

{2-[2-(1*H*-1,3-Benzimidazol-2-yl)ethylimino-methyl]-4-chlorophenolato}thiocyanatocopper(II) monohydrate**Xiao-Hang Qiu,* Jun Zhao and Xiao-Lan Tong**

Department of Chemistry, Nankai University, Tianjin 300071, People's Republic of China

Correspondence e-mail: qjxh@nankai.edu.cn

In the title compound, $[\text{Cu}(\text{C}_{16}\text{H}_{13}\text{ClN}_3\text{O})(\text{NCS})]\cdot\text{H}_2\text{O}$, the Cu^{II} atom adopts a distorted square-planar coordination with two N atoms and one O atom of the tridentate phenolate ligand, and one N atom of the thiocyanate anion. $\text{N}-\text{H}\cdots\text{S}$, $\text{O}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds give rise to a two-dimensional network.

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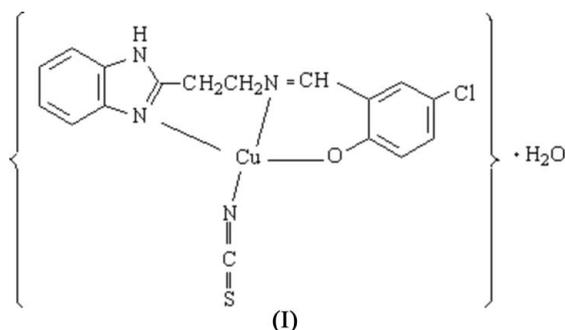
Key indicators

Single-crystal X-ray study
 $T = 294\text{ K}$
 Mean $\sigma(\text{C}-\text{C}) = 0.006\text{ \AA}$
 R factor = 0.042
 wR factor = 0.101
 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

Benzimidazole and its derivatives have attracted a great deal of attention in recent years (Qiu & Tong, 2005) due to their biological activities and their strong coordination abilities as multidentate ligands (Carcanagne *et al.*, 2002). Copper plays an important role in metalloproteins involved in electron-transfer and oxygenation reactions (Holm *et al.*, 1996). Various model complexes for such enzymes have been synthesized and their reactivity to oxygen has been investigated (Gao *et al.*, 2004). We have prepared a new Cu^{II} -benzimidazole complex, (I) (Fig. 1), and determined its crystal structure, which is presented here.



The $[\text{Cu}(\text{NCS})(\text{C}_{16}\text{H}_{13}\text{ClN}_3\text{O})]$ complex molecule adopts a distorted square-planar geometry about the Cu atom, in which the *trans* positions are occupied by atoms N2 and O1, and N1 and N4. The *trans* bond angles deviate significantly from the ideal value of 180° , O1—Cu1—N2 and N1—Cu1—N4 being $160.27(13)$ and $162.48(15)^\circ$ respectively. The sum of the *cis* bond angles at Cu1 is 365.9° , showing that the Cu atom is nearly in the mean plane of the basal donors, deviating by $0.012(6)\text{ \AA}$ from the coordination plane. The Cu—N distances in (I) (Table 1) are shorter than those reported for similar copper complexes with benzimidazole and imidazole ligands (Afreen *et al.*, 2005). The Cu—O(phenolate) bond distance of $1.893(3)\text{ \AA}$ is similar to those recorded for related tetra-coordinated Cu^{II} complexes (Akitsu & Einaga, 2005).

$\text{N}-\text{H}\cdots\text{S}$, $\text{O}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 2) result in the formation of a two-dimensional network. Notable among these interactions is the O2—

H2B···O2ⁱⁱ bond, which results in inversion symmetry-generated dimeric associations of water molecules (Fig. 2).

Experimental

An aqueous solution (5 ml) of copper(II) perchlorate (0.1 mmol) and a methanol solution (5 ml) of KSCN (0.1 mmol) were added to a methanol solution (10 ml) of 2-[2-[(5-chlorosalicylidene)amino]ethyl]-1*H*-1,3-benzimidazole (Das & Dash, 1995) (0.1 mmol). The reaction mixture was neutralized with triethylamine (0.1 mmol); the mixture was then stirred for about 2 h and filtered. The filtrate was evaporated slowly at room temperature to yield green block-shaped crystals of (I). Analysis, calculated for C₁₇H₁₃ClCuN₄O₂S: C 46.57, H 3.45, N 12.78%; found: C 46.46, H 3.47, N 12.82%.

