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Bis{μ-2-[(*E*)-(3,5-dibromo-2-oxidophenyl)methyleneamino]ethanesulfonato-$\kappa^3N,O,O':\kappa O''$}bis[methanolcopper(II)]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.016 Å
R factor = 0.071
wR factor = 0.209
Data-to-parameter ratio = 13.6

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

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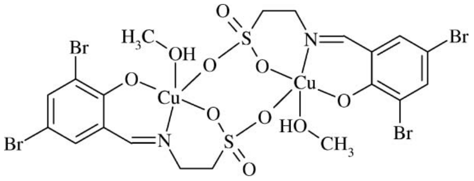
In the centrosymmetric title compound, $[Cu_2(C_9H_7Br_2NO_4S)_2(CH_3OH)_2]$, each Cu^{II} atom adopts a distorted square-pyramidal CuO_4N coordination geometry, formed by one N atom and three O atoms from two different 2-[(*E*)-(3,5-dibromo-2-oxidophenyl)methyleneamino]ethanesulfonate ligands and one O atom from a methanol molecule. Adjacent Cu^{II} atoms are linked by bridging sulfonate groups to form a dinuclear compound, with a Cu$\cdots$Cu distance of 5.41 (1) Å.

Comment

Various dicopper active sites found in copper-containing metalloenzymes have similar structural features, with three histidine donors coordinated to each of two Cu centres, and with a Cu$\cdots$Cu distance of about 3.5 Å. One prominent member of the Type III Cu proteins is catechol oxidase, which catalyzes two-electron oxidation of *ortho*-diphenols to the corresponding quinones. A number of dinuclear Cu complexes (Than *et al.*, 1999; Sreenivasulu *et al.*, 2005; Kao *et al.*, 2001) have been investigated as biomimetic catalysts for catechol oxidation by employing the most common and convenient model substrate, 3,5-di-*tert*-butylcatechol (3,5-DTBC), which can be oxidized to 3,5-di-*tert*-butylquinone (3,5-DTBQ). Here, we describe the title centrosymmetric dinuclear Cu complex, $[Cu(L)(CH_3OH)]_2$, (I), where LH_2 = 2-[(*E*)-(3,5-dibromo-2-oxidophenyl)methyleneamino]ethanesulfonic acid.



(I)

In (I), Cu^{II} is coordinated by one N atom and three O atoms from two different L^{2-} ligands, and by one O atom from a methanol molecule, forming a distorted square-pyramidal CuO_4N coordination polyhedron in which one O atom from L^{2-} lies in the apical position (Fig. 1). Sulfonate groups bridge two Cu^{II} atoms to form a dinuclear compound. The apical Cu1—O3^{i} distance [symmetry code: (i) $1 - x, 1 - y, 1 - z$] is significantly longer than the Cu1—O,N distances within the basal plane (Table 1), indicating that the bridging Cu—O interaction is a weak coordination bond (Procter *et al.*, 1968).

Experimental

A solution of taurine ($H_2N(CH_2)_2SO_3H$, 0.125 g, 1 mmol) and NaOH (0.080 g, 2 mmol) in distilled water (15 ml) was slowly added to a solution of 2,4-dibromo-6-vinylphenol (0.202 g, 1 mmol) in methanol (20 ml). The mixture was stirred for 30 min at 333 K, and this solution was then slowly added to a solution of $Cu(OAc)_2 \cdot H_2O$ (1.0 mmol, 0.199 g) in methanol (15 ml). The mixture was stirred and refluxed for 4 h at 323 K, then filtered. The filtrate was left to stand at room temperature and blue crystals were obtained in a yield of 52% (based on Cu).

Crystal data

$[Cu_2(C_9H_7Br_2NO_4S)_2(CH_4O)_2]$
$M_r = 961.24$
Triclinic, $P\overline{1}$
$a = 5.280$ (1) Å
$b = 9.374$ (2) Å
$c = 14.785$ (3) Å
$\alpha = 87.97$ (3)°
$\beta = 88.26$ (3)°
$\gamma = 74.02$ (3)°
$V = 702.8$ (2) Å^3
$Z = 1$
Mo $K\alpha$ radiation
$\mu = 7.40$ mm^{-1}
$T = 293$ (2) K
0.28 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.122$, $T_{max} = 0.228$
3971 measured reflections
2473 independent reflections
1583 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.071$
$wR(F^2) = 0.209$
$S = 1.02$
2473 reflections
182 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max} = 1.63$ e Å^{-3}
$\Delta\rho_{min} = -1.24$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.868 (7)	Cu1—O5	1.974 (7)
Cu1—N1	1.959 (9)	Cu1—O3^i	2.466 (4)
Cu1—O2	1.974 (7)		
O1—Cu1—N1	94.4 (3)	O1—Cu1—O5	88.2 (3)
O1—Cu1—O2	167.9 (3)	N1—Cu1—O5	173.6 (3)
N1—Cu1—O2	93.5 (3)	O2—Cu1—O5	83.0 (3)

Symmetry code: (i) $-x+2, -y+1, -z$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5A···O3^{ii}	0.82	2.25	2.758 (10)	121

Symmetry code: (ii) $-x+3, -y+1, -z$.

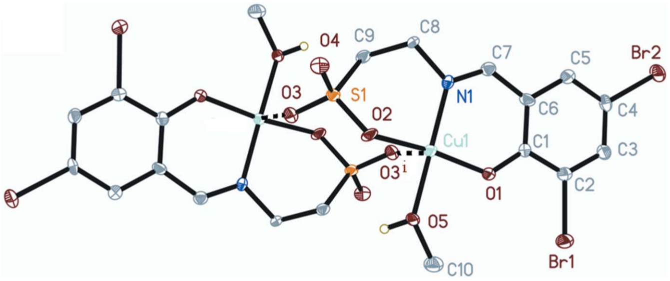


Figure 1
The molecular structure of (I), showing displacement ellipsoids at the 30% probability level for non-H atoms. Non-labelled atoms are related to labelled atoms by the symmetry operation $(1-x, 1-y, 1-z)$.

H atoms were positioned geometrically and treated as riding atoms, with C—H = 0.93–0.97 Å and O—H = 0.82 Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(C,O)$. The displacement parameters of atom C10 were restrained to approximate isotropic behaviour. The highest peak and deepest hole in the residual electron density lie 1.02 Å from atom Br1 and 1.08 Å from atom Cu1, respectively.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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