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{4-Bromo-2-[2-(methylamino)ethyliminomethyl]phenolato}thiocyanatocopper(II)

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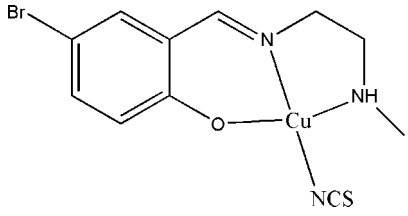
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.012 Å; R factor = 0.076; wR factor = 0.181; data-to-parameter ratio = 18.3.

In the title mononuclear copper(II) complex, [Cu($C_{10}H_{12}BrN_2O$)(NCS)], the Cu^{II} ion is coordinated by two N atoms and one O atom from a Schiff base ligand, and by one N atom from a thiocyanate anion, giving a square-planar geometry. In the crystal structure, symmetry-related molecules are linked by an N—H···S hydrogen bond.

Related literature

For related literature, see: Diao & Li (2007); Diao *et al.* (2007); Ma *et al.* (2005); Ma, Gu *et al.* (2006); Ma, Lv *et al.* (2006); Ma, Wu *et al.* (2006); Wei *et al.* (2007).



Experimental

Crystal data

[Cu($C_{10}H_{12}BrN_2O$)(NCS)]
M_r = 377.75
Monoclinic, $P2_1/n$
a = 5.952 (3) Å
b = 19.660 (3) Å
c = 12.718 (2) Å
β = 94.331 (3)°
V = 1484.0 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.30 mm^{-1}
T = 298 (2) K
0.32 × 0.32 × 0.31 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.259, T_{max} = 0.267
11246 measured reflections
2997 independent reflections
1875 reflections with $I > 2\sigma(I)$
R_{int} = 0.071

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.076
$wR(F^2)$ = 0.180
S = 1.11
2997 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.68 e Å^{-3}
$\Delta\rho_{min}$ = −0.84 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···S1^{i}	0.91	2.76	3.635 (9)	162

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2051).

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supporting information

Acta Cryst. (2008). E**64**, m878 [doi:10.1107/S1600536808016589]

{4-Bromo-2-[2-(methylamino)ethyliminomethyl]phenolato}thiocyanato-copper(II)

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S1. Comment

Recently, we have reported on teh crystal structure alanyses of some metal complexes derived from Schiff base ligands (Ma, Lv *et al.*, 2006; Ma, Gu *et al.*, 2006; Ma, Wu *et al.*, 2006; Ma *et al.*, 2005). As part of a further investigation of the structures of such complexes, the title mononuclear copper(II) complex, (I), is reported on here.

In complex (I), the Cu atom is coordinated by two nitrogen atoms and one oxygen atom from a Schiff base ligand, and by one nitrogen atom from a thiocyanate anion, giving a square planar geometry (Fig. 1). All the bond lengths and angles related to the Cu atom in the complex are within normal ranges, and comparable to the values observed in other similar copper(II) complexes (Wei *et al.*, 2007; Diao *et al.*, 2007; Diao & Li, 2007). The four coordinating atoms around the Cu centre are approximately coplanar, giving a square-planar geometry with an average deviation of 0.090 (5) Å; the Cu atom lies 0.095 (2) Å above this plane. The C8—C9—N2—C10 torsion angle is 1.5 (3)°.

In the crystal structure of compound (I) symmetry related molecules are linked by an N—H···S hydrogen bond (Table 1).

S2. Experimental

N-Methylethane-1,2-diamine (0.5 mmol, 37.0 mg) and 5-bromosalicylaldehyde (0.5 mmol, 100.5 mg) were dissolved in methanol (30 ml). The mixture was stirred for 1 h to obtain a clear yellow solution. To this solution was added with stirring a methanol solution (20 ml) of copper(II) acetate (0.5 mmol, 99.6 mg) and a methanol solution (10 ml) of ammonium thiocyanate (0.5 mmol, 38.0 mg). After keeping the resulting solution in air for a few days, blue block-shaped crystals were formed.

