Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(4-Methoxyphenyl)diphenylphosphine

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.042
wR factor = 0.104
Data-to-parameter ratio = 12.4

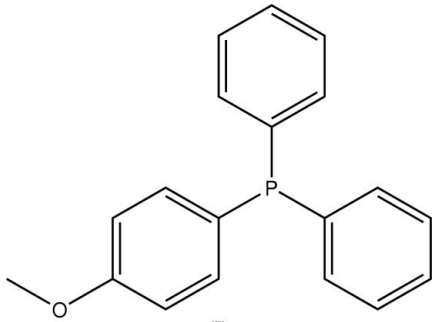
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 12 February 2007
Accepted 12 February 2007

The crystal structure of the title compound, $C_{19}H_{17}OP$, is stabilized by C—H···O and C—H···π interactions.

Comment

Triphenylphosphine, PPh_3, and its derivatives, such as compound (I), have been widely used in many areas of chemistry, especially as ligands in transition-metal-based homogeneous catalysis. Compound (I) was made as part of a larger synthetic investigation into complexes containing substituted phosphines. The structure of (I) has not previously been reported, although the structure of its corresponding oxide has been described (Whitaker *et al.*, 1995).



(I)

The molecular structure of (I) (Fig. 1) has a slightly distorted pyramidal geometry; the mean C—P—C angle (103.03°) angle is comparable with values of 102.99 and 102.8° for triphenylphosphine (Daly, 1964; Dunne & Orpen, 1991), as is the mean C—P bond length [1.831 (2) Å compared to 1.828 and 1.831 Å, respectively].

The extended structure exhibits a zigzag pattern where the molecules pack so that the methoxy groups of near neighbours pack are as far apart as possible. There is a clear intermolecular hydrogen bond [C10—H10 = 0.96 (2), H10···O^{i} = 2.694 (1), C10···O^{i} = 3.354 (3) Å and C10—H10···O^{i} 126.5 (5)°; symmetry code: (i) $1+x, y, z$] which links molecules into chains along the *a* direction. A C—H···Cπ interaction [C2—H2 = 0.98 (2), H2···C11^{ii} = 2.874 (1) Å, C2···C11^{ii} = 3.354 (5) Å and C2—H2···C11^{ii} = 165.41 (9)°; symmetry code: (ii) $\frac{3}{2}+x, -\frac{1}{2}+y, z$] is also present. A graphical representation of the extended structure is given in Fig. 2.

Experimental

Compound (I) was prepared according to a reported method (McEwan *et al.*, 1975). Crystals suitable for the diffraction study were obtained by slow cooling of a hot saturated ethanol solution.

Crystal data

$C_{19}H_{17}OP$
M_r = 292.3
Orthorhombic, *Pbca*
a = 10.8879 (4) Å
b = 11.8128 (4) Å
c = 23.9654 (14) Å
V = 3082.3 (2) Å^3
Z = 8
Mo *Kα* radiation
μ = 0.17 mm^{-1}
T = 293 (2) K
0.2 × 0.2 × 0.15 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
33037 measured reflections
3193 independent reflections
2498 reflections with $I > 2\sigma(I)$
R_{int} = 0.065

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.104
S = 1.05
3193 reflections
258 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

All H atoms were refined isotropically [C—H = 0.94 (2)–1.00 (3) Å].

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); 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: *WinGX* (Farrugia, 1999).

PJM thanks the EPSRC for a studentship.

References

Daly, J. J. (1964). *J. Chem. Soc. A*, pp. 3799–3810.
Dunne, B. J. & Orpen, A. G. (1991). *Acta Cryst.* C**47**, 345–347.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
McEwan, W. E., Shiau, W.-I., Yeh, Y.-I., Schulz, D. N., Pagilagan, R. U., Levy, J. L., Symes, C. Jr, Nelson, G. O. & Granoth, I. (1975). *J. Am. Chem. Soc.* **97**, 1787–1794.
Nonius (20008). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.

