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{4-Bromo-2-[2-(isopropylamino)ethyl- iminomethyl]phenolato}thiocyanato- copper(II)

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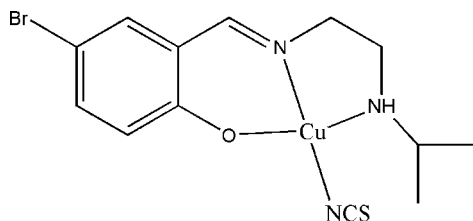
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.009$ Å; R factor = 0.056; wR factor = 0.154; data-to-parameter ratio = 19.0.

In the title mononuclear Schiff base copper(II) complex, $[\text{Cu}(\text{C}_{12}\text{H}_{16}\text{BrN}_2\text{O})(\text{NCS})]$, 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. There are long-range interactions between the Cu atom and S [3.151 (5) Å] and Br [3.929 (5) Å] atoms above and below the square plane.

Related literature

For related literature, see: Ma *et al.* (2005); Ma, Gu *et al.* (2006); Ma, Lv *et al.* (2006); Ma, Wu *et al.* (2006).



Experimental

Crystal data

$[\text{Cu}(\text{C}_{12}\text{H}_{16}\text{BrN}_2\text{O})(\text{NCS})]$
 $M_r = 405.80$

Monoclinic, $P2_1/n$
 $a = 6.161$ (2) Å

$b = 20.223$ (3) Å
 $c = 12.930$ (3) Å
 $\beta = 95.332$ (5)°
 $V = 1604.0$ (7) Å³
 $Z = 4$

Mo $K\alpha$ radiation
 $\mu = 3.98$ mm⁻¹
 $T = 298$ (2) K
 $0.40 \times 0.38 \times 0.37$ mm

Data collection

Bruker SMART 1000
diffractometer
Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)
 $T_{\text{min}} = 0.299$, $T_{\text{max}} = 0.321$
(expected range = 0.214–0.229)

11914 measured reflections
3474 independent reflections
2126 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.076$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.055$
 $wR(F^2) = 0.153$
 $S = 1.01$
3474 reflections

183 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.81$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.49$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Cu1—O1	1.903 (4)	Cu1—N3	1.959 (5)
Cu1—N1	1.932 (4)	Cu1—N2	2.075 (5)
O1—Cu1—N1	92.32 (17)	O1—Cu1—N2	171.59 (18)
O1—Cu1—N3	87.98 (19)	N1—Cu1—N2	84.45 (18)
N1—Cu1—N3	177.5 (2)	N3—Cu1—N2	94.91 (19)

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINTE* (Bruker, 2007); data reduction: *SAINTE*; 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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2226).

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supporting information

Acta Cryst. (2008). E64, m687 [doi:10.1107/S1600536808010404]

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

Jun-Ying Ma and Yin-Ting He

S1. Comment

Recently, we have reported some metal complexes derived from the 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, is reported in this paper.

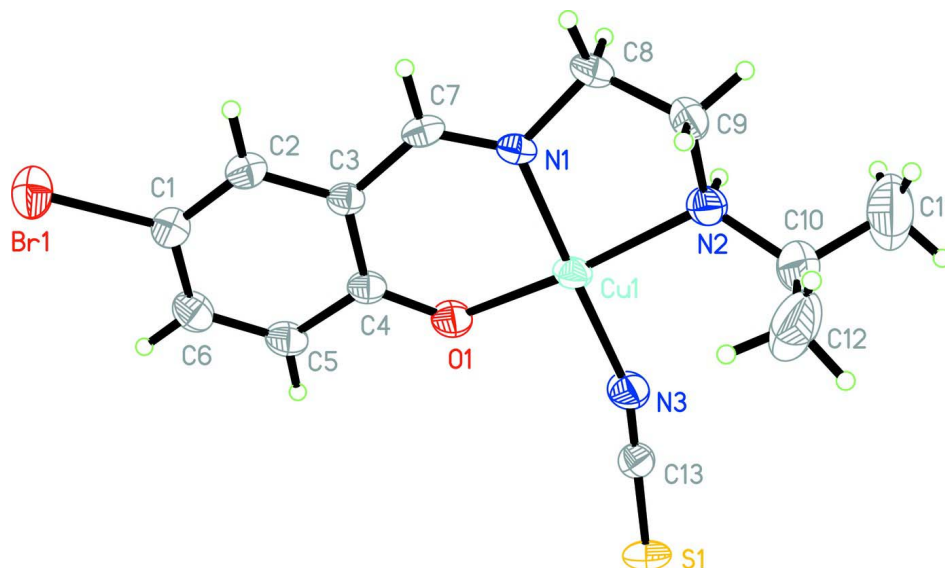
In the complex the Cu atom is coordinated by two nitrogen atoms and one oxygen atom from a Schiff base ligand, and by one nitrogen atom from a thiocyanate anion, giving a square planar geometry (Fig. 1). There exist long range interactions between the Cu and S (3.151 (5) Å; symmetry code: 1 + x, y, z) and Br (3.929 (5) Å; symmetry code: 1 - x, - y, 1 - z) atoms above and below the square plane. All the bond lengths and angles (Table 1) related to the Cu atom in the complex are within normal ranges. The four coordinating atoms around the Cu centre are approximately coplanar, giving a square-planar geometry with an average deviation of 0.047 (4) Å; the Cu atom lies 0.089 (2) Å above this plane. The C8—C9—N2—C10 torsion angle is 2.0 (3)°.

