Insecticides. Part III.† Crystal Structures of Endrin (1,2,3,4,10,10-Hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-*endo*-1,4,-*endo*-5,8-dimethanonaphthalene) and Aldrin (1,2,3,4,10,10-Hexachloro-1,4,4a,5,8,8a-hexahydro-*endo*-1,4-*exo*-5,8-dimethanonaphthalene)

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The crystal structure of endrin was determined by Patterson and Fourier methods from three-dimensional diffractometer data with 753 reflections. Z = 4 in the orthorhombic unit cell, space group, $P2_12_12_1$, a = 1530·4(2), b = 1148·6(1), and c = 820·2(1) pm. The structure was refined by least-squares to R 0·044. The crystal structure of aldrin, was determined by the symbolic addition procedure from three-dimensional diffractometer data with 1080 reflections. Z = 4 in the monoclinic unit cell, space group $P2_1/n$, a = 1080·6(1), b = 1474·3(2), c = 899·2(1) pm, β = 93·03(1)°, the structure was refined to R 0·048.

IMPORTANT wide-spectrum cyclodiene insecticides are cyclic carbon compounds having a methano-bridged structure substituted with chlorine.[1] They are produced by a Diels–Alder diene reaction from hexachlorocyclopentadiene. Many of the cyclodienes are found in their epoxidized form (*e.g.* dieldrin and endrin), or are metabolized to this form by the insect.

To investigate possible molecular criteria for the mode of action of cyclodiene insecticides,[1] the crystal structures of two active compounds, differing chiefly in geometrical isomerism, namely aldrin and endrin, have been determined.

DISCUSSION

Endrin viewed perpendicular to the plane of the gross molecule and to the line (Figure 1) through the bridgehead carbons, C(11) and C(12), and the methano-bridged chlorines, Cl(1) and Cl(2), shows six-membered rings having the *endo–endo* configuration with the epoxide oxygen lying *exo* to its adjoining ring.

At right angles to this view (Figure 2) the molecule has an approximate mirror symmetry. Only van der Waal forces hold endrin molecules in a unit cell (Figure 3).

The structure of the aldrin molecule is shown in Figures 4 and 5. The *endo–exo* configuration of the six-membered rings in the aldrin molecule is illustrated by viewing the molecule perpendicular to the line through the bridgehead carbons C(11) and C(12) and the methano-bridged chlorines Cl(1) and Cl(2). The molecule parallel to the plane of the gross molecule has mirror symmetry.

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† Part II, ref. 3.

[1] S. B. Solway, *Adv. Pest Control Research*, 1965, **6**, 85.

Figure 6 shows the packing arrangement of the aldrin molecules in the crystal.

The hexachloronorbornene moieties in both the endrin and aldrin molecules resemble each other closely. Most interatomic distances are in the expected range except the olefinic Cl–C distances, Cl(4)–C(4) and Cl(5)–C(5) (**169·4**, **169·5**, **170·6**, and **170·3** pm) are less than the normal value (**172** pm). The C–C bonds [C(**3**)–C(**4**) and C(5)–C(6)] adjacent to the double bond, are shorter than the normal C–C single bond, (**148**, **152**, **151**, and **150** pm). Nevertheless the bridged ring system of the norbornene nucleus does impose considerable strain on the tetrahedral and trigonal geometry about the respective carbon atoms, and this is shown in intra-atomic angles.

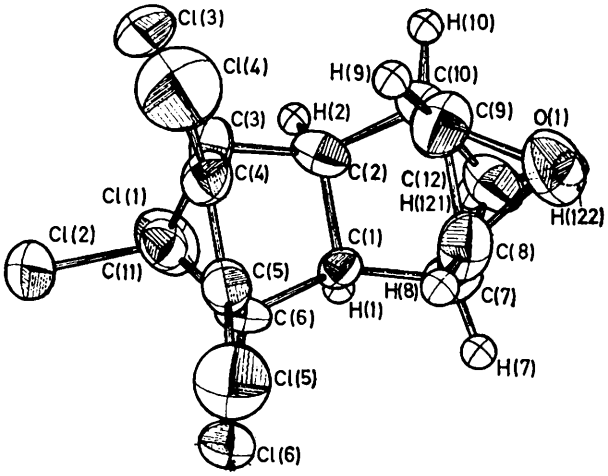

FIGURE 1 The structure of endrin viewed perpendicular to the plane of the gross molecule

