

further three cycles with anisotropic temperature factors, R was 0.081 ($R_w = 0.073$). At this stage of the calculation, a difference synthesis revealed the positions of all the H atoms which were included together with individual isotropic temperature factors in the final two cycles of refinement. Non-hydrogen atoms were held fixed. The final values of R and R_w were 0.066 and 0.050 respectively. The weights were $w^{-1} = \sigma(F)$. Neutral-atom scattering factors (Doyle & Turner, 1968) were employed. All the calculations were made using the XRAY 70 system (Stewart, Kundell & Baldwin, 1970) on an IBM 370/145 computer.*

Discussion. The heavy-atom coordinates are listed in Table 1, and H atom positional parameters and isotropic temperature factors are presented in Table 2.

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33585 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Hydrogen atom positional ($\times 10^3$) and thermal ($\text{\AA}^2 \times 10^3$) parameters, and H-X bond lengths ($X = \text{C, O}$)*

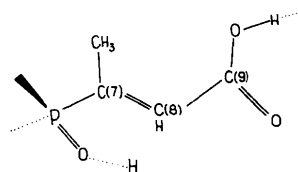
	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}	Bonded to	H-X (\AA)
H(1)	341 (7)	1059 (6)	260 (3)	212 (26)	O(2) 1.04 (3)	
H(2)	902 (8)	648 (6)	410 (4)	212 (29)	O(1) 1.58 (4)	
H(3)	1112 (8)	659 (6)	542 (4)	244 (32)	C(2) 1.12 (3)	
H(4)	1353 (7)	795 (5)	570 (3)	155 (23)	C(3) 0.99 (4)	
H(5)	1363 (6)	929 (5)	454 (3)	135 (21)	C(4) 1.04 (5)	
H(6)	1169 (6)	912 (5)	316 (3)	113 (18)	C(5) 1.07 (1)	
H(8)	547 (5)	739 (4)	206 (2)	61 (14)	C(6) 1.09 (6)	
H(101)	977 (5)	930 (5)	185 (3)	108 (18)	C(8) 1.18 (5)	
H(102)	1035 (5)	769 (4)	179 (2)	77 (15)	C(10) 1.12 (4)	
H(12)	764 (5)	1018 (5)	82 (3)	108 (19)	C(10) 1.04 (2)	
H(13)	571 (7)	1012 (6)	-60 (3)	165 (24)	C(12) 1.07 (1)	
H(14)	511 (5)	800 (4)	-138 (3)	79 (16)	C(13) 1.09 (2)	
H(15)	647 (8)	597 (7)	-72 (4)	249 (33)	C(14) 1.06 (4)	
H(16)	834 (6)	616 (5)	74 (3)	158 (24)	C(15) 1.17 (7)	
H(171)	871 (7)	36 (5)	273 (3)	189 (23)	C(16) 1.12 (4)	
H(172)	705 (7)	82 (6)	275 (4)	150 (25)	C(17) 0.93 (7)	
H(173)	831 (8)	16 (6)	362 (4)	198 (30)	C(17) 0.91 (8)	
					C(17) 1.23 (9)	

Table 3. *Bond lengths (\AA)*

P-O(1)	1.493 (1)	C(7)-C(17)	1.525 (3)
P-C(1)	1.796 (2)	C(8)-C(9)	1.510 (1)
P-C(7)	1.827 (2)	C(9)-O(2)	1.310 (1)
P-C(10)	1.827 (1)	C(9)-O(3)	1.194 (1)
C(1)-C(2)	1.410 (1)	C(10)-C(11)	1.520 (1)
C(2)-C(3)	1.431 (1)	C(11)-C(12)	1.404 (1)
C(3)-C(4)	1.415 (1)	C(12)-C(13)	1.434 (2)
C(4)-C(5)	1.402 (1)	C(13)-C(14)	1.379 (5)
C(5)-C(6)	1.405 (1)	C(14)-C(15)	1.402 (3)
C(6)-C(1)	1.402 (1)	C(15)-C(16)	1.409 (2)
C(7)-C(8)	1.333 (1)	C(16)-C(11)	1.425 (3)

Bond lengths and angles are in Tables 3 and 4. The atom numbering is shown in Fig. 1.

As expected, a considerable part of the molecule is almost flat as a result of the conjugated system of double bonds.



