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Iodotris(tri-*p*-tolylphosphine)silver(I)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
Disorder in main residue
R factor = 0.040
wR factor = 0.094
Data-to-parameter ratio = 19.6

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

In the title compound, $[AgI(C_{21}H_{21}P)_3]$, important bond distances are: Ag—P = 2.5346 (9), 2.5562 (9) and 2.5617 (9) Å, and Ag—I = 2.8683 (5) Å. The Ag^I atom is in a distorted tetrahedral environment and all bond angles are close to the ideal values.

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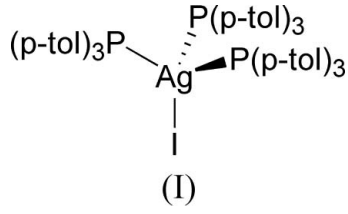
Comment

As part of our investigation of the coordination of tri-*p*-tolylphosphine to silver(I) (Meijboom, 2006; Meijboom & Muller, 2006, Meijboom *et al.*, 2006; Venter *et al.*, 2006), we report here the solid-state structure of the title compound, $[Ag\{P(4\text{-}MeC_6H_4)_3\}_3I]$, (I).



(I)

The Ag atom of (I) is coordinated by three phosphine ligands and one iodide anion, forming a distorted tetrahedral environment (Table 1). All bond angles around the Ag atom

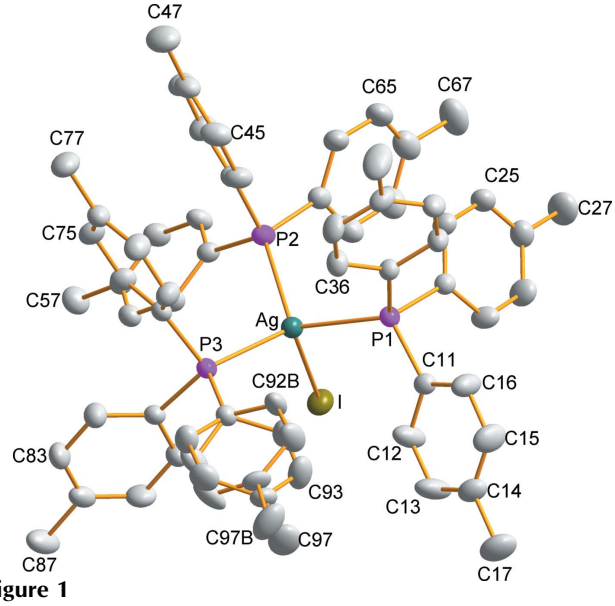


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids. H atoms have been omitted for clarity. For the C atoms, the first digit indicates the ring number and the second digit indicates the position of the atom in the ring. Some labels have been omitted for clarity, but all rings were numbered in a similar fashion.

are close to the ideal values for a tetrahedral environment. Some thermal motion of ring 1 was observed but was not regarded as large enough for disordered refinement.

Experimental

Silver(I) iodide (100 mg, 0.43 mmol) was added to a solution of tri-*p*-tolylphosphine (395 mg, 1.15 mmol) in pyridine (5 ml) and heated at 373 K for 5 min. The resulting colourless solution was cooled and the title compound crystallized on standing in quantitative yield as colourless crystals.

Crystal data

$[AgI(C_{21}H_{21}P)_3]$
M_r = 1147.81
Triclinic, $P\overline{1}$
a = 11.0426 (13) Å
b = 11.5665 (14) Å
c = 23.243 (3) Å
α = 99.292 (3)°
β = 92.174 (2)°
γ = 106.196 (2)°
V = 2802.7 (6) Å^3
Z = 2
D_x = 1.36 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.03 mm^{-1}
T = 293 (2) K
Block, colourless
0.3 × 0.26 × 0.15 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.747, T_{max} = 0.860
19391 measured reflections
13246 independent reflections
8623 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 28°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.094
S = 1.01
13246 reflections
677 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0327P)^2 + 1.1965P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag—P1	2.5346 (9)	Ag—P3	2.5617 (9)
Ag—P2	2.5562 (9)	Ag—I	2.8683 (5)
P1—Ag—P2	112.04 (3)	P1—Ag—I	102.35 (2)
P1—Ag—P3	117.65 (3)	P2—Ag—I	99.38 (2)
P2—Ag—P3	111.94 (3)	P3—Ag—I	111.51 (2)

The methyl and aromatic H atoms were placed in geometrically idealized positions (C—H = 0.92–0.98 Å) and constrained to ride on their parent atoms, with U_{iso}(H) = 1.5U_{eq}(C) for methyl H or 1.2U_{eq}(C) for aromatic H. Methyl H atoms were placed in idealized positions and the torsion angles refined to fit the electron density. The disordered tolyl substituent (C92–C97) was refined with complementary group occupancy factors; these refined to 0.648 (17)/0.352 (17).

Data collection: *SMART-NT* (Bruker, 1999); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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