

(X) and a line perpendicular thereto (Y) will remain the principal directions. This result is new, and if we measure θ and $q_{11}-q_{12}$ experimentally, we can evaluate q_{61} for a chosen crystal.

If to the same prism, a tangential stress XY is applied, we have again $B_{11}x^2+B_{22}y^2+2B_{12}xy=1$ as the equation of the elliptic section in the XY plane, where $B_{11}-B_{11}^0=B_{11}^0-B_{22}=2q_{61}\cdot XY$ and $B_{12}=- (q_{11}-q_{12})XY$. The existence of B_{12} shows that birefringence is caused by the XY plane being sheared, a result which persists even when the coefficients of x and y remain unchanged. In this case, q_{61} causes a different kind of birefringence in that n_x-n_y , which is zero before the application of stress, becomes equal to $4q_{61}\cdot XY\cdot \frac{1}{2}n_0^3$ as a result of the stress XY . This again is a new result and has been visualized by Fumi (1952) in his recent note. n_x-n_y would be zero even in the stressed crystal if $q_{61}=0$.

If, from the class of crystals C_4 , S_4 and C_{4h} , we choose one and cut a prism of the same type as above (axis of crystallographic symmetry is Z , and X and Y are in the plane perpendicular thereto) and subject it to a tangential stress ZX , according to the scheme of q 's given in this paper, we have amongst other things, $B_{23}=-q_{45}\cdot ZX$, indicating a tilt of the principal

axes in the YZ plane. This is capable of being experimentally observed. On the other hand, the same amount of stress applied as ZY will cause an equal tilt of the principal axes in the XZ plane but in the *opposite sense*.

In an actual experiment, choice of crystals belonging to the classes C_3 , C_6 , C_4 and S_4 will cause complications as they are optically active, making the observations more difficult, and may therefore be avoided.

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The Crystal Structure of Naphthalene Tetrachloride, $C_{10}H_8Cl_4$

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The values of the diamagnetic anisotropy in the monoclinic crystal of naphthalene tetrachloride were found to be

$$\begin{aligned} \chi_1-\chi_2 &= 56\cdot2 \times 10^{-6} \text{ c.g.s.e.m.u.} & \theta &= +23\cdot2^\circ (\chi_2 \wedge [100]) \\ \chi_1-\chi_3 &= 2\cdot6 \times 10^{-6} & \psi &= -0\cdot5^\circ (\chi_1 \wedge [001]) \\ \chi_3-\chi_2 &= 53\cdot5 \times 10^{-6} & & (\chi_3 \text{ along } [010]) \end{aligned}$$

These results show that the (100) plane is the plane of the molecule. The dimensions of the unit cell, which contains four molecules, each having a diad axis of symmetry, are $a=7\cdot92_5 \pm 0\cdot03$, $b=10\cdot25 \pm 0\cdot04$, $c=14\cdot25 \pm 0\cdot05$ Å, $\beta=112\cdot6 \pm 0\cdot5$. The space group is $I2/c$ and Patterson projections confirm the molecular orientation deduced from the magnetic measurements. The C-Cl bonds have the configuration 1ϵ , 2κ , 3κ , 4ϵ (deduced from electron-density projections on (100), (010) and (001)), and interatomic Cl...Cl distances agree closely with those derived from other chlorinated cyclohexane compounds. The aromatic ring has the normal C-C distances of 1.39-1.40 Å and is undistorted. Eight of the carbon atoms appear to be closely co-planar.

Introduction

The results of previous crystallographic investigations on naphthalene tetrachloride crystals are summarised by Groth (1906-19, vol. 5, p. 368). Sir W. H. Bragg

(1927) studied this substance by the X-ray method and found its lattice to be monoclinic body-centred, with four molecules per unit cell. The cell dimensions he reported, $a=7\cdot88$, $b=10\cdot30$, $c=14\cdot20$ Å, $\beta=112^\circ 40'$, agree with the data recorded by Groth except in the doubling of the c -axis length. Bragg adopted the space group C_2^4 and suggested that the molecules

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lie along the *c* axis in the same way as those of naphthalene and anthracene. Robertson (1928) confirmed Bragg's results.