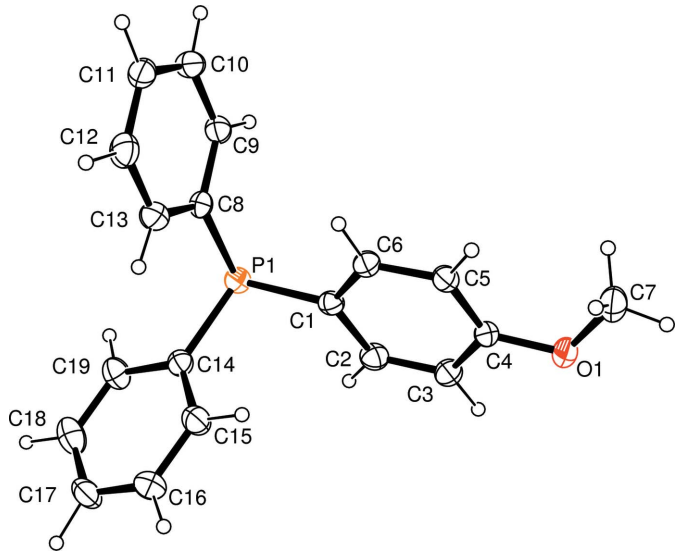


Figure 1
The structure of (I), with displacement ellipsoids drawn at the 30% probability level.

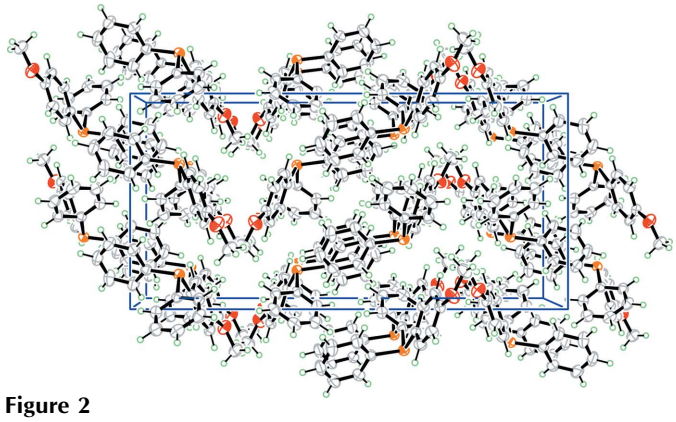


Figure 2
View normal to (100) of the extended structure of (I), showing the zigzag packing.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Whitaker, C. M., Kott, K. L. & McMahon, R. J. (1995). *J. Org. Chem.* **60**, 3499–3508.

supporting information

Acta Cryst. (2007). E**63**, o1339–o1340 [https://doi.org/10.1107/S1600536807007271]

