complex formation. The P—O—C angles are 124·1 (4) and 120·9 (4)°. The geometries of these OC_2H_5 groups do not show significant differences. The O—P—O angles are in the range of 99·1–116·3° (Table 3). The P—C bond value of 1·821 (6) Å is in good agreement with the value of 1·81 (2) Å in $(CH_3)_3PO$ (Wang, 1965).

Both enantiomers related by the centre of symmetry are hydrogen bonded forming dimers. Each molecule is involved as a donor and an acceptor in the hydrogen bond N—H···O(3), 2·990 Å (Fig. 2). H···O(3) is 2·195 Å and ∠N—H···O(3) is 168°.

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1,1-Bis(*p*-chlorophenyl)-2,2,2-trichloroethanol

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Abstract. $C_{14}H_9Cl_5O$, triclinic, $P\bar{1}$, $a = 16{\cdot}779$ (10), $b = 10{\cdot}443$ (6), $c = 9{\cdot}684$ (8) Å, $\alpha = 107{\cdot}52$ (5), $\beta = 93{\cdot}06$ (6), $\gamma = 106{\cdot}99$ (5)°, $M_r = 370{\cdot}5$, $Z = 4$, $D_x = 1{\cdot}60$ g cm^{-3}, μ(Mo $K\alpha$) = 8·6 cm^{-1}, $R = 0{\cdot}069$, 2535 observed reflexions. Two independent molecules (*A*,*B*) in the asymmetric unit differ in conformation. The difference is considered to be due to the effects of hydrogen bonding (O···O 3·00 Å) between the hydroxyl groups of two symmetry-related *A* molecules. No similar associations were found for the *B* molecules.

Introduction. Dicofol was first reported to be a highly active acaricide by Wilson & Barker (1954). It is structurally related to DDT, but has limited insecticidal activity (Gunther, Blinn & Metcalf, 1956; Metcalf & Fukuto, 1968). However, it is one of the products of the biological degradation of DDT in the environment (Metcalf, 1973). It is also known as Acarin, DTMC, FW293, Kelamite, Kelthane, and Mitigan (*PANS Pesticide Index*, 1976). Needle-shaped crystals were grown from a continuously stirred solution of the compound in *n*-hexane.

2535 reflexions with $|F_o| > 2{\cdot}5\sigma(F_o)$ were considered observed out of 4035 collected from one crystal (0·44 × 0·24 × 0·12 mm) mounted on a Syntex $P\bar{1}$ four-circle diffractometer ($2\theta_{\max} = 57°$, Mo $K\alpha$

radiation, graphite monochromator). No correction was applied for absorption [$\mu(\text{Mo } K\alpha) = 8{\cdot}6 \text{ cm}^{-1}$] or extinction.

The structure was solved by multisolution $\sum_2$ sign expansion (Sheldrick, 1976). Full-matrix least-squares isotropic refinement with rigid-body constraints imposed on the C atoms of all four benzene rings reduced R from an initial value of 0·42 to 0·16. The rigid-body constraints were removed and the refinement was completed with all non-hydrogen atoms anisotropic. This reduced R to 0·093. The H atoms were located in a difference-Fourier synthesis and were included but not refined. The final R $(= \sum||F_o| - |F_c||/\sum|F_o|)$ was 0·069 and R_w $[= (\sum w||F_o| - |F_c||^2/\sum w|F_o|^2)^{1/2}]$ was 0·073. The weighting scheme used was $w = 2{\cdot}42/[\sigma^2(F_o) + 1{\cdot}65 \times 10^{-3}(F_o)^2]$. A final difference-Fourier map revealed no peaks with intensity greater than 0·4 e Å^{-3}. Positional parameters are listed in Table 1.* The molecular conformation and numbering scheme are given in Fig. 1, and a view perpendicular to the ab plane is in Fig. 2.

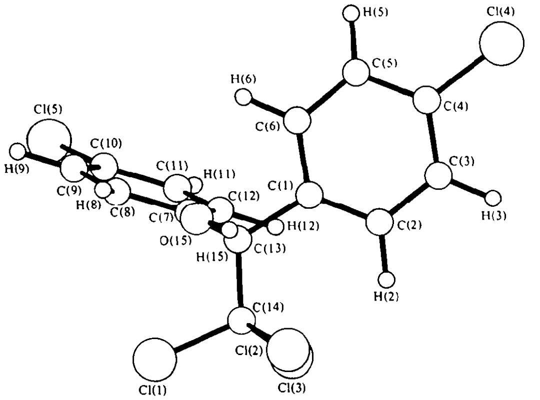

Fig. 1. Molecular conformation and numbering scheme used for the title compound (molecule A).

Discussion. Although there are two independent dicofol molecules (A,B) in the asymmetric unit, their interatomic distances and angles are not significantly different (Table 2) and are comparable with those found for p,p'-DDT (DeLacy & Kennard, 1972).

