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(Diphenylphosphoryl)(4-nitrophenyl)methanol

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The title compound, $C_{19}H_{16}NO_4P$, was obtained by the reaction of diphenylphosphine oxide and 4-nitrobenzaldehyde. Molecules are linked into chains, running along the *b* axis, by O—H···O and C—H···O intermolecular hydrogen bonds.

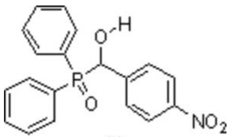
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.042
wR factor = 0.128
Data-to-parameter ratio = 14.3

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

Comment

The title compound, (I), is an analogue of (diphenylphosphinoyl)phenylmethanol, which is employed as a ligand in the rhodium-catalysed hydroformylation of alkenes, with good yields and regioselectivities (Clark *et al.*, 2002).



(I)

The molecular structure of (I) is shown in Fig. 1. Bond lengths and angles in (I) are in agreement with those reported for similar compounds (Dankowski *et al.*, 1979; Fang *et al.*, 2006). The dihedral angle between the C8-phenyl and C14-phenyl planes is 56.1 (1)°. The O3—N1—C5—C4 and O4—N1—C5—C4 torsion angles of −35.0 (2) and 144.94 (18)°, respectively, indicate that the nitro group is twisted away from the attached ring.

O—H···O and C—H···O hydrogen bonds (Table 1) involving the hydroxyl group link the molecules into a chain running along the *b* axis. In addition, O3···N1($2-x, -y, -z$) [2.849 (3) Å], O3···O3($2-x, -y, -z$) [2.896 (3) Å] and O4···O4($2-x, 1-y, -z$) [2.892 (3) Å] short contacts are observed in the crystal structure.

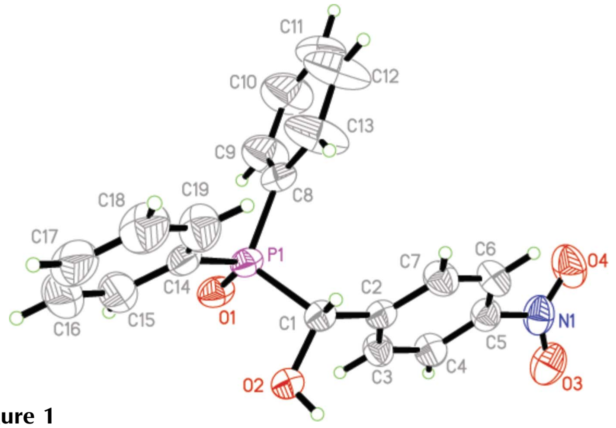


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids (arbitrary spheres for H atoms).

Experimental

To a precooled solution of 4-nitrobenzaldehyde (0.15 g, 1.0 mmol) and diphenylphosphine oxide (0.20 g, 1.0 mmol) in tetrahydrofuran (10 ml) at 273 K was added dropwise triethylamine (0.15 ml, 1.0 mmol). The cooling bath was removed and the mixture warmed to ambient temperature for 3 h. The solvent was concentrated under vacuum and the crude product was purified by column chromatography (petroleum ether–ethyl acetate, 1:1) to give the title compound as a white solid in 88% yield. Single crystals of (I) were obtained by slow evaporation of a methanol solution.

Crystal data

$C_{19}H_{16}NO_4P$
$M_r = 353.30$
Monoclinic, $P2_1/n$
$a = 11.449$ (3) Å
$b = 6.1417$ (15) Å
$c = 23.624$ (6) Å
$\beta = 94.409$ (5)°
$V = 1656.2$ (7) Å^3

$Z = 4$
$D_x = 1.417$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.19$ mm^{-1}
$T = 298$ (2) K
Needle, colourless
0.72 × 0.27 × 0.20 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{\min} = 0.875$, $T_{\max} = 0.963$

8522 measured reflections
3236 independent reflections
2800 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.020$
$\theta_{\max} = 26.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.128$
$S = 1.01$
3236 reflections
226 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0846P)^2 + 0.3649P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.35$ e Å^{-3}
$\Delta\rho_{\min} = -0.20$ e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O2—H2$A\cdots$O1$^{\rm i}$	0.82	1.93	2.696 (2)	156
C1—H1$B\cdots$O2$^{\rm i}$	0.98	2.47	3.050 (2)	117

Symmetry code: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 (aromatic) or 0.98 Å (methine), O—H = 0.82 Å, and $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C) and $1.5U_{\rm eq}$(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 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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