.73
3	23.51	-22.22
4	10.77	10.61
5	14.88	13.39
6	5.46	4.99
7	5.72	-2.17
8	4.72	-6.76
9	3.37	-1.34
h=-3, l=-5		
2	13.45	-13.33
4	7.24	-0.49
5	8.03	-7.01
6	8.00	-1.56
7	7.58	10.75
8	11.25	7.65
9	3.02	-5.02
h=-3, l=-6		
1	24.79	21.03
2	5.65	0.36
3	22.45	-16.18
4	5.99	1.64
5	7.65	2.04
6	18.30	-12.70
7	5.02	1.25
8	15.09	14.03
h=-3, l=-7		
2	16.16	-12.67
3	6.47	4.62
4	20.52	18.43
5	12.76	-10.70
6	20.49	-21.90
7	4.19	6.11
h=4, l=0		
0	13.52	12.62
1	16.79	14.70
2	4.90	2.65
3	5.32	1.21
4	7.52	1.52
h=4, l=1		
0	10.60	8.87
1	22.32	-20.18
2	9.36	9.65
3	15.56	16.49
4	9.98	-11.80
5	8.81	-8.78
h=4, l=2		
0	43.46	40.36
1	19.84	-21.97
2	26.19	-26.32
3	18.71	19.01
4	13.66	14.13
5	8.64	-8.96
h=4, l=3		
0	18.15	-12.44
1	7.98	-8.34
2	9.49	9.27
3	11.13	12.53
4	3.16	-1.31
h=4, l=4		
0	13.60	13.02
1	11.04	-8.19
2	3.95	1.62
3	4.95	5.70
h=4, l=5		
0	14.04	9.46
1	7.22	-6.06
h=4, l=-1		
0	47.42	-50.37
1	5.92	-3.31
2	22.28	26.80
3	19.42	22.68
5	12.91	-15.62
6	4.70	-0.90
7	5.03	7.18
h=4, l=-2		
0	8.28	6.77
1	8.41	-6.43
2	28.09	-29.43
4	23.67	27.24
5	7.91	8.57
6	8.64	-9.66
7	3.84	-7.35
h=4, l=-3		
0	16.15	-17.95
2	9.39	11.65
3	15.30	-12.27
4	9.20	-11.19
5	13.96	13.94
6	8.45	12.18
7	6.41	-4.10
8	2.75	-6.28
h=4, l=-4		
0	20.00	-18.81
1	30.00	34.41
2	4.48	1.90
3	40.45	-45.83
4	6.31	5.53
5	27.90	31.89
6	10.94	-6.95
7	11.73	-12.87
8	8.11	7.59
h=4, l=-5		
0	20.50	12.72
1	57.63	66.39
2	7.17	-3.03
3	42.89	-42.64
4	5.37	-1.89
5	18.35	14.60
6	5.86	0.18
7	6.13	-1.34
8	5.81	2.49
h=4, l=-6		
0	27.89	-23.91
1	9.82	-5.57
2	23.65	27.55
3	14.44	14.22
4	15.14	-10.19

TABLE 5. (Continued)