S2. Experimental

N-Isopropylethane-1,2-diamine (0.5 mmol, 51.0 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 the 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 H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H = 0.93–0.97 Å, N—H = 0.91 Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C,N})$ and $1.5U_{\text{eq}}(\text{methyl C})$.

**Figure 1**

The molecular structure at the 30% probability level ellipsoids.

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

Crystal data

[Cu(C₁₂H₁₆BrN₂O)(NCS)]

M_r = 405.80

Monoclinic, *P*2₁/*n*

Hall symbol: -*P* 2₁ *y*

a = 6.161 (2) Å

b = 20.223 (3) Å

c = 12.930 (3) Å

β = 95.332 (5)°

V = 1604.0 (7) Å³

Z = 4

F(000) = 812

D_x = 1.680 Mg m⁻³

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 1880 reflections

θ = 2.5–24.3°

μ = 3.98 mm⁻¹

T = 298 K

Block, blue

0.40 × 0.38 × 0.37 mm

Data collection

Bruker SMART 1000

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

T_{min} = 0.299, *T_{max}* = 0.321

11914 measured reflections

3474 independent reflections

2126 reflections with *I* > 2σ(*I*)

R_{int} = 0.076

θ_{\max} = 27.0°, θ_{\min} = 1.9°

h = -7→7

k = -25→25

l = -16→16

Refinement

Refinement on *F*²

Least-squares matrix: full

R [*F*² > 2σ(*F*²)] = 0.055

wR (*F*²) = 0.153

S = 1.01

3474 reflections

183 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

$$w = 1/[\sigma^2(F_o^2) + (0.0682P)^2]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$

