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Diphenyl (hydroxyphenylmethyl)phosphonate

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.004 Å
R factor = 0.051
wR factor = 0.142
Data-to-parameter ratio = 13.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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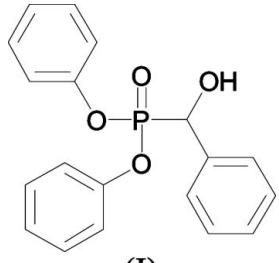
The title compound, $C_{19}H_{17}O_4P$, was obtained as colorless block-shaped crystals by the reaction of diphenyl phosphite and benzaldehyde. The crystal structure is stabilized by strong intermolecular O—H···O hydrogen bonds.

Comment

Some α-hydroxyphenymethylphosphonic esters and their derivaties are compounds of significant biological and pharmaceutical interest, affording properties such as inhibition of inositol monophosphatase (Maier & Diel, 1994). They are useful reagents for the synthesis of enol ethers and α-ketophosphonates (Babak & Rahman, 2001). Bond lengths and angles in the title compound, (I), are in agreement with the values reported in the literature (Lane *et al.*, 1996; Fang *et al.*, 2006). The hydroxy group is involved in hydrogen-bonding interactions with the phosphoryl O atom of a neighboring molecule [O···O = 2.691 (2) Å] (Table 1 and Fig. 2).



(I)

Experimental

To a solution of benzaldehyde (5.3 g, 50 mmol) and diphenyl phosphite (11.7 g, 50 mmol) in tetrahydrofuran (30 ml) at 268 K was added triethylamine (1 ml). The mixture was left to stand at ambient temperature for 24 h, during which time a precipitate separated. The precipitate was filtered off and rapidly washed with benzene (Walsh, 1959). Single crystals were obtained by crystallization from benzene and ethanol (6:1 *v*/*v*) solution.

Crystal data

$C_{19}H_{17}O_4P$
M_r = 340.30
Monoclinic, $P2_1/n$
a = 10.349 (3) Å
b = 7.881 (2) Å
c = 20.362 (6) Å
β = 102.075 (5)°
V = 1624.0 (8) Å^3
Z = 4
D_x = 1.392 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 273 (2) K
Block, colourless
0.29 × 0.20 × 0.18 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.947, T_{max} = 0.967
7898 measured reflections
2857 independent reflections
2472 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.142
S = 1.03
2857 reflections
217 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0849P)^2 + 0.3832P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1B···O4^{i}	0.82	1.87	2.691 (2)	178

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

All H atoms were placed in geometrically idealized positions and treated as riding on their parent atoms, with C—H = 0.93 Å (aromatic) or 0.98 Å (CH), O—H = 0.82 Å, and U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(O).

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* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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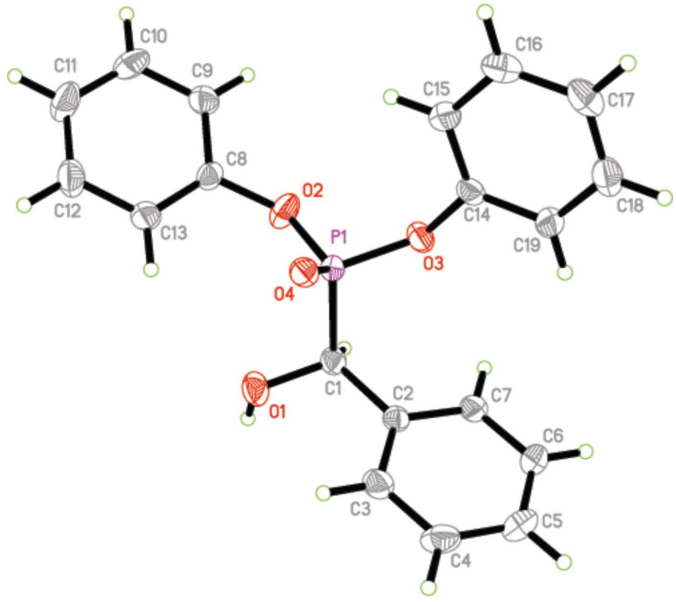

Figure 1
A molecular view of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

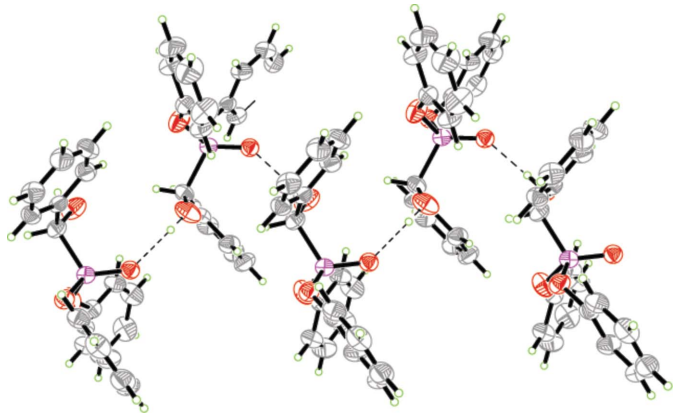

Figure 2
Packing diagram of (I), showing the O—H···O interactions as dashed lines. [Symmetry code: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.]

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