k	F_o	F_c
5	5.64	-5.75
6	7.82	-5.08
7	11.39	-5.06
8	9.07	8.88
h=4, l=-7		
0	19.00	-15.33
1	21.52	16.02
2	8.68	6.28
3	31.61	-21.73
4	12.59	9.69
5	41.12	29.86
6	16.28	-11.64
7	29.86	-24.99
8	5.75	5.66
h=4, l=-8		
0	6.08	-0.27
2	14.19	-9.08
3	6.35	1.66
4	15.48	13.01
5	8.72	5.64
7	6.98	-2.86
h=4, l=-9		
0	4.79	5.88
1	10.81	6.95
2	5.72	-2.98
3	15.43	-9.23
5	13.48	9.53
6	11.11	8.14
7	5.66	-3.99
h=4, l=-10		
1	12.46	-12.26
3	19.87	13.96
4	4.47	-2.01
5	11.87	-10.19
6	4.46	1.40
h=-4, l=0		
1	18.67	-18.65
2	35.20	-40.23
3	11.30	-9.74
4	24.40	29.62
5	18.28	20.14
7	10.37	-10.38
8	4.27	-2.28
h=-4, l=1		
1	28.23	-32.68
2	28.80	33.14
3	23.52	27.83
4	11.71	-13.15
5	4.37	-7.72
6	5.28	6.76
8	3.06	-3.72
h=-4, l=2		
1	12.88	-14.61
2	12.42	10.38
3	21.08	23.00
4	16.75	-15.06
5	11.77	-13.63
6	13.48	14.30
8	7.30	-10.37
h=-4, l=3		
1	2.78	-1.75
2	16.04	16.90
3	10.40	10.18
4	11.24	-10.62
5	14.96	-14.39
6	4.66	3.53
7	7.50	9.61
h=-4, l=4		
1	5.84	-4.66
2	30.90	32.74
3	13.98	-12.51
4	36.44	-34.27
5	11.52	9.86
6	22.97	22.91
h=-4, l=5		
1	61.92	-55.68
2	16.10	-11.41
3	28.76	26.43
5	8.38	-8.31
6	3.64	5.25
h=-4, l=6		
2	14.39	8.72
4	5.11	-3.09
5	3.38	1.16
h=-4, l=7		
1	16.75	-14.42
2	8.45	8.55
3	8.75	8.54
h=-4, l=8		
1	7.04	7.31
h=-4, l=9		
1	7.34	-5.26
h=-4, l=-1		
1	30.02	28.92
2	18.50	-21.76
3	31.44	-35.01
4	3.26	2.63
5	14.36	13.79
6	8.12	9.42
7	5.36	6.55
9	2.51	-7.74
h=-4, l=-2		
1	20.93	22.19
2	36.43	-38.32
3	15.72	-15.87
4	16.02	17.02
6	9.50	-9.60
7	4.75	9.52
8	11.32	11.56
h=-4, l=-3		
1	7.83	5.87
2	18.17	12.01
3	7.59	-5.22
4	10.55	-8.78
5	5.65	-2.02
6	7.98	-4.25
7	5.80	3.06
8	13.95	11.29
h=-4, l=-4		
1	21.70	17.65
2	30.86	-28.41
3	24.83	-23.46
4	35.57	33.25
5	16.21	14.69
6	30.00	-32.29
7	8.21	-6.75
8	19.59	22.18
9	3.88	3.54
h=-4, l=-5		
1	9.13	8.44
2	16.47	-9.83
3	5.66	-4.39
4	10.93	4.71
5	10.64	-6.35
6	9.98	-4.67
7	11.22	8.70
8	10.15	4.21
h=-4, l=-6		
1	6.68	-1.62
5	5.20	1.23
6	12.51	-9.29
7	4.27	-4.79
8	9.17	9.76
h=-4, l=-7		
5	4.71	4.31
h=5, l=0		
0	12.59	-9.14
1	14.95	-12.91
3	23.02	25.55
5	13.90	-15.75
h=5, l=1		
0	4.10	-2.23
1	3.70	-5.99
2	11.62	9.26
3	4.41	5.98
4	3.19	-1.47
5	2.93	-0.18
h=5, l=2		
1	19.23	-15.76
2	14.16	9.92
3	17.49	16.22
4	6.84	-4.97
h=5, l=3		
0	22.67	16.32
1	16.86	12.03
2	4.25	-2.40
3	5.14	-6.25
h=5, l=4		
0	4.47	1.42
1	3.80	-1.53
h=5, l=5		
0	5.25	-2.95
h=5, l=-1		
0	22.69	22.98
1	55.13	-64.56
2	16.97	-16.07
3	35.99	42.06
4	9.42	9.19
5	11.81	-12.81
h=5, l=-2		
0	20.10	-23.97
1	13.41	-13.44
2	15.33	17.92
