size. Measurements of the low-angle $11\bar{2}0$ line at 39°, which was resolved graphically into its α_1, α_2 components, also suggested a variation of a, a difference of $0{\cdot}0007 \pm 0{\cdot}0002$ A. being obtained between samples A_1 and A_3. At first sight this variation is a genuine effect, since if each sample were composed entirely of regular blocks of thickness t the $hki0$ reflexions would be pure three-dimensional reflexions and not subject to change of shape and displacement to larger θ values, as described for turbostratic material by Warren (1941) and discussed by Taylor (1942). The conclusion of the latter paper is that there is no genuine change of the a dimension for carbon layers having widths greater than a few tens of Ångström units, but the accuracy of the measurements considered is not sufficient for this paper alone to discount the genuineness of the relatively small variation shown in our curve (2). However, the theoretical work of Bradburn, Coulson & Rushbrooke (1948) does suggest that variations of this magnitude will not be found amongst particles as large as those under consideration. Measurements were made therefore of the position of the $12\bar{3}1$ line, which is a well resolved line for all but the first sample, A_1. It is necessary to assume a value of c in order to determine a from this line, but the result is very insensitive to the precise value chosen, since in the formula for calculating the spacing of this line the term involving c is less than 2 % of the a term; an error of 0·01 A. would be necessary in c in order to give an error of 0·00005 A. in a. The values obtained are shown in curve (3) of the figure and are constant to a few hundred-thousandths of an Ångström unit. With A_3, the sample with the largest particles, the mean value of a from $12\bar{3}0$ is still slightly below the value obtained from $12\bar{3}1$, but the difference here is within the estimated experimental error. Unfortunately, with A_1, the sample showing the smallest layer planes, the $12\bar{3}1$ reflexion is too diffuse for accurate measurement, on account of the simultaneous reduction of t, so that it is not possible to investigate by this method over what further range a remains constant.

From curve (3) it is concluded that the apparent displacements of the $hki0$ maxima, such as $11\bar{2}0$ and $12\bar{3}0$, are due to the increasing effect of the superposition of a two-dimensional maximum, from a proportion of turbostratic material, on what is mainly a three-dimensional reflexion. The resultant error in a would depend not only on the values of the layer dimensions and $1/\sin\theta$ (Taylor, 1942) but also on the proportions and the relative magnitudes of the structure factor for two and three-dimensional reflexions for the particular $hki0$ line. It is hoped that evidence may be obtained from intensity measurements to decide whether the actual magnitude of the displacements found can be accounted for.

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The Crystal Structure of 'Gammexane', γ-$C_6H_6Cl_6$

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The crystal structure of the γ-isomer of benzene hexachloride, the insecticide 'Gammexane', has been determined by X-ray analysis (Weissenberg diagrams) in the usual way by trial and error, starting from Patterson data and supported by repeated Fourier syntheses.

Introduction

Gammexane (m.p. 112° C.), γ-$C_6H_6Cl_6$, is monoclinic prismatic with

$$a = 8{\cdot}52,\quad b = 10{\cdot}27,\quad c = 13{\cdot}94\text{ A.},\quad \beta = 121°\,16'.$$

Cell volume 1042·6 A.^{3}. Four molecules per unit cell. Measured density = 1·85 g.cm.$^{-3}$; calculated density = 1·852 g.cm.$^{-3}$. Absent spectra: $(h0l)$ when l is odd; $(0k0)$ when k is odd. Space group $P2_1/c$. Equivalent points: (x,y,z); $(\bar{x},\bar{y},\bar{z})$; $(x,\bar{y}+\frac{1}{2},z+\frac{1}{2})$; $(\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2})$. Most crystals have well-developed diamond-shaped $(\bar{1}02)$ planes with diagonals [201] and [010]; also the planes

(110), (1$\bar{1}$0), ($\bar{1}$10), ($\bar{1}\bar{1}$0), (100), ($\bar{1}$00), (010) and (0$\bar{1}$0) often appear (crystallization from ether). All X-ray diagrams were made with crystals ground to the form of cylinders about the [010] and [201] axes and of diameter 0·080 and 0·086 cm. The unit-cell dimensions were found from rotation diagrams.

