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Structure of 1-[Ethyl(phenyl)phosphinyl]-1-phenylethanol, $C_{16}H_{19}O_2P$

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Abstract. $M_r = 274{\cdot}3$, monoclinic, space group $P2_1/c$, $Z = 4$, $a = 15{\cdot}960\ (4)$, $b = 5{\cdot}614\ (2)$, $c = 16{\cdot}418\ (4)$ Å, $\beta = 110{\cdot}06\ (2)°$, $V = 1381{\cdot}7$ Å^3, $D_m = 1{\cdot}303$, $D_x = 1{\cdot}318$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}7107$ Å, $\mu = 0{\cdot}20$ mm^{-1}, $F(000) = 584$, room temperature, m.p. 410–412 K, final $R = 0{\cdot}078$ for 2973 reflections. There are no unusual bond distances and angles. The conformation about C(10)—P is such that the two phenyl groups are in antiperiplanar orientation. The molecules form chains along the [010] direction by means of hydrogen bonding with O···O 2·758 (3), H···O 1·94 (6) Å and O···H—O 144 (6)°.

Introduction. Crystalline 1-[ethyl(phenyl)phosphinyl]-1-phenylethanol, (±)-*threo* isomer assumed, provided a convenient model compound for X-ray analysis which we decided to use to establish the stereochemistry. We are also interested in conformations and hydrogen bonding in crystals of phosphine oxide derivatives (Gałdecki & Główka, 1980*a,b,c*, 1981; Główka & Gałdecki, 1981).

Experimental. Recrystallization from a mixture of methanol and ethyl acetate (1:1). D_m by flotation. Colourless prismatic crystal 0·30 × 0·20 × 0·25 mm. Syntex $P3$ diffractometer. Unit-cell parameters from accurately measured values of 20 high-angle reflections. Empirical absorption corrections (transmission coefficients 0·908 to 0·953). $\sin\theta/\lambda \le 0{\cdot}65$ Å^{-1}. 3051 reflections measured ($0 \le h \le 20$, $0 \le k \le 7$, $-21 \le l \le 20$), all unique; 2973 considered observed with $F_o > 2\sigma(F_o)$. Four standard reflections: intensity variation <6%. Structure solved by direct methods with *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), which revealed positions of all non-hydrogen atoms. Refinement (on F) by full-matrix least squares with anisotropic temperature factors for non-hydrogen atoms. All H atoms located in difference Fourier synthesis and included in the refinement isotropically. Final $R = 0{\cdot}078$, $R_w = 0{\cdot}081$ and $S = 1{\cdot}47$ for the 2973 observed reflections; $w = 1/\sigma_F^2$. $(\Delta/\sigma)_{max}$ for non-H atoms 0·92, average value 0·33. Final difference synthesis revealed no electron density excursions exceeding 0·34 e Å^{-3}. Atomic scattering factors for neutral atoms from *International Tables for X-ray Crystallography* (1974); anomalous-dispersion corrections for non-hydrogen atoms (Cromer & Liberman, 1970). All calculations (except those using *MULTAN*) performed using the *XRAY*76 system (Stewart, 1976).

Discussion. The positional parameters and isotropic thermal parameters for the non-hydrogen atoms are in Table 1.† A view of the molecule on the xz plane and the atom-numbering system are shown in Fig. 1. The bond lengths and angles listed in Table 2 are close to those commonly observed in similar structures. The configuration around the chiral centres P and C(10) can be deduced from the Newman projection of Fig. 2. The conformation about C(10)—P is such that the two phenyl groups are in antiperiplanar orientation. The molecules are connected into chains by means of hydrogen bonds with O···O = 2·758 (3), H···O = 1·94 (6) Å and O···H—O = 144 (6)° along the [010] direction, as compared with the values found in 1-[benzyl(phenyl)phosphinyl]-1-phenylethanol (Główka & Gałdecki, 1981) (2·693, 1·76 Å, 176°), 2-hydroxy-2-methyl-1-phenylphospholane 1-oxide (Gałdecki & Główka, 1980*c*) (2·702, 1·67 Å, 174°), 2-hydroxy-1-phenylphospholane 1-oxide (Gałdecki & Główka, 1981) (2·616, 1·49 Å, 170°), and 2-hydroxy-5-hydroxymethylene-1-phenylphospholane 1-oxide (Gałdecki & Główka, 1980*d*) (2·744, 2·743, 1·83, 1·79 Å; 171, 161°).

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† Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39155 (21 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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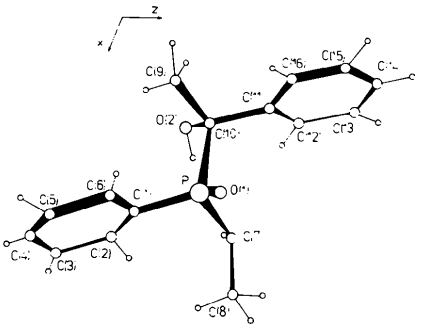

Fig. 1. View of the molecule along [010] showing the atom numbering.

