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(3,5-Dichloro-2-oxidobenzoato-κ^2O,O')-(1,10-phenanthroline-κ^2N,N')copper(II) monohydrate

Shu-Hua Zhang,* Xiao-Zhen Feng, Guang-Zhao Li, Li-Xia Jing and Zheng Liu*

Key Laboratory of Non-Ferrous Metal Materials and Processing Technology, Department of Materials and Chemical Engineering, Guilin University of Technology, Ministry of Education, Guilin 541004, People's Republic of China

Correspondence e-mail: zsh720108@21cn.com, lisa4.6@163.com

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Key indicators

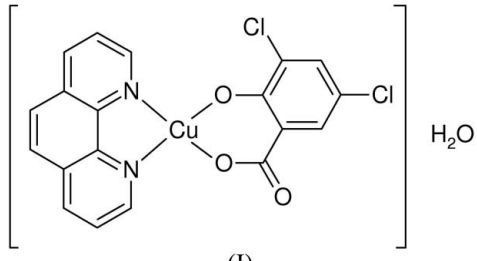
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.046
wR factor = 0.111
Data-to-parameter ratio = 12.1

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

In the title compound, $[Cu(C_7H_2Cl_2O_3)(C_{12}H_8N_2)]\cdot H_2O$, the Cu^{II} atom is coordinated in a slightly distorted square-planar geometry by two O atoms from a 3,5-dichloro-2-oxidobenzoate dianion and by two N atoms from 1,10-phenanthroline. The Cu^{II} complex and water molecules are linked into chains through O—H···O hydrogen bonds.

Comment

Metal-organic complexes containing pyridines (Stemmler *et al.*, 1995; Zhong *et al.*, 2003; Guthrie *et al.*, 1980) are of general interest for inorganic and bioinorganic chemists. The title compound, (I), is a new Cu^{II} complex prepared by reaction of 3,5-dichloro-2-hydroxybenzoic acid, 1,10-phenanthroline and copper(II) nitrate.



(I)

In (I), the Cu^{II} atom is coordinated by two O atoms from a 3,5-dichloro-2-oxidobenzoate dianion and by two N atoms from 1,10-phenanthroline in a slightly distorted square-planar geometry (Fig. 1 and Table 1). The water molecules form O—H···O hydrogen bonds (Table 2) to the carboxylate O atoms, linking the complexes into chains running along the *a* axis.

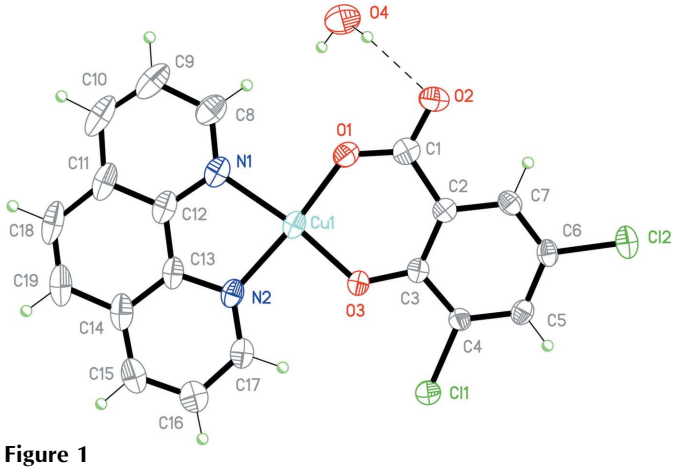


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids for non-H atoms. The dashed line indicates a hydrogen bond.

Experimental

A solution of 3,5-dichloro-2-hydroxybenzoic acid (2 mmol, 0.414 g) and potassium hydroxide (2 mmol, 0.112 g) in distilled water (15 ml) was slowly added to a solution of copper(II) nitrate (1 mmol, 0.260 g) in distilled water (10 ml). The mixture was stirred and refluxed for 2 h at room temperature. 1,10-Phenanthroline (2 mmol, 0.396 g) was added and the reaction continued for a further 2 h. The solution was filtered and the filtrate was left to stand at room temperature. Blue prisms suitable for X-ray diffration were obtained in a yield of 52% (based on copper nitrate).

