Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(Diphenylphosphoryl)(2-nitrophenyl)-methanol

Xiao-Ling Yuan, Wan-Yun Liu, Ping Huo and Guang-Quan Mei*

Key Laboratory of Jiangxi University for Applied Chemistry and Chemical Biology, Yichun 336000, People's Republic of China
Correspondence e-mail: yyhx2005@163.com

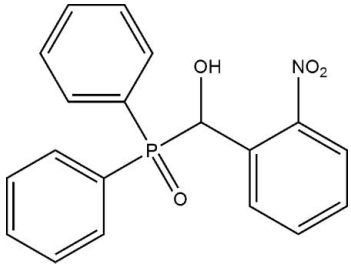
Received 13 July 2010; accepted 9 August 2010

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.029; wR factor = 0.078; data-to-parameter ratio = 14.7.

In the title compound, $C_{19}H_{16}NO_4P$, the dihedral angle between the mean planes of the phenyl rings bonded to the P atom is 75.4 (1)°. In the crystal, molecules are linked into chains running along the a axis by intermolecular O—H···O hydrogen bonds. Molecules are further connected into a three-dimensional array by weak C—H···O hydrogen bonds.

Related literature

For applications of the analogous compound (diphenylphosphinoyl)phenylmethanol in the rhodium-catalysed hydroformylation of alkenes, see: Clark *et al.* (2002). For related structures, see: Liu *et al.* (2007); Liu & Huo (2008).



Experimental

Crystal data

$C_{19}H_{16}NO_4P$
M_r = 353.30
Orthorhombic, $P2_12_12_1$
a = 5.9179 (12) Å
b = 13.917 (3) Å
c = 20.405 (4) Å
V = 1680.6 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 293 K
0.35 × 0.22 × 0.13 mm

Data collection

Bruker SMART APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.533, T_{max} = 1.000
14520 measured reflections
3311 independent reflections
3065 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.078
S = 1.05
3311 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Absolute structure: Flack (1983), 1377 Friedel pairs
Flack parameter: 0.19 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···O1^{i}	0.82	1.86	2.6483 (16)	161
C4—H4A···O3^{ii}	0.93	2.52	3.207 (2)	131
C19—H19A···O2^{iii}	0.93	2.50	3.404 (2)	164

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

The authors thank the Technical Project of the Department of Education of Jiangxi Province of China (Nos. GJJ08528 and GJJ09638) for supporting this work. We also thank the Hunan Provincial University Key Laboratory of QSAR/QSPR for providing technical assistance.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PB2037).

References

Bruker (2001). *SAINT*, *SMART* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Clark, H. J., Wang, R. & Alper, H. (2002). *J. Org. Chem.* **67**, 6224–6225.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Liu, W.-Y. & Huo, P. (2008). *Acta Cryst.* E**64**, o233.
Liu, W.-Y., Huo, P., Gao, Y.-X., Liu, P. & Zhao, Y.-F. (2007). *Acta Cryst.* E**63**, o1008–o1009.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supplementary materials

Acta Cryst. (2010). E**66**, o2331 [**doi:10.1107/S160053681003196X**]

(Diphenylphosphoryl)(2-nitrophenyl)methanol

X.-L. Yuan, W.-Y. Liu, P. Huo and G.-Q. Mei

Comment

The title compound, (I), is an analog of (diphenylphosphinoyl)phenylmethanol, which was employed as a ligand in the rhodium-catalyzed hydroformylation of alkenes, with good conversions and regioselectivities (Clark *et al.*, 2002).

The molecular structure of (I) is shown in Fig. 1. Bond lengths and angles in (I) are in agreement with those reported for similar compounds (Liu *et al.*, 2007; Liu *et al.*, 2008). The dihedral angle between the mean-planes of the phenyl rings (C8—C13) and (C14—C19) bonded to P-atoms is 53.0 (1)°. The strong O—H···O and weak C—H···O intermolecular hydrogen bonds play a significant role in stabilizing the crystal structure; see Table 1 for geometric parameters and symmetry operations. A strong O—H···O hydrogen bond involving the hydroxyl group link the molecules into a chain running along the *a* axis. Molecules are further connected into a three-dimensional array by non-classical and rather weak C—H···O intermolecular hydrogen-bonding interactions.