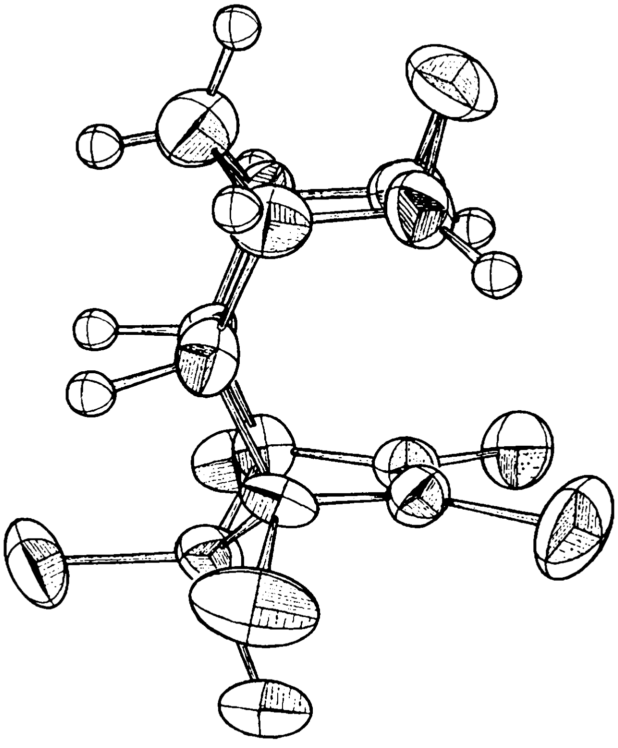

FIGURE 2 The structure of endrin viewed parallel to the plane of the gross molecule

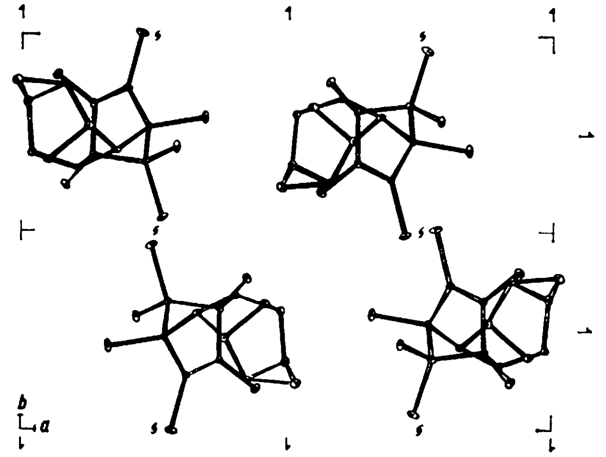

FIGURE 3 Packing of endrin in a unit cell viewed perpendicular to *c*

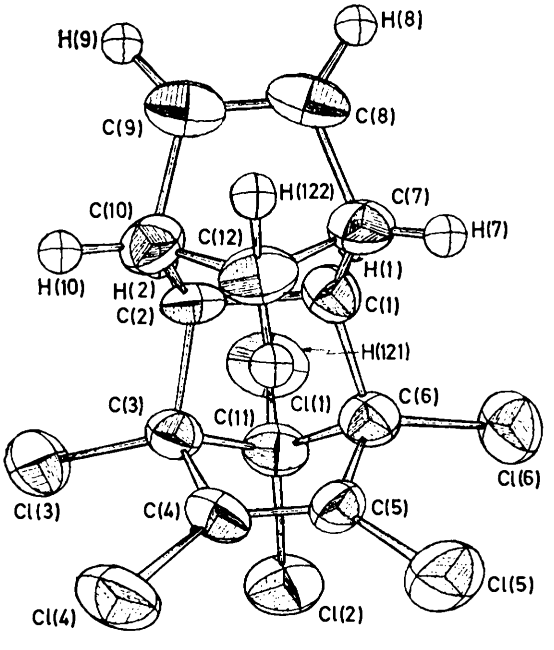

FIGURE 4 The structure of aldrin viewed perpendicular to the plane of the gross molecule

The different geometrical configurations in endrin and aldrin and the effect of the epoxide oxygen in the endrin molecule result in differences in bond lengths and angles in the unchlorinated section between the two molecules. The olefinic C(8)–C(9) distance in aldrin (**133** pm) is in the expected range as are the slightly shortened bond distances for C(7)–C(8) (**152** pm) and

C(9)–C(10) (154 pm). Distance of 152, 151, and 148 pm, for the bonds C(8)–C(9), C(7)–C(8), and C(9)–C(10) in endrin, are all significantly shorter than the normal C–C single bond distance. This is consistent with the electronegative nature of the epoxide group. Values (144 and 146 pm) for the epoxide C–O distances are close to reported epoxide ring distances. All other C–C bond distances in the unchlorinated norbornene section of both molecules are in the range of the normal C–C single bond distance.

