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

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.050
wR factor = 0.141
Data-to-parameter ratio = 18.7

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

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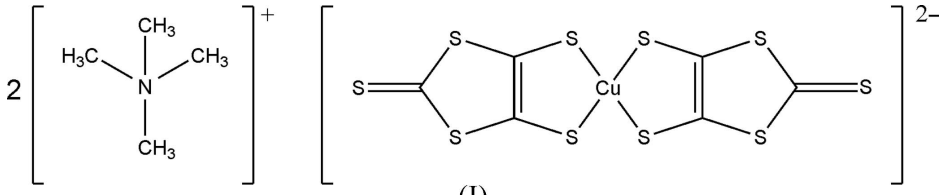
In the title compound, $(C_4H_{12}N)_2[Cu(C_3S_5)_2]$, the Cu^{II} atom lies on a centre of inversion and is coordinated by four S atoms from two 2-thioxo-1,3-dithiole-4,5-dithiolate ligands in a square-planar geometry.

Comment

Transition-metal complexes with 2-thioxo-1,3-dithiole-4,5-dithiolate (dmit) have attracted attention because of their promising conducting and optical properties (Li *et al.*, 1996; Xia *et al.*, 1997; Dai *et al.*, 2000; Sun *et al.*, 2001). In salts of these complexes, the identity of the cation influences both the molecular and crystal structures. As part of our research in this area, we report here the crystal structure of the title salt, (I).



(I)

In (I) (Fig. 1 and Table 1), dmit shows its typical chelating behaviour and Cu^{II} is coordinated by four S atoms from two dmit ligands. The CuS_4 core adopts a square-planar geometry, with Cu^{II} lying on a centre of inversion. This is similar to the tetrabutylammonium salt (Wang *et al.*, 1986), but differs from the tetraethylammonium (Wang *et al.*, 2005) and *N*-ethylpyridinium (Matsubayashi *et al.*, 1988) salts, in which the coordination geometry is distorted towards a tetrahedral arrangement.

Experimental

The title compound was prepared according to a literature procedure (Steimeck & Kirmse, 1979). Single crystals suitable for X-ray analysis were obtained by slow evaporation of an acetone solution at room temperature.

Crystal data

$(C_4H_{12}N)_2[Cu(C_3S_5)_2]$
M_r = 604.49
Monoclinic, $P2_1/c$
a = 11.440 (3) Å
b = 10.362 (3) Å
c = 12.140 (4) Å
β = 113.697 (4)°
V = 1317.8 (7) Å^3
Z = 2
D_x = 1.523 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.63 mm^{-1}
T = 293 (2) K
Prism, brown
0.36 × 0.27 × 0.07 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.596, T_{max} = 0.892
6352 measured reflections
2324 independent reflections
1889 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.141
S = 0.93
2324 reflections
124 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0871P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—S1	2.2732 (12)	Cu1—S2	2.2758 (12)
S1—Cu1—S2	91.83 (4)	Cu1—S2—C2	100.27 (14)
S1^{i}—Cu1—S2	88.17 (4)	C3—S3—C1	98.8 (2)
S1^{i}—Cu1—S1	180.0	C3—S4—C2	98.8 (2)
Cu1—S1—C1	100.43 (14)		

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

H atoms were placed in calculated positions, with C—H = 0.96 Å, and refined in riding mode, with $U_{iso}(H) = 1.5U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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*.

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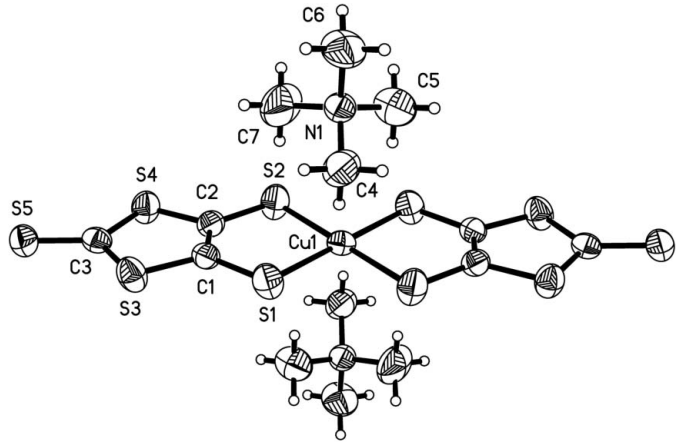

Figure 1
The molecular structure of (I), showing displacement ellipsoids drawn at the 50% probability level for non-H atoms. Unlabelled atoms are related to labelled atoms by $(-x, 1-y, 1-z)$.

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