Table 1. *Atomic parameters* ($\times 10^4$) *and isotropic temperature factors* ($\times 10^3$)

The coordinates for H(15) in both molecules correspond to positive electron density in the final difference map and may not be reliable.

	x	y	z	U (Å^2)		x	y	z	U (Å^2)
Molecule A					Molecule B				
Cl(1)	4853 (2)	1178 (4)	−1013 (4)		Cl(1)	3624 (2)	3113 (4)	1617 (4)	
Cl(2)	3075 (2)	−171 (4)	−1508 (4)		Cl(2)	3210 (2)	5682 (4)	2590 (4)	
Cl(3)	4122 (2)	−1574 (4)	−3227 (4)		Cl(3)	3853 (2)	4644 (4)	4690 (4)	
Cl(4)	1503 (2)	−2624 (5)	−9243 (4)		Cl(4)	208 (2)	5413 (4)	7532 (4)	
Cl(5)	3155 (2)	6287 (4)	−866 (4)		Cl(5)	150 (3)	804 (5)	−2923 (5)	
O(15)	4752 (4)	1174 (8)	−3990 (9)		O(15)	2382 (5)	1980 (9)	3400 (9)	
C(1)	3285 (7)	−147 (11)	−5003 (11)		C(1)	1803 (7)	3924 (12)	4205 (11)	
C(2)	3513 (7)	0 (12)	−6314 (13)		C(2)	1014 (8)	2988 (15)	4307 (14)	
C(3)	2975 (7)	−773 (13)	−7602 (14)		C(3)	548 (8)	3484 (15)	5323 (14)	
C(4)	2211 (7)	−1671 (13)	−7649 (13)		C(4)	828 (9)	4855 (14)	6242 (11)	
C(5)	1974 (8)	−1860 (14)	−6347 (15)		C(5)	1601 (7)	5782 (15)	6163 (16)	
C(6)	2505 (7)	−1099 (14)	−5051 (14)		C(6)	2076 (8)	5283 (14)	5129 (12)	
C(7)	3727 (7)	2209 (11)	−2907 (12)		C(7)	1740 (7)	2573 (13)	1528 (12)	
C(8)	4359 (7)	3462 (14)	−2280 (13)		C(8)	1389 (7)	3420 (13)	999 (13)	
C(9)	4205 (8)	4728 (12)	−1627 (13)		C(9)	901 (8)	2884 (14)	−361 (14)	
C(10)	3368 (8)	4721 (13)	−1652 (12)		C(10)	757 (8)	1501 (17)	−1170 (13)	
C(11)	2722 (8)	3506 (14)	−2313 (14)		C(11)	1095 (9)	639 (16)	−663 (16)	
C(12)	2884 (7)	2204 (13)	−2947 (13)		C(12)	1567 (8)	1188 (12)	696 (13)	
C(13)	3918 (8)	820 (12)	−3621 (12)		C(13)	2287 (7)	3204 (13)	3061 (13)	
C(14)	3980 (8)	85 (13)	−2415 (13)		C(14)	3171 (8)	4103 (13)	2967 (14)	
H(2)	4106	826	−6212	39	H(2)	815	1897	3547	54
H(3)	3085	−851	−8590	60	H(3)	−128	2832	5203	49
H(5)	1358	−2613	−6337	38	H(5)	1806	6869	6903	41
H(6)	2289	−1323	−4081	49	H(6)	2675	6035	5069	54
H(8)	5002	3513	−2129	38	H(8)	1523	4548	1682	47
H(9)	4621	5769	−1002	61	H(9)	602	3457	−890	53
H(11)	2069	3461	−2344	59	H(11)	954	−469	−1352	90
H(12)	2373	1228	−3466	43	H(12)	1799	644	1197	68
H(15)	5284	2466	−3421	37	H(15)	2635	2483	4235	76

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33657 (17 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Interatomic distances* (Å) *and angles* (°) *with estimated standard deviations in parentheses*

	A	*B*		*A*	*B*		*A*	*B*
Cl(1)–C(14)	1·780 (11)	1·763 (12)	C(5)–C(6)	1·366 (16)	1·387 (15)	C(13)–C(14)	1·593 (15)	1·530 (14)
Cl(2)–C(14)	1·788 (11)	1·777 (13)	C(6)–C(1)	1·382 (14)	1·355 (14)	C(2)–H(2)	1·07	1·09
Cl(3)–C(14)	1·766 (12)	1·807 (13)	C(1)–C(13)	1·532 (14)	1·550 (14)	C(3)–H(3)	0·97	1·12
Cl(4)–C(4)	1·728 (11)	1·743 (11)	C(7)–C(8)	1·359 (14)	1·392 (16)	C(5)–H(5)	1·10	1·08
Cl(5)–C(10)	1·733 (12)	1·757 (12)	C(8)–C(9)	1·387 (15)	1·375 (15)	C(6)–H(6)	1·08	1·10
O(15)–C(13)	1·433 (13)	1·461 (15)	C(9)–C(10)	1·401 (15)	1·361 (17)	C(8)–H(8)	1·06	1·11
C(1)–C(2)	1·384 (14)	1·426 (15)	C(10)–C(11)	1·352 (14)	1·381 (19)	C(9)–H(9)	1·07	1·10
C(2)–C(3)	1·367 (14)	1·364 (15)	C(11)–C(12)	1·425 (16)	1·363 (16)	C(11)–H(11)	1·08	1·09
C(3)–C(4)	1·338 (14)	1·363 (15)	C(12)–C(7)	1·411 (15)	1·361 (14)	C(12)–H(12)	1·10	0·99
C(4)–C(5)	1·394 (15)	1·395 (16)	C(7)–C(13)	1·542 (15)	1·547 (15)	O(15)–H(15)	1·31	0·83

