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{2-Bromo-4-chloro-6-[2-(diethylamino)-ethyliminomethyl]phenolato-κ^3N,N',O}-(thiocyanato-κN)copper(II)

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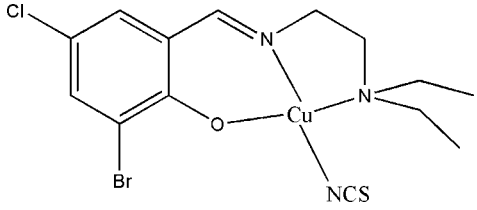
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.045; wR factor = 0.123; data-to-parameter ratio = 18.6.

In the title compound, [Cu($C_{13}H_{17}BrClN_2O$)(NCS)], the Cu atom is in a slightly distorted square-planar geometry, coordinated by the three donor atoms of the ligand and the N atom of the isothiocyanate group.

Related literature

For the biological activity of Schiff base compounds, see: Panneerselvam *et al.* (2005); Shi *et al.* (2007); Singh *et al.* (2006, 2007); Zhong *et al.* (2006).



Experimental

Crystal data

[Cu($C_{13}H_{17}BrClN_2O$)(NCS)]
M_r = 454.27
Monoclinic, $P2_1/c$
a = 8.651 (2) Å
b = 14.137 (2) Å
c = 14.145 (2) Å
β = 90.820 (2)°
V = 1729.7 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.85 mm^{-1}
T = 293 (2) K
0.17 × 0.13 × 0.13 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.561, T_{max} = 0.634
14228 measured reflections
3745 independent reflections
2784 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.123
S = 1.04
3745 reflections
201 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.92 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.902 (3)	Cu1—N3	1.945 (4)
Cu1—N1	1.940 (3)	Cu1—N2	2.073 (3)
O1—Cu1—N1	92.66 (14)	O1—Cu1—N2	168.15 (14)
O1—Cu1—N3	87.45 (14)	N1—Cu1—N2	83.93 (14)
N1—Cu1—N3	176.83 (16)	N3—Cu1—N2	95.33 (15)

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: SG2212).

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supporting information

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{2-Bromo-4-chloro-6-[2-(diethylamino)ethyliminomethyl]phenolato-κ^3N,N',O}(thiocyanato-κN)copper(II)

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S1. Comment

Schiff base compounds and metal complexes have been reported to have excellent biological activity (Shi *et al.*, 2007; Panneerselvam *et al.*, 2005, Singh *et al.*, 2006, 2007; Zhong *et al.*, 2006).

In the title compound the Cu atom is in a slightly distorted square planar geometry coordinated by the three donor atoms of the ligand and the N atom of the isothiocyanate group. (Fig. 1). The Cu atom is displaced out of the least-squares plane defined by the four donor atoms by 0.125 (2) Å. The coordination bond values (Table 1) are within normal ranges.

S2. Experimental

The title compound was obtained by the reaction of equimolar 3-bromo-5-chlorosalicylaldehyde, *N*,*N*-diethylethane-1,2-diamine, sodium thiocyanate, and copper acetate in an ethanol solution. Blue block-like single crystals were obtained by the slow evaporation of the filtrate in air.

S3. Refinement

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93–0.97Å and with U_{iso}(H) = 1.2 (1.5 for methyl groups) times U_{eq}(C).

