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Butyldiphenylphosphine oxide

Judy Caddy,[a] E. Mabel Coyanis,[b] Andreas Lemmerer,[b] Setshaba D. Khanye[b] and Bernard Omondi[b]*

[a]Project AuTEK, Mintek, Private Bag X3015, Randburg 2125, South Africa, and [b]Molecular Science Institute, School of Chemistry, University of the Witwatersrand, PO Wits, 2050 Johannesburg, South Africa

Correspondence e-mail:
bernard@chem.wits.ac.za

Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.031
wR factor = 0.084
Data-to-parameter ratio = 15.5

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

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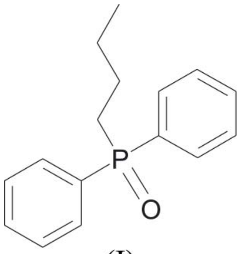
The solid state structure of the title compound, $C_{16}H_{19}OP$, an organic tertiary phosphine oxide, is stabilized mainly by C—H$\cdots\pi$ intermolecular interactions.

Comment

There has been considerable interest in studying phosphine oxides as ligands, particularly as chelating ligands for complex formation with transition metals. The title compound, (I) (Fig. 1), has the expected deformed tetrahedral arrangement around the phosphorus atom, with C—P—C angles smaller than tetrahedral and O—P—C angles larger than tetrahedral values (Table 1), and also with a normal P═O bond distance (Bye *et al.*, 1982). The dihedral angle between the mean weighted least-squares planes of the phenyl rings (atoms C5–C10 and C11–C16) is 70.62 (6)°.



(I)

In the crystal structure, molecules of (I) are connected through three C—H$\cdots\pi$ intermolecular interactions (Table 2), resulting in a two-dimensional network parallel to the *ac*

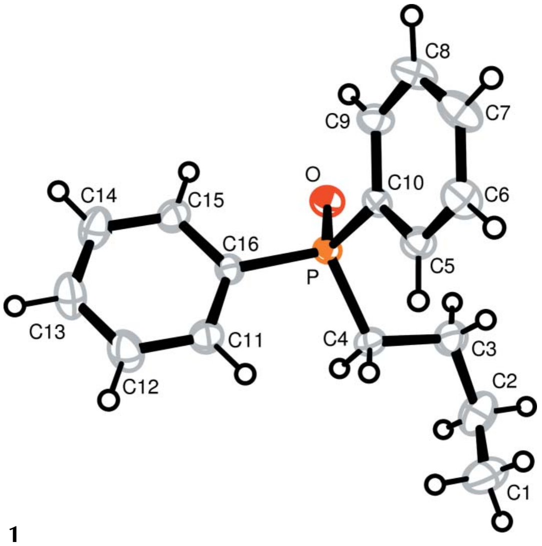


Figure 1
The molecular structure of (I), showing the atomic numbering scheme and 50% probability displacement ellipsoids.

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plane. Atom C2 in the molecule at (x, y, z) acts a donor atom *via* H2*A* and H2*B* to the phenyl rings in the molecule at ($1 + x$, y, z), thereby generating a chain along the *a* axis. The third C—H···π interaction is generated *via* atom H14 of the molecule at (x, y, z) to the C5–C10 phenyl ring of the molecule at ($-\frac{1}{2} + x$, $1 - y$, $\frac{1}{2} + z$) (Fig. 2).

Experimental

The title compound (the oxidized form of butyldiphenylphosphine) was serendipitously obtained upon exposure of the unoxidized ligand to air, during the attempted crystallization of an organometallic compound by slow evaporation from hexane.

Crystal data

$C_{16}H_{19}OP$
$M_r = 258.28$
Monoclinic, *Pn*
$a = 8.1289\ (12)$ Å
$b = 5.9814\ (9)$ Å
$c = 14.600\ (2)$ Å
$\beta = 93.326\ (3)$°
$V = 708.68\ (18)$ Å^3
$Z = 2$
$D_x = 1.210$ Mg m^{-3}
Mo *Kα* radiation
$\mu = 0.18$ mm^{-1}
$T = 173\ (2)$ K
Block, colourless
0.44 × 0.32 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
4597 measured reflections
2532 independent reflections
2474 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.021$
$\theta_{\rm max} = 28.0$°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.084$
$S = 1.06$
2532 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0541P)^2 + 0.118P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.011$
$\Delta\rho_{\rm max} = 0.34$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.19$ e Å^{-3}
Absolute structure: Flack (1983), 825 Friedel pairs
Flack parameter: −0.04 (8)

Table 1
Selected bond angles (°).

O—P—C4	115.03 (8)	O—P—C10	110.95 (8)
O—P—C16	110.89 (8)	C4—P—C10	107.95 (9)
C4—P—C16	105.27 (9)	C16—P—C10	106.23 (8)

Table 2
Hydrogen-bond geometry (Å, °).

*Cg*1 and *Cg*2 denote the centroids of the C5–C10 and C11–C16 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2*A*···*Cg*2$^{\rm i}$	0.99	2.86	3.676 (3)	153
C2—H2*B*···*Cg*1$^{\rm i}$	0.99	2.71	3.695 (3)	174
C14—H14···*Cg*1$^{\rm ii}$	0.95	2.91	3.729 (3)	145

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

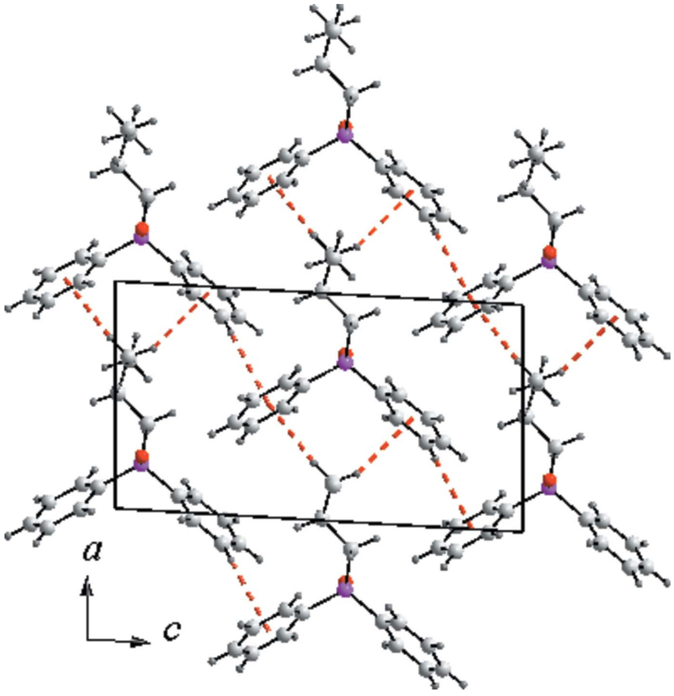

Figure 2
Packing diagram of (I), viewed down the *b* axis. C—H···π interactions are shown as red dashed lines.

C-bound H atoms were positioned geometrically, with C—H = 0.93 Å, and allowed to ride on their parent atoms, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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References

Brandenburg, K. (2006). *DIAMOND*. Version 2.1e. Crystal Impact GbR, Bonn, Germany.
Bruker (1997). *SMART* (Version 5.6) and *SAINT* (Version 5.06a). Bruker AXS Inc., Madison, Wisconsin, USA.
Bye, E., Schweizer, B. W. & Dunitz, J. D. (1982). *J. Am. Chem. Soc.* **104**, 5893–5898.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

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