Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-[2-(Diphenylphosphino)phenyliminomethyl]-*N*,*N*-dimethylaniline, a new Schiff base containing triphenylphosphine

Kai-Bin Yang, Li-Rong Lin and Rong-Bin Huang*

Department of Chemistry, Xiamen University, Xiamen 361005, People's Republic of China

Correspondence e-mail: rbhuang@xmu.edu.cn

Received 10 May 2006
Accepted 19 May 2006

The title compound, $C_{27}H_{25}N_2P$, is a Schiff base containing triphenylphosphine. The molecule has a *trans* configuration about the C=N double bond [1.277 (2) Å]. The crystal packing is stabilized by van der Waals forces.

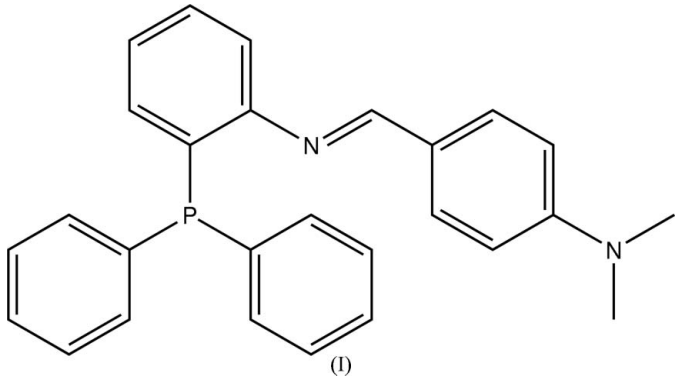
Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.056
wR factor = 0.141
Data-to-parameter ratio = 17.4

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

Comment

Schiff base ligands have various applications in the fields of synthesis and catalysis, and exhibit biological activity (Cozzi *et al.*, 2003; Qiao *et al.*, 2004; Maciejewska *et al.*, 1999; Jalil *et al.*, 2001; Li *et al.*, 2005). Some Schiff bases containing oxygen, sulfur and complexes of transition metal ions have been synthesized (Rivera *et al.*, 2006; Sah *et al.*, 2006; Sharif *et al.*, 2006) but few Schiff bases containing phosphorus have been reported. A Schiff base containing triphenylphosphine may be expected to be a useful bidentate ligand with new properties, because triphenylphosphine is a well known ligand for coordination compounds. Here we present the title compound, (I), a new Schiff base derivative containing triphenlphosphine.



(I)

In (I) (Fig. 1), all bond lengths and angles show normal values. The molecule has a *trans* configuration about the C9=N2 double bond. The crystal packing is stabilized by van der Waals forces.

Experimental

2-(Diphenylphosphino)benzenamine was prepared according to the literature method of Papathanasiou *et al.* (1997). The Schiff base was synthesized by refluxing an ethanol solution (20 ml) of 4-(dimethylamino)benzaldehyde (10 mmol) and 2-(diphenylphosphino)-benzenamine (10 mmol) for 2 h. The solution was then cooled to room temperature. Light-yellow crystals were obtained, filtered and washed with cold ethanol. Crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{27}H_{25}N_2P$
M_r = 408.46
Monoclinic, $P2_1/c$
a = 17.579 (4) Å
b = 14.419 (3) Å
c = 8.732 (2) Å
β = 100.985 (4)°
V = 2172.7 (8) Å^3
Z = 4
D_x = 1.249 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.14 mm^{-1}
T = 173 (2) K
Block, yellow
0.50 × 0.43 × 0.21 mm

Data collection

Bruker SMART APEX 2000 CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.932, T_{max} = 0.971
12521 measured reflections
4719 independent reflections
4172 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 27.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.141
S = 1.11
4719 reflections
271 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0695P)^2 + 0.8283P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

All H atoms were positioned geometrically, with C—H distances of 0.95–0.98 Å, and refined using a riding model, with U_{iso}(H) = 1.2 or 1.5U_{eq}(C).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

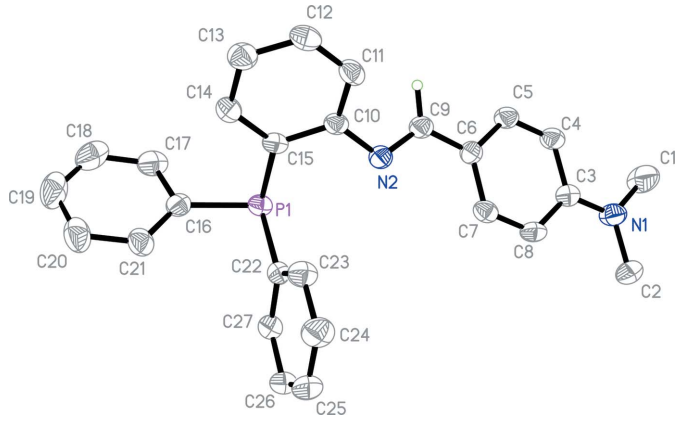


Figure 1
View of (I), with displacement ellipsoids drawn at the 50% probability level. For clarity, H atoms except for the methine H atom have been omitted.

References

Bruker (2001). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cozzi, P. G., Dolci, L. S., Garelli, A., Montalti, M., Prodi, L. & Zaccheroni, N. (2003). *New J. Chem.* **27**, 692–697.
Jalil, M. A., Fujinami, S. & Nishikawa, H. (2001). *J. Chem. Soc. Dalton Trans.* pp. 1091–1098.
Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Li, L.-Z., Zhao, C., Xu, T., Ji, H.-W., Yu, Y.-H., Guo, G.-Q. & Chao, H. (2005). *J. Inorg. Biochem.* **99**, 1076–1082.
Maciejewska, D., Pawlak, D. & Koleva, V. (1999). *J. Phys. Org. Chem.* **12**, 875–880.
Papathanasiou, P., Salem, G., Waring, P. & Willis, A. C. (1997). *J. Chem. Soc. Dalton Trans.* pp. 3435–3443.
Qiao, J., Wang, L.-D., Duan, L., Li, Y., Zhang, D.-Q. & Qiu, Y. (2004). *Inorg. Chem.* **43**, 5096–5102.
Rivera, J. M., Reyes, H., Cortes, A. & Santillan, R. (2006). *Chem. Mater.* **18**, 1174–1183.
Sah, A. K., Tanase, T. & Mikuriya, M. (2006). *Inorg. Chem.* **45**, 2083–2092.
Sharif, S., Denisov, G. S., Toney, M. D. & Limbach, H. (2006). *J. Am. Chem. Soc.* **128**, 3375–3387.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.