Weissenberg photographs were made of the (*h*0*l*)–(*h*5*l*) layer lines (Cu $K\alpha$ radiation), the (*h*0*l*), (*h*6*l*)–(*h*9*l*) layers (Mo radiation) and the first four layers of the [201] diagram (Cu $K\alpha$ radiation). Using a slightly diverging beam of copper radiation we obtained sufficiently homogeneous and congruent spots to enable the intensities to be determined with the photometer by measuring the spot-centres only. The measured values were controlled visually. The accuracy was about 10 %. The molybdenum reflexions were visually estimated.

These values were corrected for absorption, Lorentz and polarization factors and (in the case of the non-equatorial reflexions) for the inclination factor.

Structure analysis

The direct Fourier analysis with the aid of isomorphous compounds fails in this case because no such compounds exist; thus we depend on the method of trial and error. This method is rather difficult here because the form of the molecule is unknown and because all six substitutes are of equal scattering power. First we calculated a Patterson–Harker section at $y=\frac{1}{2}$. This diagram gives the co-ordinates $2x_{\mathrm{Cl}}$, $2z_{\mathrm{Cl}}$, so the implication diagram is constructed by halving the Harker co-ordinates. As it was unknown which of the maxima of the implication diagram belonged to the Fourier projection, we restricted the possibilities with the aid of several models of the molecule. The remaining possibilities were tested by calculation of the intensities (*h*0*l*). In a few cases a rather good correspondence could be obtained and repeated Fourier syntheses gave 24 clearly resolved maxima. It seemed plausible that these maxima should be chlorine maxima. Thus it was surprising we did not succeed in fitting the carbon atoms in this way. Finally, we approached the matter in another way, and after the structure had been determined we ascertained that in this case most of the maxima of the Harker diagram are non-Harker background maxima.

Two particular facts are seen in the [010] Patterson projection:

(1) Besides the centres of symmetry (0, 0), (0, $\frac{1}{4}$), (0, $\frac{1}{2}$), (0, $\frac{3}{4}$), ($\frac{1}{2}$, 0), ($\frac{1}{2}$, $\frac{1}{4}$), ($\frac{1}{2}$, $\frac{1}{2}$), ($\frac{1}{2}$, $\frac{3}{4}$), there appear to be present eight pseudo-centres of symmetry ($\frac{1}{4}$, $\frac{1}{8}$), ($\frac{1}{4}$, $\frac{3}{8}$), ($\frac{1}{4}$, $\frac{5}{8}$), ($\frac{1}{4}$, $\frac{7}{8}$), ($\frac{3}{4}$, $\frac{1}{8}$), ($\frac{3}{4}$, $\frac{3}{8}$), ($\frac{3}{4}$, $\frac{5}{8}$), ($\frac{3}{4}$, $\frac{7}{8}$). Thus our Patterson projection between $z=0$ and $z=\frac{1}{2}$ has the symmetry of the plane group $C_2{}^IB$ in the nomenclature of Patterson (1935). The whole set of symmetry centres connects eight (pseudo) equivalent maxima of the Patterson map.