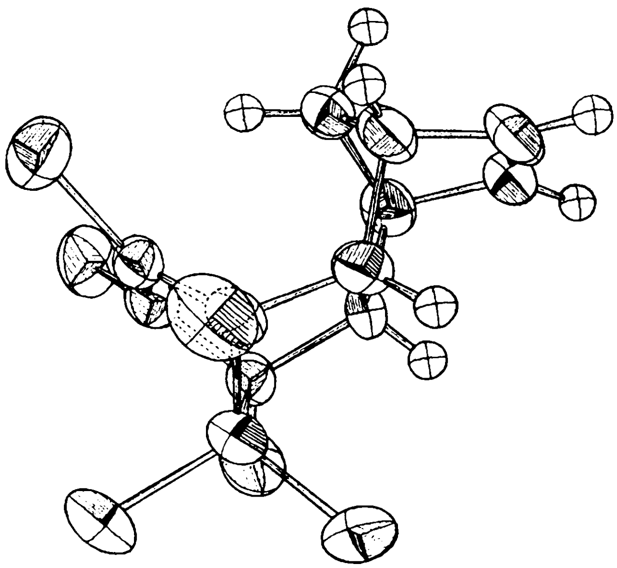

Figure 5 The structure of aldrin viewed parallel to the plane of the gross molecule

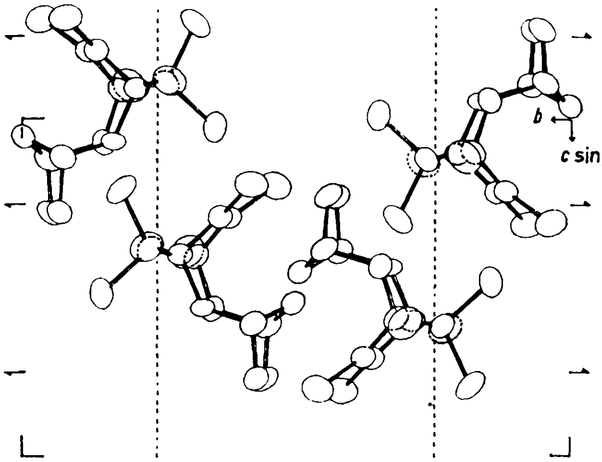

Figure 6 Packing of aldrin in a unit cell viewed perpendicular to *a*

The angles in these sections of the molecules reflect the different interactions caused by the different configuration imposed on the constraining influence of the bridged ring system.

Solway [1] has correlated biological activity with molecular structure of the cyclodiene insecticides. He found

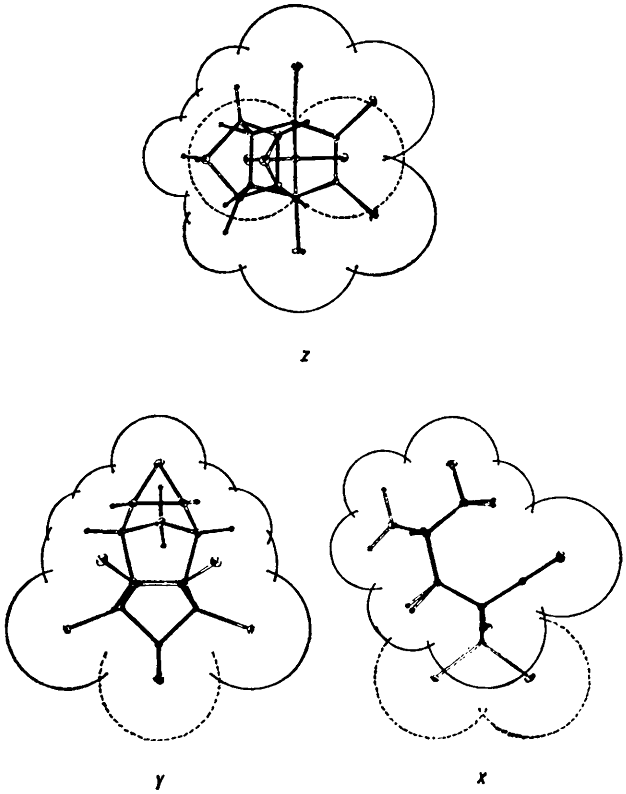

Figure 7 Three plane projections of endrin with the van der Waals circumferences drawn in