S3. Refinement

All the H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H = 0.93 - 0.97 Å, with U_{iso}(H) = 1.2 or 1.5U_{eq}(C). An unassigned maximum residual density (1.68 Å^3) was observed 1.03 Å from Br1, which is due to the tail-effects of the heavy atom Br1. The structure contains solvent accessible voids of 119 Å^3, which may perhaps accommodate a partially occupied solvent molecule.

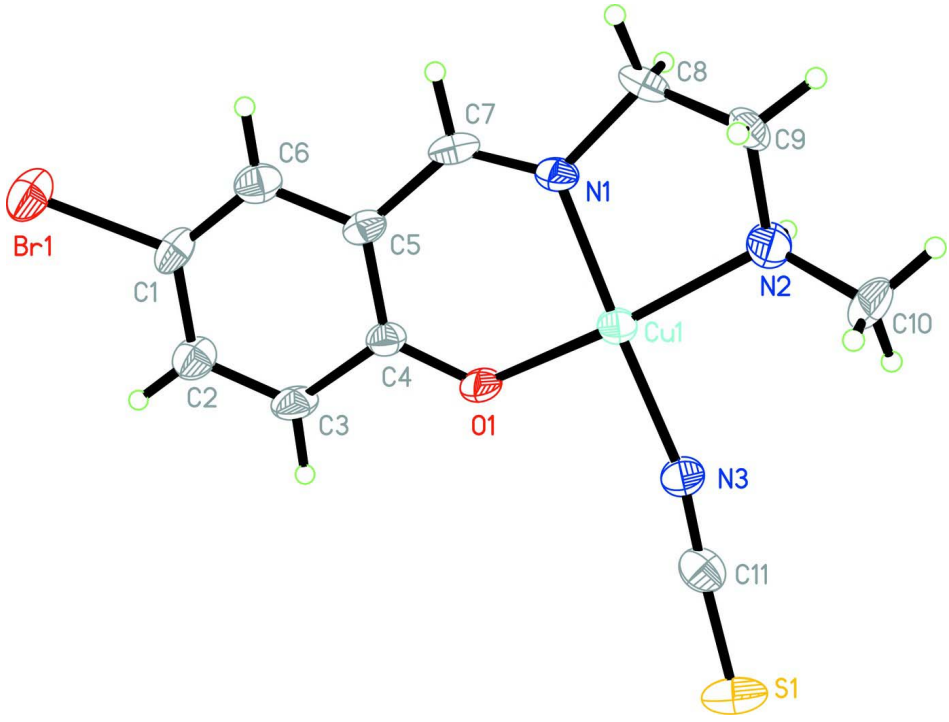

Figure 1

The molecular structure of compound (I), showing the atomic numbering scheme and the displacement ellipsoids drawn at the 30% probability level.

{4-Bromo-2-[2-(methylamino)ethyliminomethyl]phenolato}thiocyanatocopper(II)

