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(2-Hydroxy-5-methylphenyl)diphenylphosphine oxide

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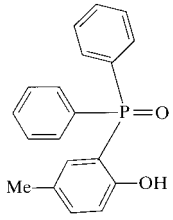
Pairs of individual molecules of the title compound, $C_{19}H_{17}O_2P$, (I), containing tetrahedrally coordinated P atoms



(I)

are connected across crystallographic inversion centres *via* complementary O—H···O═P hydrogen bonds.

Experimental

Yellow crystals of (I) were obtained when the $ReN(O–P)_2$ complex of the (2-hydroxy-5-methylphenyl)diphenylphosphine anion (O–P) was recrystallized from dimethyl sulfoxide. The phosphine oxide probably resulted from oxygen abstraction from the sulfoxide.

Crystal data

$C_{19}H_{17}O_2P$
M_r = 308.30
Monoclinic, $P2_1/n$
a = 10.730 (2) Å
b = 9.659 (2) Å
c = 15.287 (3) Å
β = 92.49 (2)°
V = 1582.9 (5) Å^3
Z = 4
D_x = 1.294 Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 20–22°
μ = 1.569 mm^{-1}
T = 293 (2) K
Block, pale yellow
0.62 × 0.25 × 0.18 mm

Data collection

Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: by integration (*ABSORP* in *NRCVAX*; Gabe *et al.*, 1989)
T_{min} = 0.539, T_{max} = 0.777
11 236 measured reflections
2994 independent reflections
2666 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 69.78°
$h = -13 \rightarrow 13$
$k = -11 \rightarrow 11$
$l = -18 \rightarrow 18$
5 standard reflections
frequency: 60 min
intensity variation: 2.2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.103
S = 1.092
2994 reflections
201 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0567P)^2 + 0.5028P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.006
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0062 (5)

Table 1
Selected geometric parameters (Å, °).

P—O	1.4950 (12)	P—C31	1.8027 (16)
P—C21	1.8004 (17)	O12—C12	1.3565 (19)
P—C11	1.8027 (17)		
O—P—C21	113.79 (7)	C12—C11—P	119.36 (12)
O—P—C11	113.98 (7)	O12—C12—C13	122.35 (15)
C21—P—C11	107.85 (7)	O12—C12—C11	118.18 (14)
O—P—C31	110.53 (7)	C26—C21—P	122.62 (13)
C21—P—C31	104.24 (7)	C22—C21—P	118.34 (13)
C11—P—C31	105.70 (7)	C32—C31—P	118.95 (13)
C16—C11—P	121.75 (12)	C36—C31—P	121.96 (12)
O—P—C11—C16	−118.04 (13)	O—P—C21—C22	41.97 (15)
C21—P—C11—C16	114.58 (13)	C11—P—C21—C22	169.46 (13)
C31—P—C11—C16	3.54 (15)	C31—P—C21—C22	−78.52 (14)
O—P—C11—C12	57.36 (14)	P—C21—C22—C23	175.05 (14)
C21—P—C11—C12	−70.02 (13)	P—C21—C26—C25	−175.69 (15)
C31—P—C11—C12	178.95 (12)	O—P—C31—C32	16.00 (16)
C16—C11—C12—O12	−176.99 (14)	C21—P—C31—C32	138.64 (14)
P—C11—C12—O12	7.47 (19)	C11—P—C31—C32	−107.79 (15)
P—C11—C12—C13	−174.09 (12)	O—P—C31—C36	−166.44 (14)
O12—C12—C13—C14	176.44 (15)	C21—P—C31—C36	−43.79 (16)
P—C11—C16—C15	175.46 (13)	C11—P—C31—C36	69.77 (16)
O—P—C21—C26	−142.81 (14)	P—C31—C32—C33	177.07 (16)
C11—P—C21—C26	−15.32 (16)	P—C31—C36—C35	−176.10 (15)
C31—P—C21—C26	96.71 (15)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O12—H12···O^{i}	0.82	1.86	2.664 (2)	166

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

H atoms were constrained to the parent sites using a riding model; C—H 0.93–0.96 Å and O—H 0.82 Å. The isotropic displacement parameters, U_{iso}, were adjusted to a value 50% (methyl and hydroxyl) or 20% (phenyl) higher than that of the parent site. A final verification of possible voids was performed using the *VOID* routine of the *PLATON* program (Spek, 1995).

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *NRC*-2 and *NRC*-2*A* (Ahmed *et al.*, 1973); program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1986); program(s) used to refine structure: *NRCVAX* (Gabe *et al.*, 1989) and *SHELXL*93 (Sheldrick, 1993); software used to prepare material for publication: *NRCVAX* and *SHELXL*93.

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