From his magnetic measurements on the crystal, Banerjee (1938) concluded that the molecular planes make angles of $\pm 76^\circ$ with the (010) plane.

Preparation of the crystals

The naphthalene tetrachloride used in the present investigation was prepared by British Drug Houses Ltd, London. Small crystals suitable for X-ray work were obtained by slow evaporation of a concentrated solution in chloroform. Evaporation of a dilute solution gave prismatic crystals large enough for goniometric and magnetic measurements. These have the habit described by Groth.

Goniometric measurements

Measurement of the interfacial angles, using a Fuess goniometer, gave the values listed in Groth. X-ray measurements confirmed the doubling of the *c* axis reported by Bragg (1927) and Robertson (1928).

Magnetic measurements

The method used for the measurement of the magnetic anisotropy was first described by Krishnan & Banerjee (1935). The quartz fibre was calibrated using a crystal of 1·3·5-triphenyl-benzene whose diamagnetic susceptibilities in the directions of the axes of its orthorhombic unit cell are known (Lonsdale, 1937). The following results were obtained for C₁₀H₈Cl₄:

$$\begin{aligned}\chi_1 - \chi_2 &= 56.2 \times 10^{-6} \text{ c.g.s.e.m.u. } \theta = +23.2^\circ \\ \chi_1 - \chi_3 &= 2.6 \times 10^{-6} \quad \psi = -0.5^\circ \\ \chi_3 - \chi_2 &= 53.6 \times 10^{-6}\end{aligned}$$

where χ_3 is the value of the diamagnetic susceptibility along the *b* axis and χ_1 and χ_2 are the values along the two principal axes, lying in the (010) plane, perpendicular to each other. θ is the angle between χ_2 and the *a* axis (positive in the obtuse β angle) and ψ is that between χ_1 and the *c* axis. The values of θ , ψ and β are related by the equation $\theta + \frac{1}{2}\pi + \psi = \beta$. The possible error in these results is estimated at about $\pm 2\%$, taking the mean of several separate determinations.

Deductions from the magnetic measurements

These results show that the crystal is magnetically almost uniaxial. The anisotropy found is that of a single benzene ring, and the molecule probably consists of a benzene ring and a cyclohexane ring which, with the four chlorine atoms, has no, or very small, effect on the values of the magnetic anisotropy. This was also expected from the coincidence of the average diamagnetic susceptibility observed by Banerjee (1938)

and the Pascal value calculated on the basis of this type of molecule. This means that χ_1 and χ_3 are in the plane of the benzene ring and χ_2 is perpendicular to it. The *b* axis is therefore in the plane of the molecule and, as the molecule itself may have an axis of symmetry, there is a great probability that the *b* axis may coincide with the long axis of the molecule. This is contrary to the structure suggested in previous work. The *c* axis is very near to χ_1 so that the (100) plane is the plane of the molecule, within the experimental error.

X-ray measurements: unit cell and space group

The value of the angle β was calculated from the goniometric measurements and from a zero-layer Weissenberg photograph taken with *b* as rotation axis. The lengths of the three axes of the unit cell were determined, using a calibrated cylindrical camera, from rotation and oscillation photographs round the axes:

$$\begin{aligned}a &= 7.925 \pm 0.03, \quad b = 10.25 \pm 0.04, \quad c = 14.25 \pm 0.05 \text{ \AA} \\ \beta &= 112.6 \pm 0.5^\circ.\end{aligned}$$

Systematic absences are *hkl* when (*h*+*k*+*l*) is odd, and *h0l* when *h* is odd or *l* is odd. Therefore the space group is either *Ic* (monoclinic domatic) or *I2/c* (monoclinic prismatic). No polarity was detected in a test for piezo-electricity. Also, all the Patterson projections along the three principal axes could be best interpreted on the assumption that the space group of the crystal is *I2/c*, and that the molecule has a diad axis of symmetry along [010]. The general equivalent positions are

$$\begin{aligned}x, y, z; \quad x, \bar{y}, \frac{1}{2}+z; \quad \frac{1}{2}+x, \frac{1}{2}+y, \frac{1}{2}+z; \quad \frac{1}{2}+x, \frac{1}{2}-y, z; \\ \bar{x}, \bar{y}, \bar{z}; \quad \bar{x}, y, \frac{1}{2}-z; \quad \frac{1}{2}-x, \frac{1}{2}-y, \frac{1}{2}-z; \quad \frac{1}{2}-x, \frac{1}{2}+y, \bar{z}.\end{aligned}$$