4	10.54	-13.58
6	11.96	14.36
7	2.43	1.30
h=5, l=-3		
0	26.48	26.14
1	11.39	-12.80
2	27.70	-25.73
3	9.55	8.97
4	14.68	13.45
5	8.93	-8.01
6	5.28	-0.67
7	8.72	9.49
h=5, l=-4		
0	17.60	-17.87
1	18.44	17.55
2	19.02	21.00
3	4.51	1.06
4	15.60	-19.08
5	10.60	-8.48
6	13.62	15.15
7	10.91	9.03
8	1.98	-7.27
h=5, l=-5		
0	4.99	0.74
1	20.72	-17.67
2	16.21	-11.39
3	19.08	15.85
4	18.47	15.46
5	6.86	-5.33
6	12.22	-10.91
7	4.75	0.32
8	6.13	6.44
h=5, l=-6		
0	27.86	-23.21
1	13.02	15.26
2	12.36	12.24
3	22.99	-22.24
4	5.13	-5.27
5	19.97	20.23
7	6.38	-9.28
8	3.38	-3.01
h=5, l=-7		
0	7.80	5.86
1	25.31	17.67
2	26.22	-22.32
3	27.62	-21.37
4	28.09	23.56
5	17.53	14.72
6	19.64	-15.72
8	9.48	9.71
h=5, l=-8		
0	15.31	10.36
1	15.66	21.72
2	7.86	-3.69
3	17.58	-20.29
4	5.51	-5.19
5	13.10	12.07
6	4.91	7.18
7	7.00	-4.05
h=5, l=-9		
0	16.68	-13.08
1	10.98	7.85
2	22.92	13.52
3	12.67	-6.55
4	8.79	-4.63
5	11.75	5.31
6	8.49	-6.07
7	8.57	-4.09
h=5, l=-10		
1	9.50	8.98
2	7.77	-3.82
3	11.56	-9.31
4	15.65	10.59
5	11.79	10.41
6	11.32	-10.77
h=-5, l=0		
1	14.25	-13.42
2	4.43	-3.75
3	14.45	16.24
4	5.22	5.76
5	7.66	-10.93
6	7.03	-3.59
7	5.46	8.99
8	6.46	5.80
h=-5, l=1		
1	48.66	56.23
2	29.05	-36.44
3	32.74	-38.52
4	25.50	29.97
5	21.02	19.87
6	13.13	-15.33
7	8.35	-5.90
8	6.00	7.61
h=-5, l=2		
1	10.47	10.87
2	12.49	11.99
3	7.11	-7.66
4	7.21	-3.61
6	5.60	1.68
h=-5, l=3		
1	14.12	14.08
2	22.36	-21.47
3	20.28	-20.39
4	8.89	8.25
5	18.13	19.10
6	4.45	3.87
7	7.10	-8.03
h=-5, l=4		
1	32.69	-35.66
2	5.71	4.69
3	24.62	27.70
4	4.98	0.31
5	6.83	-10.07
6	4.42	3.67
h=-5, l=5		
1	4.20	1.43
2	4.77	0.02
3	13.66	8.64
5	6.48	-5.64
6	2.91	1.43
h=-5, l=6		
1	8.42	-12.65
2	26.59	21.65
3	10.59	11.88
4	13.68	-10.84
5	6.11	-7.88
h=-5, l=7		
1	15.73	-10.69
2	10.69	10.44
3	9.33	5.68
4	13.28	-15.20
h=-5, l=8		
1	10.11	-15.65
2	12.95	-9.32
h=-5, l=9		
1	5.15	-6.84
h=-5, l=-1		
1	13.87	15.28
2	17.85	-18.34
3	30.73	-37.32
4	21.94	21.81
5	29.85	37.05
6	16.53	-17.38
7	14.24	-20.29
8	13.28	14.66
h=-5, l=-2		
1	22.75	18.65
2	21.52	-19.87
3	23.34	-22.42
4	18.63	17.97
5	9.25	8.19
6	13.47	-12.76
7	6.41	6.42
8	12.18	11.63
h=-5, l=-3		
1	8.56	-5.13
2	28.16	-20.53
4	14.90	8.15
6	9.31	-3.26
7	5.27	-1.01
8	11.19	5.95
h=-5, l=-4		
1	14.00	11.30
2	13.63	8.92
3	16.29	-14.15
4	21.70	-17.49
6	9.85	8.28
7	8.75	2.21
8	4.22	3.22
h=-5, l=-5		
1	4.67	-5.30
2	7.21	6.86
3	12.52	8.38
4	5.23	-3.48
5	16.21	-11.34
6	12.84	-7.33
7	8.62	4.99
8	9.18	10.06
h=-5, l=-6		
2	3.95	5.98
3	6.75	4.81
4	4.25	-3.75