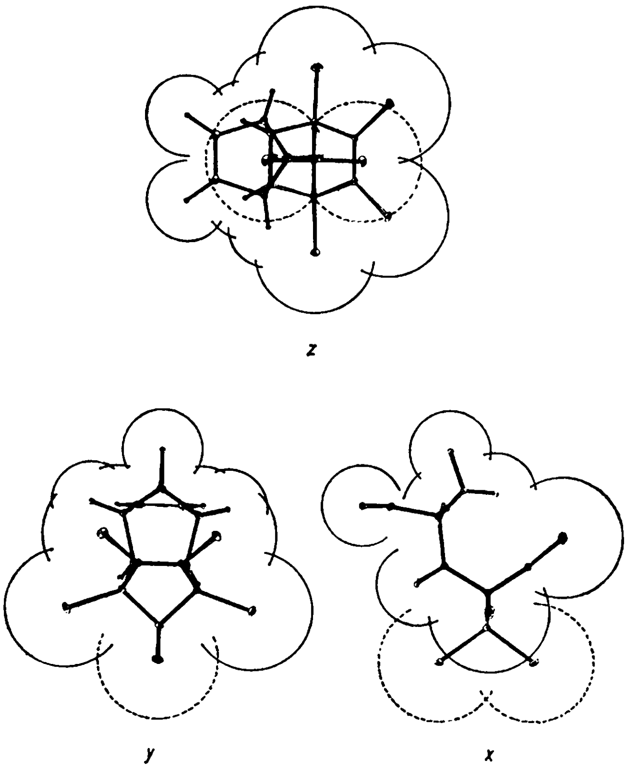

Figure 8 Three plane projections of aldrin with the van der Waals circumferences drawn in

that the overall molecular topography of these compounds is a critical factor in determining their activity. He used the projection of the Courtauld molecular models of aldrin and its analogues taken along a line joining the bridgehead atoms of the dimethanonaphthalene nucleus to correlate cyclodiene activity.

Figures 7 and 8 show the three-plane van der Waals projection of the endrin and aldrin structures. They were obtained from the atomic parameters using a thermal elipsoid plotting programme [2] (ORTEP), with a scale of one inch to the 100 pm and a view distance of infinity (parallel projection). The van der Waals circumferences of the periphery atoms in each projection were drawn in to scale.

Solway [1] has assumed that the deviations in the strained norbornene system compared to the idealized Courtauld models are either small or at least common to all the cyclodiene molecules. As discussed earlier, the deviations from tetrahedral and trigonal geometry in the dimethanonaphthalene nucleus are significant, and the deviations very similar in the two hexachloronorbornene moieties but different between the unchlorinated norbornene sections. A comparison of the van der Waals outlines of the *x* projections of the molecultes show that the Solway's models approximate to those found. The projected hexachloronorbornene moieties of both molecules superimpose almost exactly.

The relationships between the two electronegative centres with respect to distance and orientation is shown in these *x* projections. The distance in the *x* projection between the two electronegative groups [C(3)–C(6) in the hexachloronorbornene system, and a van der Waals limit on either the epoxide oxygen or the olefinic group] is similar for both endrin and aldrin (580 and 570 pm). The diameter of the bridged chlorine groups in the *x* and *y* projections (dashed lines) is 650 pm for endrin and 640 pm for aldrin. The height of the *x* and *z* projections for endrin and aldrin are 978 and 940 pm respectively.

EXPERIMENTAL

Crystal Structure of Endrin

Crystal Data.—$C_{12}H_8Cl_6O$, $M = 381$. Orthorhombic, $a = 1530·4(2)$, $b = 1148·6(1)$, $c = 820·2(1)$ pm, $U = 1·441$ nm^3, $D_m = 1·75$ (by flotation), $Z = 4$, $D_c = 1·753$, $F(000) = 760$. Space group $P2_12_12_1$. Mo-K_α radiation $\lambda = 71·07$ pm; μ(Mo-K_α) $= 11·68$ cm^{-1}.

A crystal (0·2 × 0·1 × 0·1 mm) was mounted in a general orientation on a Hilger and Watts computer-controlled four-circle diffractometer. Accurate cell dimensions and intensity data were collected as described.[3] Two octants of data were collected, hkl, $2\theta < 46°$ and $\bar{h}\bar{k}l$, $I_0 > 2\sigma(I_0)$. Both sets of data were corrected for Lorentz and polarization factors and absorption (gaussian integration with grid size 4 × 4 × 4). 753 out of 1047 independent reflections were considered observed.

Structure Determination.—Partial solution of a sharpened Patterson synthesis enabled location of two chlorine atoms. A series of Patterson syntheses were computed with the sharpening coefficient, the temperature factor *B*, reduced until two successive calculations had common features. Although a Wilson' plot suggested *B* 0·54 nm^2 the interpretable Patterson had *B* 0·24 nm^2. Successive electron-density syntheses enabled location of remaining non-hydrogen atoms.

Structure Refinement.—Full-matrix least-squares refinement, with statistical weights, reduced *R* to 0·053 and *R'* to 0·044 $[R' = (\Sigma w|F_o - F_c|^2/\Sigma w|F_o^2|)]^{\frac{1}{2}}$. During refinement, a difference-Fourier map showed the positions of all the hydrogens. A final difference-Fourier failed to reveal any prominent features. The standard deviation of an observation of unit weight, given by the expression $\{[\Sigma w||F_o| - |F_c||]^2/(n - m)\}^{\frac{1}{2}}$, where *n* is the number of observations and *m* the number of variables, was 0·797. This indicates that the errors were slightly overestimated. A plot of I_c/I_o *vs.* I_o gave an indication that two low-angle high-

