Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

{[*N*-Benzyl-*N*-(2-pyridyl)amino]methylene}-diphenylphosphine oxide

Da-Jun Cui,* Xianshun Zeng, Xuebing Leng, Fengbo Xu and Zhengzhi Zhang

National Key Laboratory of Elemento-Organic Chemistry, Nankai University, Tianjin 300071, People's Republic of China

Correspondence e-mail: cuidajun@eyou.com

Received 13 March 2003
Accepted 14 April 2003
Online 23 April 2003

Key indicators

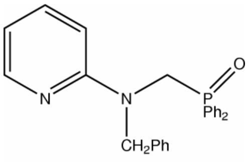
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.047
wR factor = 0.120
Data-to-parameter ratio = 14.2

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

The title compound, $Ph_2P(O)CH_2N(CH_2Ph)C_5H_4N$ or $C_{25}H_{23}N_2OP$, was obtained by reaction of $Ph_2PCH_2N(CH_2Ph)C_5H_4N$ and H_2O_2. The crystal structure shows distorted tetrahedral geometry around the P atom.

Comment

Pyridylphosphines continue to generate much interest as excellent ligands for stabilizing many transition-metal coordination and organometallic complexes (Espinet & Soulantica, 1999). One important property of these ligands is that they can stabilize metal ions in a variety of oxidation states and geometries. Hence, a metal–metal bond between an electron-rich metal (soft base) and a high oxidation-state metal (Lewis acid) is easily formed (Zhang & Cheng, 1996). Recently, we designed and synthesized a hetero-binuclear complex containing an Fe—Cu bond with a new pyridylphosphine ligand, *viz*. 2-(*N*-diphenylphosphinomethyl-*N*-cyclohexyl)-aminopyridine (Cui *et al.*, 2001).



(I)

Pyridylphosphine oxides have recently been shown to behave either as *N*(pyridyl)-donor or *N*(pyridyl),*O*-chelating ligands upon complexation with palladium(II) and platinum(II) centres (Minghetti *et al.*, 1998; Durran *et al.*, 2000). In order to study the interesting coordination potential of this kind of ligand we synthesized a new pyridylphosphine oxide $Ph_2P(O)CH_2N(CH_2Ph)C_5H_4N$ and its molecular structure has been determined by an X-ray diffraction study. The crystal structure of the title compound, (I), shows distorted tetrahedral geometry around the P atom. The P—O distance [1.4815 (18) Å] is shorter than those in other triarylphosphine oxides (Durran *et al.*, 2000; Minghetti *et al.*, 1998; Szlyk *et al.*, 1989; Bandoli *et al.*, 1970).

Experimental

The synthesis of (I) was carried out under an argon atmosphere. To a solution of $Ph_2PCH_2N(CH_2Ph)C_5H_4N$ (0.100 g, 0.252 mmol) in tetrahydrofuran (2 ml) was added aqueous H_2O_2 solution (30% *w*/*w*, 0.2 ml). The resulting solution was stirred for about 48 h, filtered to remove some insoluble material, and diethyl ether (15 ml) added. The white solid was collected by filtration and dried *in vacuo*.

DOI: 10.1107/S1600536803008304

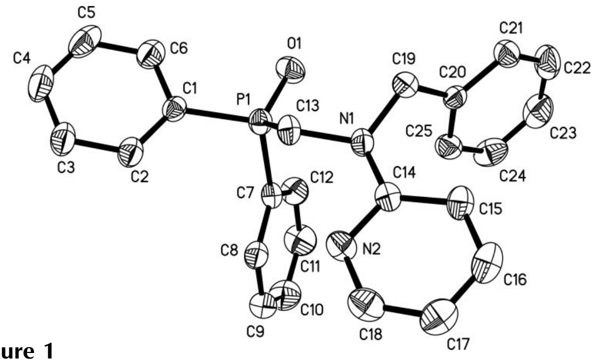


Figure 1
A view of (I), with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