Experimental

To a solution of 2-nitrobenzaldehyde (0.30 g, 2.0 mmol) and diphenylphosphine oxide (0.40 g, 2.0 mmol) in tetrahydrofuran (10 ml) at 273 K was added dropwise triethylamine (0.03 ml, 2 mmol). The cooling bath was removed and the mixture warmed to ambient temperature for 2 h. The solvent was concentrated under vacuum and the crude product was purified by recrystallization in methanol to give the title compound as a white solid in 82% yield. Single crystals of (I) were obtained by slow evaporation of a methanol solution.

Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å (aromatic), 0.98 Å (methine), O—H = 0.82 Å, and U_{iso}(H) = 1.2U_{eq}(*c*) and 1.5U_{eq}(O).

Figures

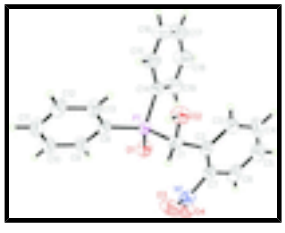


Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids (arbitrary spheres for H atoms).

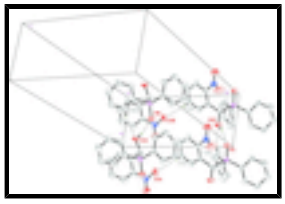


Fig. 2. Part of the packing of the title compound. Intermolecular hydrogen bonds are represented by dashed lines. H atoms not involved in hydrogen bonding have been omitted.

(Diphenylphosphoryl)(2-nitrophenyl)methanol

Crystal data

$C_{19}H_{16}NO_4P$	$F(000) = 736$
$M_r = 353.30$	$D_x = 1.396$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2ac 2ab	Cell parameters from 2260 reflections
$a = 5.9179$ (12) Å	$\theta = 3.3$–$27.5°$
$b = 13.917$ (3) Å	$\mu = 0.19$ mm^{-1}
$c = 20.405$ (4) Å	$T = 293$ K
$V = 1680.6$ (6) Å^3	Plate, colorless
$Z = 4$	0.35 × 0.22 × 0.13 mm

Data collection

Bruker APEX area-detector diffractometer	3311 independent reflections
Radiation source: fine-focus sealed tube	3065 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.028$
φ and ω scans	$\theta_{max} = 26.0°$, $\theta_{min} = 3.1°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)	$h = -7 \rightarrow 7$
$T_{min} = 0.533$, $T_{max} = 1.000$	$k = -16 \rightarrow 17$
14520 measured reflections	$l = -25 \rightarrow 25$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.029$	H-atom parameters constrained
$wR(F^2) = 0.078$	$w = 1/[\sigma^2(F_o^2) + (0.0524P)^2 + 0.0539P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} < 0.001$
3311 reflections	$\Delta\rho_{max} = 0.18$ e Å^{-3}
226 parameters	$\Delta\rho_{min} = -0.20$ e Å^{-3}
0 restraints	Absolute structure: Flack (1983), 1373 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: please supply