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Crystal data

$C_{19}H_{17}OP$
$M_r = 292.3$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 10.8879$ (4) Å
$b = 11.8128$ (4) Å
$c = 23.9654$ (14) Å
$V = 3082.3$ (2) Å^3
$Z = 8$
$F(000) = 1232$
$D_x = 1.26$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3722 reflections
$\theta = 2$–27°
$\mu = 0.17$ mm^{-1}
$T = 293$ K
Prism, colourless
0.2 × 0.2 × 0.15 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: Enraf–Nonius FR590
Graphite monochromator
Detector resolution: 9 pixels mm^{-1}
CCD rotation images, thick slices scans
33037 measured reflections
3193 independent reflections
2498 reflections with $I > 2\sigma(I)$
$R_{int} = 0.065$
$\theta_{max} = 26.5°$, $\theta_{min} = 3.1°$
$h = 0 \rightarrow 13$
$k = 0 \rightarrow 14$
$l = 0 \rightarrow 30$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.104$
$S = 1.05$
3193 reflections
258 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.041P)^2 + 1.4742P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.88214 (16)	0.57892 (14)	0.64240 (7)	0.0337 (4)
C2	0.99900 (18)	0.62695 (16)	0.64880 (8)	0.0424 (4)
C3	1.09525 (17)	0.56660 (17)	0.67109 (9)	0.0437 (5)
C4	1.07743 (16)	0.45571 (16)	0.68899 (8)	0.0375 (4)
C5	0.96335 (17)	0.40543 (16)	0.68238 (8)	0.0379 (4)
C6	0.86713 (16)	0.46720 (15)	0.65923 (8)	0.0366 (4)
C7	1.1591 (2)	0.2977 (2)	0.73846 (11)	0.0539 (5)
C8	0.62513 (15)	0.57439 (14)	0.61868 (8)	0.0349 (4)
C9	0.55593 (17)	0.56854 (16)	0.66757 (9)	0.0416 (4)
C10	0.45233 (18)	0.50101 (18)	0.67087 (9)	0.0475 (5)
C11	0.41621 (18)	0.43818 (18)	0.62500 (10)	0.0482 (5)
C12	0.4850 (2)	0.44130 (18)	0.57668 (10)	0.0510 (5)
C13	0.58858 (18)	0.50932 (17)	0.57329 (9)	0.0437 (4)
C14	0.79069 (16)	0.69045 (14)	0.54461 (8)	0.0362 (4)
C15	0.8692 (2)	0.6235 (2)	0.51312 (9)	0.0504 (5)
C16	0.8938 (2)	0.6493 (2)	0.45795 (9)	0.0592 (6)
C17	0.8404 (2)	0.7429 (2)	0.43347 (9)	0.0573 (6)
C18	0.7608 (2)	0.8086 (2)	0.46334 (10)	0.0603 (6)
C19	0.7362 (2)	0.78278 (17)	0.51891 (9)	0.0490 (5)
O1	1.17739 (12)	0.40407 (12)	0.71215 (6)	0.0501 (4)
P1	0.75715 (4)	0.67060 (4)	0.61893 (2)	0.03547 (14)
H2	1.0096 (19)	0.7059 (18)	0.6368 (9)	0.052 (6)*
H3	1.178 (2)	0.5994 (18)	0.6762 (9)	0.054 (6)*
H5	0.9490 (18)	0.3257 (18)	0.6934 (9)	0.046 (5)*
H6	0.7889 (19)	0.4305 (16)	0.6562 (8)	0.042 (5)*
H7A	1.132 (2)	0.2382 (19)	0.7117 (10)	0.056 (6)*
H7B	1.095 (2)	0.303 (2)	0.7666 (11)	0.074 (8)*
H7C	1.240 (2)	0.2778 (19)	0.7527 (10)	0.063 (6)*
H9	0.5791 (18)	0.6119 (18)	0.7006 (9)	0.050 (6)*
H10	0.402 (2)	0.4981 (19)	0.7037 (10)	0.058 (6)*
H11	0.342 (2)	0.3925 (18)	0.6269 (9)	0.058 (6)*
H12	0.463 (2)	0.3969 (18)	0.5438 (10)	0.058 (6)*
H13	0.633 (2)	0.5124 (18)	0.5387 (10)	0.056 (6)*
H15	0.909 (2)	0.560 (2)	0.5290 (11)	0.072 (7)*
H16	0.950 (2)	0.599 (2)	0.4375 (12)	0.080 (8)*
H17	0.861 (2)	0.762 (2)	0.3941 (11)	0.069 (7)*
H18	0.719 (2)	0.873 (2)	0.4464 (12)	0.089 (9)*