The special positions corresponding to point-symmetry 2 are

$$0, y, \frac{1}{4}; \quad 0, \bar{y}, \frac{3}{4}; \quad \frac{1}{2}, \frac{1}{2}+y, \frac{3}{4}; \quad \frac{1}{2}, \frac{1}{2}-y, \frac{1}{4}.$$

The density, as measured by the flotation of crystals in an aqueous solution of zinc chloride, is 1.670 g.cm.⁻³, hence there are four (calculated 3.98) molecules of C₁₀H₈Cl₄ per unit cell. Volume of the unit cell: 1068 Å³. *M* = 270.0. Absorption coefficient for X-rays ($\lambda = 1.542 \text{ \AA}$): $\mu = 94.8 \text{ cm.}^{-1}$. Total number of electrons per unit cell: *F*(000) = 544.

Observed structure factors

15° oscillation photographs with 10° overlap were taken around the *a* and *b* axes. The actual shape of the crystal made it difficult to take *c*-axis oscillation photographs on a crystal small enough for intensity measurements. The dimensions of the crystal used were 0.62, 0.19 and 0.22 mm. along the *b* axis, the *a* axis, and perpendicular to the (001) face respectively. The two sets of oscillation photographs taken gave

all the reflexions needed for projections on the (100) and the (010) planes, and these gave sufficient information about the structure. The $hk0$ reflexions recorded on the different layer lines of these two sets of photographs were used to give the (001) projection, which provided confirmation of the other two projections. The integrated intensities of the diffraction spots were estimated by visual comparison with a graduated scale of intensities prepared from the $20\bar{2}$ reflexion of the same crystal.

Absorption corrections were calculated for all the $h0l$ reflexions by the graphical method of Albrecht (1939). The calculations were laborious and it was found that the absorption corrections for most of the planes are nearly equal and that the improvements that these factors make in the observed structure factors are therefore not worth the time and effort involved. For that reason it was decided not to calculate these corrections for other crystal planes.

The values of the structure factor $|F|$ were derived from the intensity measurements by the usual formula for a mosaic crystal.

Patterson projections

In the Patterson projection parallel to the b axis there is a series of overlapping peaks lying along the c axis from which it can readily be seen that the (100) plane is the plane of the molecule. This can also be seen from the (001) Patterson projection, with another series of overlapping peaks along the b axis. This result is a confirmation of the conclusion obtained from the magnetic measurements.

The (010) Patterson projection also shows some high peaks, which must denote Cl-Cl or Cl-C vectors, or both, lying on the traces of the (400) planes. The same thing can be seen from the (001) Patterson projection, in which, besides the peaks along the b axis, there is a very high peak at the point $x = \frac{1}{2}, y = \frac{1}{2}$. From these observations it is reasonable to say that two of the four chlorine atoms in the molecule are very near to the plane of the molecule while the other two are situated on the two different sides of that plane very near to the (400) and $(\bar{4}00)$ planes. The four C-Cl bonds have either the configuration $1\varepsilon, 2\kappa, 3\kappa, 4\varepsilon$ or $1\kappa, 2\varepsilon, 3\varepsilon, 4\kappa$ where, in the usual notation, ε means normal to the mean plane of the molecule as a whole.

Solution of the (100) projection

The z co-ordinates of the atoms were found from the (100) Patterson projection, using an approximate molecular model based on the chemical formula. Examination of the intensities of the $0k0$ reflexions gave two different possible molecular positions, along the [010] axis, but comparison of the calculated and observed structure factors for $0kl$ reflexions, together with the Fourier projections, eliminated one of these.