(2) Besides the maxima at special points (0, 0), (0, $\frac{1}{2}$), ($\frac{1}{2}$, $\frac{1}{4}$), and some small ones, there are only 16 high peaks. These 16 peaks form two of the above-mentioned 8-point sets with co-ordinates ($\frac{1}{8}$, $\frac{1}{8}$), etc., and ($\frac{3}{16}$, $\frac{5}{16}$), etc. From the tables of Patterson (1935) we infer the same (psuedo) symmetry $C_2{}^IB$ for the corresponding Fourier projection. Thus the 24 chlorine atoms of our cell content form three sets of 8 points. In general two of these Fourier sets would give 16 strongest Patterson peaks, while a third Fourier set would increase this number to 48; it is therefore clear that there must exist occasional relations between these sets. For these relations there are several possibilities. First we tried the location by calculating the two Fourier sets, which by themselves give already the 16 observed Patterson peaks. There are two pairs of sets which satisfy the Patterson projection; one of these could be excluded by comparison with the Harker section at $y=\frac{1}{2}$. So in the present procedure the co-ordinates of 16 chlorine atoms would be fixed; they represent four sets of equivalent points of the class $P2_1/c$ ($\frac{5}{32}$, $\frac{7}{32}$, etc.; $\frac{11}{32}$, $\frac{1}{32}$, etc.; $\frac{1}{32}$, $\frac{3}{32}$, etc.; $\frac{15}{32}$, $\frac{5}{32}$, etc.).

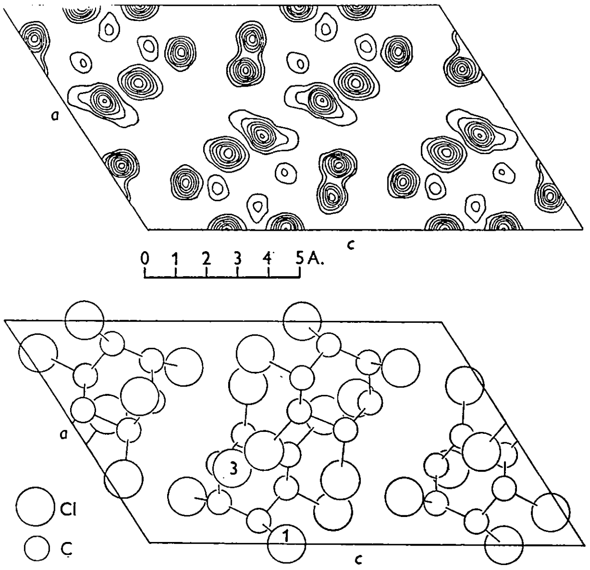

Fig. 1. Projection of the electron density along the *b* axis.

The possibility of finding the two supplementary chlorine sets and the six carbon sets was tried by repeated Fourier syntheses, starting from the 16 chlorine atoms already located. This proved to be successful. After ten successive syntheses the final [010] projection, Fig. 1, was obtained; it shows the chlorine atoms and a part of the carbon atoms resolved. Table 1 shows the agreement between calculated and observed structure factors (*h*0*l*), the former being calculated with a temperature factor $\exp[-3{\cdot}0\sin^2\theta/\lambda^2]$.

Next we tried to fit this projection with different models of the molecule $C_6H_6Cl_6$ and we found the model εεεκκκ (nomenclature of Hassel (Hassel, 1943; Hassel & Viervoll, 1947)) in good agreement. Assuming this model in the orientation just found, there remains but one undetermined *b* parameter, which fixes the model in relation to the glide symmetry plane. Its value was determined from the (0*kl*) intensities. A final [100] projection, Fig. 2, was obtained by four times repeated

