Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Chloro(2-oxidobenzaldehyde 2-thienylcarbonylhydrazone)copper(II) monohydrate

Yong Lu, Jing Chen, Wen-Shi Wu,* Jing-Cao Dai and Jian-Ming Lin

College of Materials Science, Huaqiao University, Quanzhou, Fujian 362021, People's Republic of China

Correspondence e-mail: wws@hqu.edu.cn

Received 28 March 2006
Accepted 8 May 2006

Key indicators

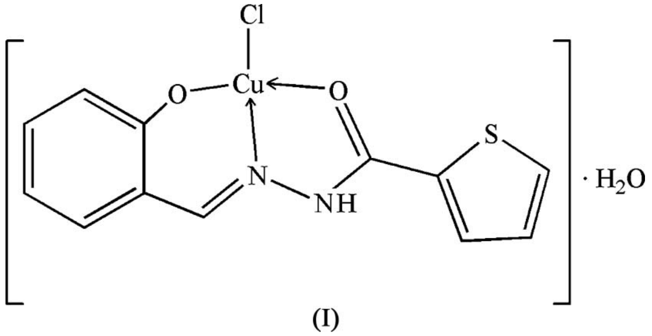
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.030
wR factor = 0.088
Data-to-parameter ratio = 17.2

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

The title complex, $[Cu(C_{12}H_9N_2O_2S)Cl]\cdot H_2O$, features a square-planar Cu^{II} centre coordinated by two O atoms and an N atom derived from the tridentate ligand, and a Cl atom. The complex molecules stack in layers which are held together by hydrogen bonds involving the water molecules of crystallization.

Comment

A number of metal–organic complexes with *N,O*-donor ligands have been widely investigated in coordination chemistry owing to their varied coordination modes and interesting reactivity (Iskander *et al.*, 2001; Kido *et al.*, 2003; Costes *et al.*, 2004). However, related complexes containing a thiophene ring are not so common (Amari *et al.*, 1993; Christidis *et al.*, 1994). In the title complex, (I) (Fig. 1 and Table 1), the Cu^{2+} cation is coordinated by an amide N, a phenoxide O and a carbonyl O atom, all derived from the tridentate ligand, and the square-planar coordination geometry is completed by a Cl atom. The five- and six-membered chelate rings are effectively planar, the mean deviation from the least-squares plane through both of them being 0.037 (18) Å. The distance of the Cl atom from this plane is 0.4565 (18) Å, indicating some distortion towards a tetrahedral geometry for the Cu^{II} centre. The thiophene ring is approximately coplanar with the above-mentioned plane, forming a dihedral angle of 8.77 (9)°.



(I)

The crystal packing is stabilized by intermolecular N—H⋯O, O—H⋯O and O—H⋯Cl hydrogen bonds, as detailed in Table 2. Stacks of complex molecules are held together *via* π–π interactions. The shortest separation between rings comprising the stack [3.4921 (12) Å] occurs between the five-membered Cu/O2/N1 chelate ring and the ring centroid of (C1–C6)^{i} [symmetry code: (i) $1 - x$, $1 - y$, $-z$]. These stacks are connected to each other *via* the aforementioned hydrogen-bonding interactions, as highlighted in Fig. 2.

Experimental

The ligand was synthesized according to the method of Wu *et al.* (2004). A mixture of $CuCl_2\cdot 2H_2O$ (1 mmol) and the ligand (1 mmol) was dissolved in methanol (20 ml), stirred at room temperature for 1 h and then filtered. The filtrate was allowed to stand at room temperature for two weeks, yielding deep-blue crystals of (I).

Crystal data

$[Cu(C_{12}H_9N_2O_2S)Cl]\cdot H_2O$
$M_r = 362.28$
Monoclinic, $P2_1/c$
$a = 11.9991\ (9)$ Å
$b = 7.1804\ (5)$ Å
$c = 16.2195\ (11)$ Å
$\beta = 92.646\ (3)^\circ$
$V = 1395.96\ (17)$ Å^3

$Z = 4$
$D_x = 1.724$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.91$ mm^{-1}
$T = 293\ (2)$ K
Prism, blue
$0.65 \times 0.55 \times 0.45$ mm

Data collection

Bruker P4 diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.370$, $T_{\max} = 0.480$ (expected range = 0.326–0.423)