The final Fourier synthesis was evaluated at inter-

vals of $b/60 = 0.171 \text{ \AA}$ and $c/120 = 0.119 \text{ \AA}$, and the resulting electron-density map is shown in Fig. 1 (Fig. 2 gives the arrangement of the molecules in this projection). The value of the reliability factor, $R = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}$, using the co-ordinate values given in Table 1, is 0.22, assuming $|F_o|$ equal to zero

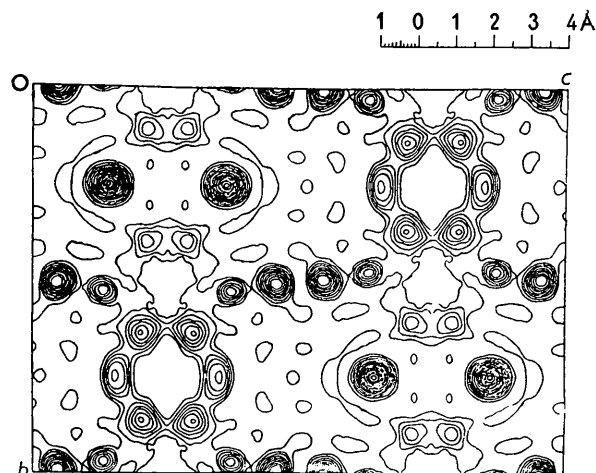


Fig. 1. Final electron-density map on (100). The contours are drawn at intervals of 1.5 e. \AA^{-2} for carbon atoms and 3 e. \AA^{-2} for chlorine atoms and the diffraction peaks round them. The lowest contour line represents 3 e. \AA^{-2} .

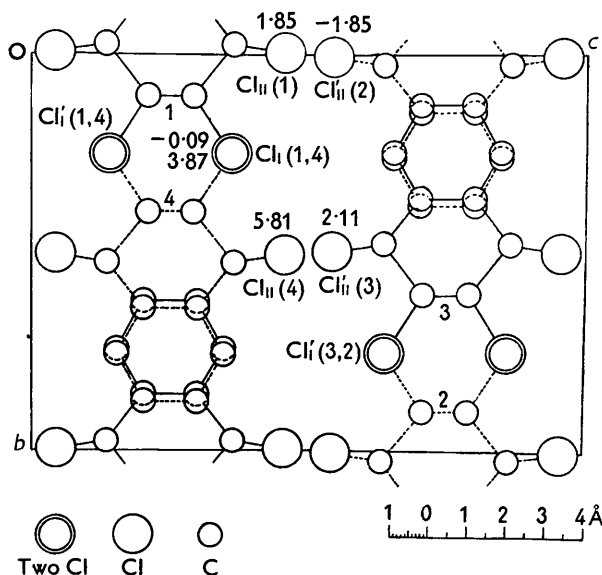


Fig. 2. Arrangement of molecules in the (100) projection. Approximate x co-ordinates are given for some atoms.

for all reflexions too weak to be recorded on the photographs. If these weak planes are excluded from the calculations, the value of R is 0.19.

There is a lack of resolution in the electron-density map due to the overlapping of the atoms in the benzene rings of two different molecules. It was not difficult, however, to find by trial the exact positions

of the centres of these atoms from the electron-density map because of the similarity of the atoms which overlapped.

Solution of the (010) projection

Successive *b*-axis Fourier syntheses were carried out and the final Fourier synthesis was evaluated at intervals of $c/120 = 0.119$ Å and $a/60 = 0.132$ Å; the final electron-density map gives the arrangement of the molecules shown in Fig. 3. The reliability factor *R* is 0.17.

The value of *R* is less for this projection than for the

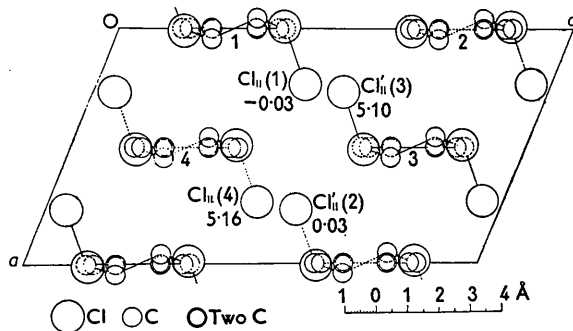


Fig. 3. Arrangement of molecules in the (010) projection. Approximate *y* co-ordinates are given for some atoms.

