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

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
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.

The title compound, $C_{36}H_{28}O_2P_2$, features weak inter- and intramolecular hydrogen bonds linking molecules into infinite chains.

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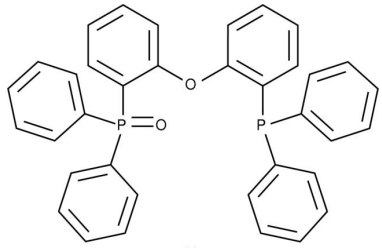
Comment

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



(I)

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].

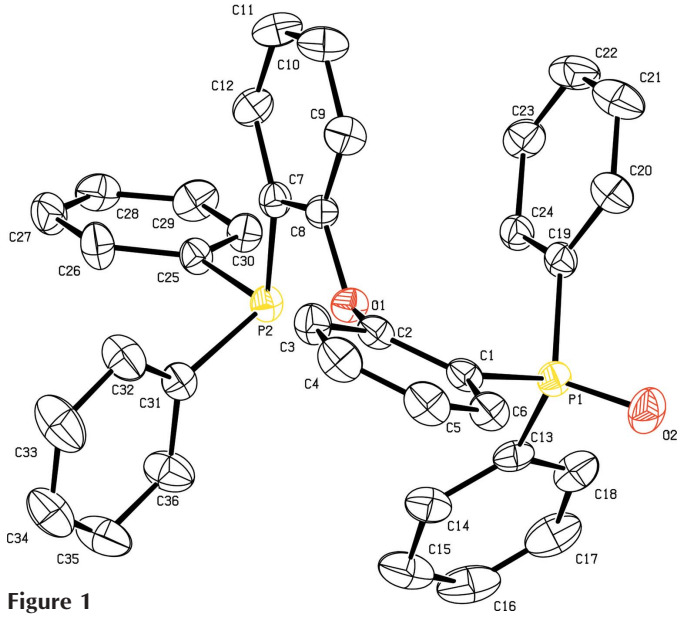


Figure 1
View of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity.

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

$C_{36}H_{28}O_2P_2$	$Z = 2$
$M_r = 554.52$	$D_x = 1.286$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 9.9316$ (7) Å	Cell parameters from 152 reflections
$b = 10.2786$ (5) Å	$\theta = 4.3$–$21.9°$
$c = 14.5778$ (10) Å	$\mu = 0.18$ mm^{-1}
$\alpha = 75.785$ (4)°	$T = 150$ (2) K
$\beta = 83.778$ (6)°	Block, colourless
$\gamma = 85.529$ (6)°	0.3 × 0.3 × 0.15 mm
$V = 1432.05$ (16) Å^3	

Data collection

Nonius KappaCCD diffractometer	$R_{int} = 0.044$
ω and φ scans	$\theta_{max} = 27.5°$
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	$w = 1/[\sigma^2(F_o^2) + (0.0396P)^2 + 0.7162P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.039$	
$wR(F^2) = 0.098$	
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.001$
6527 reflections	$\Delta\rho_{max} = 0.31$ e Å^{-3}
361 parameters	$\Delta\rho_{min} = -0.33$ e Å^{-3}
H-atom parameters constrained	

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O2	0.95	2.56	2.975 (2)	107
C27—H27···O2^{i}	0.95	2.59	3.206 (2)	123
C28—H28···O2^{i}	0.95	2.58	3.202 (2)	123

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

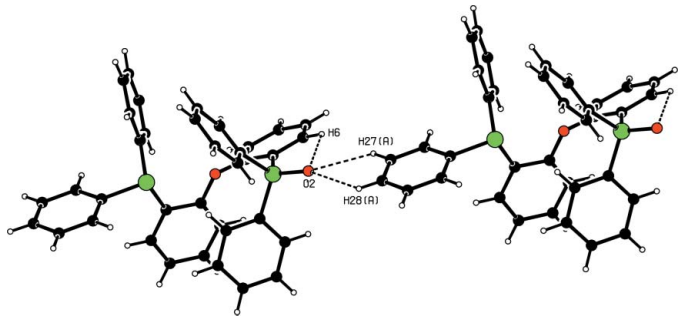


Figure 2
C—H···O hydrogen bonding (dashed lines) around the phosphine oxide. [Symmetry code: (A) $1 + x, 1 - y, z$.

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