10148 measured reflections
3187 independent reflections
2840 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.019$
$\theta_{\max} = 27.5^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.088$
$S = 1.01$
3187 reflections
185 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0564P)^2 + 0.4954P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.58$ e Å^{-3}
$\Delta\rho_{\min} = -0.34$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—Cl1	2.2111 (5)	Cu1—O2	1.9793 (14)
Cu1—O1	1.8991 (14)	Cu1—N1	1.9369 (15)
Cl1—Cu1—O1	91.98 (4)	O1—Cu1—O2	172.05 (6)
Cl1—Cu1—O2	95.61 (4)	O1—Cu1—N1	92.21 (6)
Cl1—Cu1—N1	168.50 (5)	O2—Cu1—N1	80.79 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O3$^{\rm i}$	0.86	1.98	2.767 (2)	152
O3—HW1···O1$^{\rm ii}$	0.80	2.04	2.839 (2)	173
O3—HW2···Cl1$^{\rm iii}$	0.75	2.55	3.3030 (16)	173

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

The O- and N-bound H atoms were located in a difference Fourier map and fixed in position. C-bound H atoms were included in the riding-model approximation, with C—H = 0.93 Å and $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(parent atom).

Data collection: *XSCANS* (Bruker, 1999); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Sheldrick, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

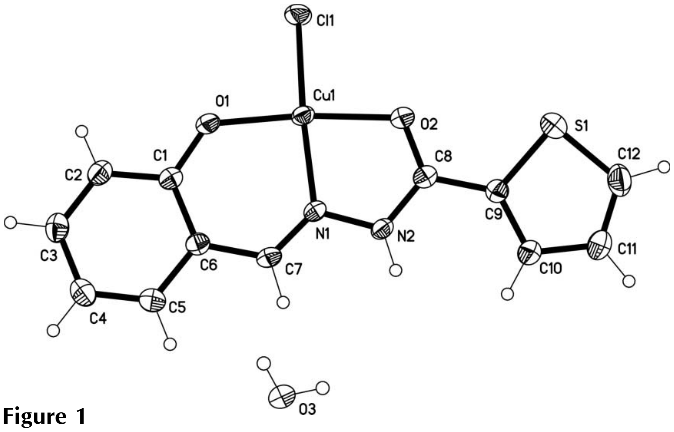


Figure 1
The molecular structure of (I), showing the atom-labelling scheme, with 30% displacement ellipsoids.

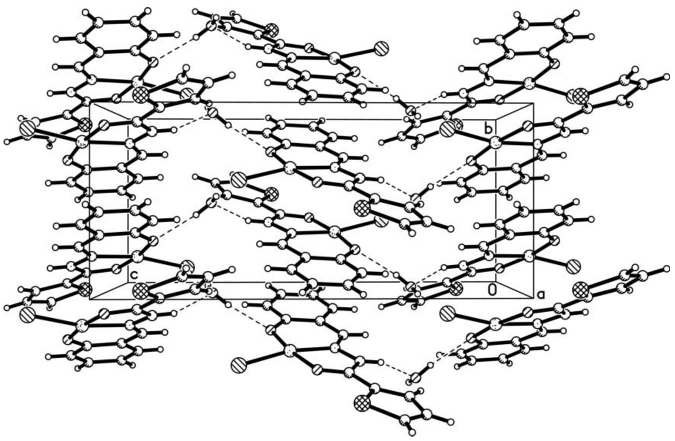


Figure 2
Packing diagram of (I), showing hydrogen bonds as dashed lines.

We are grateful for financial support from the Research Funding of Fujian Province, China (No. 2003 F006) and the National Science Foundation of Overseas Chinese Affairs Office of the State Council, China (No. 05QZR01).

References

Amari, C., Ianelli, S., Pelizzi, C., Pelizzi, G. & Predieri, G. (1993). *Inorg. Chim. Acta*, **211**, 89–94.

Bruker (1999). *XSCANS*. Version 2.10b. Bruker AXS Inc., Madison, Wisconsin, USA.

Christidis, P. C., Tossidis, I. A. & Hondroudis, C. A. (1994). *Z. Kristallogr.* **209**, 502–506.

Costes, J.-P., Clemente-Juan, J. M., Dahan, F. & Milon, J. (2004). *Inorg. Chem.* **43**, 8200–8202.

Iskander, M. F., Khalil, T. E., Haase, W., Werner, R., Svoboda, I. & Fuess, H. (2001). *Polyhedron*, **20**, 2787–2798.

Kido, T., Ikuta, Y., Sunatsuki, Y., Ogawa, Y., Matsumoto, N. & Re, N. (2003). *Inorg. Chem.* **42**, 398–408.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Sheldrick, G. M. (2000). *SHELXTL*. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.

Wu, W.-S., Feng, Y.-L., Lan, X.-R. & Huang, T.-T. (2004). *Chin. J. Appl. Chem.* **21**, 135–139.

m1292 Lu *et al.* • $[Cu(C_{12}H_9N_2O_2S)Cl]\cdot H_2O$ *Acta Cryst.* (2006). E**62**, m1291–m1292