(100) projection for two reasons. The first is that the absorption correction factor had been calculated for all the (*h*0*l*) planes only. The second is that most of the (*h*0*l*) planes have high structure factors and so the number of the reflexions too weak to be recorded was much less in the {*h*0*l*} zone than in the {0*kl*} zone.

The (001) projection

The *c*-axis Fourier synthesis was evaluated at intervals of $b/120 = 0.085$ Å and $a/60 = 0.32$ Å. The resulting electron-density map indicated the correctness of the structure although it was incomplete owing to the fact that only a small number of reflexions were included in the evaluation of the Fourier synthesis (Fig. 4 shows the arrangement of the molecules). The value of the reliability factor *R* for this projection is 0.20.

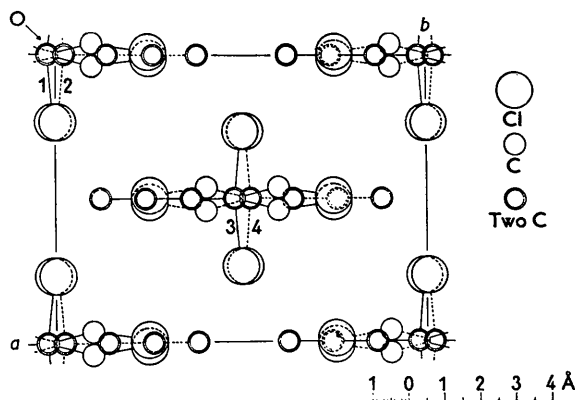


Fig. 4. Arrangement of molecules in the (001) projection.

Study of diffraction effects

Diffraction effects are clearly seen, represented by peaks and troughs that encircle the main peaks of the chlorine atoms in the electron-density map on (100) (Fig. 1). In order to find the exact positions of the centres of the carbon atoms and the exact heights of their peaks a Fourier synthesis was carried out using the calculated values of $F(0kl)$ for the chlorine atoms alone for the reflexions included in the original summation (Robertson & Woodward, 1940). All the diffraction peaks found in the original summation were also found in the new one, having nearly the same

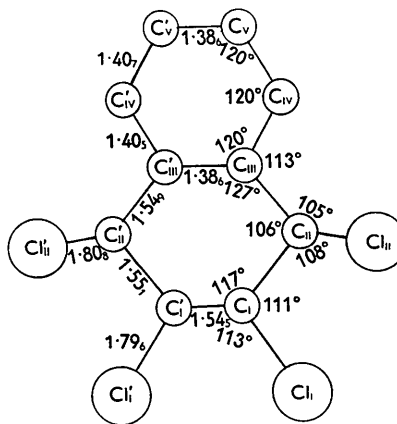


Fig. 5. Bond lengths and valency angles shown on a projection of the molecule on the plane of the benzene ring.

Table 1. Atomic co-ordinates

(Origin at centre of symmetry)

Atom	$2\pi x/a$ (°)	<i>x</i> (Å)	<i>x'</i> (Å)	$2\pi y/b$ (°)	<i>y</i> (Å)	$2\pi z/c$ (°)	<i>z</i> (Å)	<i>z'</i> (Å)
Cl _I	-4	-0.088	-0.081	90	2.563	$\pi-51$	5.106	5.140
Cl _{II}	84	1.849	1.706	-1.2	-0.034	$\pi-16.5$	6.471	5.760
Cl _I	-15.5	-0.341	-0.315	35.5	1.011	$\pi-75.5$	4.136	4.267
C _{II}	0	0	0	-7	-0.199	$\pi-49$	5.185	5.185
C _{III}	0	0	0	-50.5	-1.438	$\pi-72.5$	4.255	4.255
C _{VI}	0	0	0	-93.2	-2.654	$\pi-54.75$	4.957	4.957
C _V	0	0	0	-136	-3.873	$\pi-72.5$	4.255	4.255

