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(*R*)-(+)-2,2′-Bis(diphenylphosphinoyl)-1,1′-binaphthyl

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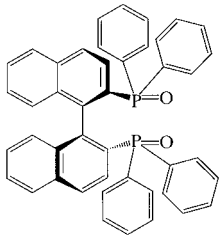
The title compound, BINAP oxide, $C_{44}H_{32}O_2P_2$, (I), was synthesized by direct oxidation of (*R*)-(+)-2,2′-bis(diphenylphosphino)-1,1′-binaphthyl (BINAP) with *tert*-butyl hydroperoxide in toluene solution. The angle between the naphthyl planes of the binaphthyl group is 94.17 (3)°.



(I)

Experimental

The title compound (BINAP oxide) was synthesized by direct oxidation of (*R*)-(+)-2,2′-bis(diphenylphosphino)-1,1′-binaphthyl (BINAP) with *tert*-butyl hydroperoxide in toluene solution. Crystals were grown from layering a toluene solution with hexanes.

Crystal data

$C_{44}H_{32}O_2P_2$	D_x = 1.279 Mg m^{-3}
M_r = 654.64	Mo $K\alpha$ radiation
Monoclinic, $P2_1$	Cell parameters from 16714 reflections
a = 9.0719 (2) Å	θ = 2.55–32.03°
b = 18.9903 (8) Å	μ = 0.166 mm^{-1}
c = 10.1528 (3) Å	T = 150 (1) K
β = 103.620 (2)°	Block cut from neeedle, colourless
V = 1699.92 (10) Å^3	0.34 × 0.30 × 0.20 mm
Z = 2	

Data collection

Nonius KappaCDD diffractometer	7746 reflections with $I > 2\sigma(I)$
φ and ω scans with κ offsets	R_{int} = 0.032
Absorption correction: multi-scan (*DENZO-SMN*; Otwinowski & Minor, 1997)	θ_{max} = 31.99°
T_{min} = 0.946, T_{max} = 0.968	$h = -13 \rightarrow 13$
16 714 measured reflections	$k = -25 \rightarrow 28$
10 057 independent reflections	$l = -15 \rightarrow 15$
	Intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0192P)^2 + 0.3419P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.052	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.099	$\Delta\rho_{max}$ = 0.32 e Å^{-3}
S = 1.021	$\Delta\rho_{min}$ = −0.37 e Å^{-3}
10 057 reflections	Absolute structure: Flack (1983); 4058 Friedel pairs
434 parameters	Flack parameter = 0.00 (6)
H-atom parameters constrained	

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SHELXTL/PC* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL/PC*; molecular graphics: *SHELXTL/PC*; software used to prepare material for publication: *SHELXTL/PC*.

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