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(2-Chlorophenyl)(diphenylphosphoryl)-methanol

Wan-Yun Liu* and Ping Huo

Department of Chemistry and Bioengineering, Yichun University, Yichun 336000, People's Republic of China
Correspondence e-mail: liuwanyun2006@tom.com

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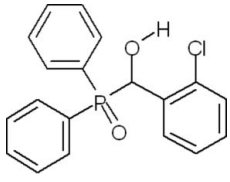
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.035; wR factor = 0.084; data-to-parameter ratio = 16.7.

The title compound, $C_{19}H_{16}ClO_2P$, was obtained by the reaction of diphenylphosphine oxide with 2-chlorobenzaldehyde. The molecule has a tetrahedral structure at the P atom. The dihedral angle between the phenyl rings attached to the P atom is 80.4 (1)°. The molecules are linked together by intermolecular O—H···O and C—H···O hydrogen-bonding interactrions. The crystal studied was an inversion twin.

Related literature

For general background, see: Clark *et al.* (2002). For related structures, see: Dankowski *et al.* (1979); Liu *et al.* (2007).



Experimental

Crystal data

$C_{19}H_{16}ClO_2P$
M_r = 342.74
Orthorhombic, $P2_12_12_1$
a = 9.0943 (4) Å
b = 10.9172 (6) Å
c = 18.0657 (12) Å
V = 1793.64 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 293 (2) K
0.57 × 0.20 × 0.10 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; (Bruker, 2001)
T_{min} = 0.844, T_{max} = 0.970
8361 measured reflections
3466 independent reflections
2494 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.084
S = 0.91
3466 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Absolute structure: Flack (1983), 1437 Friedel pairs
Flack parameter: 0.55 (8)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···O1^{i}	0.82	1.82	2.602 (2)	158
C1—H3A···O1^{i}	0.98	2.56	3.059 (2)	111
C16—H33A···O2^{ii}	0.93	2.56	3.318 (3)	139

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2343).

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supplementary materials

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(2-Chlorophenyl)(diphenylphosphoryl)methanol

W.-Y. Liu and P. Huo

Comment

The title compound is an analog of (diphenylphosphinoyl)phenylmethanol, which was employed as a ligand in the rhodiumcatalyzed hydroformylation of alkenes, with good conversions and regioselectivities (Clark *et al.*, 2002).

The molecular structure is shown in Fig. 1. Bond lengths and angles are in agreement with those reported for similar compounds (Dankowski *et al.*, 1979; Liu *et al.*, 2007). The dihedral angle between the C8-phenyl and C14-phenyl planes is 80.4 (1)°. The O—H···O and C—H···O hydrogen bonds (Table 1) involving the hydroxyl group link the molecules into a supra-molecular structure.

Experimental

To a solution of 2-chlorobenzaldehyde (0.28 g, 2.0 mmol) and diphenylphosphine oxide (0.41 g, 2.0 mmol) in tetrahydrofuran (10 ml) at 273 K was added dropwise triethylamine (0.30 ml, 2.0 mmol). The cooling bath was removed and the mixture warmed to ambient temperature for 2 h. The solvent was concentrated under vacuum and the crude product was purified by column chromatography (petroleum ether-ethyl acetate, 1:1) to give the title compound as a white solid in 85% yield. Single crystals were obtained by slow evaporation of a methanol solution.

Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å (aromatic), 0.98 Å (methine), O—H = 0.82 Å, and U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(O). The absolute structure was not determined.

Figures

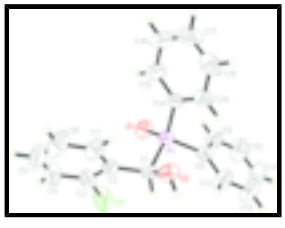


Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids (arbitrary spheres for H atoms).

