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## Key indicators

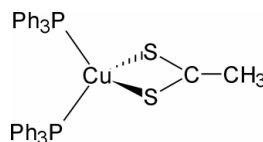
Single-crystal X-ray study  
T = 293 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.007 \text{ \AA}$   
Disorder in solvent or counterion  
R factor = 0.064  
wR factor = 0.161  
Data-to-parameter ratio = 20.4For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Bis(dithioacetato- $\kappa^2\text{S}$ )bis(triphenylphosphine- $\kappa\text{P}$ )-  
copper(I) 1.5-toluene solvate

The crystal structure of the title compound,  $[\text{Cu}(\text{C}_2\text{H}_3\text{S}_2)(\text{C}_{18}\text{H}_{15}\text{P})_2] \cdot 1.5\text{C}_7\text{H}_8$ , is reported. The compound is monomeric with the copper metal atom assuming a distorted tetrahedral geometry.

Received 16 October 2001  
Accepted 30 October 2001  
Online 10 November 2001

## Comment

We have been interested in exploring the chemistry of thio-carboxylates for many years. Recently we have synthesized and characterized a series triphenylphosphine adducts of copper(I) thioacetate and copper(I) thiobenzoate (Deivaraj *et al.*, 2000). The bis(triphenylphosphine) adduct of copper(I)-thioacetate is a dimer while the analogous thiobenzoate compound is a monomer. Similarly, the structure of  $[(\text{Ph}_3\text{P})_2\text{Cu}(\text{S}_2\text{C}-\text{C}_6\text{H}_4-\text{CH}_3)]$  is also known to be monomeric (Camus *et al.*, 1980). The title compound, (I), was obtained as a minor product of decomposition during an attempted synthesis of  $[(\text{Ph}_3\text{P})_2\text{CuGa}(\text{SC}(\text{O})\text{Me})_4]$ . Structural similarities between monothio- and dithiocarboxylates are not well understood, especially in terms of the influence of the R groups. Hence, we carried out a structural analysis of the title compound and we report here the outcome of our investigation.



(I)

The dithioacetate complex crystallizes with disordered toluene solvate molecules; the first was modelled over two positions with occupancies 0.7 and 0.3, the second over two positions with occupancies 0.25 and 0.25. The central Cu atom assumes a distorted tetrahedral geometry; it is bonded to two triphenylphosphine ligands and the dithioacetate ligand is bonded to the central metal atom in a bidentate fashion, a common bonding mode observed in dithiocarboxylate systems (Livingstone, 1987). Thus the coordination environment around the copper metal atom is  $\text{P}_2\text{S}_2$ , accounting for its distorted tetrahedral geometry.

The Cu–S distances [2.431(1) and 2.456(1) Å] observed in the title compound are comparable to those observed in the compound  $[(\text{Ph}_3\text{P})_2\text{Cu}(\text{S}_2\text{C}-\text{C}_6\text{H}_4-\text{CH}_3)]$  (Camus *et al.*, 1980). Similarly, the Cu1–P1 and Cu1–P2 distances of 2.261(1) and 2.260(1) Å are comparable to those [2.258(2) and 2.246(3) Å] observed in  $[(\text{Ph}_3\text{P})_2\text{Cu}(\text{S}_2\text{C}-\text{C}_6\text{H}_4-\text{CH}_3)]$ . The two C–S distances are 1.645(5) and 1.659(5) Å. A CSD search (Allen

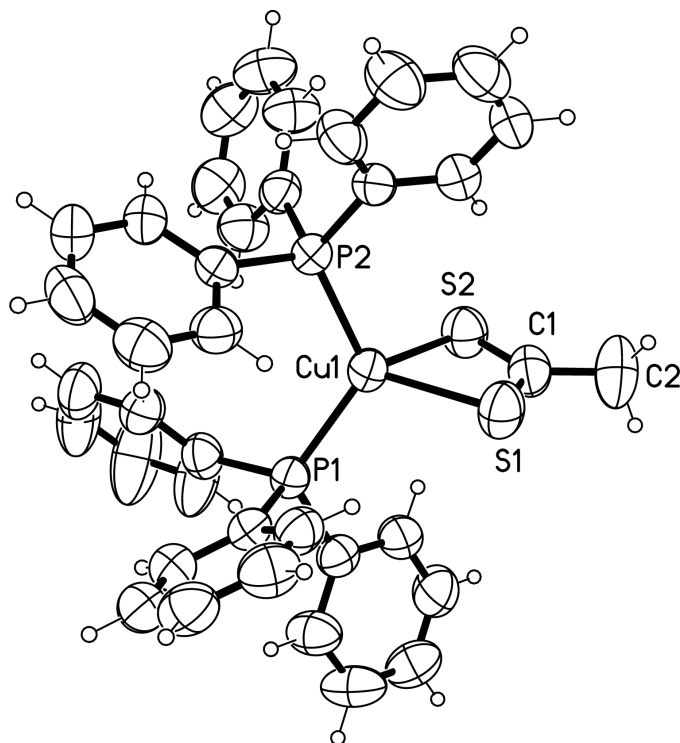


Figure 1

A view of the dithioacetate complex, showing the labelling of the non-H atoms. Displacement ellipsoids are drawn at the 50% probability level. The disordered solvent molecules have been omitted.