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 ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
P1	0.36544 (6)	0.05040 (3)	0.12304 (2)	0.02988 (11)
O1	0.13285 (17)	0.06076 (8)	0.15090 (6)	0.0399 (3)
O2	0.75302 (16)	−0.03926 (10)	0.14345 (6)	0.0448 (3)
H2A	0.8541	−0.0008	0.1517	0.067*
O3	0.3080 (3)	0.04117 (11)	0.29316 (8)	0.0683 (4)
O4	−0.0305 (2)	−0.01286 (11)	0.29317 (8)	0.0624 (4)
C1	0.5574 (2)	−0.01474 (11)	0.17954 (8)	0.0323 (3)
H1A	0.5967	0.0257	0.2172	0.039*
C2	0.4346 (3)	−0.10461 (11)	0.20185 (8)	0.0328 (3)
C3	0.4930 (3)	−0.19195 (13)	0.17376 (10)	0.0461 (4)
H3A	0.6165	−0.1948	0.1456	0.055*
C4	0.3715 (4)	−0.27538 (13)	0.18661 (12)	0.0604 (6)
H4A	0.4172	−0.3332	0.1680	0.072*
C5	0.1858 (4)	−0.27310 (14)	0.22626 (12)	0.0622 (6)
H5A	0.1040	−0.3290	0.2341	0.075*
C6	0.1201 (4)	−0.18790 (13)	0.25448 (10)	0.0524 (5)
H6A	−0.0076	−0.1856	0.2810	0.063*
C7	0.2453 (3)	−0.10560 (12)	0.24313 (8)	0.0360 (4)
C8	0.4845 (3)	0.16772 (11)	0.10671 (8)	0.0320 (3)
C9	0.3434 (3)	0.24491 (12)	0.12017 (10)	0.0455 (4)
H9A	0.2010	0.2337	0.1379	0.055*
C10	0.4114 (4)	0.33817 (13)	0.10765 (11)	0.0552 (5)
H10A	0.3158	0.3892	0.1177	0.066*
C11	0.6187 (4)	0.35558 (13)	0.08061 (10)	0.0512 (5)
H11A	0.6629	0.4183	0.0713	0.061*
C12	0.7628 (3)	0.27996 (13)	0.06705 (10)	0.0472 (5)
H12A	0.9037	0.2921	0.0487	0.057*
C13	0.6988 (3)	0.18611 (12)	0.08065 (9)	0.0408 (4)
H13A	0.7979	0.1357	0.0725	0.049*
C14	0.3674 (3)	−0.02135 (11)	0.04912 (8)	0.0349 (3)
C15	0.5420 (3)	−0.01949 (15)	0.00353 (10)	0.0496 (5)
H15A	0.6643	0.0214	0.0100	0.060*
C16	0.5353 (4)	−0.07759 (16)	−0.05106 (11)	0.0575 (5)

