2-(Diphenylphosphino)phenyl 2-(diphenylphosphinoyl)phenyl ether

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Key indicators

Single-crystal X-ray study
 $T = 150\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$
 R factor = 0.039
 wR factor = 0.098
Data-to-parameter ratio = 18.1

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, $\text{C}_{36}\text{H}_{28}\text{O}_2\text{P}_2$, features weak inter- and intramolecular hydrogen bonds linking molecules into infinite chains.

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Comment

The title compound, (I), was inadvertently obtained during an attempt to synthesize a nickel–phosphine complex.

The structure features a weak hydrogen bond between aromatic atom H6 and the phosphine oxide O atom, which a search of the Cambridge Structural Database (Version 5.26; Allen, 2002) shows to be a common feature in phenyl-substituted phosphine oxides. An additional weak (Steiner, 1996) bifurcated intermolecular hydrogen bond is also present between O2 and H27 and H28, which joins the molecules into an infinite chain along $[1\bar{1}0]$.

Figure 1
View of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity.

Experimental

A tetrahydrofuran solution of 2 equivalents of bis[2-(diphenylphosphino)phenyl] ether and bis(1,5-cyclooctadiene)nickel(0) was layered with *n*-pentane and placed in a freezer, resulting in a crop of off-white crystals after 5 d. ^{31}P NMR (162 MHz, C_6D_6): δ 22.8 (s), -17.5 (s).

Crystal data

$\text{C}_{36}\text{H}_{28}\text{O}_2\text{P}_2$	$Z = 2$
$M_r = 554.52$	$D_x = 1.286 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 9.9316$ (7) Å	Cell parameters from 152 reflections
$b = 10.2786$ (5) Å	$\theta = 4.3\text{--}21.9^\circ$
$c = 14.5778$ (10) Å	$\mu = 0.18 \text{ mm}^{-1}$
$\alpha = 75.785$ (4)°	$T = 150$ (2) K
$\beta = 83.778$ (6)°	Block, colourless
$\gamma = 85.529$ (6)°	$0.3 \times 0.3 \times 0.15 \text{ mm}$
$V = 1432.05$ (16) Å ³	

Data collection

Nonius KappaCCD diffractometer	$R_{\text{int}} = 0.044$
ω and φ scans	$\theta_{\text{max}} = 27.5^\circ$
Absorption correction: none	$h = -12 \rightarrow 12$
26296 measured reflections	$k = -13 \rightarrow 13$
6527 independent reflections	$l = -18 \rightarrow 18$
5195 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0396P)^2 + 0.7162P]$
$R[F^2 > 2\sigma(F^2)] = 0.039$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.098$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.04$	$\Delta\rho_{\text{max}} = 0.31 \text{ e Å}^{-3}$
6527 reflections	$\Delta\rho_{\text{min}} = -0.33 \text{ e Å}^{-3}$
361 parameters	
H-atom parameters constrained	

Table 1

Hydrogen-bond geometry (Å, °).

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
$\text{C6--H6}\cdots\text{O2}$	0.95	2.56	2.975 (2)	107
$\text{C27--H27}\cdots\text{O2}^i$	0.95	2.59	3.206 (2)	123
$\text{C28--H28}\cdots\text{O2}^i$	0.95	2.58	3.202 (2)	123

Symmetry code: (i) $x - 1, y + 1, z$.

Figure 2

C—H $\cdots$ O hydrogen bonding (dashed lines) around the phosphine oxide. [Symmetry code: (A) $1 + x, 1 - y, z$.]

All H atoms were placed in geometrically idealized positions (C—H = 0.95 Å) and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for all other H atoms.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DIRAX* (Duisenberg, 1992); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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