'(2-Chlorophenyl)(diphenylphosphoryl)methanol'

Crystal data

$C_{19}H_{16}ClO_2P$ F_{000} = 712

M_r = 342.74	D_x = 1.269 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 3220 reflections
a = 9.0943 (4) Å	θ = 2.5–32.6º
b = 10.9172 (6) Å	μ = 0.31 mm^{-1}
c = 18.0657 (12) Å	T = 293 (2) K
V = 1793.64 (17) Å^3	Plate, colorless
Z = 4	0.57 × 0.20 × 0.10 mm

Data collection

Bruker APEX area-detector diffractometer	3466 independent reflections
Radiation source: fine-focus sealed tube	2494 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.035
T = 293(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 2.5º
Absorption correction: multi-scan (SADABS; (Bruker, 2001)	h = −11→10
T_{min} = 0.844, T_{max} = 0.970	k = −13→13
8361 measured reflections	l = −22→19

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.035	$w = 1/[\sigma^2(F_o^2) + (0.0482P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.084	$(\Delta/\sigma)_{max} < 0.001$
S = 0.91	$\Delta\rho_{max}$ = 0.20 e Å^{-3}
3466 reflections	$\Delta\rho_{min}$ = −0.26 e Å^{-3}
208 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1437 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.55 (8)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculat-

ing *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
P1	0.39075 (6)	0.07346 (5)	0.22300 (3)	0.03563 (15)
Cl1	0.68961 (8)	0.08726 (10)	0.36635 (5)	0.0874 (3)
C1	0.4310 (2)	0.20391 (18)	0.28358 (14)	0.0371 (5)
H3A	0.5340	0.2276	0.2764	0.045*
C2	0.4092 (3)	0.1697 (2)	0.36374 (14)	0.0425 (6)
C3	0.5177 (3)	0.1153 (3)	0.40525 (16)	0.0574 (7)
C4	0.4977 (4)	0.0838 (3)	0.47859 (18)	0.0795 (9)
H26A	0.5729	0.0468	0.5054	0.095*
C5	0.3652 (5)	0.1080 (3)	0.5109 (2)	0.0929 (12)
H12A	0.3501	0.0876	0.5603	0.112*
C6	0.2538 (4)	0.1621 (3)	0.4712 (2)	0.0850 (11)
H27A	0.1637	0.1775	0.4937	0.102*
C7	0.2752 (3)	0.1935 (2)	0.39825 (17)	0.0616 (8)
H10A	0.1998	0.2308	0.3718	0.074*
C8	0.4778 (2)	0.1058 (2)	0.13569 (14)	0.0405 (6)
C9	0.5076 (3)	0.0066 (3)	0.09105 (16)	0.0575 (7)
H8A	0.4765	−0.0711	0.1053	0.069*
C10	0.5824 (4)	0.0211 (3)	0.02620 (17)	0.0771 (10)
H19A	0.6024	−0.0467	−0.0033	0.093*
C11	0.6281 (4)	0.1348 (3)	0.00437 (18)	0.0807 (10)
H21A	0.6781	0.1442	−0.0402	0.097*
C12	0.6006 (4)	0.2345 (3)	0.04770 (18)	0.0818 (10)
H20A	0.6325	0.3117	0.0331	0.098*
C13	0.5251 (3)	0.2202 (3)	0.11336 (17)	0.0641 (8)
H11A	0.5058	0.2881	0.1428	0.077*
C14	0.1961 (2)	0.0688 (2)	0.20812 (13)	0.0421 (5)
C15	0.1179 (3)	−0.0269 (3)	0.23868 (18)	0.0702 (8)
H13A	0.1659	−0.0852	0.2674	0.084*
C16	−0.0321 (4)	−0.0361 (4)	0.2266 (3)	0.0999 (12)
H33A	−0.0845	−0.1009	0.2471	0.120*
C17	−0.1028 (4)	0.0485 (4)	0.1851 (2)	0.0939 (11)
H22A	−0.2038	0.0421	0.1780	0.113*
C18	−0.0284 (3)	0.1419 (3)	0.1541 (2)	0.0795 (10)
H17A	−0.0780	0.1992	0.1253	0.095*
C19	0.1227 (3)	0.1530 (2)	0.16514 (16)	0.0590 (7)
H14A	0.1740	0.2173	0.1434	0.071*
O1	0.44309 (17)	−0.04402 (12)	0.25449 (9)	0.0471 (4)
O2	0.34008 (16)	0.30243 (12)	0.26047 (10)	0.0491 (5)
H2A	0.3910	0.3630	0.2525	0.074*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0332 (3)	0.0318 (3)	0.0419 (3)	0.0014 (3)	0.0010 (3)	0.0005 (3)
Cl1	0.0540 (4)	0.1355 (7)	0.0726 (5)	0.0196 (5)	−0.0150 (4)	0.0185 (6)
C1	0.0298 (11)	0.0323 (11)	0.0493 (14)	0.0003 (9)	0.0007 (11)	−0.0017 (11)
C2	0.0517 (14)	0.0346 (12)	0.0413 (14)	−0.0059 (11)	0.0048 (14)	−0.0053 (11)
C3	0.0652 (17)	0.0603 (18)	0.0467 (16)	−0.0005 (14)	−0.0054 (15)	−0.0049 (14)
C4	0.099 (2)	0.089 (2)	0.0506 (19)	−0.005 (2)	−0.0087 (18)	0.0145 (18)
C5	0.140 (4)	0.091 (3)	0.0477 (18)	−0.015 (3)	0.024 (2)	0.0091 (18)
C6	0.103 (3)	0.078 (2)	0.074 (2)	0.005 (2)	0.041 (2)	0.0077 (19)
C7	0.0624 (17)	0.0542 (16)	0.068 (2)	0.0005 (14)	0.0213 (16)	0.0022 (15)
C8	0.0352 (11)	0.0436 (14)	0.0427 (14)	0.0033 (10)	0.0008 (11)	−0.0010 (12)
C9	0.0623 (18)	0.0587 (17)	0.0515 (17)	0.0010 (14)	0.0121 (15)	−0.0047 (14)
C10	0.092 (3)	0.081 (2)	0.059 (2)	0.0148 (19)	0.0227 (19)	−0.0111 (17)
C11	0.095 (2)	0.091 (3)	0.056 (2)	0.014 (2)	0.032 (2)	0.0139 (18)
C12	0.106 (3)	0.0631 (19)	0.076 (2)	−0.003 (2)	0.032 (2)	0.0198 (17)
C13	0.080 (2)	0.0497 (17)	0.062 (2)	0.0061 (15)	0.0202 (17)	0.0086 (14)
C14	0.0349 (11)	0.0469 (12)	0.0446 (14)	−0.0067 (12)	0.0003 (10)	−0.0040 (13)
C15	0.0531 (16)	0.0746 (17)	0.083 (2)	−0.0208 (15)	−0.0027 (17)	0.0197 (16)
C16	0.060 (2)	0.122 (3)	0.117 (3)	−0.044 (2)	−0.001 (2)	0.021 (3)
C17	0.0360 (14)	0.143 (3)	0.103 (3)	−0.021 (2)	−0.0043 (19)	−0.006 (3)
C18	0.0530 (18)	0.099 (2)	0.086 (3)	0.0122 (18)	−0.0214 (18)	0.001 (2)
C19	0.0388 (14)	0.0696 (17)	0.069 (2)	−0.0036 (14)	−0.0068 (14)	0.0108 (14)
O1	0.0562 (10)	0.0317 (8)	0.0535 (10)	0.0105 (7)	0.0034 (9)	0.0033 (7)
O2	0.0413 (8)	0.0317 (8)	0.0743 (13)	0.0030 (6)	−0.0005 (9)	0.0047 (8)

