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Chlorobis[diphenyl(*p*-tolyl)phosphine]copper(I)

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Key indicators

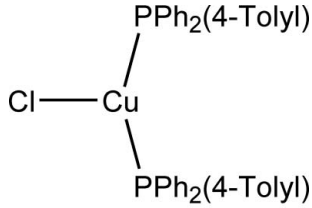
Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.007 Å
Disorder in main residue
R factor = 0.062
wR factor = 0.150
Data-to-parameter ratio = 18.2

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

The title compound, $[CuCl(C_{19}H_{17}P)_2]$, is an example of an asymmetric bisphosphine complex of copper(I). It crystallizes with a distorted trigonal–planar geometry about the copper(I) metal centre. The diphenyl(*p*-tolyl)phosphine groups adopt an eclipsed configuration in the solid state. The most important bond distances and angles include Cu—Cl = 2.2330 (12) Å, Cu—P = 2.2570 (13) Å, Cu—P (*trans* to Cl) = 2.2579 (12) Å and P—Cu—P = 126.72 (5)°.

Comment

The addition of a tertiary aryl phosphine group to a copper(I) metal centre can form a myriad of structural conformations, the cubane structure being the most widely encountered (Noren & Oskarsson, 1985). A range of substituted phosphine derivatives have also been reported (Churchill & Rotella, 1977; Bowmaker, Dyason *et al.*, 1987). The 2-tolyldiphenylphosphine derivative of copper(I) has been investigated *via* crystallographic and spectroscopic methods (Bowmaker, Engelhardt *et al.*, 1987). In the current paper we report the 4-tolyldiphenylphosphine derivative of a copper(I) chloride complex.



(I)

The title compound, (I), crystallizes in the asymmetric unit with a slightly distorted trigonal-planar geometry about the copper(I) metal centre (Fig. 1). The Cu^I atom is elevated by 0.034 (1) Å above the plane defined by the three coordinated atoms (Cl, P1, P2). The Cu—Cl and Cu—P bond distances and P—Cu—P bond angle do not significantly differ from those reported previously (Table 2).

The current study was undertaken to determine the effect of the single methyl group on the structural orientation of the complex. The 4-tolyldiphenylphosphine groups adopt an eclipsed configuration, which is typically observed for these complexes. It is interesting to note that the title compound crystallizes in the asymmetric unit in a similar fashion (Cl—Cu—P—C) to the PPh_3 derivatives (Table 2). Thus, the steric interaction of the 2-tolyl group plays a larger role in determining the packing mode of these complexes compared to the title compound.

Experimental

The title complex was synthesized by the addition of 4-tolyldiphenylphosphine (608 mg, 2.2 mmol) to a refluxing acetonitrile solution of CuCl (99 mg, 1 mmol). On cooling, crystals suitable for X-ray crystallography were obtained. Yield 540 mg (92%).

Crystal data

$[CuCl(C_{19}H_{17}P)_2]$
$M_r = 651.58$
Monoclinic, $P2_1/c$
$a = 11.5427$ (7) Å
$b = 18.1087$ (12) Å
$c = 15.4940$ (9) Å
$\beta = 102.266$ (3)°
$V = 3164.7$ (3) Å^3
$Z = 4$
$D_x = 1.368$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.90$ mm^{-1}
$T = 100$ (2) K
Block, white
0.14 × 0.12 × 0.06 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min} = 0.884$, $T_{max} = 0.948$
24407 measured reflections
6891 independent reflections
4276 reflections with $I > 2\sigma(I)$
$R_{int} = 0.076$
$\theta_{max} = 27.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.062$
$wR(F^2) = 0.150$
$S = 1.03$
6891 reflections
379 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0434P)^2 + 6.7108P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.75$ e Å^{-3}
$\Delta\rho_{min} = -0.49$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu—Cl	2.2330 (12)	Cu—P2	2.2579 (12)
Cu—P1	2.2570 (13)		
Cl—Cu—P1	114.95 (5)	P1—Cu—P2	126.72 (5)
Cl—Cu—P2	118.26 (5)		
Cl—Cu—P2—C41	−11.46 (17)	Cl—Cu—P1—C31	−113.71 (17)
Cl—Cu—P2—C61	109.55 (15)	Cl—Cu—P1—C21	127.72 (17)
Cl—Cu—P2—C51	−132.83 (16)	Cl—Cu—P1—C11	5.79 (19)

Table 2
Comparative X-ray crystallographic data for $[CuCl(PR_3)_2]$ (R = aryl group) complexes.

Compound	Cu—Cl	Cu—P	P—Cu—P	Cl—Cu—P—C
$CuCl(PPh_3)\cdot Ph$[a]	2.208	2.272	125.49	1.65
		2.260		9.71
$CuCl(PPh_3)\cdot THF$[b]	2.214	2.268	125.55	6.34
		2.256		6.37
$CuCl(PPh_2$4-Tol$)$[c]	2.233	2.257	126.72	5.79
		2.258		−11.46
$CuCl(PPh_2$2-Tol$)$[d]	2.204	2.241	126.98	25.73
		2.256		−29.70

Notes: (*a*) Bowmaker, Dyason *et al.* (1987); (*b*) Krauter & Neumuller (1996); (*c*) this work; (*d*) Bowmaker, Engelhardt *et al.* (1987).

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$ [$1.5U_{eq}(C)$ for methyl groups] and with C—H distances of 0.95 and 0.98 Å. The H atoms of the methyl group in each tolyl unit are disordered over two sites of equal occupancy.

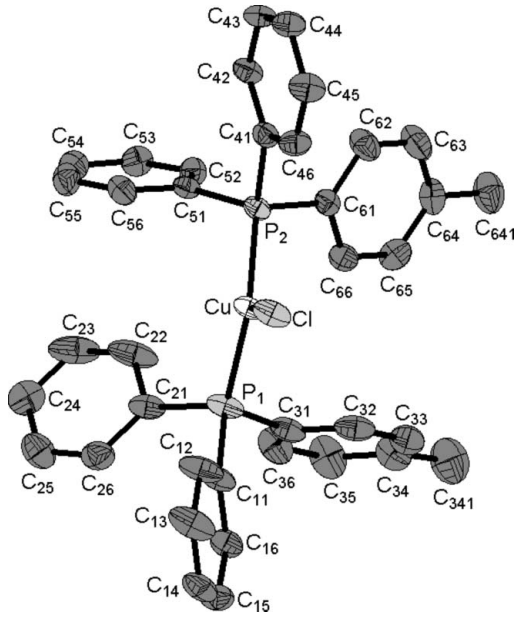


Figure 1
The molecular structure of (I), showing the numbering scheme and displacement ellipsoids (50% probability). For the carbon rings, the first digit refers to the ring number, the second digit to the atom in the ring. H atoms have been omitted for clarity.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2004); software used to prepare material for publication: *SHELXL97*.

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