TABLE 1

(*a*) Atomic parameters for endrin, with estimated standard deviations in parentheses

Atom	*x/a*	*y/b*	*z/c*	B/Å^2
Cl(1)	0·7391(2)	0·4651(2)	0·0092(4)	*
Cl(2)	0·7123(2)	0·2841(2)	−0·2208(3)	
Cl(3)	0·6589(2)	0·2082(3)	0·1718(4)	
Cl(4)	0·7793(2)	−0·0082(3)	0·0378(4)	
Cl(5)	0·9388(2)	0·1009(3)	−0·2065(4)	
Cl(6)	0·9222(2)	0·3827(2)	−0·2178(3)	
C(1)	0·9007(6)	0·3403(7)	0·1120(11)	
C(2)	0·8277(7)	0·2938(8)	0·2256(11)	
C(3)	0·7657(6)	0·2331(9)	0·0996(13)	
C(4)	0·8069(6)	0·1337(8)	0·0154(12)	
C(5)	0·8702(7)	0·1742(9)	−0·0808(12)	
C(6)	0·8709(7)	0·3058(8)	−0·0579(12)	
C(7)	0·9861(7)	0·3010(9)	0·1962(13)	
C(8)	0·9945(7)	0·1701(10)	0·1906(15)	
C(9)	0·9219(7)	0·1248(9)	0·2993(15)	
C(10)	0·8792(7)	0·2312(9)	0·3630(11)	
C(11)	0·7723(7)	0·3229(8)	−0·0437(12)	
C(12)	0·9560(9)	0·3187(10)	0·3756(13)	
O(1)	1·0143(5)	0·1141(7)	0·3436(10)	
H(1)	0·893	0·442	0·125	4·5
H(2)	0·772	0·366	0·279	4·5
H(7)	1·041	0·333	0·141	4·5
H(8)	1·007	0·124	0·096	4·5
H(9)	0·882	0·054	0·270	4·5
H(10)	0·835	0·226	0·472	4·5
H(121)	0·936	0·399	0·381	4·5
H(122)	1·004	0·283	0·457	4·5

(*b*) Anisotropic thermal parameters (× 10^4) *

Atom	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Cl(1)	78(2)	86(3)	200(6)	43(2)	−1(3)	8(4)
Cl(2)	38(1)	140(3)	162(5)	−1(2)	−17(3)	13(4)
Cl(3)	27(1)	204(5)	215(6)	−11(2)	14(3)	54(5)
Cl(4)	106(3)	68(2)	295(7)	−33(2)	−19(4)	−1(4)
Cl(5)	62(2)	118(3)	199(6)	22(2)	12(3)	−65(4)
Cl(6)	51(2)	113(3)	129(5)	−21(2)	2(3)	34(4)
C(1)	25(5)	65(9)	94(17)	−5(5)	9(9)	−26(11)
C(2)	55(6)	55(9)	108(16)	−2(6)	12(10)	5(12)
C(3)	26(5)	88(10)	156(18)	8(6)	−15(9)	11(14)
C(4)	38(6)	57(10)	131(19)	−7(6)	−6(9)	−4(12)
C(5)	34(5)	79(10)	113(19)	4(6)	−6(9)	−5(12)
C(6)	39(6)	59(9)	101(17)	−2(6)	21(8)	18(11)
C(7)	42(6)	73(11)	134(23)	−1(6)	19(10)	−30(14)
C(8)	43(6)	103(14)	170(28)	4(7)	−17(12)	−22(17)
C(9)	45(7)	61(10)	244(24)	−4(7)	−14(12)	17(15)
C(10)	50(6)	91(12)	106(17)	−1(7)	2(9)	14(13)
C(11)	41(6)	62(8)	138(18)	2(6)	−13(9)	23(12)
C(12)	80(8)	82(10)	144(22)	−11(8)	−13(12)	21(14)
O(1)	68(6)	112(8)	224(18)	13(5)	−29(8)	51(11)

* Defined as $T = \exp - (\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)$.

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[2] C. J. Johnson, ORTEP plotting program.

[3] T. P. DeLacy and C. H. L. Kennard, preceding paper.