Crystal data

$[Cu(C_{10}H_{12}BrN_2O)(NCS)]$
$M_r = 377.75$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 5.952$ (3) Å
$b = 19.660$ (3) Å
$c = 12.718$ (2) Å
$\beta = 94.331$ (3)°
$V = 1484.0$ (8) Å^3
$Z = 4$
$F(000) = 748$
$D_x = 1.691$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1708 reflections
$\theta = 2.5$–25.3°
$\mu = 4.30$ mm^{-1}
$T = 298$ K
Block, blue
0.32 × 0.32 × 0.31 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.259$, $T_{max} = 0.267$
11246 measured reflections
2997 independent reflections
1875 reflections with $I > 2\sigma(I)$
$R_{int} = 0.071$
$\theta_{max} = 26.5°$, $\theta_{min} = 2.6°$
$h = -7 \rightarrow 7$
$k = -24 \rightarrow 24$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.076$
$wR(F^2) = 0.181$
$S = 1.11$
2997 reflections
164 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0672P)^2 + 4.7203P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.68$ e Å^{-3}
$\Delta\rho_{min} = -0.84$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.77313 (15)	0.20764 (5)	0.04645 (8)	0.0407 (3)
N1	1.0514 (10)	0.1635 (3)	0.0963 (5)	0.0392 (15)
N2	0.8291 (12)	0.2634 (4)	0.1796 (7)	0.058 (2)
H2A	0.7645	0.2393	0.2304	0.070*
N3	0.4927 (12)	0.2539 (4)	0.0002 (6)	0.053 (2)
O1	0.7104 (8)	0.1410 (3)	−0.0588 (4)	0.0460 (14)
S1	0.0695 (4)	0.29376 (15)	−0.0863 (2)	0.0664 (8)
Br1	1.31654 (16)	−0.06412 (5)	−0.23999 (9)	0.0633 (4)
C1	1.1328 (13)	0.0028 (4)	−0.1792 (7)	0.044 (2)
C2	0.9203 (14)	0.0131 (4)	−0.2253 (8)	0.049 (2)
H2	0.8712	−0.0121	−0.2845	0.059*
C3	0.7799 (13)	0.0596 (4)	−0.1860 (7)	0.047 (2)
H3	0.6360	0.0657	−0.2184	0.057*
C4	0.8518 (13)	0.0994 (4)	−0.0946 (6)	0.0367 (18)
C5	1.0688 (12)	0.0860 (4)	−0.0492 (6)	0.0369 (18)
C6	1.2068 (14)	0.0376 (4)	−0.0913 (7)	0.045 (2)
H6	1.3497	0.0291	−0.0592	0.054*
C7	1.1533 (13)	0.1183 (4)	0.0480 (7)	0.042 (2)
H7	1.2941	0.1047	0.0773	0.051*
C8	1.1509 (15)	0.1902 (5)	0.1982 (7)	0.052 (2)
H8A	1.3140	0.1889	0.1997	0.062*
H8B	1.1038	0.1625	0.2557	0.062*
C9	1.0734 (14)	0.2612 (5)	0.2099 (7)	0.051 (2)
H9A	1.1028	0.2760	0.2824	0.061*
H9B	1.1531	0.2912	0.1650	0.061*

C10	0.7370 (17)	0.3305 (6)	0.1855 (10)	0.083 (4)
H10A	0.8001	0.3526	0.2482	0.125*
H10B	0.5763	0.3276	0.1874	0.125*
H10C	0.7728	0.3562	0.1248	0.125*
C11	0.3146 (15)	0.2696 (4)	−0.0378 (7)	0.048 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0271 (5)	0.0511 (6)	0.0429 (6)	0.0011 (4)	−0.0028 (4)	−0.0086 (5)
N1	0.028 (3)	0.047 (4)	0.041 (4)	−0.004 (3)	−0.006 (3)	−0.001 (3)
N2	0.040 (4)	0.062 (5)	0.070 (5)	−0.001 (4)	−0.005 (4)	−0.022 (4)
N3	0.030 (4)	0.069 (5)	0.058 (5)	0.008 (3)	−0.006 (3)	−0.015 (4)
O1	0.025 (3)	0.055 (4)	0.056 (4)	0.006 (3)	−0.009 (2)	−0.012 (3)
S1	0.0412 (13)	0.0813 (18)	0.0744 (18)	0.0000 (13)	−0.0115 (12)	0.0316 (15)
Br1	0.0480 (6)	0.0520 (6)	0.0910 (8)	0.0037 (4)	0.0131 (5)	−0.0149 (5)
C1	0.036 (4)	0.030 (4)	0.068 (6)	0.003 (3)	0.014 (4)	−0.002 (4)
C2	0.035 (5)	0.045 (5)	0.066 (6)	−0.005 (4)	0.001 (4)	−0.009 (4)
C3	0.029 (4)	0.047 (5)	0.064 (6)	0.000 (4)	−0.014 (4)	−0.007 (4)
C4	0.031 (4)	0.033 (4)	0.044 (5)	0.001 (3)	−0.006 (3)	−0.002 (4)
C5	0.029 (4)	0.040 (4)	0.041 (5)	0.004 (3)	0.004 (3)	0.013 (4)
C6	0.042 (5)	0.037 (4)	0.057 (5)	0.000 (4)	−0.002 (4)	0.007 (4)
C7	0.028 (4)	0.043 (5)	0.055 (5)	0.003 (4)	−0.007 (4)	0.015 (4)
C8	0.048 (5)	0.065 (6)	0.039 (5)	−0.011 (4)	−0.017 (4)	−0.003 (4)
C9	0.039 (5)	0.075 (6)	0.038 (5)	−0.006 (4)	−0.002 (4)	−0.022 (5)
C10	0.051 (6)	0.092 (8)	0.106 (9)	0.038 (6)	−0.005 (6)	−0.039 (7)
C11	0.042 (5)	0.051 (5)	0.050 (5)	−0.015 (4)	−0.001 (4)	−0.004 (4)