Geometric parameters (Å, °)

P1—O1	1.4816 (15)	C9—H8A	0.9300
P1—C14	1.792 (2)	C10—C11	1.367 (4)
P1—C8	1.800 (3)	C10—H19A	0.9300
P1—C1	1.833 (2)	C11—C12	1.364 (4)
Cl1—C3	1.741 (3)	C11—H21A	0.9300
C1—O2	1.420 (2)	C12—C13	1.380 (4)
C1—C2	1.509 (3)	C12—H20A	0.9300
C1—H3A	0.9800	C13—H11A	0.9300
C2—C3	1.374 (4)	C14—C19	1.375 (3)
C2—C7	1.393 (3)	C14—C15	1.379 (3)
C3—C4	1.381 (4)	C15—C16	1.385 (4)
C4—C5	1.364 (5)	C15—H13A	0.9300
C4—H26A	0.9300	C16—C17	1.351 (5)
C5—C6	1.374 (5)	C16—H33A	0.9300
C5—H12A	0.9300	C17—C18	1.346 (5)
C6—C7	1.375 (4)	C17—H22A	0.9300
C6—H27A	0.9300	C18—C19	1.394 (4)
C7—H10A	0.9300	C18—H17A	0.9300
C8—C9	1.378 (3)	C19—H14A	0.9300