H16A	0.6521	−0.0753	−0.0815	0.069*
C17	0.3564 (4)	−0.13884 (15)	−0.06060 (11)	0.0591 (5)
H17A	0.3526	−0.1784	−0.0973	0.071*
C18	0.1833 (4)	−0.14165 (17)	−0.01602 (12)	0.0643 (6)
H18A	0.0624	−0.1833	−0.0225	0.077*
C19	0.1878 (3)	−0.08300 (14)	0.03839 (11)	0.0515 (5)
H19A	0.0689	−0.0849	0.0682	0.062*
N1	0.1687 (3)	−0.01963 (11)	0.27860 (7)	0.0446 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.02187 (17)	0.03298 (19)	0.0348 (2)	−0.00254 (14)	0.00264 (15)	0.00331 (17)
O1	0.0241 (5)	0.0443 (6)	0.0512 (7)	−0.0008 (5)	0.0076 (5)	0.0058 (5)
O2	0.0226 (5)	0.0599 (8)	0.0520 (8)	−0.0028 (5)	0.0049 (5)	−0.0046 (6)
O3	0.0721 (9)	0.0642 (9)	0.0686 (10)	−0.0235 (8)	0.0197 (8)	−0.0319 (9)
O4	0.0511 (8)	0.0733 (9)	0.0628 (10)	0.0023 (7)	0.0212 (7)	−0.0041 (8)
C1	0.0243 (7)	0.0376 (8)	0.0349 (8)	−0.0013 (6)	0.0013 (6)	0.0010 (7)
C2	0.0309 (7)	0.0336 (8)	0.0338 (8)	0.0009 (6)	−0.0053 (6)	0.0038 (7)
C3	0.0444 (9)	0.0395 (9)	0.0545 (11)	0.0069 (8)	−0.0028 (9)	−0.0016 (8)
C4	0.0753 (14)	0.0295 (8)	0.0763 (15)	0.0073 (10)	−0.0113 (13)	−0.0023 (9)
C5	0.0727 (14)	0.0372 (10)	0.0766 (16)	−0.0154 (10)	−0.0069 (12)	0.0133 (10)
C6	0.0526 (10)	0.0496 (10)	0.0549 (12)	−0.0129 (9)	0.0043 (10)	0.0149 (9)
C7	0.0380 (8)	0.0343 (8)	0.0355 (9)	−0.0040 (7)	−0.0001 (7)	0.0050 (7)
C8	0.0307 (7)	0.0333 (8)	0.0320 (8)	−0.0040 (6)	0.0008 (6)	0.0027 (6)
C9	0.0440 (8)	0.0400 (8)	0.0525 (11)	0.0002 (7)	0.0113 (9)	−0.0016 (8)
C10	0.0632 (12)	0.0354 (9)	0.0670 (14)	0.0054 (8)	0.0124 (10)	−0.0033 (9)
C11	0.0618 (11)	0.0381 (9)	0.0537 (11)	−0.0095 (9)	0.0003 (10)	0.0091 (8)
C12	0.0411 (9)	0.0485 (10)	0.0520 (12)	−0.0127 (8)	0.0048 (8)	0.0100 (9)
C13	0.0319 (8)	0.0401 (9)	0.0504 (11)	−0.0016 (7)	0.0052 (7)	0.0049 (8)
C14	0.0337 (7)	0.0370 (8)	0.0340 (8)	−0.0019 (7)	−0.0047 (7)	0.0027 (7)
C15	0.0442 (9)	0.0607 (11)	0.0438 (10)	−0.0113 (9)	0.0031 (8)	−0.0067 (9)
C16	0.0590 (12)	0.0719 (14)	0.0416 (11)	−0.0029 (10)	0.0068 (9)	−0.0070 (10)
C17	0.0732 (13)	0.0576 (11)	0.0465 (11)	−0.0026 (11)	−0.0087 (11)	−0.0119 (9)
C18	0.0615 (13)	0.0644 (13)	0.0670 (15)	−0.0209 (11)	−0.0051 (11)	−0.0163 (11)
C19	0.0440 (10)	0.0567 (11)	0.0536 (12)	−0.0134 (8)	0.0012 (8)	−0.0056 (9)
N1	0.0501 (9)	0.0478 (8)	0.0359 (8)	−0.0031 (7)	0.0117 (7)	0.0011 (6)

Geometric parameters (Å, °)

P1—O1	1.4961 (11)	C8—C13	1.398 (2)
P1—C14	1.8091 (17)	C9—C10	1.383 (2)
P1—C8	1.8093 (15)	C9—H9A	0.9300
P1—C1	1.8550 (16)	C10—C11	1.367 (3)
O2—C1	1.4140 (18)	C10—H10A	0.9300
O2—H2A	0.8200	C11—C12	1.382 (3)
O3—N1	1.2180 (19)	C11—H11A	0.9300
O4—N1	1.219 (2)	C12—C13	1.388 (2)
C1—C2	1.516 (2)	C12—H12A	0.9300