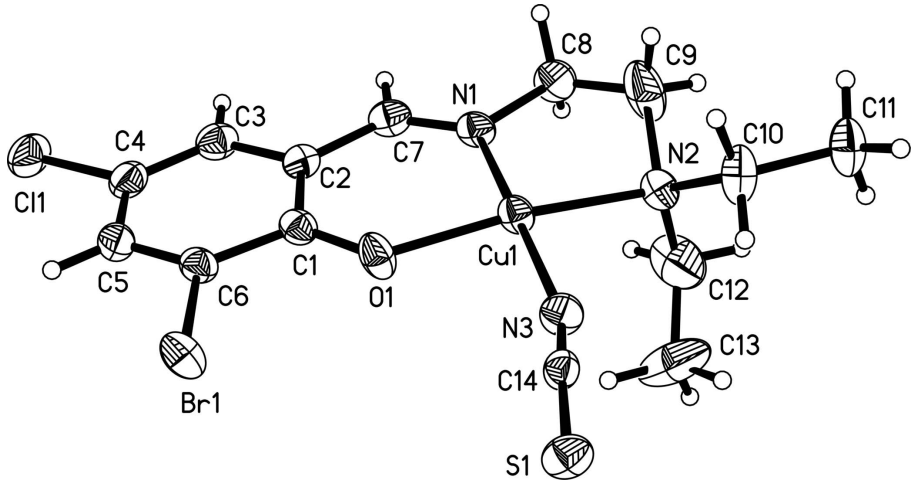

Figure 1

The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.

{2-Bromo-4-chloro-6-[2-(diethylamino)ethyliminomethyl]phenolato-\k^3*N*,*N*′,*O*}(thiocyanato-*κN*)copper(II)

Crystal data

[Cu($C_{13}H_{17}BrClN_2O$)(NCS)]
M_r = 454.27
Monoclinic, $P2_1/c$
a = 8.651 (2) Å
b = 14.137 (2) Å
c = 14.145 (2) Å
β = 90.820 (2)°
V = 1729.7 (5) Å^3
Z = 4
$F(000)$ = 908
D_x = 1.744 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3721 reflections
θ = 2.5–25.3°
μ = 3.85 mm^{-1}
T = 293 K
Block, blue
0.17 × 0.13 × 0.13 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.561, T_{max} = 0.634
14228 measured reflections
3745 independent reflections
2784 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 27.0°, θ_{min} = 2.0°
h = −11→10
k = −18→17
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.123
S = 1.04
3745 reflections
201 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
$w = 1/[\sigma^2(F_o^2) + (0.0599P)^2 + 1.7229P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.92 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cu1	0.13650 (6)	0.16708 (3)	0.07012 (3)	0.03921 (16)
O1	−0.0067 (4)	0.2249 (2)	−0.0153 (2)	0.0503 (8)
N1	0.1195 (4)	0.2692 (3)	0.1611 (2)	0.0424 (8)
N2	0.3230 (4)	0.1260 (3)	0.1541 (2)	0.0436 (8)
N3	0.1631 (4)	0.0684 (3)	−0.0241 (3)	0.0478 (9)