Table 1. *Calculated and observed structure factors* F_{h0l}

$h0l$	$F_{\text{calc.}}$	$F_{\text{obs.}}$	$h0l$	$F_{\text{calc.}}$	$F_{\text{obs.}}$	$h0l$	$F_{\text{calc.}}$	$F_{\text{obs.}}$	$h0l$	$F_{\text{calc.}}$	$F_{\text{obs.}}$
100	$\overline{15}$	15	304	30	40	406	14	15	$\bar{1},0,14$	7	< 10
$\bar{1}02$	$\overline{65}$	68	$\bar{5}08$	33	34	1,0,10	$\overline{13}$	15	3,0,10	23	15
002	$\bar{2}$	10	008	$\overline{35}$	30	602	$\overline{40}$	34	$\bar{5},0,16$	12	< 10
$\bar{2}02$	45	43	500	34	30	$\bar{8}06$	42	34	$\bar{6},0,16$	28	20
102	$\overline{18}$	25	206	$\overline{11}$	< 10	$\bar{8}08$	$\overline{22}$	25	$\bar{9}02$	$\overline{36}$	30
200	$\overline{48}$	46	$\bar{6}06$	28	20	$\bar{1},0,12$	$\overline{24}$	30	$\bar{4},0,16$	$\bar{2}$	< 10
$\bar{1}04$	25	25	$\bar{6}04$	12	< 10	308	$\overline{21}$	25	$\overline{10},0,8$	0	< 10
$\bar{2}04$	$\overline{110}$	105	$\bar{3},0,10$	9	10	700	28	30	606	33	30
004	18	15	$\bar{4},0,10$	1	< 10	$\bar{7},0,12$	$\overline{12}$	15	704	5	< 10
$\bar{3}02$	$\overline{162}$	145	$\bar{2},0,10$	2	< 10	$\bar{8}04$	$\bar{7}$	< 10	$\overline{10},0,10$	$\overline{17}$	10
$\bar{3}04$	$\bar{4}$	< 10	$\bar{6}08$	$\overline{21}$	15	$\bar{8},0,10$	12	20	$\bar{7},0,16$	$\overline{21}$	10
202	$\overline{84}$	90	$\bar{6}02$	$\overline{13}$	20	$\bar{5},0,14$	$\bar{4}$	< 10	$\bar{9},0,14$	3	< 10
300	21	37	108	$\overline{60}$	62	$\bar{4},0,14$	$\bar{2}$	< 10	2,0,12	18	15
104	31	34	$\bar{5},0,10$	25	25	$\bar{8},0,12$	3	< 10	0,0,14	$\overline{24}$	15
$\bar{2}06$	$\overline{56}$	62	$\bar{1},0,10$	$\overline{24}$	34	0,0,12	$\bar{9}$	< 10	$\bar{3},0,16$	20	15
$\bar{1}06$	52	54	404	$\overline{101}$	105	2,0,10	41	34	$\overline{10},0,6$	$\bar{7}$	< 10
$\bar{3}06$	$\overline{31}$	43	502	$\overline{37}$	30	$\bar{8}02$	$\overline{15}$	15	508	$\overline{25}$	15
$\bar{4}04$	64	65	306	35	43	$\bar{6},0,14$	14	15	802	5	< 10
$\bar{4}02$	$\overline{11}$	10	$\bar{6},0,10$	1	< 10	$\bar{3},0,14$	$\overline{37}$	30	$\overline{10},0,12$	$\overline{12}$	10
006	50	49	$\bar{7}06$	$\overline{11}$	< 10	604	23	20	$\bar{8},0,16$	18	10
$\bar{4}06$	42	37	600	24	20	506	$\overline{22}$	20	4,0,10	$\overline{16}$	10
302	24	30	$\bar{7}04$	29	34	$\bar{9}08$	$\overline{48}$	37	$\bar{2},0,16$	17	10
204	11	< 10	$\bar{7}08$	$\overline{18}$	20	702	33	25	$\overline{10},0,4$	$\overline{19}$	10
400	8	15	0,0,10	22	20	$\bar{9}06$	$\bar{1}$	< 10	900	11	10
$\bar{3}08$	$\overline{90}$	90	208	29	34	$\bar{7},0,14$	$\overline{31}$	37	$\overline{10},0,14$	$\bar{3}$	< 10
$\bar{2}08$	$\overline{82}$	75	$\bar{4},0,12$	55	75	$\bar{2},0,14$	$\overline{13}$	10	1,0,14	$\bar{8}$	< 10
$\bar{5}04$	$\overline{71}$	65	$\bar{3},0,12$	$\overline{23}$	15	$\bar{9},0,10$	$\bar{2}$	< 10	$\bar{9},0,16$	8	10
106	86	85	$\bar{5},0,12$	58	55	408	$\overline{10}$	< 10	0,0,16	$\overline{21}$	15
$\bar{4}08$	3	10	$\bar{7}02$	55	51	1,0,12	28	20	2,0,16	10	20
$\bar{5}06$	84	80	$\bar{7},0,10$	17	20	$\bar{9}04$	$\bar{8}$	< 10	$\bar{6},0,18$	$\overline{11}$	10
$\bar{1}08$	48	46	$\bar{2},0,12$	11	< 10	800	4	< 10	$\bar{7},0,18$	$\overline{21}$	10
$\bar{5}02$	$\overline{24}$	30	$\bar{6},0,12$	$\overline{23}$	25	$\bar{9},0,12$	16	15			
402	$\bar{7}$	< 10	504	$\overline{13}$	< 10	$\bar{8},0,14$	$\overline{45}$	42			