H19	0.682 (2)	0.829 (2)	0.5403 (11)	0.074 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0361 (9)	0.0355 (9)	0.0295 (9)	−0.0016 (7)	0.0002 (7)	−0.0015 (7)
C2	0.0430 (10)	0.0386 (10)	0.0456 (11)	−0.0083 (8)	−0.0001 (9)	0.0042 (9)
C3	0.0345 (9)	0.0487 (11)	0.0478 (12)	−0.0089 (8)	−0.0030 (8)	0.0036 (9)
C4	0.0330 (9)	0.0484 (10)	0.0310 (9)	0.0007 (8)	−0.0006 (7)	0.0026 (8)
C5	0.0375 (9)	0.0394 (10)	0.0369 (10)	−0.0027 (8)	0.0004 (8)	0.0060 (8)
C6	0.0324 (9)	0.0381 (9)	0.0394 (10)	−0.0041 (8)	−0.0014 (8)	0.0019 (8)
C7	0.0493 (12)	0.0561 (13)	0.0562 (15)	0.0059 (10)	−0.0108 (11)	0.0140 (11)
C8	0.0329 (8)	0.0353 (9)	0.0365 (9)	0.0064 (7)	−0.0008 (7)	0.0039 (8)
C9	0.0417 (10)	0.0447 (10)	0.0383 (11)	0.0049 (8)	0.0006 (8)	0.0029 (8)
C10	0.0395 (10)	0.0541 (12)	0.0488 (12)	0.0041 (9)	0.0060 (9)	0.0129 (10)
C11	0.0362 (10)	0.0496 (11)	0.0589 (14)	−0.0026 (9)	−0.0049 (9)	0.0137 (10)
C12	0.0509 (12)	0.0514 (12)	0.0507 (13)	−0.0054 (10)	−0.0109 (10)	−0.0003 (10)
C13	0.0445 (10)	0.0477 (11)	0.0389 (11)	−0.0005 (9)	0.0001 (9)	0.0009 (9)
C14	0.0361 (9)	0.0362 (9)	0.0364 (10)	−0.0032 (7)	−0.0016 (7)	0.0019 (7)
C15	0.0529 (12)	0.0579 (13)	0.0403 (12)	0.0119 (10)	0.0049 (9)	0.0061 (10)
C16	0.0555 (13)	0.0841 (17)	0.0381 (12)	0.0065 (12)	0.0068 (10)	0.0028 (12)
C17	0.0648 (14)	0.0713 (15)	0.0358 (12)	−0.0179 (12)	−0.0029 (10)	0.0124 (11)
C18	0.0805 (16)	0.0524 (12)	0.0480 (13)	0.0008 (12)	−0.0137 (12)	0.0142 (10)
C19	0.0590 (12)	0.0426 (11)	0.0453 (12)	0.0068 (10)	−0.0047 (10)	0.0031 (9)
O1	0.0346 (7)	0.0616 (9)	0.0541 (9)	−0.0001 (6)	−0.0068 (6)	0.0148 (7)
P1	0.0389 (3)	0.0329 (2)	0.0346 (3)	0.00217 (18)	0.0016 (2)	−0.00096 (18)

Geometric parameters (Å, º)

C1—C6	1.390 (2)	C9—H9	0.98 (2)
C1—C2	1.402 (2)	C10—C11	1.384 (3)
C1—P1	1.8279 (18)	C10—H10	0.96 (2)
C2—C3	1.375 (3)	C11—C12	1.380 (3)
C2—H2	0.98 (2)	C11—H11	0.97 (2)
C3—C4	1.392 (3)	C12—C13	1.387 (3)
C3—H3	0.99 (2)	C12—H12	0.98 (2)
C4—O1	1.366 (2)	C13—H13	0.96 (2)
C4—C5	1.386 (3)	C14—C19	1.386 (3)
C5—C6	1.392 (3)	C14—C15	1.388 (3)
C5—H5	0.99 (2)	C14—P1	1.8331 (19)
C6—H6	0.96 (2)	C15—C16	1.383 (3)
C7—O1	1.420 (3)	C15—H15	0.94 (2)
C7—H7A	1.00 (2)	C16—C17	1.380 (3)
C7—H7B	0.98 (3)	C16—H16	0.98 (3)
C7—H7C	0.97 (2)	C17—C18	1.366 (3)
C8—C13	1.390 (3)	C17—H17	1.00 (3)
C8—C9	1.395 (3)	C18—C19	1.392 (3)
C8—P1	1.8325 (18)	C18—H18	0.97 (3)