Table 2. Comparison of observed and calculated structure factors

hkl	$ F_o $	F_c	hkl	$ F_o $	F_c	hkl	$ F_o $	F_c
000	—	+544	011	30	-24	086	17	+27
002	41	-41	013	44	-60	088	—	-3
004	64	-65	015	46	+63	0,8,10	57	-53
006	65	+71	017	43	+23	0,8,12	41	-36
008	25	-14	019	64	-55	091	—	-6
0,0,10	83	-79	0,1,11	—	+16	093	—	-17
0,0,12	70	-69	0,1,13	19	+26	095	42	+36
0,0,14	24	+25	020	17	+5	097	—	+12
2,0,14	46	+45	022	85	+113	099	15	-28
2,0,12	16	+11	024	95	+117	0,9,11	28	+12
2,0,10	24	+8	026	58	-64	0,10,0	—	-2
208	90	+64	028	81	-70	0,10,2	34	+37
206	100	+82	0,2,10	19	0	0,10,4	41	+48
204	88	-82	0,2,12	55	-33	0,10,6	38	-27
202	194	-176	0,2,14	49	-49	0,10,8	34	-36
200	169	+154	031	67	+70	0,11,1	45	+27
20 $\bar{2}$	190	-190	033	52	+42	0,11,3	29	+20
204	144	-170	035	57	-59	0,11,5	28	-22
20 $\bar{6}$	88	+85	037	—	0	0,11,7	17	+3
208	57	+61	039	50	+42	0,11,9	26	+24
2,0, $\bar{10}$	36	+21	0,3,11	—	-7	0,12,0	42	+53
2,0, $\bar{12}$	—	+2	0,3,13	40	-30	0,12,2	41	+17
2,0, $\bar{14}$	79	+77	040	131	+149	110	87	+74
4,0,12	33	-24	042	95	+94	310	13	+8
4,0,10	56	-59	044	92	-91	510	44	+40
408	39	-17	046	39	+38	710	18	-22
406	16	+18	048	—	+32	910	10	+20
404	30	-41	0,4,10	121	-111	220	193	-181
402	39	-39	0,4,12	34	-33	420	13	-4
400	187	+205	051	58	-62	620	69	-78
40 $\bar{2}$	42	+36	053	25	+3	330	22	-11
40 $\bar{4}$	56	-47	055	39	+41	530	22	+34
40 $\bar{6}$	70	+85	057	—	0	730	20	-19
40 $\bar{8}$	22	+11	059	—	-20	240	12	-14
4,0, $\bar{10}$	45	-61	0,5,11	—	0	440	103	+100
4,0, $\bar{12}$	64	-85	0,5,13	22	+25	640	—	+4
608	36	+34	060	23	-10	840	19	+41
606	48	+52	062	61	+74	350	14	-14
604	10	-18	064	59	+72	550	28	+29
602	60	-56	066	45	-42	260	105	-121
600	32	+39	068	59	-55	170	37	+19
60 $\bar{2}$	60	-54	0,6,10	—	-2	280	32	+30
60 $\bar{4}$	91	-113	0,6,12	35	-21	190	—	+3
60 $\bar{6}$	34	+15	0,6,14	39	-41	2,10,0	60	-69
60 $\bar{8}$	18	+35	071	56	+44	1,11,0	22	+8
6,0, $\bar{10}$	17	+8	073	37	+30			
6,0, $\bar{12}$	—	0	075	33	-35			
6,0, $\bar{14}$	41	+66	077	—	-3			
804	13	-24	079	42	+40			
802	10	-20	0,7,11	—	-8			
800	45	+57	0,7,13	29	-25			
80 $\bar{2}$	23	+38	080	92	+130			
80 $\bar{4}$	—	-11	082	—	+11			
80 $\bar{6}$	29	+37	084	34	-27			
80 $\bar{8}$	34	+32						
8,0, $\bar{10}$	27	-28						

heights. The exact positions of the centres of the peaks representing the carbon atoms were then calculated, with an allowance for the diffraction effects.