Table 2. *Calculated and observed structure factors* F_{0kl}

$0kl$	$F_{\text{calc.}}$	$F_{\text{obs.}}$	$0kl$	$F_{\text{calc.}}$	$F_{\text{obs.}}$	$0kl$	$F_{\text{calc.}}$	$F_{\text{obs.}}$	$0kl$	$F_{\text{calc.}}$	$F_{\text{obs.}}$
011	14	< 10	046	$\overline{41}$	37	068	$\overline{27}$	15	0,6,11	$\bar{7}$	< 10
002	$\bar{3}$	10	063	24	20	085	24	25	0,1,13	$\bar{6}$	< 10
012	28	20	055	43	37	092	9	< 10	0,11,3	$\bar{7}$	< 10
020	$\overline{69}$	75	037	$\overline{48}$	57	059	14	15	0,2,13	10	< 10
021	34	37	008	$\overline{35}$	30	077	$\bar{5}$	< 10	098	1	< 10
022	$\overline{26}$	25	018	39	34	093	$\overline{41}$	40	0,5,12	$\overline{12}$	< 10
013	$\overline{114}$	95	064	$\overline{19}$	20	0,4,10	26	25	0,3,13	$\bar{4}$	< 10
031	$\bar{4}$	< 10	071	45	40	0,1,11	$\bar{1}$	< 10	0,8,10	$\bar{5}$	< 10
023	6	< 10	028	$\overline{13}$	< 10	086	37	37	0,7,11	$\bar{6}$	< 10
004	18	15	056	$\overline{49}$	54	0,2,11	10	< 10	099	4	< 10
032	$\overline{10}$	< 10	072	$\bar{6}$	< 10	094	7	< 10	0,6,12	4	< 10
014	16	20	047	$\overline{17}$	10	078	11	< 10	0,12,0	18	15
033	2	< 10	065	$\overline{20}$	25	069	15	20	0,12,1	$\overline{15}$	10
024	19	20	073	$\overline{29}$	34	0,3,11	21	20	0,4,13	$\overline{21}$	20
040	$\overline{100}$	85	038	8	< 10	095	$\overline{27}$	20	0,0,14	$\overline{24}$	15
041	$\overline{57}$	57	019	$\overline{28}$	25	0,10,0	$\overline{11}$	< 10	0,1,14	$\bar{9}$	15
042	$\overline{62}$	50	057	$\overline{10}$	< 10	0,10,1	$\overline{22}$	15	0,12,2	3	< 10
015	75	80	074	$\overline{43}$	57	0,5,10	$\bar{9}$	< 10	0,2,14	7	< 10
034	30	20	066	$\bar{7}$	25	087	36	25	0,5,13	$\overline{20}$	15
025	30	34	048	$\bar{9}$	< 10	0,10,2	$\bar{4}$	< 10	0,12,3	$\bar{1}$	< 10
043	$\overline{45}$	40	080	60	55	0,4,11	$\overline{14}$	< 10	0,8,11	11	10
051	15	< 10	029	$\overline{36}$	40	0,10,3	$\overline{12}$	< 10	0,3,14	6	< 10
006	50	48	081	35	30	0,0,12	$\overline{10}$	< 10	0,9,10	$\bar{6}$	< 10
035	$\overline{39}$	55	082	$\overline{20}$	30	096	8	< 10	0,7,12	$\overline{19}$	20
016	77	80	075	76	110	0,1,12	26	20	0,4,14	18	15
044	18	20	039	44	46	079	$\overline{20}$	15	0,6,13	4	< 10
052	2	< 10	083	20	15	0,2,12	$\bar{5}$	< 10	0,1,15	7	< 10
026	34	46	058	$\overline{16}$	15	0,6,10	26	20	0,13,1	7	< 10
053	30	40	067	$\overline{16}$	10	088	$\overline{16}$	20	0,5,14	5	< 10
045	$\overline{22}$	25	0,0,10	22	20	0,5,11	$\bar{1}$	< 10	0,9,11	15	15
036	41	46	0,1,10	27	20	0,3,12	21	15	0,8,12	$\bar{7}$	< 10
060	70	60	076	$\bar{7}$	< 10	097	$\bar{5}$	< 10	0,13,3	2	< 10
061	5	< 10	049	$\bar{3}$	< 10	0,11,1	$\overline{23}$	20	0,7,13	$\overline{10}$	15
054	21	20	084	9	< 10	0,4,12	$\overline{21}$	20	0,6,14	$\overline{10}$	< 10
017	$\bar{6}$	< 10	0,2,10	5	< 10	0,7,10	$\bar{6}$	< 10	0,0,16	$\overline{22}$	15
062	$\overline{28}$	30	091	0	< 10	0,11,2	$\overline{10}$	< 10			
027	$\bar{7}$	< 10	0,3,10	17	10	089	11	< 10			

