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Chloro[tris(*p*-methoxyphenyl)phosphine]gold(I)

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Key indicators

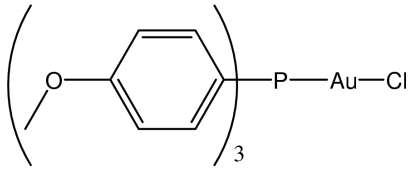
Single-crystal X-ray study
T = 223 K
Mean σ(C–C) = 0.005 Å
R factor = 0.028
wR factor = 0.064
Data-to-parameter ratio = 24.5

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

The Au atom in the title compound, $(p\text{-MeOC}_6\text{H}_4)_3\text{PAuCl}$ or $[\text{AuCl}(\text{C}_7\text{H}_7\text{O}_3\text{P})]$, exhibits a linear geometry so that the Au—Cl bond length is 2.2885 (9) Å, Au—P is 2.2333 (8) Å and the angle at gold is 175.94 (3)°.

Comment

As expected, an effectively linear geometry is found for the Au atom in $(p\text{-MeOC}_6\text{H}_4)_3\text{PAuCl}$, (I) (Fig. 1), with the angle at gold being 175.94 (3)°. The Au—Cl and Au—P distances in (I) are 2.2885 (9) and 2.2333 (8) Å, respectively. The Au donor atom parameters found in (I) are equal, within experimental error, to those found in the unsubstituted analogue, *viz.* $(\text{C}_6\text{H}_5)_3\text{PAuCl}$ (Baenziger *et al.*, 1976), for which the Au—Cl and Au—P distances are 2.279 (3) and 2.235 (3) Å, respectively. The aromatic rings are almost symmetrically disposed as seen in the sequence of dihedral angles of 68.76 (16), 73.48 (16) and 78.66 (15)° for the C1–C6, C8–C13 and C15–C20 rings, respectively. There is no evidence for π...π interactions in the lattice but arguably there are two C—H$\cdots\pi$ contacts involving methyl-H atoms of note. Thus, C7—H7*c* is 3.07 Å from the ring centroid of C8^{i}–C13^{i} with an angle at H7*c* of 175° [symmetry code: (i) $1-x, y, \frac{1}{2}-z$]. Similarly, C14—H14*b* is 3.09 Å from the ring centroid of C1^{ii}–C6^{ii} with 166° being the angle at the H14*b* atom [symmetry code: (ii) $\frac{1}{2}-x, -\frac{1}{2}+y, \frac{1}{2}-z$]. A close C—H$\cdots$O contact is also noted, so that C14—H14*a* is 2.58 Å from O3^{iii} with a C14$\cdots$O3^{iii} distance of 3.430 (5) Å, and the angle subtended at H14*a* is 146°; [symmetry code: (iii) $\frac{1}{2}+x, -\frac{1}{2}-y, \frac{1}{2}+z$].



(I)

Experimental

The title compound was prepared from the reaction between $\text{HAuCl}_4.3\text{H}_2\text{O}$ and $(p\text{-MeOC}_6\text{H}_4)_3\text{P}$ (Strem Chemicals Inc.) in accord with the literature procedure of Al-Saády *et al.* (1985) and had spectroscopic characteristics as reported in the literature (Decker *et al.*, 1999). Colourless crystals were obtained from the layering of ethanol into a concentrated CH_2Cl_2 solution of the compound.

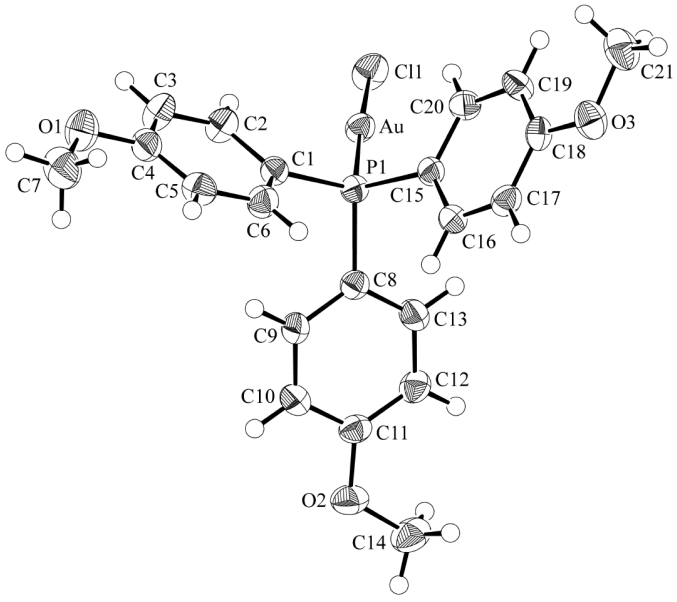


Figure 1
The molecular structure and crystallographic numbering scheme for (I). Displacement ellipsoids are shown at the 50% probability level (Johnson, 1976).

Crystal data

$[AuCl(C_7H_7O_3P)]$	D_x = 1.887 Mg m^{-3}
M_r = 584.76	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 16 893 reflections
a = 14.2875 (4) Å	θ = 2.0–30.0°
b = 14.5396 (4) Å	μ = 7.37 mm^{-1}
c = 20.2212 (6) Å	T = 223 (2) K
β = 101.504 (1)°	Block, colourless
V = 4116.3 (2) Å^3	0.42 × 0.26 × 0.10 mm
Z = 8	

Data collection

Bruker SMART CCD diffractometer	6001 independent reflections
ω scans	4896 reflections with $I > 2\sigma(I)$
Absorption correction: empirical (*SADABS*; Bruker, 2000)	R_{int} = 0.040
T_{min} = 0.114, T_{max} = 0.478	θ_{max} = 30.0°
16 893 measured reflections	$h = -18 \rightarrow 20$
	$k = -18 \rightarrow 20$
	$l = -28 \rightarrow 27$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.028	$w = 1/[\sigma^2(F_o^2) + (0.0317P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.064	$(\Delta/\sigma)_{max}$ = 0.002
S = 0.95	$\Delta\rho_{max}$ = 1.38 e Å^{-3}
6001 reflections	$\Delta\rho_{min}$ = −0.71 e Å^{-3}
245 parameters	

The C-bound H atoms were placed in geometrically calculated positions and included in the final refinement as riding with an overall displacement parameter, U_{iso}, with U_{iso} for CH and 1.5U_{iso} for CH_3. The residual electron-density peak is located in the vicinity of the Au atom.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SHELXTL* (Bruker, 2000); program(s) used to solve structure: *PATTY* in *DIRDIF*92 (Beurskens *et al.*, 1992); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXTL*.

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