$$\Delta\rho_{\max} = 0.81 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.49 \text{ e } \text{\AA}^{-3}$$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.26493 (10)	0.20760 (3)	0.47898 (5)	0.0450 (2)
N1	0.5364 (7)	0.1721 (2)	0.5425 (3)	0.0408 (10)
N2	0.3292 (7)	0.2854 (2)	0.5819 (4)	0.0534 (12)
H2A	0.2664	0.2729	0.6397	0.064*
N3	-0.0164 (8)	0.2425 (3)	0.4201 (4)	0.0616 (14)
O1	0.2003 (6)	0.1286 (2)	0.4022 (3)	0.0551 (10)
S1	-0.4273 (2)	0.25260 (9)	0.31058 (11)	0.0566 (4)
Br1	0.80195 (10)	-0.08910 (3)	0.28530 (5)	0.0677 (3)
C1	0.6219 (9)	-0.0194 (3)	0.3274 (4)	0.0475 (13)
C2	0.6939 (9)	0.0269 (3)	0.3994 (4)	0.0466 (13)
H2	0.8364	0.0245	0.4299	0.056*
C3	0.5578 (8)	0.0781 (2)	0.4285 (4)	0.0382 (12)
C4	0.3387 (8)	0.0829 (3)	0.3822 (4)	0.0418 (12)
C5	0.2699 (9)	0.0321 (3)	0.3099 (4)	0.0532 (15)
H5	0.1270	0.0326	0.2795	0.064*
C6	0.4065 (10)	-0.0175 (3)	0.2836 (5)	0.0552 (15)
H6	0.3554	-0.0499	0.2365	0.066*
C7	0.6414 (9)	0.1221 (3)	0.5099 (4)	0.0436 (12)
H7	0.7808	0.1140	0.5413	0.052*
C8	0.6326 (9)	0.2117 (3)	0.6316 (4)	0.0544 (15)
H8A	0.7902	0.2077	0.6376	0.065*
H8B	0.5801	0.1957	0.6955	0.065*
C9	0.5675 (9)	0.2829 (3)	0.6140 (4)	0.0536 (15)
H9A	0.6006	0.3081	0.6773	0.064*
H9B	0.6478	0.3019	0.5602	0.064*
C10	0.2371 (15)	0.3525 (4)	0.5575 (6)	0.092 (2)
H10	0.0818	0.3447	0.5376	0.111*
C11	0.242 (2)	0.3952 (5)	0.6475 (9)	0.150 (4)
H11A	0.2122	0.3697	0.7072	0.225*
H11B	0.1328	0.4290	0.6354	0.225*
H11C	0.3828	0.4154	0.6596	0.225*
C12	0.319 (2)	0.3811 (5)	0.4651 (7)	0.152 (5)

H12A	0.2246	0.4165	0.4396	0.228*
H12B	0.3221	0.3477	0.4125	0.228*
H12C	0.4633	0.3979	0.4824	0.228*
C13	-0.1851 (9)	0.2472 (3)	0.3741 (4)	0.0457 (13)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0348 (4)	0.0592 (5)	0.0396 (4)	0.0019 (3)	-0.0042 (3)	-0.0043 (3)
N1	0.038 (2)	0.048 (3)	0.035 (2)	-0.006 (2)	-0.0057 (18)	0.002 (2)
N2	0.051 (3)	0.066 (3)	0.044 (3)	0.010 (2)	0.007 (2)	-0.005 (2)
N3	0.042 (3)	0.079 (4)	0.061 (3)	0.011 (3)	-0.008 (2)	-0.015 (3)
O1	0.036 (2)	0.066 (3)	0.061 (3)	0.0002 (19)	-0.0087 (17)	-0.011 (2)
S1	0.0407 (8)	0.0800 (11)	0.0466 (8)	-0.0024 (8)	-0.0086 (6)	0.0161 (8)
Br1	0.0639 (5)	0.0571 (4)	0.0838 (5)	-0.0015 (3)	0.0157 (4)	-0.0128 (3)
C1	0.043 (3)	0.045 (3)	0.055 (3)	-0.004 (3)	0.007 (3)	0.000 (3)
C2	0.043 (3)	0.046 (3)	0.050 (3)	-0.002 (3)	-0.001 (2)	0.007 (3)
C3	0.039 (3)	0.038 (3)	0.037 (3)	-0.004 (2)	0.000 (2)	0.005 (2)
C4	0.037 (3)	0.046 (3)	0.041 (3)	-0.006 (2)	-0.001 (2)	0.004 (2)
C5	0.040 (3)	0.062 (4)	0.054 (4)	-0.009 (3)	-0.011 (3)	-0.007 (3)
C6	0.058 (4)	0.052 (4)	0.054 (4)	-0.013 (3)	0.001 (3)	-0.007 (3)
C7	0.038 (3)	0.048 (3)	0.044 (3)	0.001 (3)	-0.003 (2)	0.015 (3)
C8	0.049 (3)	0.063 (4)	0.048 (3)	-0.006 (3)	-0.013 (3)	-0.009 (3)
C9	0.056 (4)	0.057 (4)	0.049 (3)	-0.002 (3)	0.006 (3)	-0.014 (3)
C10	0.121 (7)	0.082 (5)	0.073 (5)	0.032 (5)	0.002 (5)	-0.017 (4)
C11	0.248 (14)	0.083 (7)	0.124 (9)	0.029 (7)	0.039 (9)	-0.018 (6)
C12	0.280 (15)	0.099 (7)	0.084 (6)	0.089 (9)	0.055 (8)	0.028 (6)
C13	0.046 (3)	0.049 (3)	0.043 (3)	0.002 (3)	0.007 (3)	0.002 (3)