5	7.92	-3.43
6	4.46	1.18
7	2.69	-2.04
h=6, l=0		
0	28.08	27.87
1	5.44	-2.76
2	16.45	-16.36
3	5.34	-4.80
4	4.54	7.96
h=6, l=1		
0	16.61	-15.42
1	10.91	-8.24
2	5.49	4.61
3	8.10	7.62
h=6, l=2		
1	18.59	17.49
2	5.11	-2.74
3	8.70	-7.71
h=6, l=3		
0	14.67	-10.35
1	8.98	10.12
2	8.52	8.65
h=6, l=4		
0	13.61	11.14
h=6, l=-1		
0	17.58	-17.82
1	9.45	-11.10
2	25.79	25.24
3	8.00	9.27
4	15.03	-15.64
5	2.91	-5.26
h=6, l=-2		
3	7.48	6.47
5	4.30	-1.70
6	3.12	-3.35
h=6, l=-3		
0	11.50	-9.70
1	39.26	-44.76
2	11.76	8.39
3	36.87	41.64
4	7.07	-6.41
5	17.22	-20.57
6	11.52	10.35
7	3.62	8.78
h=6, l=-4		
0	14.92	-11.95
1	43.41	-51.40
2	4.77	4.51
3	23.51	23.49
4	5.81	-4.30
5	5.40	-0.27
6	11.39	9.44
7	3.27	-2.32
h=6, l=-5		
0	7.05	-10.02
2	4.27	1.14
3	4.67	-2.39
5	6.04	0.69
6	13.02	11.80
7	9.90	6.73
h=6, l=-6		
0	18.18	12.71
1	28.11	-26.50
2	21.49	-17.18
3	20.70	16.87
4	5.58	3.17
5	16.13	-12.35
6	7.33	6.75
7	11.54	10.08
h=6, l=-7		
0	6.95	5.68
1	19.99	15.46
2	6.80	4.98
3	14.17	-13.40
4	17.79	-17.35
6	12.93	16.02
7	4.98	2.98
h=6, l=-8		
0	6.82	6.82
2	9.43	5.50
3	12.56	7.71
5	13.55	-9.85
6	5.88	-5.34
7	11.32	6.53
h=6, l=-9		
0	7.83	-4.28
1	17.43	14.77
3	19.18	-13.87
4	9.43	6.36
5	10.57	10.32
6	9.04	-5.95
h=6, l=-10		
2	19.67	-11.11
4	16.76	11.53
h=-6, l=0		
1	16.09	14.33
2	30.26	-31.19
3	20.78	-22.68
4	12.86	14.31
5	10.74	10.90
6	5.48	-3.25
8	6.35	5.87
h=-6, l=1		
1	18.00	19.36
2	6.48	-6.06
3	31.00	-36.51
4	10.45	10.41
5	26.06	30.96
6	5.32	-4.49
7	6.53	-9.03
8	5.19	5.85
h=-6, l=2		
1	12.14	-9.21
2	15.36	-13.00
3	10.24	-8.66
4	16.66	16.03
5	22.02	23.71
6	8.41	-5.71
7	13.77	-16.52
h=-6, l=3		
1	11.13	14.32
2	9.20	-9.65
3	5.91	4.16
4	19.87	20.72
6	12.60	-12.79
7	2.98	3.29
h=-6, l=4		
1	42.15	48.22
2	7.16	2.38
3	28.25	-32.23
4	9.05	9.14
5	23.62	21.61
6	4.93	-6.34
h=-6, l=5		
1	4.77	-1.82
2	9.62	9.18
3	10.30	7.74
4	5.11	1.16
5	5.64	-4.66
6	5.10	-4.68
h=-6, l=6		
1	29.21	23.98
2	6.04	-0.76
3	18.07	-12.66
4	6.62	-4.09
5	7.69	5.21
h=-6, l=7		
1	17.80	-12.88
2	6.83	-7.69
3	9.01	9.09
h=-6, l=8		
2	5.69	3.40
h=-6, l=9		
1	14.40	-13.73
h=-6, l=-1		
1	5.51	2.79
2	21.57	22.95
4	18.97	-24.10
5	11.46	-10.17
6	6.57	11.24
7	10.73	9.38
8	6.34	3.47
h=-6, l=-2		
1	26.39	-22.77
2	8.71	-7.28
3	17.06	14.80
4	14.39	10.29
5	6.69	-3.86
6	14.55	-12.14
8	9.43	10.20
h=-6, l=-3		
1	7.25	-9.50
2	11.86	9.60
3	5.74	2.15
4	11.35	-12.03
6	12.49	12.16
7	6.17	1.10
8	6.69	-8.98
h=-6, l=-4		
1	12.50	-10.92
2	17.35	-12.30
3	11.85	7.68
4	8.54	4.98
5	12.67	-7.77
6	4.88	0.70