Fourier syntheses. Contrary to the [010] projection, the [100] projection must be corrected for diffraction effects as we could not measure all (0*kl*) reflexions. The unobservable F_{0kl} structure factors were calculated with the preliminary values of the co-ordinates, and the corresponding Fourier terms were included in the series. Table 2 shows the comparison of calculated and observed structure factors (0*kl*).

The final co-ordinates are given in Table 3.

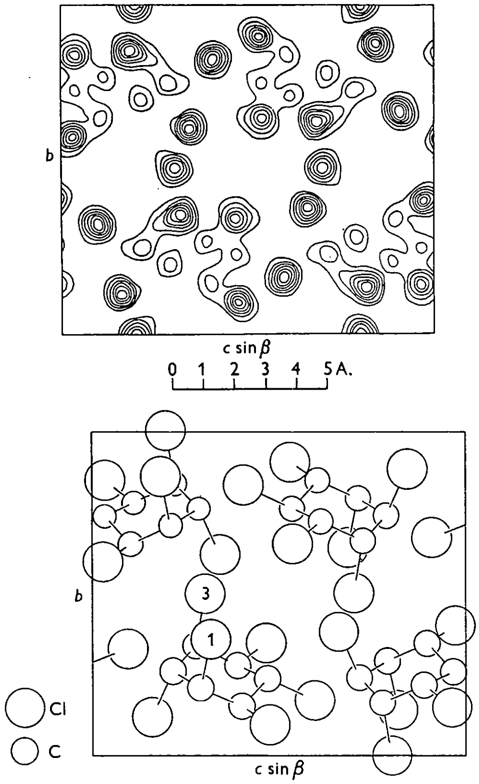

Fig. 2. Projection of the electron density on a plane perpendicular to the *a* axis.