Br1	−0.22122 (6)	0.25006 (4)	−0.17829 (3)	0.05842 (18)
Cl1	−0.33341 (16)	0.58720 (9)	0.00426 (11)	0.0698 (4)
S1	0.10508 (13)	−0.05745 (9)	−0.17046 (8)	0.0502 (3)
C1	−0.0783 (5)	0.3037 (3)	−0.0054 (3)	0.0410 (9)
C2	−0.0611 (5)	0.3662 (3)	0.0729 (3)	0.0422 (9)
C3	−0.1405 (5)	0.4526 (3)	0.0746 (3)	0.0518 (11)
H3	−0.1269	0.4932	0.1258	0.062*
C4	−0.2375 (5)	0.4777 (3)	0.0021 (3)	0.0530 (11)
C5	−0.2594 (5)	0.4179 (4)	−0.0741 (3)	0.0520 (11)
H5	−0.3259	0.4352	−0.1234	0.062*
C6	−0.1840 (5)	0.3339 (3)	−0.0770 (3)	0.0423 (9)
C7	0.0380 (5)	0.3446 (3)	0.1520 (3)	0.0481 (11)
H7	0.0437	0.3887	0.2007	0.058*
C8	0.2151 (6)	0.2587 (4)	0.2462 (3)	0.0635 (15)
H8A	0.2973	0.3053	0.2463	0.076*
H8B	0.1528	0.2689	0.3018	0.076*
C9	0.2793 (9)	0.1661 (4)	0.2487 (4)	0.087 (2)
H9A	0.2051	0.1239	0.2774	0.104*
H9B	0.3707	0.1671	0.2891	0.104*
C10	0.3261 (6)	0.0234 (3)	0.1647 (4)	0.0616 (13)
H10A	0.3399	−0.0041	0.1026	0.074*
H10B	0.2257	0.0034	0.1868	0.074*
C11	0.4495 (6)	−0.0183 (4)	0.2313 (4)	0.0676 (15)
H11A	0.5491	0.0064	0.2151	0.101*
H11B	0.4503	−0.0859	0.2251	0.101*
H11C	0.4265	−0.0015	0.2953	0.101*
C12	0.4629 (7)	0.1734 (6)	0.1237 (5)	0.098 (2)
H12A	0.4500	0.2405	0.1354	0.118*
H12B	0.5472	0.1519	0.1642	0.118*
C13	0.5091 (7)	0.1627 (7)	0.0301 (5)	0.117 (3)
H13A	0.5228	0.0968	0.0164	0.175*
H13B	0.6049	0.1955	0.0211	0.175*
H13C	0.4314	0.1885	−0.0116	0.175*
C14	0.1359 (4)	0.0175 (3)	−0.0848 (3)	0.0380 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0451 (3)	0.0384 (3)	0.0339 (3)	−0.0012 (2)	−0.0085 (2)	−0.0047 (2)
O1	0.069 (2)	0.0402 (17)	0.0409 (17)	0.0084 (15)	−0.0189 (14)	−0.0043 (13)
N1	0.045 (2)	0.051 (2)	0.0313 (17)	−0.0048 (17)	−0.0055 (15)	−0.0080 (15)
N2	0.044 (2)	0.043 (2)	0.0443 (19)	−0.0070 (16)	−0.0090 (15)	0.0003 (15)
N3	0.051 (2)	0.051 (2)	0.0413 (19)	0.0001 (17)	−0.0050 (16)	−0.0100 (17)
Br1	0.0689 (3)	0.0642 (3)	0.0418 (3)	−0.0017 (2)	−0.0130 (2)	0.0037 (2)
Cl1	0.0715 (9)	0.0532 (7)	0.0852 (9)	0.0218 (6)	0.0219 (7)	0.0123 (7)
S1	0.0508 (6)	0.0547 (7)	0.0451 (6)	−0.0034 (5)	−0.0002 (5)	−0.0178 (5)
C1	0.043 (2)	0.040 (2)	0.040 (2)	−0.0047 (18)	0.0020 (17)	0.0054 (18)
C2	0.042 (2)	0.043 (2)	0.042 (2)	0.0003 (18)	0.0053 (18)	−0.0017 (18)

C3	0.058 (3)	0.043 (3)	0.055 (3)	0.001 (2)	0.012 (2)	−0.003 (2)
C4	0.051 (3)	0.048 (3)	0.061 (3)	0.011 (2)	0.016 (2)	0.010 (2)
C5	0.045 (3)	0.059 (3)	0.052 (3)	0.006 (2)	0.006 (2)	0.016 (2)
C6	0.042 (2)	0.047 (2)	0.038 (2)	−0.0041 (19)	0.0026 (17)	0.0073 (18)
C7	0.051 (3)	0.050 (3)	0.043 (2)	−0.007 (2)	0.0018 (19)	−0.013 (2)
C8	0.055 (3)	0.096 (4)	0.039 (2)	0.008 (3)	−0.015 (2)	−0.013 (2)
C9	0.134 (6)	0.071 (4)	0.055 (3)	0.032 (4)	−0.044 (3)	−0.016 (3)
C10	0.054 (3)	0.043 (3)	0.087 (4)	0.008 (2)	−0.026 (3)	−0.004 (2)
C11	0.062 (3)	0.058 (3)	0.082 (4)	0.014 (3)	−0.027 (3)	0.001 (3)
C12	0.057 (4)	0.145 (7)	0.090 (5)	−0.029 (4)	−0.017 (3)	0.032 (4)
C13	0.060 (4)	0.196 (9)	0.095 (5)	−0.015 (5)	0.020 (4)	−0.066 (6)
C14	0.032 (2)	0.040 (2)	0.042 (2)	0.0029 (17)	−0.0011 (16)	0.0012 (18)

Geometric parameters (Å, º)

