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[5-Bromo-*N*-(2-pyridylethylsulfanylethyl)-salicylideneiminato-κ^4N,N',O,S]copper(II) perchlorate

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Key indicators

Single-crystal X-ray study
T = 113 K
Mean σ(C–C) = 0.006 Å
R factor = 0.039
wR factor = 0.107
Data-to-parameter ratio = 15.0

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

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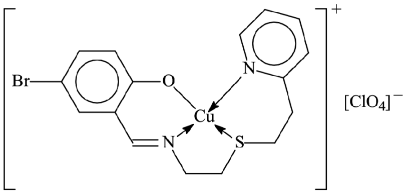
The Cu atom in the title compound, [Cu($C_{16}H_{16}BrN_2OS$)]-ClO_4, exists in a distorted square-planar geometry. The compound exists as discrete ions.

Comment

The structural chemistry of the metal complexes derived from tetradentate Schiff bases that are synthesized by condensing two formula units of salicyldehyde with one formula unit of a diamine has been documented for a wide range of metal systems. The large number of such Schiff bases contrasts with only a few that have been prepared from salicyladehyde (which provides the O and N donor sites) and an amine that possesses both an *N*-heterocycle and a thioether linkage (and which provides the S and N donor sites), owing to the relative difficulty of obtaining such amines. One example of such a metal complex, [*N*-2-[(5′-methylimidazolyl-4′-yl)methylthio]-ethylsalicylideneiminato]copper perchlorate, has the metal atom in a square-planar geometry which is distorted towards a tetrahedron, owing to a weaker Cu—S bond (Bailey *et al.*, 1988). The present study of the title copper complex of (2-pyridylethylthio)ethyl-5-bromosalicylideneimine, (I), continues a recent structural study of the nickel monoperchlorate complex of the deprotonated iodo analogue of the ligand. In that compound, the metal atoms in the two independent cations showed a distorted square-planar coordination (Daneshvar *et al.*, 2003).



(I)

The Cu atom in (I) also displays such a distorted geometry (Fig. 1). The distortion arises from the somewhat long Cu—S bond [2.332 (1) Å], but there are no significant differences in bond distances between the present Cu complex and the reported Ni complexes. There are no important interactions between the Cu atom and the perchlorate anion.

Experimental

To a stirred solution of 5-bromosalicylaldehyde (0.20 g, 1 mmol) in ethanol (5 ml) was added a solution of 1-(2-pyridyl)-3-thia-5-aminopentane (0.18 g, 1 mmol) in ethanol (5 ml). The yellow solution was heated for 1 h to afford a yellow solid. The compound was collected and recrystallized from a chloroform–ethanol (1:2 *v*/*v*) mixture in nearly quantitative yield (m.p. 342 K). Analysis, calculated for

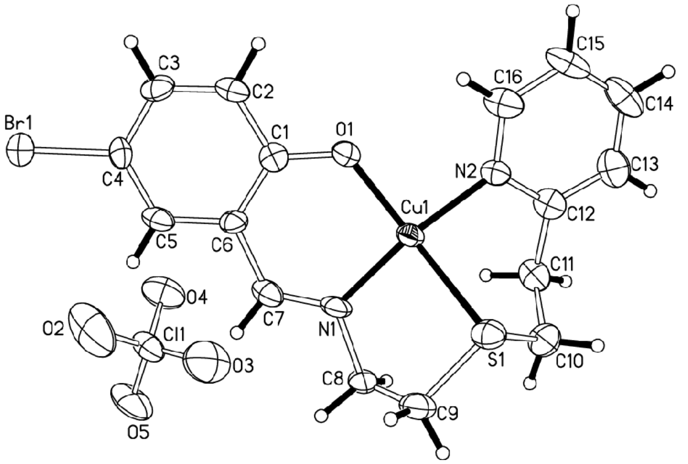


Figure 1
A view of the structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 75% probability level and H atoms are shown as small spheres of arbitrary radii.

$C_{16}H_{17}N_2OS$: C 52.60, H 4.69, N 7.66%; found: C 52.50; H 4.70; N 7.60%. A solution of this organic reagent (0.37 g, 1 mmol) in absolute ethanol (10 ml) was treated with a methanol solution (1 ml) of 1 *M* sodium hydroxide. Copper perchlorate hexahydrate (0.37 g, 1 mmol) was added to the solution to give a dark-green solution. The solution was briefly heated. The crystals of (I) which separated were collected and purified by recrystallization from methanol.

Crystal data

$[Cu(C_{16}H_{16}BrN_2OS)]ClO_4$
$M_r = 527.27$
Monoclinic, $P2_1/n$
$a = 9.9542$ (6) Å
$b = 8.8479$ (6) Å
$c = 21.223$ (1) Å
$\beta = 102.263$ (1)°
$V = 1826.5$ (2) Å^3
$Z = 4$
$D_x = 1.917$ Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 5071 reflections
$\theta = 2.5$–26.4°
$\mu = 3.68$ mm^{-1}
$T = 113$ (2) K
Plate, blue
0.45 × 0.43 × 0.15 mm

Data collection

Siemens *P*4 diffractometer with CCD area-detector
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.145$, $T_{max} = 0.576$
9902 measured reflections
3657 independent reflections
2645 reflections with $I > 2\sigma(I)$
$R_{int} = 0.057$
$\theta_{max} = 26.5°$
$h = -12 \rightarrow 12$
$k = -11 \rightarrow 11$
$l = -23 \rightarrow 26$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.107$
$S = 0.99$
3657 reflections
244 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0558P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.72$ e Å^{-3}
$\Delta\rho_{min} = -1.49$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	1.904 (3)	Cu1—O1	1.866 (3)
Cu1—N2	1.966 (3)	Cu1—S1	2.332 (1)
N1—Cu1—O1	96.2 (1)	N2—Cu1—O1	92.9 (1)
N1—Cu1—N2	157.4 (1)	N2—Cu1—S1	91.7 (1)
N1—Cu1—S1	87.5 (1)	O1—Cu1—S1	157.9 (1)

The aromatic (C—H = 0.95 Å) and aliphatic (C—H = 0.99 Å) H atoms were positioned geometrically, and were included in the refinement in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$. The final difference Fourier map had a large peak near the Br atom (at 0.79 Å). and the deepest hole was 0.13 Å from the Cu atom

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); 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.

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