TABLE 1 (*Continued*)

(*c*) Interatomic distances (pm); estimated standard deviations: Cl–C 0·5, C–C and C–O 1 , and C–H 10 pm

Cl(1)–C(11)	176·6	Cl(2)–C(11)	177·5
Cl(3)–C(3)	176·2	Cl(6)–C(6)	176·5
Cl(4)–C(4)	169·4	Cl(5)–C(5)	169·5
C(1)–C(2)	155		
C(2)–C(3)	157	C(6)–C(1)	152
C(3)–C(4)	148	C(5)–C(6)	152
C(4)–C(5)	133		
C(1)–C(7)	155	C(10)–C(2)	155
C(7)–C(8)	151	C(9)–C(10)	148
C(8)–C(9)	152		
C(3)–C(11)	157	C(6)–C(11)	153
C(7)–C(12)	156	C(10)–C(12)	155
C(8)–O(1)	144	C(9)–O(1)	146
H(1)–C(1)	120	H(2)–C(2)	130
H(2)–C(7)	100	H(10)–C(10)	110
H(8)–C(8)	100	H(9)–C(9)	100
H(121)–C(12)	100	H(122)–C(12)	110

(*d*) Interatomic angles (deg.); estimated standard deviations: 0·5°, those involving H atoms, 8°

C(2)–C(1)–C(6)	104·1	C(1)–C(2)–C(3)	101·2
C(2)–C(1)–C(7)	103·9	C(1)–C(2)–C(10)	103·3
C(6)–C(1)–C(7)	126·0	C(3)–C(2)–C(10)	125·5
H(1)–C(1)–C(2)	103	H(2)–C(2)–C(1)	118
H(1)–C(1)–C(6)	108	H(2)–C(2)–C(3)	96
H(1)–C(1)–C(7)	109	H(2)–C(2)–C(10)	113
Cl(6)–C(6)–C(1)	114·7	Cl(3)–C(3)–C(2)	114·4
Cl(6)–C(6)–C(11)	115·6	Cl(3)–C(3)–C(11)	114·8
Cl(6)–C(6)–C(5)	114·0	Cl(3)–C(3)–C(4)	115·4
C(1)–C(6)–C(11)	101·2	C(2)–C(3)–C(11)	99·4
C(1)–C(6)–C(5)	112·0	C(2)–C(3)–C(4)	113·2
C(11)–C(6)–C(5)	97·5	C(11)–C(3)–C(4)	97·5
Cl(5)–C(5)–C(6)	124·3	Cl(4)–C(4)–C(3)	125·9
Cl(5)–C(5)–C(4)	129·4	Cl(4)–C(4)–C(5)	125·6
C(6)–C(5)–C(4)	106·2	C(3)–C(4)–C(5)	108·5
C(12)–C(7)–C(1)	97·6	C(12)–C(10)–C(2)	97·7
C(12)–C(7)–C(8)	100·6	C(12)–C(10)–C(9)	102·9
C(1)–C(7)–C(8)	110·5	C(2)–C(10)–C(9)	110·5
H(7)–C(7)–C(1)	113	H(10)–C(10)–C(2)	107
H(7)–C(7)–C(8)	106	H(10)–C(10)–C(9)	120
H(7)–C(7)–C(12)	128	H(10)–C(10)–C(12)	116
C(7)–C(8)–C(9)	105·2	C(10)–C(9)–C(8)	104·4
C(7)–C(8)–O(1)	115·8	C(10)–C(9)–O(1)	114·1
C(9)–C(8)–O(1)	59·3	C(8)–C(9)–O(1)	57·9
H(8)–C(8)–C(7)	127	H(9)–C(9)–C(10)	118
H(8)–C(8)–C(9)	116	H(9)–C(9)–C(8)	124
H(8)–C(8)–O(1)	114	H(9)–C(9)–O(1)	124
Cl(1)–C(11)–C(6)	115·0	H(121)–C(12)–C(7)	105
Cl(1)–C(11)–C(3)	114·0	H(121)–C(12)–C(10)	113
Cl(2)–C(11)–C(6)	114·6	H(122)–C(12)–C(7)	110
Cl(2)–C(11)–C(3)	114·6	H(122)–C(12)–C(10)	108
Cl(1)–C(11)–Cl(2)	106·5	H(121)–C(12)–H(122)	123
C(6)–C(11)–C(3)	92·1	C(7)–C(12)–C(10)	94·4
C(8)–O(1)–C(9)	62·9		

intensity reflections were seriously effected by extinction. They were removed before the final cycle of refinement. No correction was applied for anomalous dispersion. The atomic parameters are listed in Table 1. Observed and calculated structure factor amplitudes for both compounds are listed in Supplementary Publication No. SUP 20475 (10 pp., 1 microfiche).†

Crystal Structure of Aldrin

Crystal Data.—$C_{12}H_8Cl_6$, M = 365. Monoclinic, a = 1080·6(1), b = 1474·3(2), c = 899·2(1) pm, β = 93·03(1)°, U = 1·408 nm^3, D_m = 1·73 (flotation), Z = 4, D_c = 1·719, $F(000)$ = 728. Space group $P2_1/n$ (C^5_{2h}, No. 14). μ(Mo-K_α) = 11·68 cm^{-1}.