Crystal data

[Cu(C ₁₆ H ₁₃ ClN ₃ O)(NCS)]·H ₂ O	$V = 896.7 (5) \text{ \AA}^3$
$M_r = 438.38$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.624 \text{ Mg m}^{-3}$
$a = 8.685 (3) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 8.946 (3) \text{ \AA}$	$\mu = 1.50 \text{ mm}^{-1}$
$c = 12.395 (4) \text{ \AA}$	$T = 294 (2) \text{ K}$
$\alpha = 79.660 (6)^\circ$	Block, green
$\beta = 71.659 (5)^\circ$	$0.26 \times 0.24 \times 0.22 \text{ mm}$
$\gamma = 82.709 (5)^\circ$	

Data collection

Bruker SMART CCD area-detector diffractometer	4372 measured reflections
φ and ω scans	3121 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	2051 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.704$, $T_{\max} = 0.733$	$R_{\text{int}} = 0.024$
	$\theta_{\text{max}} = 25.0^\circ$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.042$	$w = 1/[\sigma^2(F_o^2) + (0.0468P)^2]$
$wR(F^2) = 0.101$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{\text{max}} = 0.002$
3121 reflections	$\Delta\rho_{\text{max}} = 0.44 \text{ e \AA}^{-3}$
235 parameters	$\Delta\rho_{\text{min}} = -0.39 \text{ e \AA}^{-3}$

Table 1

Selected bond lengths (Å).

Cu1—O1	1.893 (3)	Cu1—N2	1.966 (3)
Cu1—N4	1.955 (3)	Cu1—N1	1.974 (3)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N3—H3···S1 ⁱ	0.86	2.62	3.440 (3)	159
O2—H2A···O1 ⁱ	0.85	2.03	2.869 (5)	169
O2—H2B···O2 ⁱⁱ	0.85	2.39	3.027 (8)	133
C7—H7···O2 ⁱⁱⁱ	0.93	2.42	3.336 (6)	167

Symmetry codes: (i) $-x, -y + 1, -z + 1$; (ii) $-x, -y + 2, -z + 2$; (iii) $-x + 1, -y + 1, -z + 1$.

The water H atoms were located in a difference map, relocated in idealized positions (O—H = 0.85 Å) and refined as riding. C- and N-bound H atoms were included in calculated positions (C—H = 0.93–

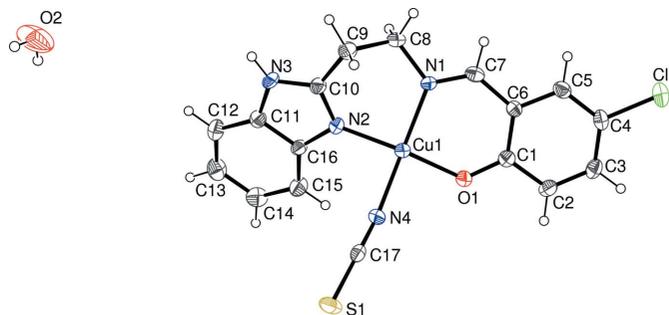


Figure 1

A view of (I), showing 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

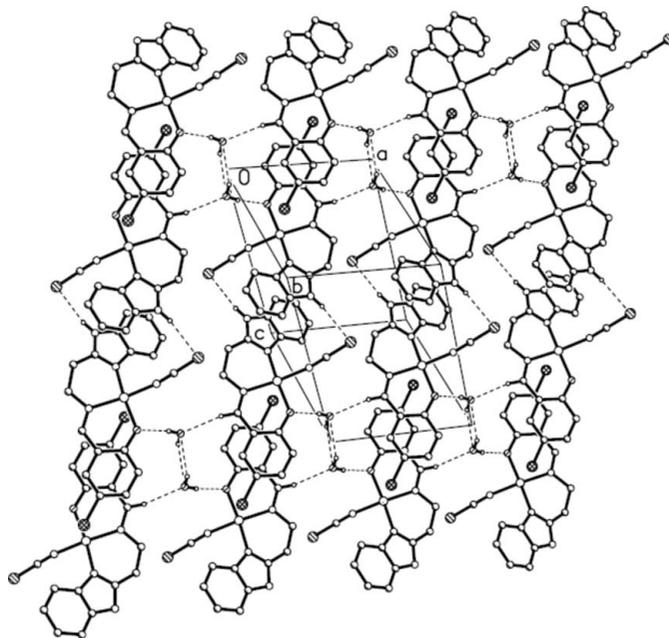


Figure 2

A packing diagram of (I), with hydrogen bonds indicated by dashed lines. H atoms not involved in hydrogen bonding have been omitted.

0.98 Å and N—H = 0.86–0.90 Å) and refined as riding. The constraint $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$ was applied in all cases.

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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