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

Duncan M. Tooke,[a]* Jos Wilting,[b] Dieter Vogt[b] and Anthony L. Spek[a]

[a]Bijvoet Center for Biomolecular Research, Crystal and Structural Chemistry, Utrecht University, Padualaan 8, 3584 CH Utrecht, The Netherlands, and [b]Schuit Institute of Catalysis, PO Box 513, 5600 MB Eindhoven, The Netherlands

Correspondence e-mail: d.m.tooke@chem.uu.nl

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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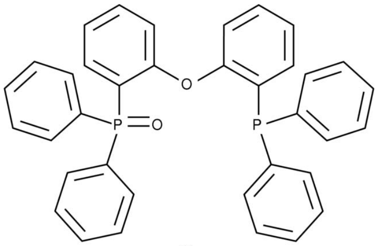
Comment

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$\overline{1}$0].

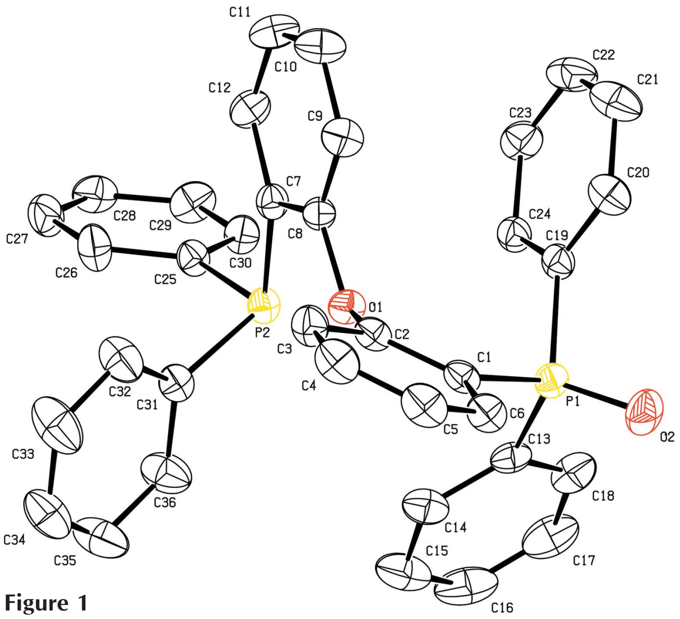


Figure 1
View of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity.

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

$C_{36}H_{28}O_2P_2$
$M_r = 554.52$
Triclinic, $P\overline{1}$
$a = 9.9316$ (7) Å
$b = 10.2786$ (5) Å
$c = 14.5778$ (10) Å
$\alpha = 75.785$ (4)°
$\beta = 83.778$ (6)°
$\gamma = 85.529$ (6)°
$V = 1432.05$ (16) Å^3

$Z = 2$
$D_x = 1.286$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 152 reflections
$\theta = 4.3$–21.9°
$\mu = 0.18$ mm^{-1}
$T = 150$ (2) K
Block, colourless
0.3 × 0.3 × 0.15 mm

Data collection

Nonius KappaCCD diffractometer
ω and φ scans
Absorption correction: none
26296 measured reflections
6527 independent reflections
5195 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.044$
$\theta_{\rm max} = 27.5°$
$h = -12 \rightarrow 12$
$k = -13 \rightarrow 13$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.098$
$S = 1.04$
6527 reflections
361 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0396P)^2 + 0.7162P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.31$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.33$ e Å^{-3}

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$^{\rm i}$	0.95	2.59	3.206 (2)	123
C28—H28···O2$^{\rm i}$	0.95	2.58	3.202 (2)	123

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

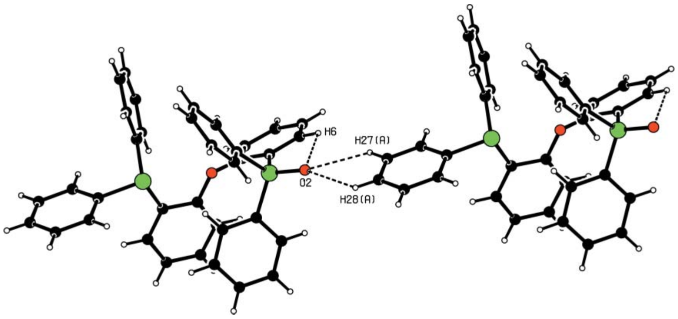


Figure 2
C—H···O hydrogen bonding (dashed lines) around the phosphine oxide. [Symmetry code: (A) $1 + x, 1 - y, z$.

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