TABLE 2

(*a*) Atomic parameters for aldrin, with estimated standard deviations in parentheses

Atom	x/a	y/b	z/c	B/Å^2
Cl(1)	0·1999(2)	0·6477(1)	0·0178(2)	*
Cl(2)	0·1902(2)	0·6834(1)	−0·2943(2)	
Cl(3)	0·4722(2)	0·7298(1)	−0·1218(2)	
Cl(4)	0·4105(2)	0·9181(1)	−0·3099(2)	
Cl(5)	0·1023(2)	0·9611(1)	−0·3048(2)	
Cl(6)	−0·0293(2)	0·8025(1)	−0·1073(2)	
C(1)	0·1807(6)	0·8484(4)	0·0640(7)	
C(2)	0·3227(6)	0·8311(4)	0·0603(7)	
C(3)	0·3344(6)	0·7897(4)	−0·0991(7)	
C(4)	0·3023(7)	0·8624(5)	−0·2127(7)	
C(5)	0·1835(7)	0·8786(4)	−0·2099(7)	
C(6)	0·1310(6)	0·8189(5)	−0·0930(8)	
C(7)	0·1782(6)	0·9494(5)	0·1160(8)	
C(8)	0·2298(8)	0·9430(5)	0·2760(8)	
C(9)	0·3506(8)	0·9276(5)	0·2732(8)	
C(10)	0·3829(6)	0·9226(5)	0·1085(8)	
C(11)	0·2127(7)	0·7347(5)	−0·1153(7)	
C(12)	0·2914(7)	0·9943(5)	0·0471(7)	
H(1)	0·141	0·806	0·143	3·5
H(2)	0·353	0·787	0·132	3·3
H(7)	0·102	0·970	0·095	3·9
H(8)	0·180	0·942	0·372	4·5
H(9)	0·412	0·908	0·366	4·1
H(10)	0·473	0·933	0·098	3·3
H(121)	0·281	1·003	−0·060	3·5
H(122)	0·312	1·066	0·115	3·5

(*b*) Anisotropic thermal parameters (× 10^4)

Atom	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Cl(1)	190(3)	36(1)	177(3)	−11(1)	28(3)	7(2)
Cl(2)	165(3)	67(1)	145(3)	−3(1)	−3(3)	−44(2)
Cl(3)	109(2)	74(1)	161(4)	38(2)	16(2)	−19(2)
Cl(4)	133(3)	76(1)	121(3)	−17(1)	48(2)	7(2)
Cl(5)	142(3)	69(1)	136(3)	30(2)	−9(2)	15(2)
Cl(6)	81(2)	77(1)	203(4)	−17(1)	8(2)	−29(2)
C(1)	78(8)	37(4)	117(12)	−2(5)	18(7)	−7(6)
C(2)	100(9)	42(5)	57(10)	2(5)	−3(7)	−3(6)
C(3)	83(8)	43(4)	85(11)	14(5)	10(8)	−2(6)
C(4)	87(9)	40(4)	94(11)	−9(5)	32(8)	−2(6)
C(5)	77(9)	41(4)	86(11)	15(5)	−10(8)	−4(6)
C(6)	82(7)	41(4)	107(12)	−10(5)	1(8)	−17(8)
C(7)	101(9)	48(5)	102(12)	11(5)	−6(8)	−22(6)
C(8)	146(11)	50(5)	108(14)	0(6)	33(10)	−29(6)
C(9)	137(11)	42(5)	103(13)	−1(6)	15(10)	−10(6)
C(10)	82(8)	48(5)	108(12)	−11(6)	−9(8)	−10(7)
C(11)	112(9)	38(4)	111(12)	0(6)	10(8)	−15(6)
C(12)	116(9)	37(4)	99(10)	−9(6)	−6(8)	−9(6)

* Defined as footnote to Table 1.

(*c*) Interatomic distances (pm); estimated standard deviations Cl–C 0·5, C–C 1, and C–H 10 pm

Cl(1)–C(11)	176·5	Cl(2)–C(11)	178·4
Cl(3)–C(3)	175·3	Cl(6)–C(6)	174·8
Cl(4)–C(4)	170·6	Cl(5)–C(5)	170·3
C(1)–C(2)	156		
C(2)–C(3)	157	C(6)–C(1)	155
C(3)–C(4)	151	C(5)–C(6)	150
C(4)–C(5)	131		
C(1)–C(7)	156	C(10)–C(2)	155
C(7)–C(8)	152	C(9)–C(10)	154
C(8)–C(9)	133		
C(3)–C(11)	155	C(6)–C(11)	154
C(7)–C(12)	155	C(10)–C(12)	153
H(1)–C(1)	110	H(2)–C(2)	100
H(7)–C(7)	90	H(10)–C(10)	100
H(8)–C(8)	100	H(9)–C(9)	110
H(121)–C(12)	100	H(122)–C(12)	120

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† See note about Supplementary Publications in Notice to Authors No. 7 in *J. Chem. Soc.* (*A*), 1970, Issue No. 20.

