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## Key indicators

Single-crystal X-ray study  
*T* = 293 K  
Mean  $\sigma(\text{C}-\text{C})$  = 0.005 Å  
*R* factor = 0.043  
*wR* factor = 0.084  
Data-to-parameter ratio = 13.1For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Diisopropyl [(2-hydroxy-1-naphthyl)-  
methyl]phosphonate

The bond lengths and angles in the title compound,  $\text{C}_{17}\text{H}_{23}\text{PO}_4$ , are in accordance with anticipated values. There are two conformers in the asymmetric unit. They differ from each other in the orientation of the C and P tetrahedra. Analysis of the structure does not reveal any significant differences between the bond distances and angles of the molecules in the asymmetric unit. In the crystal structure, the conformers are linked by  $\text{O}-\text{H}\cdots\text{O}=\text{P}$  and  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds.

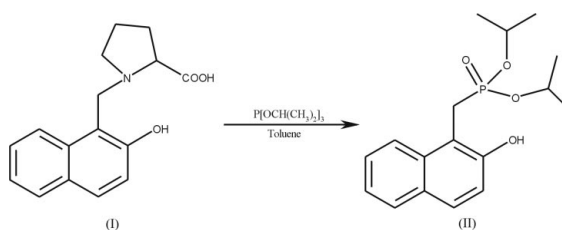
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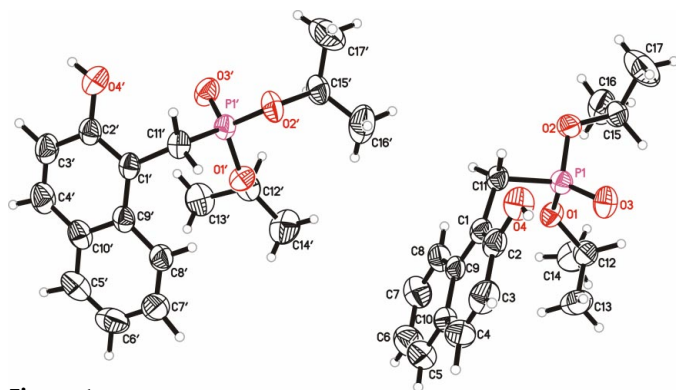
## Comment

Phosphorus derivatives are an important class of biologically active compounds (Kabacnik, 1987). The reaction of phenolic Mannich bases with trialkoxyphosphites leads to methylphosphonate derivatives of phenols (Ivanov & Valitova, 1967; Hahn & Weglewski, 1968; Rupp & Heiner, 1982). In our investigations, we used a  $\beta$ -naphthol derivative of L-proline, (I), and triisopropyl phosphite. In this paper, we present the results of X-ray crystallographic analysis of the title compound, (II).



The presence of a stereogenic centre in derivative (I) creates the possibility of stereoselective synthesis of chiral phosphorous derivatives; this is still under investigation.

The title compound crystallizes in space group  $P2_1$ , with two nearly centrosymmetrically related molecules in the asymmetric unit. The two independent conformers, *A* and *B*, are shown in Fig. 1. In conformer *A*, the dihedral angle between planes  $\text{C}2-\text{C}1-\text{C}11$  and  $\text{C}1-\text{C}11-\text{P}1$  is  $88.2(3)^\circ$ , while in the conformer *B* it is  $-88.6(3)^\circ$ . The  $-\text{CPO}(\text{OC}_3\text{H}_7)_2$  and hydroxynaphthyl groups in the two conformers are therefore twisted by  $-178.6(2)$  and  $-179.4(2)^\circ$ . Analysis of the structure does not reveal significant differences in the bond distances and angles of the two molecules in the asymmetric unit. The most significant differences in bond length between the two conformers are  $0.026(4)$  and  $0.023(5)$  Å for  $\text{C}1-\text{C}2$  and  $\text{C}2-\text{C}3$ , respectively. The 2-hydroxynaphthyl group is nearly planar. The torsion angles which most deviate from  $0^\circ$  or  $180^\circ$  are  $\text{C}9-\text{C}1-\text{C}2-\text{O}4$  [ $-177.3(3)^\circ$ ] and  $\text{C}9'-\text{C}1'-\text{C}2'-\text{O}4'$  [ $177.3(2)^\circ$ ] (Table 1). The bond lengths and angles in the structure are in accordance with anticipated values



**Figure 1**

The molecular structure of the title compound, showing the two independent conformers, *A* and *B*, in the asymmetric unit. Displacement ellipsoids are drawn at the 50% probability level.