Table 1. *Fractional positional parameters* ($\times 10^5$) *and equivalent isotropic temperature factors* ($Å^2 \times 10^3$) *for the non-hydrogen atoms*

$U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	U_{eq}
P	28386 (4)	42555 (11)	20320 (4)	21·3 (3)
O(1)	28186 (14)	17636 (34)	23439 (13)	31 (1)
O(2)	17989 (14)	80634 (35)	14082 (13)	32 (1)
C(1)	31474 (18)	43142 (47)	10696 (15)	26 (1)
C(2)	36074 (18)	61878 (51)	8752 (19)	31 (1)
C(3)	38502 (22)	61212 (66)	1390 (21)	42 (1)
C(4)	36010 (24)	42142 (70)	−4200 (19)	43 (2)
C(5)	31387 (24)	23370 (58)	−2362 (21)	40 (1)
C(6)	29071 (20)	23724 (56)	5093 (19)	32 (1)
C(7)	36118 (18)	61281 (47)	28201 (17)	28 (1)
C(8)	45584 (24)	51829 (65)	31398 (23)	45 (2)
C(9)	10706 (18)	43978 (55)	9885 (17)	32 (1)
C(10)	17320 (16)	57551 (45)	17429 (16)	25 (1)
C(11)	14561 (17)	58138 (48)	25439 (16)	24 (1)
C(12)	16831 (20)	76904 (51)	31226 (20)	32 (1)
C(13)	14652 (23)	77113 (60)	38724 (22)	40 (2)
C(14)	9945 (21)	58350 (71)	40502 (20)	21 (2)
C(15)	7458 (23)	39457 (65)	34645 (23)	43 (2)
C(16)	9846 (20)	39198 (49)	27321 (20)	33 (1)

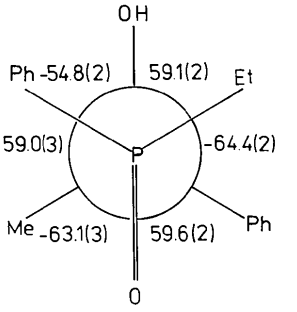

Fig. 2. Newman projection of the molecule along C(10)—P. Torsion angles are in degrees.

Table 2. *Bond lengths* (Å) *and angles* (°)

P—O(1)	1·494 (3)	C(1)—P—C(10)	106·70 (12)
P—C(1)	1·809 (4)	C(7)—P—C(10)	106·06 (13)
P—C(7)	1·791 (3)	P—C(1)—C(2)	122·77 (22)
P—C(10)	1·865 (3)	P—C(1)—C(6)	117·82 (23)
C(1)—C(2)	1·381 (5)	C(2)—C(1)—C(6)	119·41 (28)
C(1)—C(6)	1·393 (4)	C(1)—C(2)—C(3)	120·60 (28)
C(2)—C(3)	1·391 (6)	C(2)—C(3)—C(4)	119·82 (35)
C(3)—C(4)	1·377 (5)	C(3)—C(4)—C(5)	120·17 (35)
C(4)—C(5)	1·378 (6)	C(4)—C(5)—C(6)	120·28 (30)
C(5)—C(6)	1·395 (6)	C(1)—C(6)—C(5)	119·67 (30)
C(7)—C(8)	1·515 (5)	P—C(7)—C(8)	113·76 (22)
C(9)—C(10)	1·527 (4)	P—C(10)—O(2)	108·59 (19)
C(10)—C(11)	1·524 (5)	P—C(10)—C(9)	108·18 (19)
C(10)—O(2)	1·426 (4)	P—C(10)—C(11)	108·60 (16)
C(11)—C(12)	1·381 (4)	O(2)—C(10)—C(9)	105·26 (20)
C(11)—C(16)	1·397 (5)	O(2)—C(10)—C(11)	113·27 (22)
C(12)—C(13)	1·389 (6)	C(9)—C(10)—C(11)	112·76 (24)
C(13)—C(14)	1·382 (6)	C(10)—C(11)—C(12)	121·66 (27)
C(14)—C(15)	1·395 (6)	C(10)—C(11)—C(16)	120·76 (25)
C(15)—C(16)	1·381 (6)	C(12)—C(11)—C(16)	117·55 (30)
		C(11)—C(12)—C(13)	121·98 (30)
O(1)—P—C(1)	111·14 (13)	C(12)—C(13)—C(14)	120·02 (31)
O(1)—P—C(7)	113·11 (12)	C(13)—C(14)—C(15)	118·73 (35)
O(1)—P—C(10)	112·34 (13)	C(14)—C(15)—C(16)	120·68 (34)
C(1)—P—C(7)	107·08 (14)	C(11)—C(16)—C(15)	121·01 (28)

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