C1—H1A	0.9800	C13—H13A	0.9300
C2—C3	1.387 (2)	C14—C19	1.384 (2)
C2—C7	1.402 (2)	C14—C15	1.390 (2)
C3—C4	1.391 (3)	C15—C16	1.377 (3)
C3—H3A	0.9300	C15—H15A	0.9300
C4—C5	1.365 (3)	C16—C17	1.373 (3)
C4—H4A	0.9300	C16—H16A	0.9300
C5—C6	1.374 (3)	C17—C18	1.370 (3)
C5—H5A	0.9300	C17—H17A	0.9300
C6—C7	1.384 (2)	C18—C19	1.378 (3)
C6—H6A	0.9300	C18—H18A	0.9300
C7—N1	1.470 (2)	C19—H19A	0.9300
C8—C9	1.388 (2)		
O1—P1—C14	112.08 (7)	C10—C9—H9A	119.5
O1—P1—C8	109.96 (7)	C8—C9—H9A	119.5
C14—P1—C8	109.99 (7)	C11—C10—C9	120.14 (18)
O1—P1—C1	111.99 (7)	C11—C10—H10A	119.9
C14—P1—C1	104.15 (7)	C9—C10—H10A	119.9
C8—P1—C1	108.49 (7)	C10—C11—C12	119.96 (17)
C1—O2—H2A	109.5	C10—C11—H11A	120.0
O2—C1—C2	110.46 (13)	C12—C11—H11A	120.0
O2—C1—P1	107.20 (11)	C11—C12—C13	120.53 (17)
C2—C1—P1	107.24 (10)	C11—C12—H12A	119.7
O2—C1—H1A	110.6	C13—C12—H12A	119.7
C2—C1—H1A	110.6	C12—C13—C8	119.72 (16)
P1—C1—H1A	110.6	C12—C13—H13A	120.1
C3—C2—C7	116.01 (15)	C8—C13—H13A	120.1
C3—C2—C1	118.65 (15)	C19—C14—C15	118.46 (16)
C7—C2—C1	124.84 (14)	C19—C14—P1	117.98 (14)
C2—C3—C4	121.67 (18)	C15—C14—P1	123.54 (12)
C2—C3—H3A	119.2	C16—C15—C14	120.60 (17)
C4—C3—H3A	119.2	C16—C15—H15A	119.7
C5—C4—C3	120.57 (18)	C14—C15—H15A	119.7
C5—C4—H4A	119.7	C17—C16—C15	120.1 (2)
C3—C4—H4A	119.7	C17—C16—H16A	120.0
C4—C5—C6	119.74 (18)	C15—C16—H16A	120.0
C4—C5—H5A	120.1	C18—C17—C16	120.00 (19)
C6—C5—H5A	120.1	C18—C17—H17A	120.0
C5—C6—C7	119.51 (18)	C16—C17—H17A	120.0
C5—C6—H6A	120.2	C17—C18—C19	120.23 (19)
C7—C6—H6A	120.2	C17—C18—H18A	119.9
C6—C7—C2	122.46 (16)	C19—C18—H18A	119.9
C6—C7—N1	115.23 (15)	C18—C19—C14	120.63 (19)
C2—C7—N1	122.30 (14)	C18—C19—H19A	119.7
C9—C8—C13	118.62 (15)	C14—C19—H19A	119.7
C9—C8—P1	115.32 (12)	O3—N1—O4	122.76 (16)
C13—C8—P1	126.04 (13)	O3—N1—C7	118.48 (14)
C10—C9—C8	121.00 (16)	O4—N1—C7	118.75 (16)

O1—P1—C1—O2	167.18 (10)	C13—C8—C9—C10	0.6 (3)
C14—P1—C1—O2	45.86 (12)	P1—C8—C9—C10	−177.73 (17)
C8—P1—C1—O2	−71.28 (12)	C8—C9—C10—C11	1.1 (3)
O1—P1—C1—C2	48.55 (13)	C9—C10—C11—C12	−1.4 (3)
C14—P1—C1—C2	−72.77 (12)	C10—C11—C12—C13	0.0 (3)
C8—P1—C1—C2	170.09 (11)	C11—C12—C13—C8	1.7 (3)
O2—C1—C2—C3	−14.0 (2)	C9—C8—C13—C12	−1.9 (3)
P1—C1—C2—C3	102.53 (15)	P1—C8—C13—C12	176.16 (14)
O2—C1—C2—C7	174.47 (14)	O1—P1—C14—C19	−21.10 (16)
P1—C1—C2—C7	−69.03 (19)	C8—P1—C14—C19	−143.75 (14)
C7—C2—C3—C4	−0.7 (3)	C1—P1—C14—C19	100.16 (15)
C1—C2—C3—C4	−172.97 (17)	O1—P1—C14—C15	160.53 (15)
C2—C3—C4—C5	1.8 (3)	C8—P1—C14—C15	37.87 (17)
C3—C4—C5—C6	−0.9 (3)	C1—P1—C14—C15	−78.22 (16)
C4—C5—C6—C7	−1.0 (3)	C19—C14—C15—C16	0.2 (3)
C5—C6—C7—C2	2.2 (3)	P1—C14—C15—C16	178.53 (16)
C5—C6—C7—N1	−176.57 (18)	C14—C15—C16—C17	−0.7 (3)
C3—C2—C7—C6	−1.3 (3)	C15—C16—C17—C18	0.5 (4)
C1—C2—C7—C6	170.47 (17)	C16—C17—C18—C19	0.1 (4)
C3—C2—C7—N1	177.34 (16)	C17—C18—C19—C14	−0.7 (3)
C1—C2—C7—N1	−10.9 (3)	C15—C14—C19—C18	0.5 (3)
O1—P1—C8—C9	−1.93 (16)	P1—C14—C19—C18	−177.97 (17)
C14—P1—C8—C9	121.97 (14)	C6—C7—N1—O3	150.69 (18)
C1—P1—C8—C9	−124.70 (14)	C2—C7—N1—O3	−28.0 (2)
O1—P1—C8—C13	179.93 (14)	C6—C7—N1—O4	−28.1 (2)
C14—P1—C8—C13	−56.18 (17)	C2—C7—N1—O4	153.19 (17)
C1—P1—C8—C13	57.15 (17)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2A···O1^{i}	0.82	1.86	2.6483 (16)	161.
C4—H4A···O3^{ii}	0.93	2.52	3.207 (2)	131.
C19—H19A···O2^{iii}	0.93	2.50	3.404 (2)	164.