7	10.26	6.43
8	2.43	-1.48
h=-6, l=-5		
1	4.01	-4.88
2	10.80	9.53
3	8.06	7.12
4	20.91	-18.95
5	11.91	-9.73
6	17.07	18.86
7	7.64	7.67
h=7, l=0		
0	7.86	-3.10
1	21.41	23.66
3	11.03	-12.94
h=7, l=1		
0	9.56	8.35
1	11.06	11.21
2	4.60	-4.74
3	9.59	10.53
h=7, l=2		
0	8.60	7.30
1	4.72	2.79
2	8.50	-8.77
h=7, l=3		
0	3.94	-2.15
h=7, l=-1		
0	14.00	14.83
1	18.76	18.98
2	7.27	-8.50
3	8.19	-5.73
4	8.24	8.65
h=7, l=-2		
0	32.93	-29.47
1	6.96	-4.69
2	18.37	16.39
3	10.95	10.71
h=7, l=-3		
0	5.65	4.95
1	30.26	-29.47
2	19.96	-18.83
3	6.48	6.34
4	17.45	18.96
5	13.02	9.87
6	5.58	-7.17
h=7, l=-4		
0	15.27	-12.27
1	4.97	2.49
2	12.56	8.13
3	17.03	-12.55
4	15.19	-11.18
5	11.94	9.40
6	13.10	13.17
h=7, l=-5		
0	16.05	11.04
1	11.40	-11.49
2	9.69	-6.80
3	10.17	11.37
4	6.56	-1.24
5	7.60	-10.03
6	6.29	4.08
7	3.43	8.26
h=7, l=-6		
0	25.96	-20.40
1	34.58	-31.61
2	18.35	24.39
3	26.39	22.80
4	24.59	-23.82
5	12.27	-11.05
6	14.61	17.03
7	2.97	4.38
h=-7, l=0		
1	21.30	-23.06
3	6.96	9.37
4	13.61	-16.94
5	5.51	-4.34
6	16.43	19.35
7	10.84	8.61
8	5.91	-9.35
h=-7, l=1		
1	25.07	-26.06
2	25.50	-26.01
3	7.48	8.10
4	21.40	19.53
5	10.13	10.11
6	8.78	-3.90
7	8.41	-10.37
h=-7, l=2		
1	18.57	-18.05
2	19.56	36.72
3	27.50	24.65
5	14.11	-14.24
7	4.08	5.79
h=-7, l=3		
1	34.39	33.08
3	22.67	-24.34
5	12.59	13.77
6	4.90	-4.58
h=-7, l=4		
1	12.93	7.94
2	12.47	10.49
3	18.85	-16.85
4	5.90	-5.69
5	19.59	18.16
h=-7, l=5		
1	4.60	5.23
2	20.16	-16.13
3	5.19	-5.91
4	15.84	15.06
5	10.51	11.45
6	5.41	-5.34
h=-7, l=6		
1	27.20	21.49
2	7.31	4.49
3	11.41	-8.56
4	12.49	10.30
5	7.39	6.01
h=-7, l=-1		
1	3.64	-6.07
2	11.93	-8.07
4	3.64	1.44
5	3.76	-3.97
7	7.63	6.68
8	2.07	1.67
h=-7, l=-2		
1	6.50	-9.14
3	16.48	17.55
4	14.13	-9.75
5	21.37	-22.15
6	12.64	11.88
7	15.17	17.21
8	5.75	-8.44
h=-7, l=-3		
1	17.87	-16.05
2	10.33	6.50
3	19.92	17.81
4	9.10	-7.62
5	15.23	-12.86
6	5.95	5.54
7	6.51	4.83
h=-7, l=-4		
2	4.56	2.26
3	3.56	2.08
5	3.82	-1.64
6	6.70	0.86
7	2.12	1.85
h=8, l=0		
0	13.66	11.11
1	9.69	10.50
2	11.95	-12.33
h=8, l=1		
0	10.11	-9.05
1	3.75	2.80
h=8, l=2		
0	5.45	6.03
h=8, l=-1		
1	6.48	-1.83
2	4.89	-5.02
3	2.90	1.73
h=8, l=-2		
0	7.20	1.83
1	16.39	15.88
2	12.65	-9.00
3	14.06	-14.38
4	10.57	10.10
h=8, l=-3		
0	16.28	15.02
1	22.38	18.40
2	17.08	-18.62
3	13.21	-10.11
4	13.04	14.39
h=8, l=-4		
0	14.95	12.27
1	9.36	5.92
2	7.74	-8.65
3	6.60	-3.92
4	7.00	5.04
5	5.64	2.38
h=8, l=-5		
0	19.59	-14.22
1	12.47	7.91
2	14.63	10.02
3	5.17	-2.75
6	3.00	-3.14
h=8, l=-6		
0	20.53	-14.81