Geometric parameters (Å, º)

Cu1—O1	1.890 (5)	C2—H2	0.9300
Cu1—N1	1.934 (6)	C3—C4	1.439 (11)
Cu1—N3	1.952 (7)	C3—H3	0.9300
Cu1—N2	2.024 (7)	C4—C5	1.399 (10)
N1—C7	1.262 (10)	C5—C6	1.390 (11)
N1—C8	1.479 (10)	C5—C7	1.446 (12)
N2—C10	1.432 (12)	C6—H6	0.9300
N2—C9	1.476 (11)	C7—H7	0.9300
N2—H2A	0.9100	C8—C9	1.481 (12)
N3—C11	1.172 (11)	C8—H8A	0.9700
O1—C4	1.282 (9)	C8—H8B	0.9700
S1—C11	1.612 (10)	C9—H9A	0.9700
Br1—C1	1.911 (8)	C9—H9B	0.9700
C1—C6	1.356 (12)	C10—H10A	0.9600
C1—C2	1.368 (12)	C10—H10B	0.9600
C2—C3	1.358 (12)	C10—H10C	0.9600
O1—Cu1—N1	92.3 (3)	C6—C5—C4	121.6 (8)

O1—Cu1—N3	89.5 (3)	C6—C5—C7	116.9 (7)
N1—Cu1—N3	178.1 (3)	C4—C5—C7	121.4 (7)
O1—Cu1—N2	168.3 (3)	C1—C6—C5	119.9 (8)
N1—Cu1—N2	83.4 (3)	C1—C6—H6	120.1
N3—Cu1—N2	94.7 (3)	C5—C6—H6	120.1
C7—N1—C8	120.0 (7)	N1—C7—C5	125.2 (7)
C7—N1—Cu1	126.0 (5)	N1—C7—H7	117.4
C8—N1—Cu1	113.9 (5)	C5—C7—H7	117.4
C10—N2—C9	112.8 (8)	N1—C8—C9	108.4 (7)
C10—N2—Cu1	120.2 (7)	N1—C8—H8A	110.0
C9—N2—Cu1	107.4 (5)	C9—C8—H8A	110.0
C10—N2—H2A	105.0	N1—C8—H8B	110.0
C9—N2—H2A	105.0	C9—C8—H8B	110.0
Cu1—N2—H2A	105.0	H8A—C8—H8B	108.4
C11—N3—Cu1	166.5 (7)	N2—C9—C8	108.1 (7)
C4—O1—Cu1	126.5 (5)	N2—C9—H9A	110.1
C6—C1—C2	120.7 (8)	C8—C9—H9A	110.1
C6—C1—Br1	121.4 (6)	N2—C9—H9B	110.1
C2—C1—Br1	117.9 (7)	C8—C9—H9B	110.1
C3—C2—C1	121.1 (8)	H9A—C9—H9B	108.4
C3—C2—H2	119.4	N2—C10—H10A	109.5
C1—C2—H2	119.4	N2—C10—H10B	109.5
C2—C3—C4	120.6 (7)	H10A—C10—H10B	109.5
C2—C3—H3	119.7	N2—C10—H10C	109.5
C4—C3—H3	119.7	H10A—C10—H10C	109.5
O1—C4—C5	125.7 (7)	H10B—C10—H10C	109.5
O1—C4—C3	118.1 (7)	N3—C11—S1	177.5 (9)
C5—C4—C3	116.1 (7)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···S1^{i}	0.91	2.76	3.635 (9)	162

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