	A	*B*		*A*	*B*
Cl(1)–C(14)–Cl(2)	105·8 (8)	108·0 (8)	C(6)–C(1)–C(13)	126·2 (10)	126·8 (10)
Cl(1)–C(14)–Cl(3)	108·8 (8)	106·8 (8)	C(2)–C(1)–C(13)	116·0 (10)	113·9 (9)
Cl(2)–C(14)–Cl(3)	108·9 (8)	106·6 (8)	C(7)–C(8)–C(9)	122·4 (10)	120·7 (11)
Cl(1)–C(14)–C(13)	110·0 (8)	110·9 (8)	C(8)–C(9)–C(10)	118·8 (10)	118·6 (13)
Cl(2)–C(14)–C(13)	113·3 (8)	114·4 (8)	C(9)–C(10)–C(11)	120·6 (11)	121·6 (12)
Cl(3)–C(14)–C(13)	109·9 (8)	109·8 (8)	C(10)–C(11)–C(12)	120·3 (11)	118·7 (13)
Cl(4)–C(4)–C(5)	118·0 (9)	120·9 (9)	C(11)–C(12)–C(7)	119·1 (10)	121·5 (13)
Cl(4)–C(4)–C(3)	123·4 (10)	118·6 (10)	C(12)–C(7)–C(8)	118·8 (10)	118·8 (11)
Cl(5)–C(10)–C(9)	120·0 (9)	119·3 (10)	C(8)–C(7)–C(13)	121·2 (10)	119·6 (11)
Cl(5)–C(10)–C(11)	119·5 (10)	119·0 (10)	C(12)–C(7)–C(13)	120·0 (10)	121·6 (12)
C(1)–C(2)–C(3)	120·4 (10)	119·3 (12)	C(1)–C(13)–O(15)	109·5 (10)	108·2 (11)
C(2)–C(3)–C(4)	122·0 (10)	120·9 (12)	C(1)–C(13)–C(14)	113·9 (8)	117·3 (10)
C(3)–C(4)–C(5)	118·6 (11)	120·5 (11)	C(1)–C(13)–C(7)	112·0 (9)	109·6 (10)
C(4)–C(5)–C(6)	120·1 (11)	118·7 (12)	C(7)–C(13)–O(15)	108·4 (9)	104·5 (10)
C(5)–C(6)–C(1)	121·1 (11)	121·3 (11)	C(7)–C(13)–C(14)	108·8 (9)	109·6 (10)
C(6)–C(1)–C(2)	117·7 (10)	119·2 (10)	C(14)–C(13)–O(15)	104·0 (8)	106·5 (10)

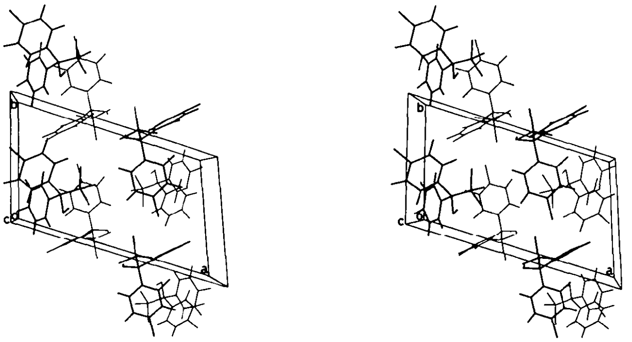

Fig. 2. Stereoview perpendicular to the *ab* plane.

However, the angles between the normals to the benzene rings differ markedly (*A* 86·4°, *B* 76·7°). The intramolecular distances between the hydroxyl O(15) and two terminal Cl atoms are dissimilar in *A* (2·88, 3·08 Å) and similar in *B* (2·98, 2·99 Å). Torsion angles about O(15), determined in a projection down C(13)–C(14), show considerable distortion for *A* [−68·9° Cl(1), 50·8° Cl(3)] compared with those of *B* [−58·5° Cl(1), 59·3° Cl(3)]. Also, the angles between the benzene rings and the plane containing C(1), C(13), C(7) are 57·6, 52·2° for *A* and 35·5, 86·2° for *B*.

These differences may be interpreted as the effects of intermolecular hydrogen bonding involving hydroxyl groups of symmetry-related *A* molecules, with an O···O distance of 3·00 Å. No similar contacts were observed for the *B* group of molecules.

The angle C(6)–C(1)–C(13) [126·2 (10), 126·8 (10)°] for both molecules is significantly different from the expected trigonal planar angle. This distortion is not unusual among the DDT analogues and is not considered to be due to the effects of the presence of the hydroxyl group on the *β*-C.

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