Geometric parameters (Å, °)

Cu1—O1	1.903 (4)	C4—C5	1.426 (7)
Cu1—N1	1.932 (4)	C5—C6	1.372 (8)
Cu1—N3	1.959 (5)	C5—H5	0.9300
Cu1—N2	2.075 (5)	C6—H6	0.9300
N1—C7	1.292 (6)	C7—H7	0.9300
N1—C8	1.481 (6)	C8—C9	1.507 (8)
N2—C9	1.489 (7)	C8—H8A	0.9700
N2—C10	1.493 (9)	C8—H8B	0.9700
N2—H2A	0.9100	C9—H9A	0.9700
N3—C13	1.152 (6)	C9—H9B	0.9700
O1—C4	1.300 (6)	C10—C11	1.448 (11)
S1—C13	1.639 (6)	C10—C12	1.458 (12)
Br1—C1	1.905 (5)	C10—H10	0.9800
C1—C2	1.364 (7)	C11—H11A	0.9600
C1—C6	1.394 (8)	C11—H11B	0.9600
C2—C3	1.406 (7)	C11—H11C	0.9600
C2—H2	0.9300	C12—H12A	0.9600

C3—C4	1.428 (7)	C12—H12B	0.9600
C3—C7	1.436 (7)	C12—H12C	0.9600
O1—Cu1—N1	92.32 (17)	N1—C7—C3	124.6 (5)
O1—Cu1—N3	87.98 (19)	N1—C7—H7	117.7
N1—Cu1—N3	177.5 (2)	C3—C7—H7	117.7
O1—Cu1—N2	171.59 (18)	N1—C8—C9	108.5 (5)
N1—Cu1—N2	84.45 (18)	N1—C8—H8A	110.0
N3—Cu1—N2	94.91 (19)	C9—C8—H8A	110.0
C7—N1—C8	120.1 (4)	N1—C8—H8B	110.0
C7—N1—Cu1	126.3 (3)	C9—C8—H8B	110.0
C8—N1—Cu1	113.5 (3)	H8A—C8—H8B	108.4
C9—N2—C10	115.9 (5)	N2—C9—C8	108.5 (5)
C9—N2—Cu1	106.1 (3)	N2—C9—H9A	110.0
C10—N2—Cu1	120.5 (4)	C8—C9—H9A	110.0
C9—N2—H2A	104.2	N2—C9—H9B	110.0
C10—N2—H2A	104.2	C8—C9—H9B	110.0
Cu1—N2—H2A	104.2	H9A—C9—H9B	108.4
C13—N3—Cu1	162.4 (5)	C11—C10—C12	116.1 (9)
C4—O1—Cu1	126.3 (3)	C11—C10—N2	113.2 (7)
C2—C1—C6	119.7 (5)	C12—C10—N2	112.3 (6)
C2—C1—Br1	122.8 (4)	C11—C10—H10	104.6
C6—C1—Br1	117.5 (4)	C12—C10—H10	104.6
C1—C2—C3	121.6 (5)	N2—C10—H10	104.6
C1—C2—H2	119.2	C10—C11—H11A	109.5
C3—C2—H2	119.2	C10—C11—H11B	109.5
C2—C3—C4	120.1 (5)	H11A—C11—H11B	109.5
C2—C3—C7	118.1 (5)	C10—C11—H11C	109.5
C4—C3—C7	121.8 (5)	H11A—C11—H11C	109.5
O1—C4—C5	118.8 (5)	H11B—C11—H11C	109.5
O1—C4—C3	125.2 (5)	C10—C12—H12A	109.5
C5—C4—C3	116.0 (5)	C10—C12—H12B	109.5
C6—C5—C4	122.4 (5)	H12A—C12—H12B	109.5
C6—C5—H5	118.8	C10—C12—H12C	109.5
C4—C5—H5	118.8	H12A—C12—H12C	109.5
C5—C6—C1	120.2 (5)	H12B—C12—H12C	109.5
C5—C6—H6	119.9	N3—C13—S1	178.7 (6)
C1—C6—H6	119.9		