1	27.86	-22.92
3	11.58	10.60
4	14.82	12.41
6	6.06	-8.38
h=9, l=0		
0	10.65	-6.42
1	8.88	-6.84
h=9, l=-1		
0	10.95	8.40
2	6.48	-5.15
h=9, l=-2		
1	15.04	13.60
3	3.17	-4.83
h=9, l=-3		
0	18.12	17.57
1	4.43	-1.71
2	13.67	-13.11
3	7.75	5.05
4	7.85	8.55
h=9, l=-4		
0	15.28	-5.97
1	6.62	6.43
2	6.39	2.05
3	4.77	-4.69
4	4.78	1.24
5	1.46	3.26
h=9, l=-5		
0	14.66	12.15
1	7.30	8.40
2	25.71	-22.94
3	6.73	-6.25
4	18.79	21.00
h=9, l=-6		
0	23.13	17.45
1	5.77	5.71
2	19.74	-17.47
3	7.71	-4.35
4	10.68	9.21
5	4.40	1.04
h=-9, l=0		
1	12.55	8.16
2	13.02	9.56
4	11.65	-6.09
5	6.17	-5.54
6	5.19	2.11
h=-9, l=1		
1	8.85	6.98
2	7.32	-6.33
3	10.25	-9.46
4	4.40	3.41
5	7.82	6.87
h=-9, l=2		
1	21.30	-19.46
3	17.83	18.28
5	9.84	-11.94
6	5.58	5.24
h=-9, l=3		
1	6.44	-6.61
2	19.26	-19.38
3	12.62	11.94
4	14.67	14.45
5	10.63	-10.07
6	4.09	-4.29
h=-9, l=4		
1	14.28	-11.34
2	9.91	2.91
3	17.28	13.88
4	4.50	3.37
5	12.69	-10.37
6	3.53	-3.94
h=-9, l=5		
1	8.97	-11.92
3	13.83	12.61
4	5.54	-4.48
5	9.62	-7.83
h=-9, l=6		
2	15.78	-12.19
3	7.28	11.01
4	9.56	7.80
h=-9, l=-1		
1	6.81	8.54
3	3.00	-3.10
4	2.93	2.99
5	2.69	3.12
6	2.19	-4.62
h=-9, l=-2		
2	7.41	7.33
3	2.90	1.03
5	4.47	3.83
h=10, l=-1		
0	10.35	-10.25
1	2.50	-3.35
h=10, l=-2		
0	7.98	-8.85
1	11.58	-10.91
2	3.79	5.53
h=10, l=-3		
0	10.63	-7.05
2	3.77	5.01
3	2.64	-3.69
h=10, l=-4		
0	13.12	5.62
1	6.78	-3.91
2	8.66	-5.26
3	4.27	-0.22
h=10, l=-5		
0	15.31	12.23
1	13.33	11.77
2	6.21	-3.52
3	4.78	-6.43
4	3.52	-3.32
h=10, l=-6		
0	9.36	7.32
1	6.74	-4.37
3	11.04	6.32
h=-10, l=0		
1	3.25	2.82
3	10.48	-9.31
h=-10, l=1		
1	4.09	-0.13
2	4.27	6.65
3	7.33	3.89
h=-10, l=2		
1	13.93	13.66
2	12.26	9.19
3	6.05	-8.15
h=-10, l=3		
1	4.14	2.05
2	13.03	9.28
3	7.93	3.27
4	6.29	-3.37
5	9.54	-6.53
h=-10, l=4		
1	15.93	9.50
3	12.38	-7.44
4	10.91	-6.30
5	3.79	2.14
h=-10, l=5		
1	15.30	-12.29
2	14.06	-12.22
3	10.64	11.51
4	3.69	6.06
5	5.81	-10.14
h=-10, l=6		
1	5.32	2.82
2	14.26	-10.87
4	9.36	8.91
h=-10, l=-1		
3	8.62	-11.36
4	6.69	-7.82
h=11, l=-2		
0	10.33	-15.24
h=11, l=-3		
0	11.69	6.68
1	3.99	0.68
h=11, l=-4		
0	11.73	-10.66
1	6.05	2.50
2	14.48	16.59
h=11, l=-5		
0	10.46	-8.42
1	4.64	-1.49
2	8.43	8.16
h=11, l=-6		
0	7.72	-5.41
1	4.25	4.11
2	5.23	6.85
h=-11, l=2		
1	7.73	7.17
2	21.45	23.65
4	14.07	-17.59
h=-11, l=3		
1	10.07	8.58
2	3.22	1.13
3	12.16	-10.32
4	5.15	-6.10
h=-11, l=5		
1	5.06	6.18
2	6.63	7.75
3	3.37	-7.22
4	3.21	-4.68
h=-11, l=6		
1	4.40	-3.93
2	5.11	3.77
3	5.51	4.03
h=-12, l=5		
1	3.04	-3.46