TABLE 2 (*Continued*)

(*d*) Interatomic angles (deg.); estimated standard deviation: 0·5°, those involving H atoms, 8°

C(2)–C(1)–C(6)	103·3	C(1)–C(2)–C(3)	102·1
C(2)–C(1)–C(7)	101·3	C(1)–C(2)–C(10)	104·2
C(6)–C(1)–C(7)	122·0	C(3)–C(2)–C(10)	122·9
H(1)–C(1)–C(2)	111	H(2)–C(2)–C(1)	113
H(1)–C(1)–C(6)	109	H(2)–C(2)–C(3)	108
H(1)–C(1)–C(7)	110	H(2)–C(2)–C(10)	107
Cl(6)–C(6)–C(1)	113·6	Cl(3)–C(3)–C(2)	114·3
Cl(6)–C(6)–C(11)	116·8	Cl(3)–C(3)–C(11)	116·7
Cl(6)–C(6)–C(5)	116·0	Cl(3)–C(3)–C(4)	116·5
C(1)–C(6)–C(11)	99·9	C(2)–C(3)–C(11)	100·4
C(1)–C(6)–C(5)	110·4	C(2)–C(3)–C(4)	108·4
C(11)–C(6)–C(5)	98·1	C(11)–C(3)–C(4)	98·4
Cl(5)–C(5)–C(6)	124·4	Cl(4)–C(4)–C(3)	123·4
Cl(5)–C(5)–C(4)	127·0	Cl(4)–C(4)–C(5)	128·4
C(6)–C(5)–C(4)	108·3	C(3)–C(4)–C(5)	107·9
C(12)–C(7)–C(1)	105·1	C(12)–C(10)–C(2)	104·8
C(12)–C(7)–C(8)	98·5	C(12)–C(10)–C(9)	98·4
C(1)–C(7)–C(8)	102·3	C(2)–C(10)–C(9)	101·7
H(7)–C(7)–C(1)	112	H(10)–C(10)–C(2)	120
H(7)–C(7)–C(8)	120	H(10)–C(10)–C(9)	111
H(7)–C(7)–C(12)	117	H(10)–C(10)–C(12)	118
C(7)–C(8)–C(9)	107·8	C(10)–C(9)–C(8)	107·1
H(8)–C(8)–C(7)	127	H(9)–C(9)–C(10)	125
H(8)–C(8)–C(9)	124	H(9)–C(9)–C(8)	127
Cl(1)–C(11)–C(6)	115·6	H(121)–C(12)–C(7)	114
Cl(1)–C(11)–C(3)	114·5	H(121)–C(12)–C(10)	119
Cl(2)–C(11)–C(6)	114·0	H(122)–C(12)–C(7)	107
Cl(2)–C(11)–C(3)	112·5	H(122)–C(12)–C(10)	108
Cl(1)–C(11)–Cl(2)	107·0	H(121)–C(12)–H(122)	113
C(6)–C(11)–C(3)	93·2	C(7)–C(12)–C(10)	93·7

A plate-shaped crystal (0·3 × 0·2 × 0·07 mm) was mounted in a general orientation on a Hilger and Watts computer-controlled four-circle diffractometer. 1080 out of 1400 independent reflections, collected up to $2\theta < 40°$, were considered observed. During data collection, the intensity of the standard reflections were reduced by 40%, and the data were rescaled accordingly.

Structure Solution.—The structure was determined by the symbolic-addition phase-determining technique using the largest 170 E values. The six chlorine atoms were located from an E map calculated with all the 170 phased E values. Successive electron-density syntheses enabled location of the carbon atoms.

Structure Refinement.—Full-matrix least-squares refinement with statistical weights reduced R to 0·048 and R' to 0·045. During refinement, a difference-Fourier synthesis revealed the positions of all the hydrogens. A final difference-Fourier was completely featurless. The standard deviation of an observation of unit weight was 1·063, (calc. 1·00). A plot of I_c/I_0 *vs.* I_0 gave no indication of serious extinction effects for low-angle high-intensity reflections. The atomic co-ordinates and temperature factors are listed in Table 2. Scattering factors used were those for chlorine, carbon,[4] and hydrogen.[5] No correction was applied for anomalous dispersion.

All calculations were carried out with local versions of standard programmes.[6]

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[4] 'International Tables for *X*-Ray Crystallography,' vol. III, Kynoch Press, Birmingham, 1962.

[5] R. F. Stewart, E. R. Davidson, and W. T. Simpson, *J. Chem. Phys.*, 1965, **42**, 3175.

[6] FAME–MAGIC (Symbolic Addition), Dewar and Stone, modified by R. C. Seccombe, (1970); PREFOUR (Structure Factor), FOURIER, J. Blount, 1966; ORFLS (Full-Matrix Least-Squares), W. R. Busing, K. O. Martin, and H. A. Levy, 1964.