The shortening of the C(8)-C(9) bond is noticeable (1.510 \AA). The angle between the plane of the carboxyl group and the plane of the double bond C(7)=C(8) is about 13° (Table 5). The planar fragments of the molecules having the same configuration, linked into long chains along the screw axis by means of hydrogen bonding, are nearly parallel to each other (Fig. 2). Phenyl and benzyl substituents fill the space between the pseudolayers formed from the chains. It is interesting that the antiplanar C=C-C=O conformation is observed; this was found in none of the

Table 4. *Bond angles ($^\circ$)*

P-C(7)-C(8)	113.64 (20)	C(7)-C(8)-C(9)	127.50 (14)
P-C(7)-C(17)	117.09 (18)	C(8)-C(7)-C(17)	129.26 (19)
P-C(10)-C(11)	109.85 (2)	C(8)-C(9)-O(2)	117.48 (5)
P-C(1)-C(2)	116.28 (2)	C(8)-C(9)-O(3)	119.51 (9)
P-C(1)-C(6)	122.52 (5)	O(2)-C(9)-O(3)	122.89 (8)
C(1)-P-O(1)	112.48 (2)	C(10)-C(11)-C(12)	119.18 (1)
C(1)-P-C(7)	104.96 (5)	C(10)-C(11)-C(16)	120.71 (7)
C(1)-P-C(10)	106.06 (3)	C(11)-C(12)-C(13)	118.93 (18)
O(1)-P-C(7)	113.17 (8)	C(12)-C(13)-C(14)	120.01 (3)
O(1)-P-C(10)	112.93 (1)	C(13)-C(14)-C(15)	121.68 (28)
C(7)-P-C(10)	106.61 (7)	C(14)-C(15)-C(16)	118.88 (32)
C(1)-C(2)-C(3)	119.11 (4)	C(15)-C(16)-C(11)	120.42 (12)
C(2)-C(3)-C(4)	119.46 (6)	C(16)-C(11)-C(12)	120.08 (8)
C(3)-C(4)-C(5)	119.88 (4)		
C(4)-C(5)-C(6)	121.07 (3)	C(9)-O(2)-H(1)	106.54 (39)
C(5)-C(6)-C(1)	119.24 (5)	P-O(1)...H(1)	139.50 (44)
C(6)-C(1)-C(2)	121.19 (5)		

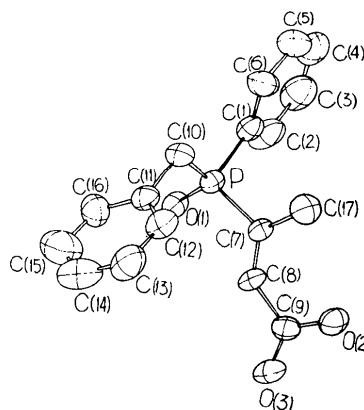


Fig. 1. A view of the molecule and the numbering of the atoms (ORTEP, Johnson, 1965).

Table 5. *Least-squares planes*(a) Coefficients in $AX + BY + CZ = D$, referred to the crystallographic axes

	A	B	C	D
Plane (I): C(1)–(6)	–5.4781	8.1277	7.3993	3.3573
Plane (II): C(11)–(16)	–8.4425	–1.7010	11.7144	–7.2596
Plane (III): C(9), O(2), O(3)	–1.7832	–4.9288	15.0220	–1.7504
Plane (IV): C(7), C(8), C(9)	–1.4942	–2.9696	16.1538	0.4260
Plane (V): C(7), C(8), C(17)	–1.5827	–2.7563	16.2813	0.5846
Plane (VI): P, C(7), C(8)	–1.6546	–2.5742	16.3819	0.7201

(b) Deviations of the atoms from the planes (Å)

	(I)	(II)	(III)	(IV)	(V)	(VI)
P	0.0431			0.0703	0.0320	
C(1)	0.0042					
C(2)	0.0013					
C(3)	–0.0090					
C(4)	0.0120					
C(5)	–0.0072					
C(6)	–0.0012					
C(7)		–0.0632				
C(8)		0.0933				
C(9)						0.0505
C(10)	–0.0432					
C(11)	0.0004					
C(12)	0.0010					
C(13)	–0.0029					
C(14)	0.0037					
C(15)	–0.0025					
C(16)	0.0003					
C(17)			–0.0267			0.0230
H(1)		–0.1734				

(c) Angles between planes (°)

(III)/(IV)	11.85	(III)/(VI)	13.89
(III)/(V)	12.93		

previously examined $R\text{-CH}_2\text{-CH}_2\text{-COOH}$ monocarboxylic acids and was only rarely present in α,β -unsaturated ones (Leiserowitz, 1976). A similar arrangement has only been found in *trans*-cinnamic acid (Ladell, McDonald & Schmidt, 1956) and fumaric acid (Brown, 1966; Bednowitz & Post, 1966). A synplanar conformation is more usually found.

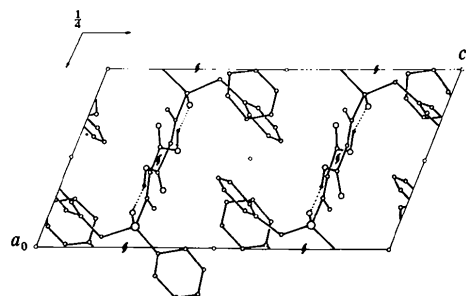


Fig. 2. The packing of the molecules in the racemic crystal.

As in the organic phosphorus compounds of the type $R_3P=O$ previously studied, a deformation of the P coordination tetrahedron (comprising an increase in the $O=P-C$ and a simultaneous decrease in the $C-P-C$ valency angles) is found. In the crystal studied the mean values of these angles are about 106 and 113° .

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