No reason was found, from the new summation, for the difference in the heights of the two carbon peaks representing C_I and C_{II} which are 9 and 10.5 e.Å⁻², respectively. Two recent papers on naphthalene

(Abrahams, Robertson & White, 1949) and anthracene (Sinclair, Robertson & Mathieson, 1950) have reported a similar observation and have suggested that it is due to thermal agitation. If the molecules were imagined to be rigid bodies vibrating about their centres, the effect of this vibration would be most marked on the outlying atoms and would consequently

give rise to this slight blurring effect. This may also explain the fact that the height of the peak representing Cl_{II} is more than half the height of the peak representing two Cl_I atoms (Fig. 1).

Atomic co-ordinates

In any case of ambiguity due to poor resolution, the co-ordinates that gave best agreement between calculated and observed structure factors were chosen. The results are given in Table 1, where the co-ordinates x, y, z are expressed (a) in angular measure and (b) in Ångström units, all referred to the monoclinic axial directions. They are also expressed (c) in orthogonal co-ordinates x', y, z' referred to the a', b and c axes, where a' is an axis chosen perpendicular to the b and c crystal axes.

These orthogonal co-ordinates were used in calculating the interatomic distances and valency angles, and are derived from the monoclinic crystal co-ordinates by the relations

$$x' = x \sin \beta, \quad z' = z + x \cos \beta.$$

The co-ordinates are given in Table 1 only for the atoms in one half of the initial molecule situated between $z = \frac{1}{4}$ and $z = \frac{1}{2}$. If the co-ordinates of any atom in that half of the molecule are (x, y, z) , then those of the identical atom in the other half derived from it by the operation of the twofold rotation axis are $(-x, y, \frac{1}{2} - z)$.

The interatomic distances and valency angles are shown in Fig. 5. The (C-Cl)_{I, I'} bonds are of the α -, and the (C-Cl)_{II, II'} bonds are of the ϵ -type.

Table 2 gives a comparison between calculated and observed $|F|$ values for the three axial zones.

Discussion of the structure

The coincidence of the molecular plane as found from both the magnetic and X-ray measurements is striking. From the electron-density projections along the three axes it was found that the six carbon atoms constituting the benzene ring, together with the next two carbon atoms in the cyclohexane ring, C_{II} and C'_{II}, are coplanar to within experimental error.

The four chlorine atoms in the molecule were found to have the configuration $1\epsilon, 2\alpha, 3\alpha, 4\epsilon$.

The average length of the six C-C bonds in the benzene ring, 1.40 Å, is very close to the standard value of 1.39 Å for the aromatic bond length. The C_{III}-C'_{III} bond common to the benzene and cyclohexane rings has the length 1.39 Å, which implies that the attachment of the benzene ring to the rest of the naphthalene tetrachloride molecule has not changed

the character of its bonds. This result confirms the similar conclusion drawn from the values of the molecular magnetic anisotropy, which are simply those of one benzene ring.

The average length of the C-C bonds in the cyclohexane ring, excluding that of the common C_{III}-C'_{III} bond, is 1.55 Å. This may be compared with 1.54 Å, the standard value for the length of the aliphatic C-C bond.

The average length of the C-Cl bonds is 1.80 Å, in good agreement with previously recorded values (Clews & Cochran, 1948; Hassel & Wang Lund, 1949; Vloten, Kruissink, Stijk & Bijvoet, 1950; Pasternak, 1951).

The valency angles in the benzene ring are all 120°. The two valency angles in the cyclohexane ring adjacent to the benzene ring, that is C_{II}-C_{III}-C'_{III} and C'_{II}-C'_{III}-C_{III}, are both 127°, which is unusually large.

The intermolecular distances are all equal to, or higher than, the usual van der Waals type. The shortest intermolecular Cl...Cl distance is 3.85 Å, the shortest Cl...C distance is 3.72 Å, while the shortest C...C distance is 3.89 Å (Lasheen, 1952).

The short Cl...Cl distances between atoms in the same molecule, found to be 3.21 Å for Cl_I...Cl_{II} and Cl'_I...Cl'_{II} and 3.16 Å for Cl_I...Cl'_I, are in good agreement with those (3.18, 3.19, 3.20 and 3.22 Å) recorded for the crystal structure of Gammexane (Vloten, Kruissink, Stijk & Bijvoet, 1950).

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