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A dinuclear chloro(triphenylphosphito)copper(I) complex, di-μ_2-chloro-bis[bis(triphenylphosphito)-copper(I)]

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.008 Å
R factor = 0.052
wR factor = 0.146
Data-to-parameter ratio = 17.7

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

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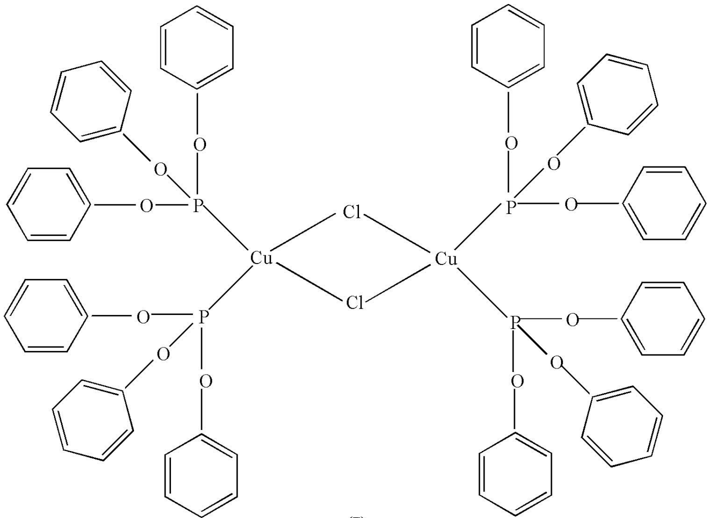
The title compound, $[Cu_2Cl_2(C_{18}H_{15}O_3P)_4]$, is a centrosymmetric dinuclear complex, where each Cu^I atom has a distorted tetrahedral coordination involving two triphenylphosphite ligands and two bridging Cl^- anions. The molecular structure and packing are stabilized by C—H···O and C—H···π interactions.

Comment

The presence of electronegative substituents on a phosphine ligand in a metal complex is known to cause a decrease in the metal–phosphorus bond length compared with that in a corresponding aryl– or alkyl–phosphine complex (Cotton, 1964). This shortening has been ascribed to several different causes, such as lower steric requirements due to a smaller cone angle in fluorophosphines and phosphites, and contraction of the phosphorus lone-pair donor orbital (Rudolph & Parry, 1967). In the course of our studies of new dinuclear chloro(triphenylphosphite) complexes, we have synthesized the title compound, (I), and report its structure here.



(I)

Compound (I) is a centrosymmetric complex consisting of two Cu^I ions, four triphenylphosphite ligands and two Cl^- anions. The coordination of the Cu^I ions is best described as distorted tetrahedral. Each Cu^I ion is coordinated by two triphenylphosphite ligands and two bridging Cl^- anions. The average Cu—Cl bond length [2.3703 (10) Å] is significantly shorter than the average values of 2.402 Å found in $[Cu_2Cl_2(PPh_3)_4]$ (Balogh-Hergovich *et al.*, 1998) and 2.392 Å found in $[CuCl(P(OPh)_3)]_4$ (Pike *et al.*, 1999). The average Cu—P bond length [2.2370 (11) Å] is intermediate between