C8—C13	1.380 (3)	O2—H2A	0.8200
C9—C10	1.364 (4)		
O1—P1—C14	110.54 (11)	C10—C9—H8A	119.7
O1—P1—C8	111.42 (10)	C8—C9—H8A	119.7
C14—P1—C8	107.99 (11)	C9—C10—C11	120.3 (3)
O1—P1—C1	112.28 (10)	C9—C10—H19A	119.8
C14—P1—C1	107.99 (10)	C11—C10—H19A	119.8
C8—P1—C1	106.42 (11)	C12—C11—C10	120.2 (3)
O2—C1—C2	113.15 (18)	C12—C11—H21A	119.9
O2—C1—P1	107.26 (15)	C10—C11—H21A	119.9
C2—C1—P1	110.76 (15)	C11—C12—C13	119.6 (3)
O2—C1—H3A	108.5	C11—C12—H20A	120.2
C2—C1—H3A	108.5	C13—C12—H20A	120.2
P1—C1—H3A	108.5	C12—C13—C8	120.6 (3)
C3—C2—C7	117.7 (2)	C12—C13—H11A	119.7
C3—C2—C1	122.4 (2)	C8—C13—H11A	119.7
C7—C2—C1	119.9 (2)	C19—C14—C15	118.8 (2)
C2—C3—C4	122.4 (3)	C19—C14—P1	123.04 (18)
C2—C3—Cl1	120.0 (2)	C15—C14—P1	118.1 (2)
C4—C3—Cl1	117.5 (3)	C14—C15—C16	120.0 (3)
C5—C4—C3	118.6 (3)	C14—C15—H13A	120.0
C5—C4—H26A	120.7	C16—C15—H13A	120.0
C3—C4—H26A	120.7	C17—C16—C15	120.4 (3)
C4—C5—C6	120.7 (3)	C17—C16—H33A	119.8
C4—C5—H12A	119.6	C15—C16—H33A	119.8
C6—C5—H12A	119.6	C18—C17—C16	120.6 (3)
C5—C6—C7	120.2 (3)	C18—C17—H22A	119.7
C5—C6—H27A	119.9	C16—C17—H22A	119.7
C7—C6—H27A	119.9	C17—C18—C19	120.1 (3)
C6—C7—C2	120.4 (3)	C17—C18—H17A	120.0
C6—C7—H10A	119.8	C19—C18—H17A	120.0
C2—C7—H10A	119.8	C14—C19—C18	120.1 (3)
C9—C8—C13	118.6 (3)	C14—C19—H14A	120.0
C9—C8—P1	116.43 (19)	C18—C19—H14A	120.0
C13—C8—P1	124.8 (2)	C1—O2—H2A	109.5
C10—C9—C8	120.6 (3)		
O1—P1—C1—O2	−162.66 (13)	C14—P1—C8—C13	98.3 (2)
C14—P1—C1—O2	−40.54 (17)	C1—P1—C8—C13	−17.4 (3)
C8—P1—C1—O2	75.19 (16)	C13—C8—C9—C10	0.1 (4)
O1—P1—C1—C2	−38.74 (18)	P1—C8—C9—C10	−175.5 (3)
C14—P1—C1—C2	83.38 (18)	C8—C9—C10—C11	−0.4 (5)
C8—P1—C1—C2	−160.89 (15)	C9—C10—C11—C12	0.7 (6)
O2—C1—C2—C3	−153.6 (2)	C10—C11—C12—C13	−0.6 (6)
P1—C1—C2—C3	85.9 (2)	C11—C12—C13—C8	0.3 (5)
O2—C1—C2—C7	26.2 (3)	C9—C8—C13—C12	0.0 (4)
P1—C1—C2—C7	−94.3 (2)	P1—C8—C13—C12	175.1 (3)
C7—C2—C3—C4	0.3 (4)	O1—P1—C14—C19	−165.4 (2)
C1—C2—C3—C4	−179.9 (3)	C8—P1—C14—C19	−43.2 (2)

