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{2-[2-(1*H*-1,3-Benzimidazol-2-yl)ethyliminomethyl]-4-bromophenolato}thiocyanatocopper(II) methanol solvate

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In the title compound, $[Cu(NCS)(C_{16}H_{13}BrN_3O)]\cdot CH_4O$, the Cu^{II} center forms a distorted square coordination with two N atoms and one O atom of the ligand 2-{2-[(5-bromosalicylidene)amino]ethyl}-1*H*-1,3-benzimidazole, and one N atom of the thiocyanate anion. The distortion is quite large, with an O—Cu—N angle of 150.83 (10)° and an N—Cu—N angle of 149.17 (12)°. Methanol molecules link the salicylidene groups *via* hydrogen bonds.

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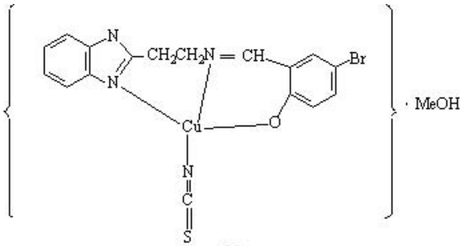
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.034
wR factor = 0.098
Data-to-parameter ratio = 13.3

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

Comment

The coordination behaviour of chelating ligands incorporating benzimidazole groups has been investigated extensively in recent years (Sanni *et al.*, 1988). Copper is an important trace element for plants and animals. Investigations of the coordination chemistry of copper(II) continue to be stimulated by interest in developing models for copper proteins and in understanding the factors which cause the seemingly infinite variety of distortions from regular stereochemistry observed in Cu^{II} complexes (Fenton, 1992). In the present work, we have prepared a new Cu^{II} benzimidazole complex, (I), and determined its crystal structure.



(I)

A distorted square is formed around the Cu^{II} atom, in which diagonal positions are occupied by atoms N2 and O1, and atoms N1 and N4 (Fig. 1). The Cu—O and Cu—N bond lengths are shorter than those recorded for other benzimidazole complexes (Gupta *et al.*, 2001), and the *trans* bond angles deviate from the expected value of 180° (Table 1). The sum of the *cis* bond angles at atom Cu1 is 375.34°, showing that the metal ion is not in the mean plane of the donors; atom Cu1 deviates by 0.0 (5) Å from the coordination plane. There is an N—H···S hydrogen bond between the imidazole group and the thiocyanate anion of an adjacent Cu^{II} complex. Methanol molecules also link the complexes *via* C—H···O and O—H···O hydrogen bonds (Table 2 and Fig. 2).

Experimental

The title compound was prepared by adding a methanol solution (5 ml) of copper(II) chloride (0.1 mmol) and a methanol sulution

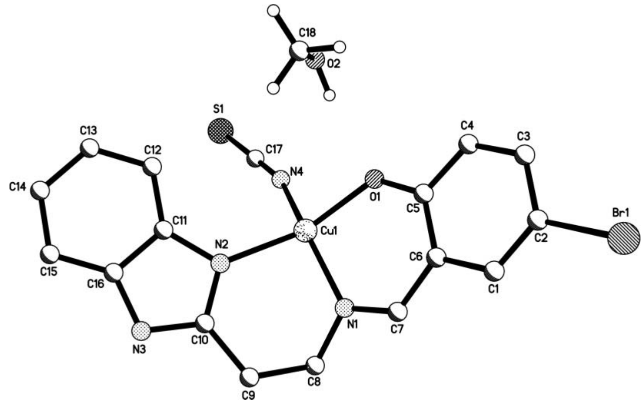


Figure 1
A view of (I). Displacement ellipsoids are drawn at the 30% probability level.

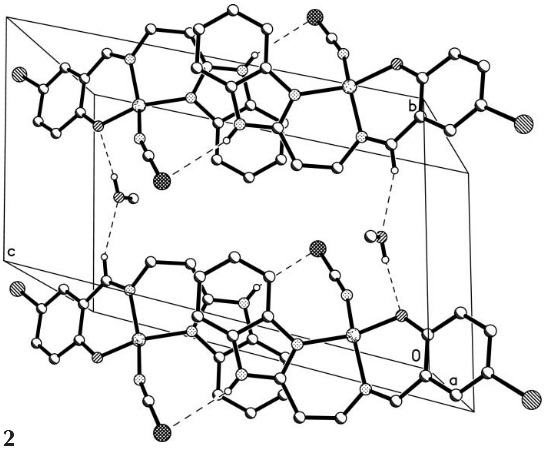


Figure 2
A packing diagram of (I) viewed along the *a* axis. Hydrogen bonds are shown by dashed lines.

(5 ml) of KSCN (0.1 mmol) to a methanol solution (10 ml) of 2-{2-[(5-bromosalicylidene)amino]ethyl}-1*H*-1,3-benzimidazole (Das & Dash, 1995) (0.1 mmol) and neutralizing the reaction mixture with triethylamine (0.1 mmol). The mixture was stirred for about 2 h and filtered. The filtrate was evaporated slowly at room temperture to yield green block-shaped crystals of (I). Analysis calculated for $C_{18}H_{17}BrCuN_4O_2S$: C 43.51, H 3.45, N 11.28%; found: C 43.48, H 3.46, N 11.35%.

Crystal data

$[Cu(NCS)(C_{16}H_{13}BrN_3O)]\cdot CH_4O$
$M_r = 496.87$
Triclinic, $P\overline{1}$
$a = 7.4111$ (16) Å
$b = 8.7821$ (19) Å
$c = 15.545$ (3) Å
$\alpha = 75.292$ (3)°
$\beta = 84.626$ (2)°
$\gamma = 78.163$ (3)°
$V = 956.9$ (4) Å^3
$Z = 2$
$D_x = 1.725$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2585 reflections
$\theta = 2.44$–25.03°
$\mu = 3.36$ mm^{-1}
$T = 293$ (2) K
Block, green
0.48 × 0.34 × 0.20 mm

Data collection

Bruker APEX-II CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.220$, $T_{max} = 0.511$
5142 measured reflections
3334 independent reflections
2802 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 25.0°$
$h = -8 \rightarrow 8$
$k = -10 \rightarrow 8$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.098$
$S = 1.06$
3334 reflections
250 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0603P)^2 + 0.2902P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.62$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.889 (2)	Cu1—N4	1.946 (3)
Cu1—N1	1.931 (3)	Cu1—N2	1.978 (2)
O1—Cu1—N1	94.94 (10)	C7—N1—Cu1	123.7 (2)
O1—Cu1—N4	93.45 (11)	C8—N1—Cu1	117.69 (19)
N1—Cu1—N4	149.17 (12)	C10—N2—Cu1	126.0 (2)
O1—Cu1—N2	150.83 (10)	C11—N2—Cu1	127.5 (2)
N1—Cu1—N2	92.00 (10)	C17—N4—Cu1	163.9 (3)
N4—Cu1—N2	94.95 (11)	C5—O1—Cu1	125.56 (19)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1	0.82	2.03	2.840 (5)	171
C7—H7···O2^{i}	0.93	2.39	3.289 (6)	162
N3—H3*A*···S1^{ii}	0.74 (3)	2.69 (3)	3.406 (3)	161 (3)

Symmetry codes: (i) $x, y-1, z$; (ii) $-x+1, -y, -z+1$.

The N-bound H atom was refined freely. Other H atoms were included in calculated positions and refined with fixed displacement parameters riding on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(C_{methyl},O)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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, 1998); software used to prepare material for publication: *SHELXTL*.

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