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N-[2-(Diphenylphosphanyl)benzylidene]-4-methylaniline

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Key indicators

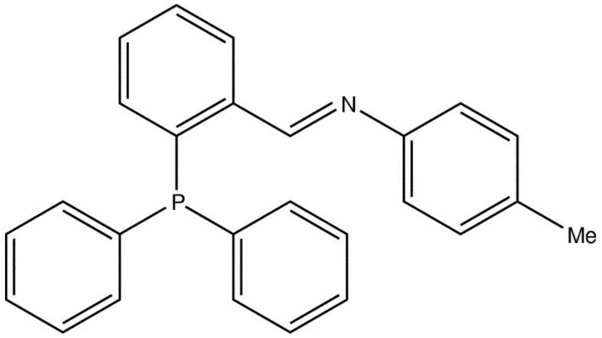
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.067
wR factor = 0.140
Data-to-parameter ratio = 14.7

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

The title compound, $C_{26}H_{22}NP$, is a Schiff base derived from triphenylphosphine with a 4-methylphenylamine group attached to one of the benzene rings of the phosphine in the *o*-position. The azomethine C=N bond length is 1.259 (3) Å and the dihedral angle between the benzene ring and its 4-methylphenylamine substituent is 40.02 (2) Å. The geometry at the P atom is approximately tetrahedral.

Comment

Schiff bases derived from phosphines are relatively scarce. An example is *N*-benzylidene-3-(diphenylphosphino)-1-propanamine (Xie *et al.*, 2001), a diphenylphosphine system with an *N*-benzylidene-1-propanamine Schiff base group bound to the P atom by the terminal carbon of the propylamine fragment. The presence of both P and N atoms as soft and hard electron donors, respectively, is attractive from the point of view of heterometallic complexation, but also as potential catalysts, providing active sites for an incoming substrate (Elliott *et al.*, 1999).



(I)

The title compound, (I), is a triphenylphosphine derivative in which one of the benzene rings is substituted in the *ortho* position with a 4-methylphenylamine group (Fig. 1). Bond lengths and angles in the molecule are in normal ranges (Allen *et al.*, 1987), with an azomethine C7=N1 bond length of 1.259 (3) Å and an approximately tetrahedral geometry around P1 (Table 1). The methylene-*p*-toluidine fragment, C1–C6/N1/C7, is planar, with a maximum deviation of 0.040 (4) Å for atom N1. Its least-squares plane is at an angle of 40.0 (2)° with respect to benzene ring C9–C10 to which it is bound. This benzene ring also makes dihedral angles of 85.98 (18) and 87.1 (2)° with benzene rings C15–C20 and C21–C26, respectively. There is one weak intramolecular hydrogen bond, C8—H8*A*$\cdots$P1 (Table 2), which contributes to the stability of the molecule.

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Experimental

2-(Diphenylphosphino)benzaldehyde (0.939 g, 3.23 mmol) and *p*-toluidine (0.398 g, 3.72 mmol) were dissolved in 100 ml of an MeOH–CH_2Cl_2 (3:1 *v*/*v*) mixture and stirred under N_2 for 4 h. After standing overnight at room temperature, the solution was concentrated to a small volume (*ca* 5 ml) and kept at 253 K for 24 h. A yellow crystalline solid, (I) (yield 75%), was obtained and washed with cold ethanol. Crystals suitable for X-ray analysis were obtained by recrystallization from ethanol (m.p. 394.2–395.4 K). Analysis calculated: C 82.3, H 5.84, N 3.69%; found: C 81.8, H 5.62, N 3.51%.

Crystal data

$C_{26}H_{22}NP$
$M_r = 379.42$
Monoclinic, $P2_1/c$
$a = 13.938$ (4) Å
$b = 10.414$ (3) Å
$c = 19.311$ (4) Å
$\beta = 131.108$ (13)°
$V = 2112.0$ (10) Å^3
$Z = 4$

$D_x = 1.193$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2598 reflections
$\theta = 1.9$–25.0°
$\mu = 0.14$ mm^{-1}
$T = 298$ (2) K
Block, pale yellow
0.47 × 0.17 × 0.15 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.936$, $T_{\max} = 0.979$
15172 measured reflections

3724 independent reflections
2686 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.049$
$\theta_{\max} = 25.0°$
$h = -16 \rightarrow 16$
$k = -12 \rightarrow 12$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.067$
$wR(F^2) = 0.140$
$S = 1.19$
3724 reflections
253 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0425P)^2 + 0.7448P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.21$ e Å^{-3}
$\Delta\rho_{\min} = -0.14$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

P1—C21	1.820 (3)	P1—C14	1.837 (3)
P1—C15	1.825 (3)	N1—C6	1.423 (4)
C21—P1—C15	102.18 (13)	C15—P1—C14	103.14 (13)
C21—P1—C14	101.49 (13)		

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C8—H8*A*⋯P1	0.93	2.60	3.059 (4)	111

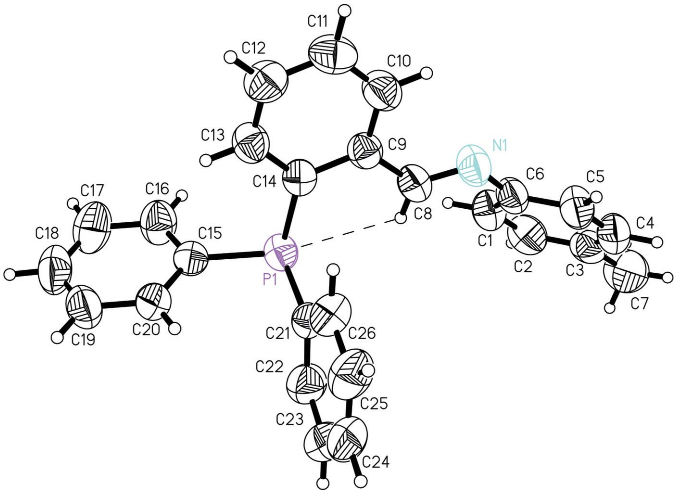

Figure 1
The molecular structure of the title compound, (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The intramolecular hydrogen bond is drawn as a dashed line.

After their location in a difference map, all H atoms were placed at ideal positions and allowed to ride on the parent C atoms, with C—H = 0.93–0.96 Å and $U_{\rm iso}$(H) = 1.2 $U_{\rm eq}$(CH_2 and aromatic) or 1.5$U_{\rm eq}$(CH_3).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L. Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Elliott, M. E., Kimmerling, T. S., Zhu, L. Z., Storhoff, B. N. & Huffman, J. H. (1999). *Polyhedron*, **18**, 1603–1608.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Xie, T., Li, Y. -Z., Li, B. -J., Shi, L., Wang, L. -F., Gao, S. -Y. & Liang, Y. -M (2001). *Acta Cryst.* E**57**, o858–o859.