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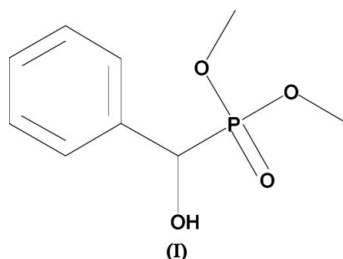
## Key indicators

Single-crystal X-ray study  
 $T = 273$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å  
 $R$  factor = 0.067  
 $wR$  factor = 0.186  
Data-to-parameter ratio = 17.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Dimethyl [hydroxy(phenyl)methyl]-  
phosphonateThe title compound,  $\text{C}_9\text{H}_{13}\text{O}_4\text{P}$ , has been obtained by the reaction of dimethyl phosphite and benzaldehyde. In the crystal structure, intermolecular  $\text{O}-\text{H} \cdots \text{O}$  hydrogen bonds link the molecules into infinite chains.

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## Comment

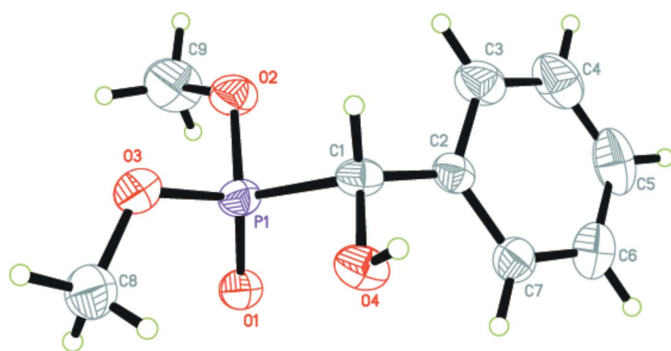
Some  $\alpha$ -hydroxyphenylmethylphosphonic esters and their derivatives are compounds of significant biological and pharmaceutical interest, for example as inhibitors of inositol monophosphatase (Maier & Diel, 1994). They are useful reagents for the synthesis of enol ethers and  $\alpha$ -ketophosphonates (Babak & Rahman, 2001).Bond lengths and angles in the title compound, (I), are in agreement with the values reported for related compounds (Smaardijk *et al.*, 1985; Aras *et al.*, 2003). The hydroxy unit is involved in a hydrogen-bonding interaction with the phosphoryl O atom of a neighboring molecule (Table 1 and Fig. 2).

## Experimental

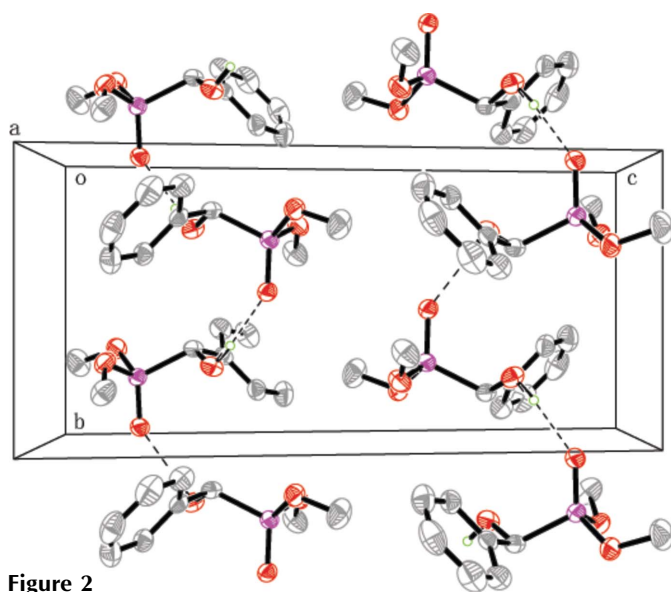
To a solution of benzaldehyde (5.3 g, 50 mmol) and dimethyl phosphite (5.5 g, 50 mmol) in tetrahydrofuran (30 ml) at 268 K was added ammonia (16 ml, 25% aqueous). The mixture was left to stand at ambient temperature for 3 h, during which time a precipitate separated. The precipitate was filtered off and rapidly washed with cold diethyl ether (Martine *et al.*, 1995). Single crystals were obtained by crystallization from dichloromethane and petroleum ether (1:6 *v/v*).

## Crystal data

 $\text{C}_9\text{H}_{13}\text{O}_4\text{P}$   
 $M_r = 216.16$   
Monoclinic,  $P2_1/n$   
 $a = 8.400$  (3) Å  
 $b = 7.737$  (3) Å  
 $c = 16.477$  (6) Å  
 $\beta = 98.949$  (7)°  
 $V = 1057.8$  (7) Å<sup>3</sup>  
 $Z = 4$  $D_x = 1.357$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
Cell parameters from 1831 reflections  
 $\theta = 2.3$ – $25.6$ °  
 $\mu = 0.25$  mm<sup>-1</sup>  
 $T = 273$  (2) K  
Chunk, colorless  
 $0.46 \times 0.20 \times 0.18$  mm

**Figure 1**

The molecular structure of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are drawn as spheres of arbitrary radii.

**Figure 2**

Packing, showing the O—H...O hydrogen bonds as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

#### Data collection

Bruker SMART APEX area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Bruker, 2001)  
 $T_{\min} = 0.895$ ,  $T_{\max} = 0.957$   
 5687 measured reflections

2179 independent reflections  
 1728 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.044$   
 $\theta_{\text{max}} = 26.5^\circ$   
 $h = -10 \rightarrow 10$   
 $k = -9 \rightarrow 9$   
 $l = -12 \rightarrow 20$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.067$   
 $wR(F^2) = 0.186$   
 $S = 1.09$   
 2179 reflections  
 127 parameters  
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.1044P)^2 + 0.0871P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.49 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.33 \text{ e } \text{\AA}^{-3}$

**Table 1**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O4-H4B\cdots O1^i$	0.82	1.88	2.689 (3)	168

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 = 0.95 (aromatic) or 0.98 (CH and CH<sub>3</sub>), O—H = 0.82  $\text{\AA}$  and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{aromatic C, CH, O})$  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 ViewerPro (Accelrys, 2001); software used to prepare material for publication: SHELXL97.

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