(Tahar *et al.*, 1996; Langley *et al.*, 1996). In these compounds, there is a characteristic pattern of torsion angles and of the orientation of the C and P tetrahedra (Ružić-Toroš & Kojić-Prodić, 1987). The aromatic system and O2 or O2' are *anti* to each other [O2–P1–C11–C1 = 178.6 (2) and O2'–P1'–C11'–C1' = 179.4 (2)°], while the P–C bond is perpendicular to the plane of the hydroxynaphthyl group in both conformers (Benedetto *et al.*, 1997). No H atoms were located in the region of O3 or O3'. In the crystal structure, conformers *A* and *B* are linked by O–H···O=P hydrogen bonds, leading to dimerization (Fig. 2). Those dimers are joined by weak C–H···O hydrogen bonds (Table 2).

## Experimental

A solution of compound (I) and P[OCH(CH<sub>3</sub>)<sub>2</sub>]<sub>3</sub> was heated to reflux in toluene for 4 h. The resulting solution was evaporated and acetonitrile was added. After 24 h, compound (II) crystallized with a yield of 75%. The melting point is 398–399 K.

### Crystal data

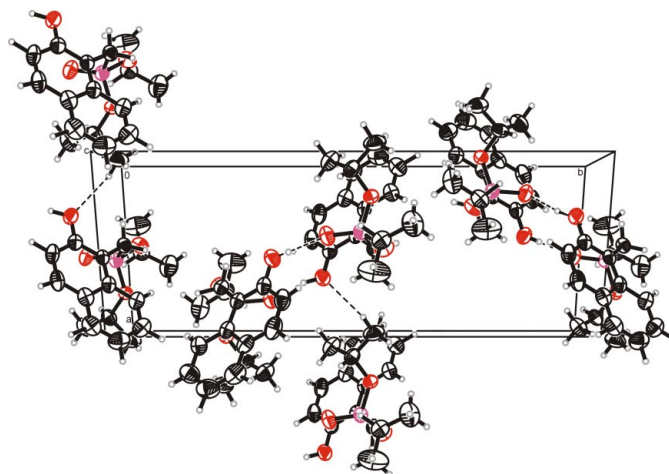
C <sub>17</sub> H <sub>23</sub> PO <sub>4</sub>	$D_x = 1.231 \text{ Mg m}^{-3}$
$M_r = 322.32$	Mo $K\alpha$ radiation
Monoclinic, $P2_1$	Cell parameters from 6056 reflections
$a = 9.166 (1) \text{ \AA}$	$\theta = 3.6\text{--}25.0^\circ$
$b = 22.484 (2) \text{ \AA}$	$\mu = 0.17 \text{ mm}^{-1}$
$c = 9.579 (1) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 118.21 (1)^\circ$	Irregular, colourless
$V = 1739.7 (3) \text{ \AA}^3$	$0.20 \times 0.15 \times 0.10 \text{ mm}$
$Z = 4$	

### Data collection

Oxford Diffraction Xcalibur diffractometer	6056 independent reflections
$\omega$ scans	4614 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.029$
$T_{\text{min}} = 0.966$ , $T_{\text{max}} = 0.979$	$\theta_{\text{max}} = 25.0^\circ$
10929 measured reflections	$h = -10 \rightarrow 10$
	$k = -26 \rightarrow 26$
	$l = -11 \rightarrow 6$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0387P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.043$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.084$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.00$	$\Delta\rho_{\text{max}} = 0.15 \text{ e \AA}^{-3}$
6056 reflections	$\Delta\rho_{\text{min}} = -0.21 \text{ e \AA}^{-3}$
463 parameters	Absolute structure: Flack (1983)
All H-atoms parameters refined	Flack parameter = 0.00 (8)



**Figure 2**

Crystal packing of the title compound. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines.

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

C1–C2	1.366 (4)	C1'–C2'	1.385 (4)
C2–C3	1.418 (5)	C2'–C3'	1.403 (4)
C14–C12–C13	113.1 (3)	C14'–C12'–C13'	113.9 (3)
C9–C1–C2–O4	–177.3 (3)	C9'–C1'–C2'–O4'	177.3 (2)
C2–C1–C11–P1	88.2 (3)	C2'–C1'–C11'–P1'	–88.6 (3)
O2–P1–C11–C1	–178.6 (2)	O2'–P1'–C11'–C1'	–179.4 (2)

**Table 2**

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

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
O4–H4A···O3 <sup>i</sup>	0.80 (4)	1.88 (4)	2.683 (3)	178 (4)
O4'–H4C···O3 <sup>ii</sup>	0.89 (4)	1.80 (4)	2.669 (3)	166 (3)
C3'–H3B···O3 <sup>ii</sup>	1.02 (3)	2.59 (3)	3.318 (5)	128 (2)

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

H atoms bonded to the terminal CH<sub>3</sub> groups were refined using a riding model. The coordinates of the remaining H atoms were refined freely.

Data collection: *CrysAlisCCD* (Oxford Diffraction, 2002); cell refinement: *CrysAlisRED* (Oxford Diffraction, 2002); data reduction: *CrysAlisRED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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