TABLE 6. THE DEVIATIONS FROM THE MEAN PLANE (in Å)

Atom	Deviation	Atom	Deviation
Cl_3	0.044	C_2	0.011
Cl_4	−0.021	C_3	−0.021
Cl_5	0.008	C_4	−0.002
Cl_6	0.040	C_5	−0.009
C_1	−0.024	C_6	−0.024

$Z = z\sin\alpha\sin\beta^*$. The deviations of the atoms from this best plane are given in Table 6. Since the bond angles, Cl_4-C_5-C_2 (or Cl_5-C_6-C_3) and C_5-C_2-C_3 (or C_6-C_3-C_2), are both considerably larger than 120°, the two adjacent chlorine atoms, Cl_4 and Cl_5, maintain a distance of 3.28 Å. This value turns out to be extremely small considering the van der Waals radius of chlorine atoms, 1.80 Å.[6] It is an interesting fact that the planar configuration is achieved in spite of such very close contact.

The mean length of the two double bonds, C_2-C_5 and C_3-C_6, is 1.35 Å, while the C_2-C_3 distance is

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6) L. Pauling, "The Nature of the Chemical Bond," Cornell University Press, Ithaca (1940).

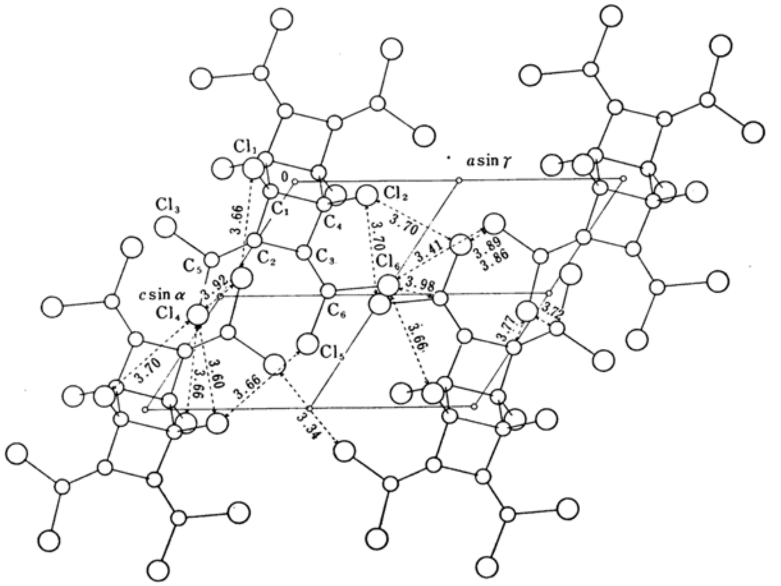

Fig. 5. The crystal structure projected along the *b* axis.