Cu1—O1	1.902 (3)	C5—C6	1.356 (6)
Cu1—N1	1.940 (3)	C5—H5	0.9300
Cu1—N3	1.945 (4)	C7—H7	0.9300
Cu1—N2	2.073 (3)	C8—C9	1.422 (7)
O1—C1	1.283 (5)	C8—H8A	0.9700
N1—C7	1.284 (6)	C8—H8B	0.9700
N1—C8	1.458 (5)	C9—H9A	0.9700
N2—C12	1.454 (7)	C9—H9B	0.9700
N2—C10	1.457 (6)	C10—C11	1.532 (6)
N2—C9	1.507 (7)	C10—H10A	0.9700
N3—C14	1.143 (5)	C10—H10B	0.9700
Br1—C6	1.884 (4)	C11—H11A	0.9600
Cl1—C4	1.757 (5)	C11—H11B	0.9600
S1—C14	1.628 (4)	C11—H11C	0.9600
C1—C6	1.421 (6)	C12—C13	1.397 (9)
C1—C2	1.421 (6)	C12—H12A	0.9700
C2—C3	1.402 (6)	C12—H12B	0.9700
C2—C7	1.433 (6)	C13—H13A	0.9600
C3—C4	1.363 (6)	C13—H13B	0.9600
C3—H3	0.9300	C13—H13C	0.9600
C4—C5	1.381 (7)		
O1—Cu1—N1	92.66 (14)	C9—C8—N1	109.3 (4)
O1—Cu1—N3	87.45 (14)	C9—C8—H8A	109.8
N1—Cu1—N3	176.83 (16)	N1—C8—H8A	109.8
O1—Cu1—N2	168.15 (14)	C9—C8—H8B	109.8
N1—Cu1—N2	83.93 (14)	N1—C8—H8B	109.8
N3—Cu1—N2	95.33 (15)	H8A—C8—H8B	108.3
C1—O1—Cu1	127.9 (3)	C8—C9—N2	115.3 (5)
C7—N1—C8	118.1 (4)	C8—C9—H9A	108.4
C7—N1—Cu1	126.7 (3)	N2—C9—H9A	108.4
C8—N1—Cu1	115.1 (3)	C8—C9—H9B	108.4
C12—N2—C10	118.3 (5)	N2—C9—H9B	108.4

C12—N2—C9	108.0 (5)	H9A—C9—H9B	107.5
C10—N2—C9	106.7 (4)	N2—C10—C11	117.3 (4)
C12—N2—Cu1	110.2 (3)	N2—C10—H10A	108.0
C10—N2—Cu1	110.5 (3)	C11—C10—H10A	108.0
C9—N2—Cu1	101.5 (3)	N2—C10—H10B	108.0
C14—N3—Cu1	160.4 (3)	C11—C10—H10B	108.0
O1—C1—C6	119.3 (4)	H10A—C10—H10B	107.2
O1—C1—C2	125.4 (4)	C10—C11—H11A	109.5
C6—C1—C2	115.3 (4)	C10—C11—H11B	109.5
C3—C2—C1	120.6 (4)	H11A—C11—H11B	109.5
C3—C2—C7	117.4 (4)	C10—C11—H11C	109.5
C1—C2—C7	122.0 (4)	H11A—C11—H11C	109.5
C4—C3—C2	120.7 (4)	H11B—C11—H11C	109.5
C4—C3—H3	119.7	C13—C12—N2	118.8 (6)
C2—C3—H3	119.7	C13—C12—H12A	107.6
C3—C4—C5	120.3 (4)	N2—C12—H12A	107.6
C3—C4—Cl1	120.1 (4)	C13—C12—H12B	107.6
C5—C4—Cl1	119.6 (4)	N2—C12—H12B	107.6
C6—C5—C4	119.9 (4)	H12A—C12—H12B	107.1
C6—C5—H5	120.0	C12—C13—H13A	109.5
C4—C5—H5	120.0	C12—C13—H13B	109.5
C5—C6—C1	123.1 (4)	H13A—C13—H13B	109.5
C5—C6—Br1	119.8 (3)	C12—C13—H13C	109.5
C1—C6—Br1	117.1 (3)	H13A—C13—H13C	109.5
N1—C7—C2	125.2 (4)	H13B—C13—H13C	109.5
N1—C7—H7	117.4	N3—C14—S1	177.3 (4)
C2—C7—H7	117.4		