Table 3. *Final co-ordinates*

	x	y	z
Cl_1	0·002 ± 0·002	0·353 ± 0·003	0·320 ± 0·001
Cl_2	0·210 ± 0·002	0·122 ± 0·003	0·156 ± 0·001
Cl_3	0·339 ± 0·002	0·503 ± 0·003	0·301 ± 0·001
Cl_4	0·716 ± 0·002	0·350 ± 0·003	0·467 ± 0·001
Cl_5	0·576 ± 0·002	0·169 ± 0·003	0·594 ± 0·001
Cl_6	0·147 ± 0·002	0·100 ± 0·003	0·474 ± 0·001
C_1	0·100 ± 0·005	0·217 ± 0·006	0·290 ± 0·003
C_2	0·186 ± 0·005	0·258 ± 0·006	0·221 ± 0·003
C_3	0·368 ± 0·005	0·339 ± 0·006	0·271 ± 0·003
C_4	0·498 ± 0·005	0·281 ± 0·006	0·389 ± 0·003
C_5	0·408 ± 0·005	0·239 ± 0·006	0·458 ± 0·003
C_6	0·258 ± 0·005	0·144 ± 0·006	0·399 ± 0·003

The *x* and *z* co-ordinates were refined by the method of least squares (Hughes, 1941). The (0*kl*) intensities had to be taken from different diagrams, no crystals about [100] being available, so the *y* co-ordinates could be determined only with less accuracy. We estimate the accuracy of x_{Cl} and z_{Cl} to be about 0·02 A.; of y_{Cl} about 0·03 A.; of x_C and z_C about 0·04 A.; of y_C about 0·06 A.

Discussion of the structure

Fig. 3 shows the shape and the dimensions of the molecule. The carbon ring is of the chair form and the chlorine configuration, as already mentioned, proves to be of type $\epsilon\epsilon\epsilon\kappa\kappa\kappa$. Thus the molecule is shown to be not isomorphous with the molecule of meso-inosite (type $\epsilon\kappa\kappa\kappa\kappa\kappa$), contrary to a suggestion by Slade (1945 *a*, *b*). Moreover, it has been generally supposed that steric hindrance would not allow chlorine atoms in 1,3 positions both to have the ϵ configuration (Slade, 1945*a*, *b*; Daasch, 1947). This too is disposed of by our results.

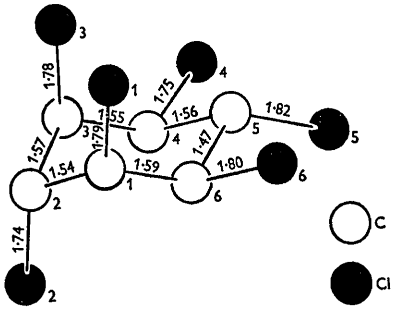

Fig. 3. Schematic model of the molecule showing bond lengths in Ångström units.

The steric hindrance causes only a bending out of the 1,3 C–Cl bonds in question (see Fig. 1 where the projections of these bonds are seen to be of unequal length). The number of isomers is now no longer restricted to five; and as a matter of fact Hassel recently announced the preparation of a sixth isomer (Bastiansen & Hassel, 1947; Hassel & Ottar, 1947). In the crystal the molecule of 'Gammexane' proves to be not quite symmetrical. The lines Cl_1–Cl_3, Cl_4–Cl_6, C_1–C_3, C_4–C_6 are not parallel; there are deviations from parallelism up to 4° in each co-ordinate. These we believe to be real as we found a symmetrical molecule to be inconsistent with the observed intensities.

The shortest intra-molecular Cl–Cl distance amounts to 3·20 A. for the '*ortho*' distances: Cl_3–Cl_4, Cl_4–Cl_5, Cl_5–Cl_6 and Cl_1–Cl_6. Unexpectedly the distance Cl_1–Cl_3 proves to be somewhat larger, namely 3·39 A. The close approach of the latter chlorine atoms is obvious from the distortion of the structure and thus these atoms might be expected to have the smaller distance. However, a possible explanation of the reverse situation might be seen in the fact that the *ortho* distances, too, are smaller than the normal Cl–Cl distance (3·6–3·8 A.), and these chlorine atoms in the *ortho* position might be displaceable with more difficulty than those in 1(ϵ)3(ϵ) position. We think the difference to be real in view of the supposed accuracy of the parameters and the fact that all *ortho* distances are found to be equal (3·22; 3·21; 3·19; 3·18 A. against 3·39 A. for Cl_1–Cl_3). A three-dimensional analysis, however, on the basis of more accurate intensities would be desirable to confirm the conclusion. For the shortest intermolecular Cl–Cl distance we found the same value of 3·4 A. Most angles show but small deviations from the tetrahedral angle 109°; only the angle between the bonds C_1–C_2 and C_2–C_3 amounts to 123° (see Table 4).

