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Tribenzylphosphine oxide

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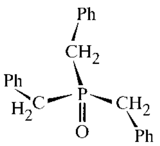
The title compound, $(C_6H_5CH_2)_3PO$, is an organic tertiary phosphine oxide. The molecule has threefold symmetry, with the P—O bond along the threefold axis. Main dimensions include P—O 1.488 (4), P—C 1.823 (3) Å and O—P—C 114.7 (1)°. The crystals were accidentally obtained when preparing complexes of nickel(II) with dibenzylphosphine.

Comment

The title compound, (I), is an organic phosphorus compound that belongs to a type of tertiary phosphine oxides. In the final stages of the synthesis of dihalogenobis(tribenzylphosphine)-nickel(II) complexes (Pérez *et al.*, 1998), (I) was isolated as colourless needles, possibly formed by an oxidation process due to atmospheric oxygen. The P—O distance agrees with the mean distance of 1.50 Å calculated by Bye *et al.* (1982), based on 62 Ph_3PO fragments. The P—C and C—C distances are similar to those found in compounds with tribenzylphosphine groups (Kilbourn & Powell, 1975). The two torsion angles P1—C3—C4—C*i* (*i* = 5 and 9) show that the three benzyl groups differ by aproximatelly 180°. The molecules are packed at normal van der Waals distances.



(I)

Experimental

In the recrystallization of dihalogenobis(tribenzylphosphine)-nickel(II) from dichloromethane–butanol (1:1) under an oxygen atmosphere (Pérez *et al.*, 1998), colorless needles of the title compound were obtained.

Crystal data

$C_{21}H_{21}OP$
$M_r = 320.35$
Trigonal, $R3$
$a = 16.685\ (2)$ Å
$c = 5.468\ (1)$ Å
$V = 1318.3\ (3)$ Å^3
$Z = 3$
$D_x = 1.211$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 30 reflections
$\theta = 13.80–27.92°$
$\mu = 0.160$ mm^{-1}
$T = 293$ K
Prism, colourless
0.56 × 0.32 × 0.20 mm

Data collection

Stoe Stadi-4 four-circle diffractometer
ω scans
Absorption correction: ψ scan (*EMPIR*; Stoe & Cie, 1992)
$T_{min} = 0.913$, $T_{max} = 0.969$
5177 measured reflections
578 independent reflections
558 reflections with $F^2 > 2\sigma(F^2)$

$R_{int} = 0.0347$
$\theta_{max} = 24.88°$
$h = -19 \rightarrow 19$
$k = -19 \rightarrow 19$
$l = 0 \rightarrow 6$
2 standard reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.088$
$S = 1.068$
578 reflections
70 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0568P)^2 + 0.3906P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.11$ e Å^{-3}
$\Delta\rho_{min} = -0.12$ e Å^{-3}
Absolute structure: Flack (1983)
Flack parameter = 0.1 (2)

Table 1
Selected geometric parameters (Å, °).

P1—O1	1.488 (4)	C4—C3	1.508 (6)
P1—C3	1.823 (3)		
O1—P1—C3	114.7 (1)	C3—C4—C9	120.9 (4)
C3—C4—C5	120.4 (3)	P1—C3—C4	114.3 (2)
O1—P1—C3—C4	65.0 (3)	C9—C4—C3—P1	−86.7 (4)
C5—C4—C3—P1	93.6 (4)		

H atoms were calculated geometrically and included in the refinement, but were restrained to ride on their parent atoms. The isotropic displacement parameters of the H atoms were fixed to $1.3U_{eq}$ of their parent atoms.

Data collection: *DIF*4 (Stoe & Cie, 1992); cell refinement: *DIF*4; data reduction: *REDU*4 (Stoe & Cie, 1992); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *PARST* (Nardelli, 1983, 1995) and *PARSTCIF* (Nardelli, 1991).

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