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Diisopropyl (hydroxyphenylmethyl)phosphonate

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.005 Å
R factor = 0.061
wR factor = 0.158
Data-to-parameter ratio = 15.4

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

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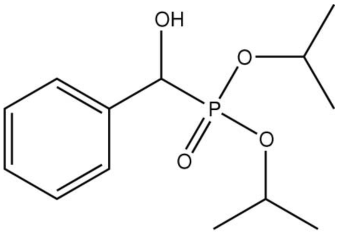
The title compound, $C_{13}H_{21}O_4P$, was obtained by the reaction of diisopropyl phosphite and benzaldehyde. The crystal structure is stabilized by strong intermolecular O—H···O hydrogen bonds.

Comment

Some α-hydroxyphenymethylphosphonic acids and their derivatives display various interesting biological properties, such as inhibition of inositol monophosphatase (Maier & Diel, 1994). Bond lengths and angles in the title compound, (I), are in agreement with the values reported in the literature (Fang *et al.*, 2005). The crystal packing is stabilized by strong intermolecular O···O hydrogen-bonding interactions (Table 1 and Fig. 2).



(I)

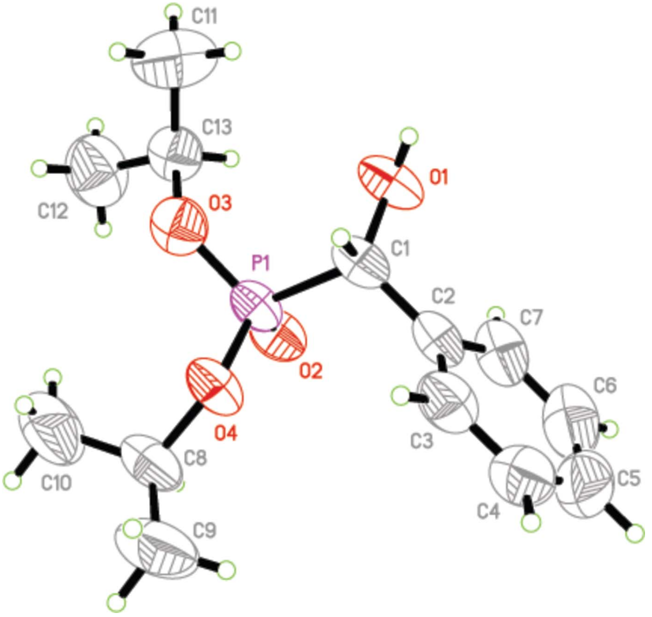


Figure 1
A view of the molecule of (I), with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

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Experimental

To a solution of benzaldehyde (5.3 g, 50 mmol) and diisopropyl phosphite (8.3 g, 50 mmol) in tetrahydrofuran (30 ml) at 268 K was added aqueous ammonia (16 ml). The mixture was left to stand at ambient temperature for 2 h, during which time a precipitate separated. The precipitate was filtered off and washed rapidly with cold diethyl ether (Drescher *et al.*, 1995). Single crystals were obtained by crystallization of a dichloromethane–petroleum ether (1:6 *v*/*v*) solution.

Crystal data

$C_{13}H_{21}O_4P$
$M_r = 272.27$
Monoclinic, $P2_1/n$
$a = 9.680\ (3)$ Å
$b = 8.579\ (3)$ Å
$c = 18.007\ (6)$ Å
$\beta = 100.217\ (6)^\circ$
$V = 1471.7\ (8)$ Å^3
$Z = 4$

$D_x = 1.229$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2266 reflections
$\theta = 2.2$–25.1°
$\mu = 0.19$ mm^{-1}
$T = 273\ (2)$ K
Block, colourless
0.49 × 0.21 × 0.11 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{\min} = 0.912$, $T_{\max} = 0.979$
7150 measured reflections

2591 independent reflections
2136 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.025$
$\theta_{\max} = 25.0^\circ$
$h = -10 \rightarrow 11$
$k = -8 \rightarrow 10$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.061$
$wR(F^2) = 0.158$
$S = 1.09$
2591 reflections
168 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.076P)^2 + 0.5611P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.38$ e Å^{-3}
$\Delta\rho_{\min} = -0.19$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2$^{\rm i}$	0.82	1.89	2.705 (3)	176

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

The H atoms were positioned geometrically (C—H = 0.93, 0.98 and 0.96 Å for phenyl, methine and methyl H atoms, respectively, and O—H = 0.82 Å) and were included in the refinement in the riding-model approximation. $U_{\rm iso}$(H) values were set equal to $xU_{\rm eq}$ of the carrier atom, where x = 1.5 for methyl and x = 1.2 for all other H atoms.

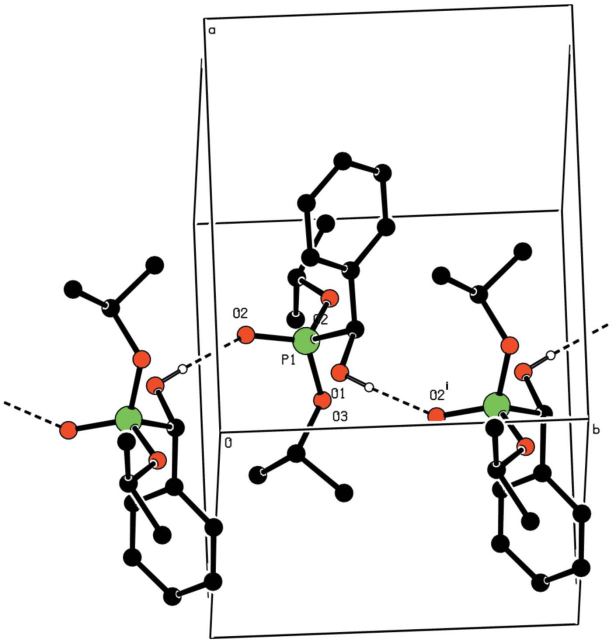

Figure 2
Packing diagram of the title compound, (I), showing the O—H···O interactions as dashed lines. H atoms not involved in hydrogen bonding have been omitted. [Symmetry code: (i) $x - \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$.]

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

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