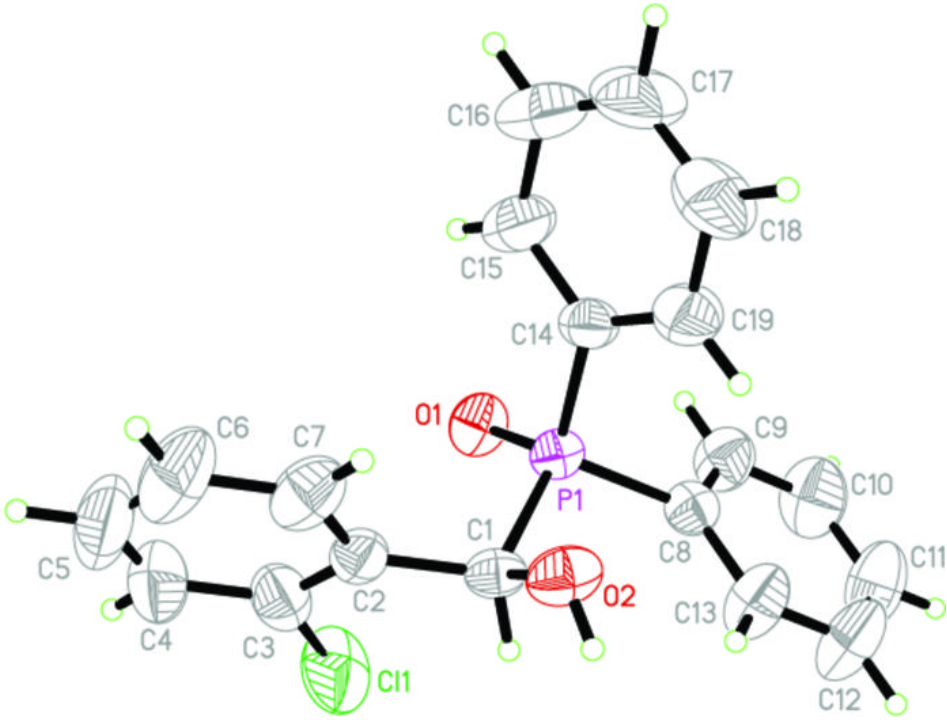
C7—C2—C3—Cl1	−178.04 (19)	C1—P1—C14—C19	71.5 (2)
C1—C2—C3—Cl1	1.8 (3)	O1—P1—C14—C15	11.7 (2)
C2—C3—C4—C5	−0.2 (5)	C8—P1—C14—C15	133.8 (2)
Cl1—C3—C4—C5	178.2 (3)	C1—P1—C14—C15	−111.5 (2)
C3—C4—C5—C6	0.3 (5)	C19—C14—C15—C16	−0.8 (5)
C4—C5—C6—C7	−0.5 (5)	P1—C14—C15—C16	−178.0 (3)
C5—C6—C7—C2	0.7 (5)	C14—C15—C16—C17	−0.2 (6)
C3—C2—C7—C6	−0.6 (4)	C15—C16—C17—C18	1.0 (6)
C1—C2—C7—C6	179.6 (3)	C16—C17—C18—C19	−0.7 (6)
O1—P1—C8—C9	35.1 (2)	C15—C14—C19—C18	1.1 (4)
C14—P1—C8—C9	−86.4 (2)	P1—C14—C19—C18	178.1 (2)
C1—P1—C8—C9	157.82 (19)	C17—C18—C19—C14	−0.4 (5)
O1—P1—C8—C13	−140.1 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2A···O1^{i}	0.82	1.82	2.602 (2)	158
C1—H3A···O1^{i}	0.98	2.56	3.059 (2)	111
C16—H33A···O2^{ii}	0.93	2.56	3.318 (3)	139

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+1/2; (ii) −*x*, *y*−1/2, −*z*+1/2.

Fig. 1


C17
C16
C18
C15
C19
C14
O1
C6
C7
C9
P1
C10
C1
C8
C11
C5
O2
C2
C13
C4
C3
Cl1
C12