Table 4. *Interbond angles*

(Calculated for the parameter values of Table 3.)

$C_1-C_2-C_3=123°$	$C_4-C_5-C_6=113°$
$Cl_2-C_2-C_1=109°$	$Cl_5-C_5-C_4=112°$
$Cl_2-C_2-C_3=107°$	$Cl_5-C_5-C_6=108°$
$C_2-C_3-C_4=105°$	$C_5-C_6-C_1=107°$
$Cl_3-C_3-C_2=112°$	$Cl_6-C_6-C_5=114°$
$Cl_3-C_3-C_4=103°$	$Cl_6-C_6-C_1=104°$
$C_3-C_4-C_5=117°$	$C_6-C_1-C_2=107°$
$Cl_4-C_4-C_3=116°$	$Cl_1-C_1-C_6=114°$
$Cl_4-C_4-C_5=115°$	$Cl_1-C_1-C_2=111°$

Optical data

By means of the Federow method we measured the orientation of the polarization ellipsoid. Refractive indices were measured by immersion methods. We found:

$n_\alpha=1{\cdot}62$; $n_\beta=1{\cdot}64$; $n_\gamma=1{\cdot}67$.
Optical axial angle $=60°$.
Optic sign +.
$n_\gamma=b$; $\angle(a, n_\alpha)=107°$; $\angle(a, n_\beta)=17°$; $\angle(c, n_\alpha)=15°$; $\angle(c, n_\beta)=75°$.

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Patterson and Fourier Projections of Single Molecules of Haemoglobin

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The one-dimensional Patterson synthesis and several one-dimensional Fourier syntheses of a single molecule of haemoglobin are computed on the basis of X-ray data published by Perutz. Conclusions on the shape of the molecule are drawn from the Fourier projections, and modifications of Perutz's model of the molecule are suggested.

It is a well-known fact that proteins, if they crystallize at all, do so with varying amounts of water and that the unit-cell dimensions depend on the amount. It has so far been generally assumed (see, for example, Crowfoot (1938), Bernal & Fankuchen (1941), Boyes-Watson, Davidson & Perutz (1947), Bernal & Carlisle (1948)) that in the wet crystals the protein molecules are separated from each other throughout by layers of water. To explain the perfect arrangement of the molecules in these crystals it was then necessary (Bernal & Fankuchen, 1941) to assume long-range forces acting between the molecules. However, these assumptions are not necessary unless it is taken for granted that each molecule lies completely within the boundaries of one unit cell, in the dry crystal. Short-range forces may be responsible for the order in wet crystals as well, if each molecule stretches through two or more unit cells of the dry crystal (see below). This seems more satisfactory in view of the striking fact that the molecules must be much better aligned in wet than in dry crystals, as the former give far better photographs than the latter.

Following these considerations, it was thought promising to concentrate first on the shape of the protein molecule. Elsewhere (Dornberger-Schiff, 1949) the principle of a method has been outlined for the calculation of the Patterson function or the electron density of *single molecules* from the observed intensities or structure factors of different crystals of the same substance with varying water content. This method can therefore be used to give the shape of the molecule and thus to decide about the necessity of assuming long-range forces; sufficient data were available to apply it to haemoglobin and to yield Fourier and Patterson projections of a single molecule on to a line parallel to the c' axis (normal to a and b). (The full details of the method used are to be described in another paper.)

Only the intensities and F values of the $(00l)$ reflexions of the crystals in different states of swelling and shrinkage were required, for, as Boyes-Watson *et al.*