*et al.*, 1991) indicates that the normal range of C—S distances in similar compounds is 1.640–1.790 Å. The fact that the two C—S distances are almost equal and fall in the lower end of the normal range observed in similar compounds suggests that the C—S bond has acquired partial double-bond character owing to delocalization of electrons.

The P2—Cu1—P1 and S1—Cu1—S2 angles are 119.64 (4) and 71.92 (4)° respectively. The P—Cu—S angles range from 107.09 (4) to 120.2 (4)°. These angles clearly illustrate the extent of distortion in the tetrahedral geometry around the copper metal atom. The S—Cu—S bond angle, 71.92 (4)°, is comparable to the bite angle observed in the compound [(Ph<sub>3</sub>P)<sub>2</sub>Cu(S<sub>2</sub>C—C<sub>6</sub>H<sub>4</sub>—CH<sub>3</sub>)] [73.5(1)°]; such a bite angle is common in dicarboxylate compounds. However, the O—Cu—S bite angle observed in [(Ph<sub>3</sub>P)<sub>2</sub>Cu(SC(O)Ph)] is much smaller [65.19 (6)°] owing to geometry constraints.

In conclusion, the molecular structure of the title compound is a monomer, similar to its tolyl derivative (Camus *et al.*, 1980). However, the corresponding monothioacetate compound is dimeric in the solid state.

## Experimental

The title compound was obtained as a minor product during an attempted synthesis of bimetallic compounds of the type [(Ph<sub>3</sub>P)<sub>2</sub>CuGa(SC(O)Me)<sub>4</sub>] by reacting appropriate amounts of [(Ph<sub>3</sub>P)<sub>2</sub>CuNO<sub>3</sub>] with Ga(NO<sub>3</sub>)<sub>3</sub>·H<sub>2</sub>O and Na<sup>+</sup>·MeC(O)S<sup>-</sup>. Bright-red single crystals of the title compound were obtained from a toluene solution of the compound stored at 268 K for nearly two days.

## Crystal data

C<sub>48.50</sub>H<sub>45</sub>CuP<sub>2</sub>S<sub>2</sub>  
*M<sub>r</sub>* = 817.44  
 Monoclinic, *P*2<sub>1</sub>/*n*  
*a* = 10.8877 (2) Å  
*b* = 24.1232 (4) Å  
*c* = 16.7066 (2) Å  
 $\beta$  = 95.772 (1)°  
*V* = 4365.68 (12) Å<sup>3</sup>  
*Z* = 4

*D<sub>x</sub>* = 1.244 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 Cell parameters from 8192 reflections  
 $\theta$  = 2.1–25.0°  
 $\mu$  = 0.70 mm<sup>-1</sup>  
*T* = 293 (2) K  
 Blocks, cut, red  
 0.40 × 0.32 × 0.24 mm

## Data collection

SMART CCD diffractometer  
 $\omega$  scans  
 Absorption correction: empirical (SADABS; Sheldrick, 2000)  
*T<sub>min</sub>* = 0.751, *T<sub>max</sub>* = 0.845  
 23356 measured reflections  
 8735 independent reflections

6380 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.028  
 $\theta_{max}$  = 26.4°  
*h* = -13 → 12  
*k* = -30 → 24  
*l* = -19 → 20

## Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.064  
*wR* (*F*<sup>2</sup>) = 0.161  
*S* = 1.10  
 8735 reflections  
 428 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0566P)^2 + 4.3706P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} < 0.001$   
 $\Delta\rho_{max} = 0.66 \text{ e \AA}^{-3}$   
 $\Delta\rho_{min} = -0.48 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Cu1—P2	2.2600 (10)	S1—C1	1.645 (5)
Cu1—P1	2.2614 (10)	S2—C1	1.659 (5)
Cu1—S1	2.4314 (12)	C1—C2	1.527 (6)
Cu1—S2	2.4556 (12)		
P2—Cu1—P1	119.64 (4)	S1—Cu1—S2	71.92 (4)
P2—Cu1—S1	118.14 (5)	C1—S1—Cu1	84.26 (15)
P1—Cu1—S1	110.96 (4)	C1—S2—Cu1	83.19 (15)
P2—Cu1—S2	107.09 (4)	C2—C1—S1	119.4 (4)
P1—Cu1—S2	120.21 (4)		

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Bruker, 1997); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

Financial support for this research to JJV from the National University of Singapore (R-143-000-084-112) is gratefully acknowledged.

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