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Iodo(1-methyl-2-mercaptoimidazole-κS)-bis(triphenylphosphine-κP)copper(I)

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.007 Å
R factor = 0.052
wR factor = 0.124
Data-to-parameter ratio = 20.4

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

The heterocyclic ligand in the title copper(I) iodide adduct, $[CuI(C_4H_6N_2S)(C_{18}H_{15}P)_2]$, coordinates to the metal atom through the S atom; the Cu atom is in a tetrahedral environment.

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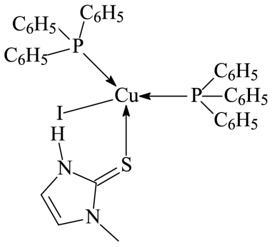
Comment

Our interest in mixed-ligand copper(I) complexes with heterocyclic mercaptans and triarylphosphines stems from our studies on the coordination compounds of the coinage metals; such complexes are photoluminescent materials (Li *et al.*, 2003). The property is also exhibited by the copper(I) iodide complex with the 2-mercapto-1-methylimidazole/triphenylphosphine pair of ligands, (I).



(I)

The Cu atom in (I) is in a tetrahedral environment (Fig. 1). A distorted tetrahedral geometry is also found in the phosphine adducts of copper(I) halides (Aslanidis *et al.*, 1993, 1998; Aslanidis, Cox, Divanidis & Tsipis, 2002; Aslanidis, Cox, Karagiannidis *et al.*, 2002; Cox *et al.*, 2000; Karagiannidis *et al.*, 1990; Lecomte *et al.*, 1989; Skoulika *et al.*, 1991). The Cu—I and Cu—S distances in (I) are similar to those observed in bis(triphenylphosphine)(pyrimidine-2-thione)copper(I) iodide (Aslanidis *et al.*, 1993), and bis(triphenylphosphine)(benzimidazole-2-thione)copper(I) iodide and bis(triphenylphosphine)(benzothiazole-2-thione)copper(I) iodide (Aslanidis, Cox, Karagiannidis *et al.*, 2002).

Experimental

Triphenylphosphine (0.11 g, 0.4 mmol) was added to a dichloromethane suspension of cuprous iodide (0.038 g, 0.2 mmol). After stirring for 0.5 h, 1-methylimidazole-2-mercaptan (0.023 g, 0.2 mmol) was added. The mixture was stirred for another hour to afford a colorless solution. The adduct was precipitated from solution by diethyl ether. Slow diffusion of diethyl ether into a dichloromethane solution of the powder led to well formed crystals.

Crystal data

$[CuI(C_4H_6N_2S)(C_{18}H_{15}P)_2]$
$M_r = 829.15$
Orthorhombic, *Pccn*
$a = 22.203$ (1) Å
$b = 17.877$ (1) Å
$c = 18.487$ (1) Å
$V = 7337.6$ (7) Å^3
$Z = 8$
$D_x = 1.501$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4458 reflections
$\theta = 2.2$–20.8°
$\mu = 1.61$ mm^{-1}
$T = 296$ (2) K
Block, colorless
0.28 × 0.22 × 0.15 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{\min} = 0.660$, $T_{\max} = 0.785$
43 051 measured reflections
8738 independent reflections
6085 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.066$
$\theta_{\max} = 28.1°$
$h = -17 \rightarrow 29$
$k = -22 \rightarrow 23$
$l = -24 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.124$
$S = 1.05$
8738 reflections
428 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0571P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.52$ e Å^{-3}
$\Delta\rho_{\min} = -0.53$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

I1—Cu1	2.6811 (5)	Cu1—P2	2.288 (1)
Cu1—P1	2.284 (1)	Cu1—S1	2.369 (1)
P1—Cu1—P2	125.72 (4)	P2—Cu1—S1	106.75 (4)
P1—Cu1—S1	102.99 (4)	P2—Cu1—I1	103.41 (3)
P1—Cu1—I1	104.63 (3)	S1—Cu1—I1	113.70 (3)

The aromatic H atoms were placed in calculated positions [C—H = 0.93 Å and $U_{\rm iso} = 1.2U_{\rm eq}$(C)] in the riding-model approximation. The torsion angle of the methyl group was refined [C—H = 0.96 Å and $U_{\rm iso} = 1.5U_{\rm eq}$(C)]. The nitrogen-bound H atom was located and refined with a distance restraint of N—H = 0.85 (1) Å. This atom is not involved in any hydrogen-bonding interaction.

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.

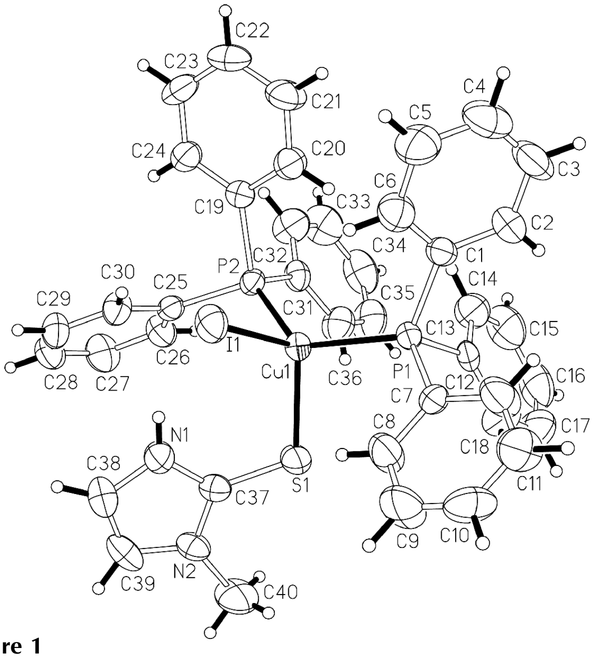


Figure 1
*ORTEP*II (Johnson, 1976) plot of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

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