Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Orotato(1,10-phenanthroline)copper(II)

Xing Li, Rong Cao,* Wenhua Bi, Daofeng Sun and Maochun Hong

State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Fuzhou, Fujian 350002, People's Republic of China

Correspondence e-mail: lix@ms.fjirsm.ac.cn

Received 26 March 2003
Accepted 2 April 2003
Online 9 April 2003

Hydrothermal reaction of CuO, orotic acid and 1,10-phenanthroline in an aqueous solution resulted in the title compound, [Cu(orotate)(phen)] or [Cu($C_5H_2N_2O_4$)($C_{12}H_8N_2$)], with a mononuclear structure. The coordination geometry around the Cu^{II} atom is distorted square planar. Through weak intermolecular Cu$\cdots$O interactions and N—H$\cdots$O hydrogen bonds, the crystal structure extends into a two-dimensional framework.

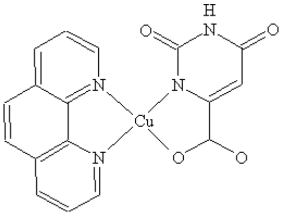
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.038
wR factor = 0.106
Data-to-parameter ratio = 10.9

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

Comment

The design and synthesis of novel inorganic–organic hybrid coordination complexes have attracted the attention of many chemists in recent years owing to their potential applications, such as selective guest absorption (Gardner *et al.*, 1995), gas storage (Li *et al.*, 1999), and heterogeneous catalysis (Dong *et al.*, 2000). In the past, many complexes have been synthesized and characterized (Harvey *et al.*, 2000). In this paper, we report the title compound, (I), a new copper coordination compound, [Cu(orotate)(phen)].



(I)

The Cu atom is four-coordinated by two N atoms from phenanthroline, and carboxylato O and N atoms from the orotate (Fig. 1). The coordination geometry of the Cu atom

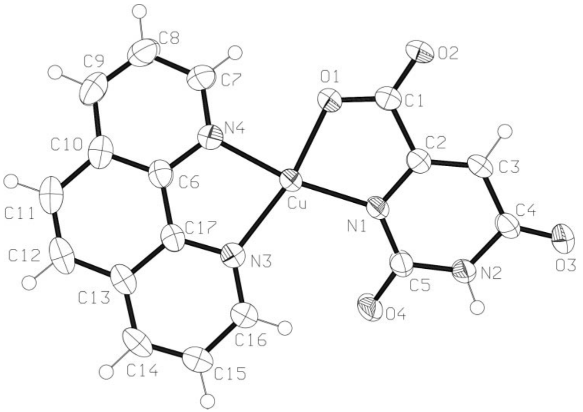


Figure 1
A view of the molecular structure of (I), showing 50% displacement ellipsoids for non-H atoms.

can be regarded as distorted square planar (Table 1). Through weak intermolecular Cu$\cdots$O interactions and N—H$\cdots$O hydrogen bonds, the crystal structure extends into a two-dimensional framework (Fig. 2). The distances Cu—O2($1-x$, $1-y$, $-z$) and Cu—O4($2-x$, $1-y$, $-z$) are 2.737 (3) and 2.771 (3) Å, respectively.

Experimental

A mixture of CuO (0.2 mmol, 0.015 g), 1,10-phenanthroline (0.2 mmol, 0.04 g), orotic acid (0.3 mmol, 0.05 g) and H_2O (15 ml) was sealed in a 25 ml Teflon-lined stainless steel reactor and heated at 453 K for 72 h. After cooling, blue crystals of (I) were obtained (yield 68%).

Crystal data

$[Cu(C_5H_2N_2O_4)(C_{12}H_8N_2)]$
$M_r = 397.83$
Monoclinic, $P2_1/n$
$a = 8.6703$ (2) Å
$b = 7.8597$ (2) Å
$c = 21.5279$ (2) Å
$\beta = 90.916$ (1)°
$V = 1466.85$ (5) Å^3
$Z = 4$

$D_x = 1.801$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 80 reflections
$\theta = 1.9$–25.0°
$\mu = 1.52$ mm^{-1}
$T = 293$ (2) K
Block, blue
0.58 × 0.26 × 0.06 mm

Data collection

Siemens SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.682$, $T_{max} = 0.913$
5179 measured reflections

2560 independent reflections
2127 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 25.0°$
$h = -9 \rightarrow 10$
$k = -9 \rightarrow 7$
$l = -20 \rightarrow 25$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.106$
$S = 1.08$
2560 reflections
235 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0483P)^2 + 1.9946P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.43$ e Å^{-3}
$\Delta\rho_{min} = -0.52$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu—O1	1.949 (2)	Cu—N4	2.004 (3)
Cu—N1	1.998 (3)	Cu—N3	2.083 (3)
O1—Cu—N1	81.97 (10)	O1—Cu—N3	165.97 (11)
O1—Cu—N4	87.76 (11)	N1—Cu—N3	110.06 (11)
N1—Cu—N4	168.99 (12)	N4—Cu—N3	80.65 (11)

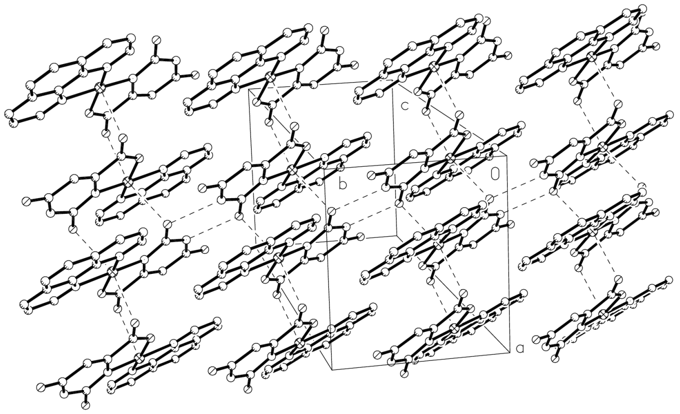


Figure 2
The crystal structure of (I), viewed approximately along the *c* axis.

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N2—H2$A\cdots$O4^{i}	0.86	2.07	2.895 (4)	161

Symmetry code: (i) $-x, 2-y, -z$.

For all H atoms the positions were generated geometrically (C—H bond fixed at 0.96 Å), and isotropic displacement parameters were assigned. The H atoms were allowed to ride on their respective parent C atoms.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1994); program(s) used to solve structure: *SHELXTL* (Siemens, 1994); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

This work was supported by the Natural Science Foundation of China and the Natural Science Foundation of Fujian Province.

References

Dong, Y. B., Smith, M. D. & zur Loye, H. C. (2000). *Solid State Sci.* **2**, 335–341.
Gardner, G. B., Venkataraman, D., Moore, J. S. & Lee, S. (1995). *Nature (London)*, **374**, 792–795.
Harvey, M., Baggio, S., Suescun, L. & Baggio, R. F. (2000). *Acta Cryst.* C**56**, 811–813.
Li, H., Eddaoudi, M., O'Keeffe, M. & Yaghi, O. M. (1999). *Nature (London)*, **402**, 276–279.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Siemens (1994). *SAINT* and *SHELXTL*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Acta Cryst. (2003). E**59**, m228–m229 Xing Li *et al.* • $[Cu(C_5H_2N_2O_4)(C_{12}H_8N_2)]$ **m229**