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Key indicators

Single-crystal X-ray study
 $T = 273$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.060
 wR factor = 0.178
Data-to-parameter ratio = 19.5For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

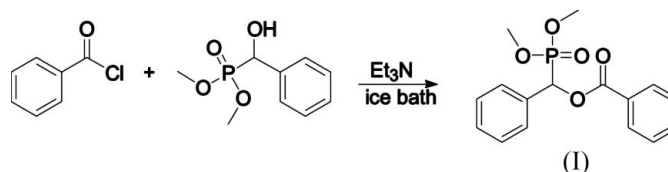
(Dimethoxyphosphoryl)(phenyl)methyl benzoate

The title compound, $\text{C}_{16}\text{H}_{17}\text{O}_5\text{P}$, was obtained by the reaction
of benzoyl chloride and dimethyl (hydroxyphenylmethyl)-
phosphonate. The molecular packing is stabilized by van der
Waals forces.

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Comment

The title compound, (I), was synthesized for a study of its
antimicrobial activity against *Bacillus subtilis*. The hydroxy-
phosphonic acid derivative was found to have moderate
antimicrobial activity (inhibition zone = 7.5 mm). The crystal
packing is stabilized by van der Waals forces, and bond lengths
and angles in (I) are in agreement with the values reported in
the literature (Smaardijk *et al.*, 1985; Deron *et al.*, 2002).

Experimental

(Hydroxyphenylmethyl)phosphonic acid dimethyl ester, $\text{C}_6\text{H}_5\text{CH}-$
 $(\text{OH})\text{P}(\text{O})(\text{OCH}_3)_2$, was prepared according to the procedure of
Fang *et al.* (2006). This ester (1.08 g, 5 mmol) was dissolved in dry
tetrahydrofuran (20 ml) to which triethylamine (0.7 ml) was added,
and the solution was added dropwise to benzoyl chloride (0.7 g,
5 mmol) in the same solvent (10 ml). After completion of the reac-
tion, the precipitate was separated and the filtrate was extracted with
ethyl acetate, dried over anhydrous MgSO_4 and concentrated under
vacuum. The residual liquid was purified by column chromatography
to give the title compound. Single crystals of (I) suitable for X-ray
analysis were obtained by slow evaporation of a petroleum ether-
ethyl acetate solution (10:1 v/v).

Crystal data

$\text{C}_{16}\text{H}_{17}\text{O}_5\text{P}$	$Z = 8$
$M_r = 320.27$	$D_x = 1.324$ Mg m $^{-3}$
Orthorhombic, $Pbca$	Mo $K\alpha$ radiation
$a = 9.400$ (2) Å	$\mu = 0.19$ mm $^{-1}$
$b = 10.739$ (2) Å	$T = 273$ (2) K
$c = 31.821$ (7) Å	Chunk, colorless
$V = 3212.2$ (12) Å 3	$0.42 \times 0.19 \times 0.11$ mm

Data collection

Bruker APEX area-detector diffractometer	18166 measured reflections 3871 independent reflections 2947 reflections with $I > 2\sigma(I)$
φ scans	$R_{\text{int}} = 0.070$
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$\theta_{\text{max}} = 28.3^\circ$
$T_{\text{min}} = 0.924$, $T_{\text{max}} = 0.979$	

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.060$
 $wR(F^2) = 0.178$
 $S = 1.04$
 3871 reflections
 199 parameters
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0984P)^2 + 0.4253P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.42 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.41 \text{ e } \text{Å}^{-3}$

All H atoms were placed in geometrically idealized positions and treated as riding on their parent atoms, with C–H = 0.93 (aromatic), 0.98 (CH) or 0.96 Å (CH₃), and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{aromatic C, CH})$ or $1.5U_{\text{eq}}(\text{methyl C})$.

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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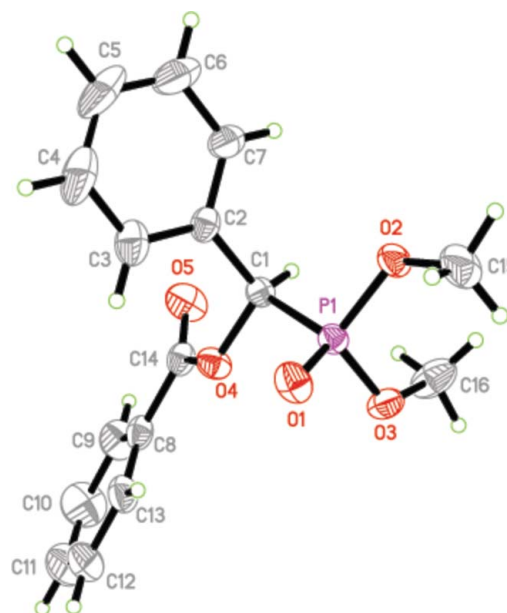


Figure 1
 View of the molecular structure of (I) with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

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