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*+1, *y*−1/2, −*z*+1/2; (iii) *x*−1, *y*, *z*.

Fig. 1

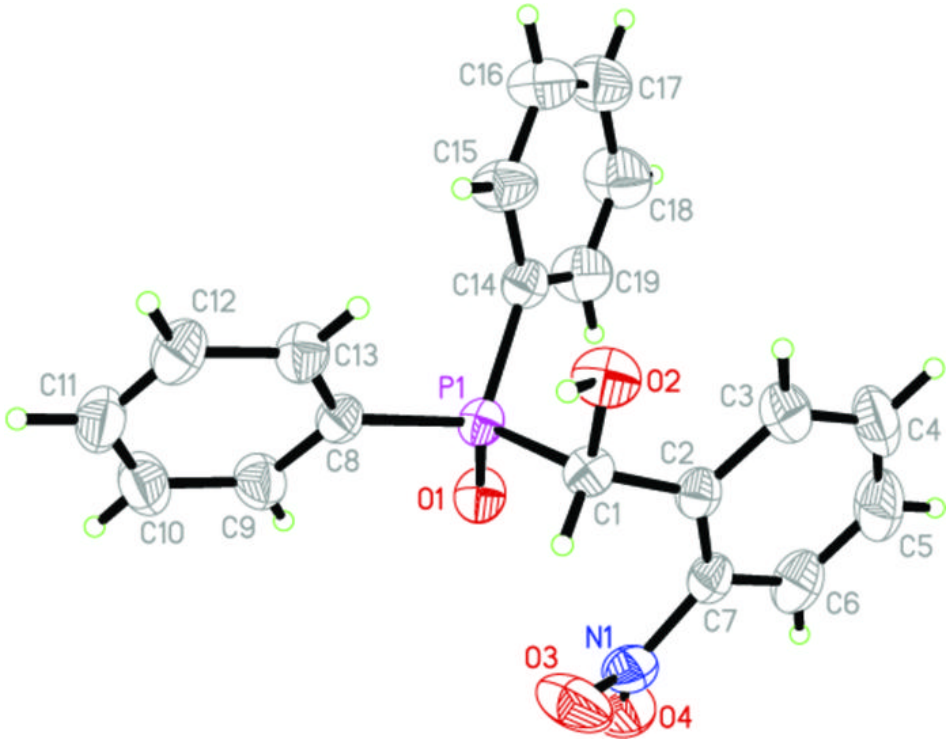

C16
C17
C15
C18
C14
C19
C12
C13
C11
P1
O2
C3
C4
C8
C2
O1
C1
C10
C9
C5
C6
C7
N1
O3
O4

Fig. 2