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Chloro[pyrimidine-2(1*H*)-thione-κ*S*]bis(triphenylphosphine-κ*P*)copper(**I**)

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The pyrimidine-2-mercaptan ligand in the title copper(I) chloride adduct, $[CuCl(C_4H_4N_2S)(C_{18}H_{15}P)_2]$, coordinates to the metal atom through the doubly bonded S atom, the ligand being in the thione form. The coordination geometry of the Cu atom is tetrahedral.

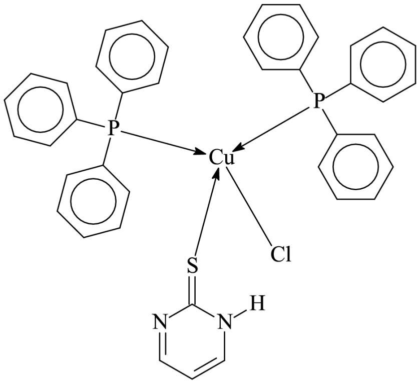
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.043
wR factor = 0.113
Data-to-parameter ratio = 18.8

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

Comment

An earlier study on the complex of copper(I) iodide with both phosphine and a heterocyclic mercaptan has shown that the 1-methyl-2-mercaptoimidazole donor ligand exists in the thione form in the adduct, the donor ligand coordinating through the doubly bonded S atom (Li *et al.*, 2004). The present bis(triphenylphosphine)cuprous chloride complex, (I), with 2-mercatopyrimidine also features such a bonding feature of the donor ligand (Fig. 1).



(I)

The amino H atom forms an intramolecular hydrogen bond to the Cl atom [$N\cdots Cl = 3.049\ (2)$ Å]. The Cu atom exists in a tetrahedral environment. The Cu—S, Cu—P and Cu—Cl distances compare well with those found in tetrahedral complexes having the $CuClP_2S$ core (Aslanidis *et al.*, 1998, 2002; Cox *et al.*, 1999; Lobana *et al.*, 1989; Skoulika *et al.*, 1991; Voutsas *et al.*, 1995).

Experimental

To a suspension of cuprous chloride (0.026 g, 0.25 mmol) in ethanol was added 2-mercaptopyrimidine (0.030 g, 0.25 mmol). The red precipitate that formed was collected and washed with ethanol. The compound was suspended in acetone together with triphenylphosphine (0.065 g, 0.25 mmol). After being stirred briefly, the mixture turned clear orange. The filtered solution, when set aside, yielded regularly shaped crystals.

Crystal data

[$\text{CuCl}(\text{C}_4\text{H}_4\text{N}_2\text{S})(\text{C}_{18}\text{H}_{15}\text{P})_2$]
M_r = 735.68
Monoclinic, $P2_1/c$
a = 14.4631 (8) Å
b = 10.1438 (6) Å
c = 24.393 (1) Å
β = 94.564 (1)°
V = 3567.4 (3) Å^3
Z = 4

D_x = 1.370 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4756 reflections
θ = 2.3–24.3°
μ = 0.87 mm^{-1}
T = 298 (2) K
Block, orange
0.20 × 0.19 × 0.13 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{\min}$ = 0.688, $T_{\max}$ = 0.896
21 086 measured reflections

8258 independent reflections
6403 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
$\theta_{\max}$ = 28.0°
$h = -18 \rightarrow 18$
$k = -6 \rightarrow 12$
$l = -32 \rightarrow 32$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.113
S = 1.01
8258 reflections
428 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0603P)^2 + 0.562P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$ = 0.001
$\Delta\rho_{\max}$ = 0.64 e Å^{-3}
$\Delta\rho_{\min}$ = −0.24 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—P1	2.2899 (6)	Cu1—S1	2.3875 (7)
Cu1—P2	2.2978 (6)	Cu1—Cl1	2.3664 (7)
P1—Cu1—P2	122.45 (2)	P2—Cu1—S1	112.70 (3)
P1—Cu1—S1	102.31 (3)	P2—Cu1—Cl1	98.77 (2)
P1—Cu1—Cl1	111.76 (2)	Cl1—Cu1—S1	108.58 (3)

The aromatic H atoms were placed at calculated positions [C—H = 0.93 Å and $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$] and were included in the refinement in the riding-model approximation. The nitrogen-bound H atom was located and refined with an N—H distance restraint of 0.85 (1) Å.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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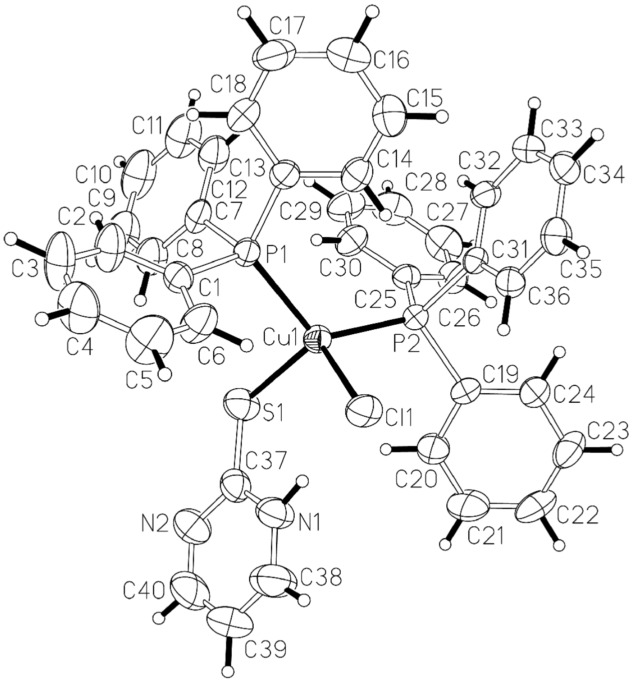

Figure 1
*ORTEP*II (Johnson, 1976) plot of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii.

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