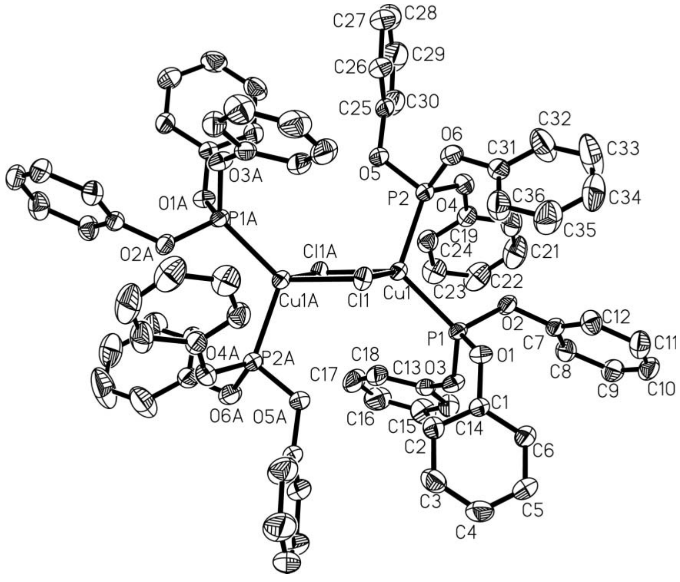


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Suffix A denotes symmetry operator ($-x$, 1 $-$ y, $-z$). H atoms have been omitted for clarity.

those observed in $[Cu_2Cl_2(PPh_3)_4]$ (2.287 Å) and $[CuCl(P(OPh)_3)]_4$ (2.156 Å).

It is interesting to note that the molecular structure and packing of (I) are stabilized by intra- and intermolecular C—H$\cdots\pi$ interactions between the aromatic H atoms and the centroids of the phenyl rings (Table 2). In addition, an intermolecular C—H$\cdots$Cl hydrogen-bond interaction is observed.

Experimental

The title compound was prepared by the reaction of copper dichloride dihydrate (1.3 mmol) with triphenylphosphite (2.1 mmol) in a water–ethanol (1:1, 10 ml) solution at 273 K. Single crystals of (I) suitable for X-ray measurements were obtained by recrystallization from acetone at room temperature.

Crystal data

$[Cu_2Cl_2(C_{18}H_{15}O_3P)_4]$
$M_r = 1439.06$
Monoclinic, $C2/c$
$a = 28.455$ (6) Å
$b = 13.737$ (3) Å
$c = 19.396$ (4) Å
$\beta = 115.46$ (3)°
$V = 6845$ (3) Å^3
$Z = 4$
$D_x = 1.396$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 4$–26°
$\mu = 0.85$ mm^{-1}
$T = 295$ (2) K
Block, blue
0.35 × 0.25 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: none
14736 measured reflections
7383 independent reflections
4751 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.065$
$\theta_{\rm max} = 27.0°$
$h = -36 \rightarrow 36$
$k = -16 \rightarrow 0$
$l = -23 \rightarrow 23$
3 standard reflections every 100 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.146$
$S = 1.07$
7383 reflections
416 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0719P)^2 + 0.8853P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 1.11$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.61$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.00067 (10)

Table 1
Selected geometric parameters (Å, °).

Cu1—P1	2.2321 (11)	Cu1—Cl1	2.3584 (10)
Cu1—P2	2.2420 (11)	Cl1—Cu1$^{\rm i}$	2.3822 (9)
P1—Cu1—P2	115.21 (4)	P2—Cu1—Cl1$^{\rm i}$	102.17 (3)
P1—Cu1—Cl1	106.44 (4)	Cl1—Cu1—Cl1$^{\rm i}$	94.90 (3)
P2—Cu1—Cl1	110.82 (4)	Cu1—Cl1—Cu1$^{\rm i}$	85.10 (3)
P1—Cu1—Cl1$^{\rm i}$	125.28 (4)		

Symmetry code: (i) $-x, 1-y, -z$.

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

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the rings C25–C30, C13–C17 and C7–C12, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C18—H18$A\cdots$Cl1$^{\rm i}$	0.93	2.73	3.408 (4)	130
C3—H3$A\cdots Cg1^{\rm i}$	0.93	2.84	3.640 (2)	145
C10—H10$A\cdots Cg2^{\rm ii}$	0.93	2.80	3.605 (2)	146
C28—H28$A\cdots Cg3^{\rm iii}$	0.93	2.80	3.605 (2)	146

Symmetry codes: (i) $-x, 1-y, -z$; (ii) $\frac{1}{2}-x, y-\frac{1}{2}, \frac{1}{2}-z$; (iii) $-x, -y, -z$.

H atoms were positioned geometrically (C—H = 0.93 Å) and allowed to ride on their parent atoms, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$. The highest peak is located 0.94 Å from atom Cu1.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1990); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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