Crystal data

$[Cu(C_7H_2Cl_2O_3)(C_{12}H_8N_2)]\cdot H_2O$
$M_r = 466.75$
Monoclinic, $P2_1/c$
$a = 4.6955\ (15)$ Å
$b = 20.383\ (3)$ Å
$c = 18.439\ (2)$ Å
$\beta = 97.105\ (2)^\circ$
$V = 1751.2\ (6)$ Å^3
$Z = 4$
$D_x = 1.770$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.58$ mm^{-1}
$T = 298\ (2)$ K
Prism, blue
0.57 × 0.16 × 0.09 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.466$, $T_{max} = 0.871$
7173 measured reflections
3071 independent reflections
2051 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 25.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.111$
$S = 1.03$
3071 reflections
253 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0425P)^2 + 1.4793P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.42$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.871 (3)	Cu1—N1	2.002 (4)
Cu1—O3	1.856 (3)	Cu1—N2	1.988 (4)
O3—Cu1—O1	95.30 (13)	O3—Cu1—N1	171.82 (15)
O3—Cu1—N2	90.06 (14)	O1—Cu1—N1	92.14 (16)
O1—Cu1—N2	173.22 (14)	N2—Cu1—N1	82.28 (17)

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H1···O2	0.85	2.10	2.922 (5)	164
O4—H2···O2^{i}	0.85	2.17	2.988 (6)	162

Symmetry code: (i) $x-1, y, z$.

H atoms of the water molecule were located in a difference Fourier map. The O—H distances were normalized to 0.85 Å and the H atoms were allowed to ride on the O atom, with $U_{iso}(H) = 1.5U_{eq}(O)$. All other H atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); 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, 1997); software used to prepare material for publication: *SHELXTL*.

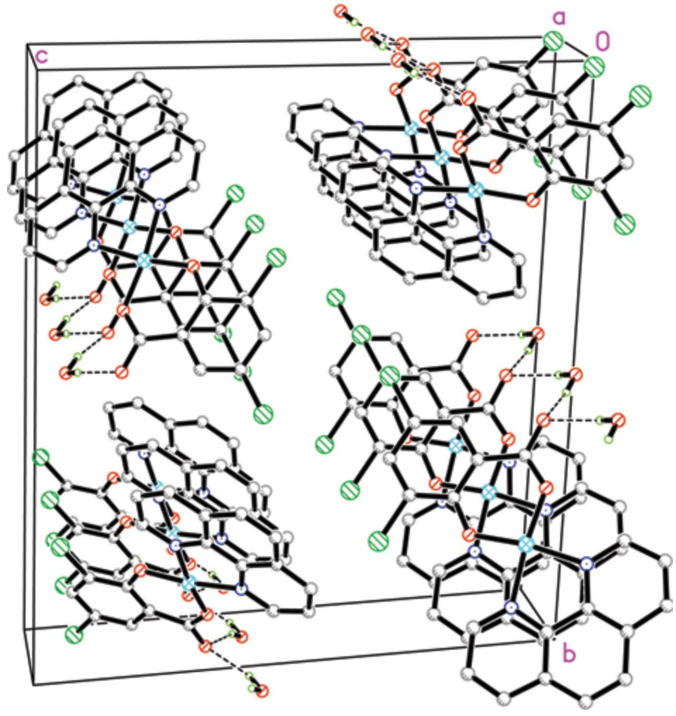


Figure 2
View of the packing of (I), showing hydrogen-bonded chains running along *a*. Hydrogen bonds are shown as dashed lines and H atoms not included in hydrogen bonding have been omitted.

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