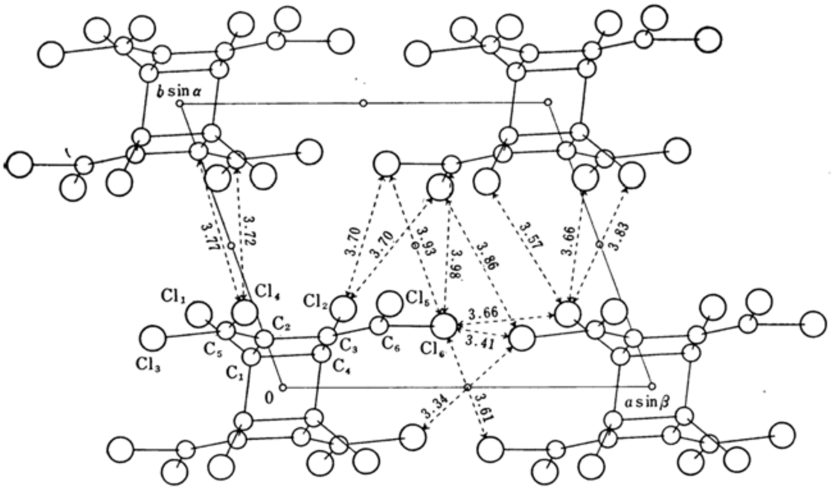

Fig. 6. The crystal structure projected along the *c* axis.

1.47 Å. These values are in good agreement with those in 1, 3-butadiene, 1.35 and 1.46 Å[7] respectively. The average distance of the four C-Cl bonds of the chloroethylene-type is 1.70 Å; this value is also in accord with that in 1, 1-dichloroethylene, 1.69 Å.[8]

Insofar as the molecule has a center of symmetry, the central four-membered ring should be exactly planar. The plane through this ring is described by the equation:

$$0.3095X + 0.5692Y - 0.7616Z = 0$$

The central ring makes an angle of about 115° with the plane of the conjugated system.

The C_1-C_4 and C_1-$C_{4'}$ distances are 1.60 and 1.54 Å respectively, the former being somewhat larger than the normal single-bond distance. The corresponding values are found to be 1.585 and 1.555 Å in tetraphenylcyclobutane[9] and 1.60 and 1.58 Å in octachlorocyclobutane[10]. Accordingly, the values found in the present experiment are reasonable considering their standard deviations. The mean length of the two C-Cl bonds of the chloromethane-type is 1.74 Å; this value is in good accordance with that in octachlorocyclobutane,[10] 1.74 Å.

Since half of the atoms in the molecule are

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[7] V. Schomaker and L. Pauling, *J. Am. Chem. Soc.*, **61**, 1769 (1939).

[8] L. O. Brockway, J. Y. Beach and L. Pauling, *J. Am. Chem. Soc.*, **57**, 2693 (1935).

[9] J. D. Dunitz, *Acta Cryst.*, **2**, 1 (1949).

[10] T. B. Owen and J. L. Hoard, *ibid.*, **4**, 172 (1951).

chlorine, some of the chlorine atoms are expected to approach one another much more closely than twice the van der Waals radius. The intramolecular Cl-Cl distances smaller than 3.60 Å are listed in Table 7.

TABLE 7. THE INTRAMOLECULAR Cl-Cl DISTANCES SHORTER THAN 3.60 Å (in Å)

$Cl_3 \cdots Cl_4$	2.84
$Cl_5 \cdots Cl_6$	2.85
$Cl_4 \cdots Cl_5$	3.28
$Cl_1 \cdots Cl_3$	3.32
$Cl_2 \cdots Cl_6$	3.32
$Cl_1 \cdots Cl_2$	3.36

The arrangement of the molecules in the crystal is shown in Figs. 5 and 6. The intermolecular distances smaller than 4.0 Å are also given in these figures. Since the carbon atoms are surrounded by the chlorine atoms in the same molecule, no intermolecular contacts are found between the carbon atoms, and only a few between the carbon and chlorine atoms. Two intermolecular Cl-Cl distances smaller than 3.6 Å are found in the crystal—3.41 and 3.34 Å. Both of these are distances between the chlorine atoms attached to the ethylenic group. A value of 3.39 Å has lately been reported as an intermolecular Cl-Cl distance of the same kind.[11] Such a close approach may be related to the fact that a portion of the electrons in the outermost shell of the chlorine atom is displaced toward the ethylenic group; hence, the outermost shell is no longer complete.

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[11] Y. Nishi, Y. Sasada, T. Ashida and M. Kakudo, This Bulletin, **39**, 818 (1966).