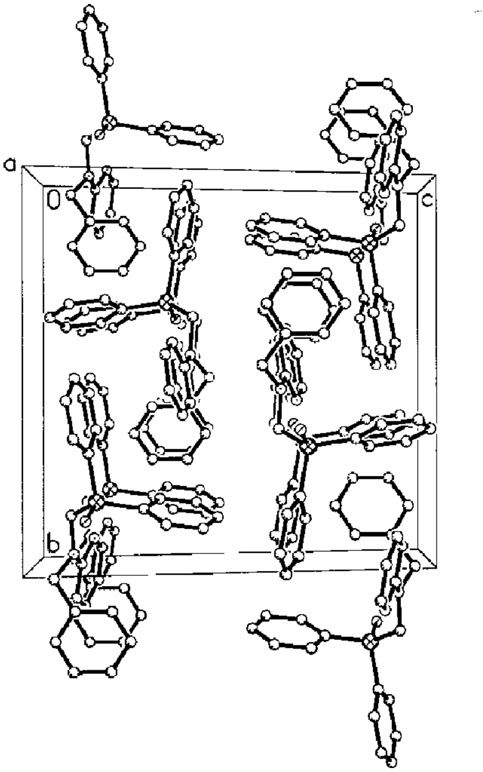


Figure 2
A view of the packing arrangement in the unit cell of (I).

Crystal data

$C_{25}H_{23}N_2OP$
$M_r = 398.42$
Monoclinic, $P2_1/n$
$a = 9.256$ (3) Å
$b = 14.834$ (5) Å
$c = 15.957$ (5) Å
$\beta = 104.979$ (6)°
$V = 2116.5$ (12) Å^3
$Z = 4$

$D_x = 1.250$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 573 reflections
$\theta = 1.9$–25.0°
$\mu = 0.15$ mm^{-1}
$T = 293$ (2) K
Plate, white
0.20 × 0.15 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
$T_{\min} = 0.971$, $T_{\max} = 0.985$
8613 measured reflections

3727 independent reflections
2051 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.062$
$\theta_{\max} = 25.0°$
$h = -11 \rightarrow 7$
$k = -17 \rightarrow 15$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.120$
$S = 0.97$
3727 reflections
262 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.009$
$\Delta\rho_{\max} = 0.31$ e Å^{-3}
$\Delta\rho_{\min} = -0.26$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

P1—O1	1.4815 (18)	P1—C13	1.804 (2)
P1—C7	1.799 (3)	P1—C1	1.808 (3)
O1—P1—C7	111.44 (11)	O1—P1—C1	111.55 (12)
O1—P1—C13	114.16 (12)	C7—P1—C1	107.96 (12)
C7—P1—C13	108.12 (12)	C13—P1—C1	103.14 (12)

All H atoms were located geometrically and refined in calculated positions using a riding model.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998) and *SHELXTL* (Bruker, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

This work was supported by the National Natural Science Foundation of China (No. 20102003).

References

Bandoli, G., Bortolozzo, G., Clemente, D. A., Croatto, U. & Panattoni, C. (1970). *J. Chem. Soc. A*, pp. 2778–2780.

Bruker (1997). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (1998). *SMART* (Version 5.00) and *SAINT* (Version 5.00). Bruker AXS Inc., Madison, Wisconsin, USA.

Cui, D.-J., Li, Q.-S., Xu, F.-B., Leng, X.-B. & Zhang, Z.-Z. (2001). *Organometallics*, **20**, 4126–4128.

Durran, S. E., Smith, M. B., Slawin, A. M. Z. & Steed, J. W. (2000). *J. Chem. Soc. Dalton Trans.* pp. 2771–2778.

Espinet, P. & Soulantica, K. (1999). *Coord. Chem. Rev.***193–195**, 499–556.

Minghetti, G., Stoccoro, S., Cinellu, M. A., Zucca, A., Manassero, M. & Sansoni, M. (1998). *J. Chem. Soc. Dalton Trans.* pp. 4119–4126.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (1997). *SHELXL*97 and *SHELXS*97. University of Göttingen, Germany.

Szlyk, E., Zhang, Z.-Y., Palenik, G. J., Palenik, R. C. & Colgate, S. O. (1989). *Acta Cryst.* C**45**, 1234–1236.

Zhang, Z.-Z. & Cheng, H. (1996). *Coord. Chem. Rev.* **147**, 1–39.