C9—C10	1.384 (3)	C19—H19	0.95 (3)
C6—C1—C2	117.35 (16)	C9—C10—H10	122.2 (14)
C6—C1—P1	124.37 (13)	C12—C11—C10	119.9 (2)
C2—C1—P1	118.02 (13)	C12—C11—H11	120.3 (14)
C3—C2—C1	121.63 (17)	C10—C11—H11	119.8 (14)
C3—C2—H2	121.1 (13)	C11—C12—C13	120.4 (2)
C1—C2—H2	117.3 (13)	C11—C12—H12	121.8 (13)
C2—C3—C4	120.08 (17)	C13—C12—H12	117.8 (13)
C2—C3—H3	122.6 (13)	C12—C13—C8	120.49 (19)
C4—C3—H3	117.3 (12)	C12—C13—H13	118.9 (13)
O1—C4—C5	124.71 (17)	C8—C13—H13	120.6 (13)
O1—C4—C3	115.75 (16)	C19—C14—C15	118.05 (19)
C5—C4—C3	119.54 (17)	C19—C14—P1	116.57 (15)
C4—C5—C6	119.70 (17)	C15—C14—P1	125.33 (14)
C4—C5—H5	121.2 (12)	C16—C15—C14	120.9 (2)
C6—C5—H5	119.1 (12)	C16—C15—H15	118.2 (16)
C1—C6—C5	121.67 (17)	C14—C15—H15	120.9 (16)
C1—C6—H6	120.8 (11)	C17—C16—C15	120.1 (2)
C5—C6—H6	117.5 (11)	C17—C16—H16	122.2 (16)
O1—C7—H7A	112.3 (13)	C15—C16—H16	117.7 (16)
O1—C7—H7B	110.5 (15)	C18—C17—C16	120.0 (2)
H7A—C7—H7B	106 (2)	C18—C17—H17	121.1 (14)
O1—C7—H7C	104.2 (14)	C16—C17—H17	118.9 (14)
H7A—C7—H7C	108.7 (19)	C17—C18—C19	119.9 (2)
H7B—C7—H7C	115 (2)	C17—C18—H18	121.4 (17)
C13—C8—C9	118.38 (17)	C19—C18—H18	118.7 (17)
C13—C8—P1	124.76 (14)	C14—C19—C18	121.0 (2)
C9—C8—P1	116.85 (14)	C14—C19—H19	118.4 (16)
C10—C9—C8	121.1 (2)	C18—C19—H19	120.6 (16)
C10—C9—H9	117.8 (12)	C4—O1—C7	117.65 (15)
C8—C9—H9	121.1 (13)	C1—P1—C8	102.56 (8)
C11—C10—C9	119.7 (2)	C1—P1—C14	103.10 (8)
C11—C10—H10	118.1 (14)	C8—P1—C14	103.44 (8)
C6—C1—C2—C3	−0.3 (3)	C14—C15—C16—C17	0.3 (4)
P1—C1—C2—C3	173.97 (16)	C15—C16—C17—C18	−1.6 (4)
C1—C2—C3—C4	−1.3 (3)	C16—C17—C18—C19	1.7 (4)
C2—C3—C4—O1	−177.96 (18)	C15—C14—C19—C18	−0.9 (3)
C2—C3—C4—C5	2.3 (3)	P1—C14—C19—C18	176.67 (17)
O1—C4—C5—C6	178.64 (18)	C17—C18—C19—C14	−0.4 (3)
C3—C4—C5—C6	−1.6 (3)	C5—C4—O1—C7	−9.4 (3)
C2—C1—C6—C5	1.0 (3)	C3—C4—O1—C7	170.80 (19)
P1—C1—C6—C5	−172.91 (15)	C6—C1—P1—C8	−4.60 (18)
C4—C5—C6—C1	0.0 (3)	C2—C1—P1—C8	−178.47 (14)
C13—C8—C9—C10	−0.9 (3)	C6—C1—P1—C14	−111.83 (16)
P1—C8—C9—C10	177.97 (14)	C2—C1—P1—C14	74.29 (16)
C8—C9—C10—C11	−0.1 (3)	C13—C8—P1—C1	−90.17 (17)

C9—C10—C11—C12	1.4 (3)	C9—C8—P1—C1	91.05 (15)
C10—C11—C12—C13	−1.7 (3)	C13—C8—P1—C14	16.80 (17)
C11—C12—C13—C8	0.6 (3)	C9—C8—P1—C14	−161.97 (14)
C9—C8—C13—C12	0.6 (3)	C19—C14—P1—C1	−160.33 (15)
P1—C8—C13—C12	−178.14 (15)	C15—C14—P1—C1	17.01 (19)
C19—C14—C15—C16	1.0 (3)	C19—C14—P1—C8	93.10 (16)
P1—C14—C15—C16	−176.35 (18)	C15—C14—P1—C8	−89.55 (18)