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Key indicators

Single-crystal X-ray study
 T = 295 K
 Mean $\sigma(C-C)$ = 0.007 Å
 R factor = 0.047
 wR factor = 0.137
 Data-to-parameter ratio = 17.0

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

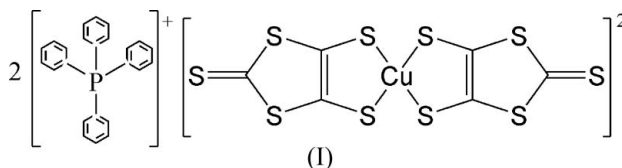
**Bis(tetraphenylphosphonium) bis(2-thioxo-
 1,3-dithiole-4,5-dithiolato)cuprate(II)**

In the title complex, $(C_{24}H_{20}P)_2[Cu(C_3S_5)_2]$, the Cu^{II} ion is coordinated by four S atoms from two 2-thioxo-1,3-dithiole-4,5-dithiolate ligands in a distorted planar geometry. The anion possesses C_2 symmetry with the metal ion lying on a twofold axis.

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Comment

Transition metal–dmit salts (dmit is 2-thioxo-1,3-dithiole-4,5-dithiolate) have attracted much attention because of their promising conduction and optical properties (Li *et al.*, 1996; Xia *et al.*, 1997; Dai *et al.*, 2000; Sun *et al.*, 2001). As part of our investigations on metal-organic materials, the title compound, (I), was prepared and analysed crystallographically.



The structure of (I) consists of $[Cu(dmit)_2]^{2-}$ anions and tetraphenylphosphonium cations (Fig. 1). The anion has C_2 symmetry. The Cu^{II} ion is located on a twofold axis and is coordinated by four S atoms from two dmit ligands in a distorted planar geometry (Table 1). The dihedral angle between the dmit planes is $24.0(1)^\circ$. The Cu^{II} ion deviates by $0.070(1)$ Å from the mean plane defined by the two dmit ligands.

Experimental

Dmit(COPh)₂ (0.816 g, 2 mmol) was treated with an excess of sodium methylate (0.5 M) in MeOH (20 ml) at room temperature with stirring. To the resulting red solution, solutions of CuCl₂·2H₂O (0.170 g, 1 mmol) in MeOH (20 ml) and then tetraphenylphosphonium bromide (1.005 g, 2.4 mmol) in MeOH (20 ml) were added. The resulting precipitate was washed with MeOH and then dissolved in acetone. Single crystals of (I) suitable for X-ray structure analysis were obtained by slow evaporation of the solution at room temperature.

Crystal data

$(C_{24}H_{20}P)_2[Cu(C_3S_5)_2]$	Z = 4
$M_r = 1134.94$	$D_x = 1.436$ Mg m ⁻³
Monoclinic, C2/c	Mo K α radiation
$a = 20.255(3)$ Å	$\mu = 0.91$ mm ⁻¹
$b = 12.6669(17)$ Å	T = 295(2) K
$c = 20.499(2)$ Å	Prism, dark red
$\beta = 93.772(10)^\circ$	$0.36 \times 0.34 \times 0.30$ mm
$V = 5248.2(12)$ Å ³	

Data collection

Bruker P4 diffractometer
 ω scans
 Absorption correction: ψ scan
 (XSCANS; Bruker, 1996)
 $T_{\min} = 0.710$, $T_{\max} = 0.765$
 6171 measured reflections
 5167 independent reflections

3172 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.031$
 $\theta_{\text{max}} = 26.0^\circ$
 3 standard reflections
 every 97 reflections
 intensity decay: 1%

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.137$
 $S = 1.03$
 5167 reflections
 304 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0617P)^2 + 1.9578P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.41 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.56 \text{ e } \text{\AA}^{-3}$
 Extinction correction: SHELXTL
 Extinction coefficient: 0.0036 (2)

Table 1

Selected geometric parameters (\AA , $^\circ$).

S4—Cu1	2.2837 (11)	S5—Cu1	2.2751 (11)
S5 ⁱ —Cu1—S5	166.73 (7)	S5—Cu1—S4	92.10 (4)
S5—Cu1—S4 ⁱ	89.80 (4)	S4 ⁱ —Cu1—S4	163.49 (7)

Symmetry code: (i) $-x + 1, y, -z + \frac{3}{2}$.

All H atoms were positioned geometrically and refined using a riding model with C—H = 0.93 \AA , with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: XSCANS (Bruker, 1996); cell refinement: XSCANS; data reduction: SHELXTL (Bruker, 1997); program(s) used to solve structure: SIR97 (Altomare *et al.*, 1999); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: WinGX (Farrugia, 1999).

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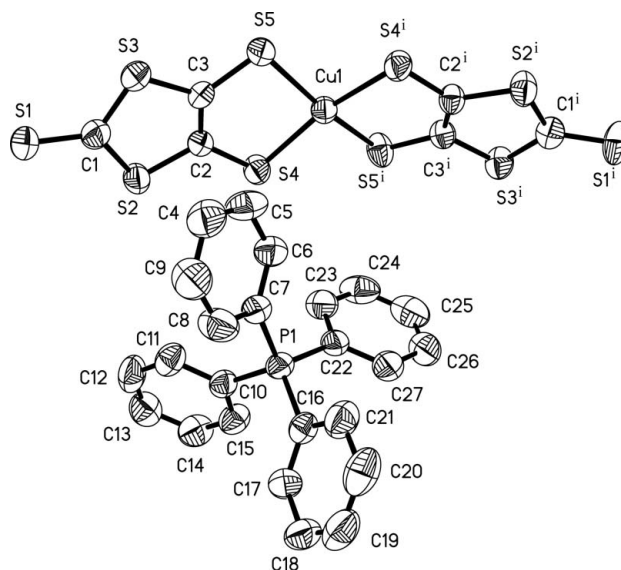


Figure 1

The structures of anion and cation in (I). Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity. [Symmetry code: (i) $1 - x, y, \frac{3}{2} - z$.]

References

- Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
- Bruker (1996). XSCANS. Version 2.2. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (1997). SHELXTL. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
- Dai, J., Bian, G. Q., Wang, X., Xu, Q. F., Zhou, M. Y., Munakata, M., Maekawa, M., Tong, M. H., Sun, Z. R. & Zeng, H. P. (2000). *J. Am. Chem. Soc.* **122**, 11007–11008.
- Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
- Li, H., Huang, C. H., Xu, J., Li, T., Zhao, X. & Xia, X. (1996). *J. Chem. Soc. Faraday Trans.* **92**, 2585–2592.
- Sun, Z. R., Tong, M. H., Zeng, H. P., Ding, L. G., Wang, Z. G., Xu, Z. Z., Dai, J. & Bian, G. Q. (2001). *Chem. Phys. Lett.* **342**, 323–327.
- Xia, W. S., Huang, C. H. & Zhou, D. J. (1997). *Langmuir*, **13**, 80–84.