Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Bis(3-bromo-1-oxidoanthraquinone-κ^2O^1,O^9)-bis(pyridine-κN)copper(II) dihydrate

Hapipah M. Ali, Siti Nadiah Abdul Halim, Saha Koushik and Seik Weng Ng*

Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Received 22 June 2005
Accepted 23 June 2005
Online 30 June 2005

The Cu atom in the title compound, $[Cu(C_{14}H_6BrO_3)_2(C_5H_5N)_2]\cdot 2H_2O$, lies on a center of inversion; it is chelated by the bromo-substituted hydroxyanthroquinone molecule and is coordinated by the pyridine molecules in an all-*trans* octahedral geometry.

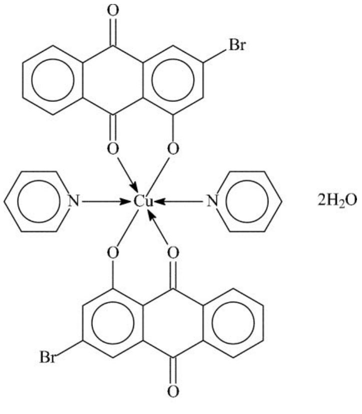
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.007 Å
R factor = 0.048
wR factor = 0.144
Data-to-parameter ratio = 15.0

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

Comment

Our previous study has documented the structure of the zinc derivative of a bromo-substituted 1-hydroxyanthraquinone anion (Ali *et al.*, 2005). This zinc complex crystallizes from pyridine as a bis-pyridine adduct in an all-*trans* octahedral enviroment. The corresponding title copper complex, (I), adopts the identical geometry, but the compound crystallizes as a dihydrate (Fig. 1). The Cu atom lies on a special position of $\overline{1}$ site symmetry; the chelating O atoms form a square, and the N atoms of the heterocyle occupy the other two octahedral sites. Hydrogen bonds (Table 2) link the molecule to the uncoordinated water molecule to give rise to a linear chain.



(I)

Experimental

3-Bromo-1-hydroxyanthraquinone (0.50 g, 1.65 mmol) and copper acetate monohydrate (0.16 g, 0.82 mmol) were heated in ethanol for several hours. The solid that was isolated upon removal of the solvent was recrystallized from pyridine to furnish brown prisms.

Crystal data

$[Cu(C_{14}H_6BrO_3)_2(C_5H_5N)_2]\cdot 2H_2O$
M_r = 861.97
Triclinic, $P\overline{1}$
a = 8.8121 (8) Å
b = 10.0253 (9) Å
c = 10.1720 (9) Å
α = 69.474 (1)°
β = 80.252 (1)°
γ = 81.477 (1)°
V = 825.6 (1) Å^3

Z = 1
D_x = 1.734 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2123 reflections
θ = 2.4–25.4°
μ = 3.14 mm^{-1}
T = 295 (2) K
Prism, brown
0.36 × 0.18 × 0.18 mm

Data collection

Bruker SMART area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
$T_{\min} = 0.347$, $T_{\max} = 0.568$
6931 measured reflections
3565 independent reflections
2240 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.029$
$\theta_{\max} = 27.2°$
$h = -10 \rightarrow 11$
$k = -12 \rightarrow 12$
$l = -12 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.144$
$S = 1.01$
3565 reflections
238 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0832P)^2 + 0.0828P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.85$ e Å^{-3}
$\Delta\rho_{\min} = -0.47$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.932 (3)	Cu1—O2	2.229 (3)
Cu1—N1	2.077 (4)		
O1—Cu1—O1$^{\rm i}$	180	O2—Cu1—O2$^{\rm i}$	180
O1—Cu1—O2	86.3 (1)	O2—Cu1—N1	91.4 (1)
O1—Cu1—O2$^{\rm i}$	93.7 (1)	O2—Cu1—N1$^{\rm i}$	88.6 (1)
O1—Cu1—N1	90.8 (1)	N1—Cu1—N1$^{\rm i}$	180
O1—Cu1—N1$^{\rm i}$	89.2 (1)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H1*w*1···O1	0.86 (1)	2.23 (4)	2.948 (5)	142 (6)
O1*w*—H1*w*2···O3$^{\rm ii}$	0.86 (1)	2.25 (4)	3.018 (6)	149 (6)

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

The C-bound H atoms were positioned geometrically (C—H = 0.93 Å) and were included in the refinement in the riding-model approximation, with $U_{\rm iso}(\rm H) = 1.2U_{\rm eq}(\rm C)$. The water H atoms were located in a difference Fourier map, and were refined with distance restraints of O—H = 0.85 (1) Å and H···H = 1.39 (1) Å.

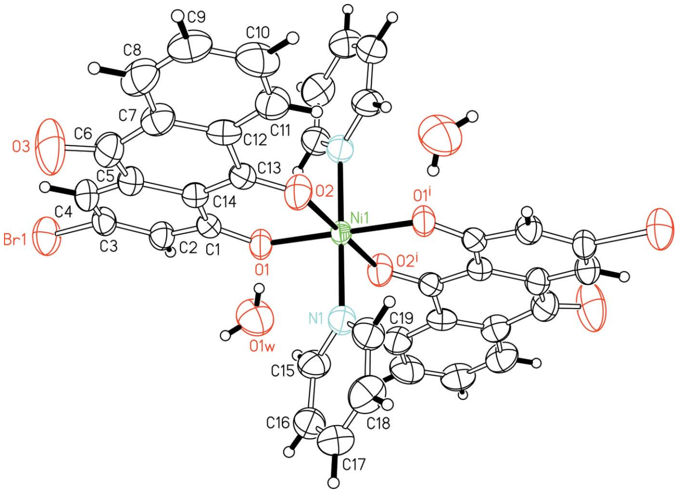


Figure 1
ORTEPII plot (Johnson, 1976) of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii. The Cu atom lies at the center of inversion ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$) [symmetry code: (i) $1-x, 1-y, 1-z$].

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

The authors thank the Ministry of Science, Technology and the Environment for supporting this study (grant No. IPRA 33–02-03–3055). We thank Mr Xiao-Long Feng of Sun Yat-Sen University for the diffraction measurements.

References

Ali, H. M., Abdul Halim, S. N., Koushik, S., Lajis, N. Hj., Basirun, W. J. & Ng, S. W. (2005). *Acta Cryst.* E**61**, m691–m692.
Bruker (1999). *SADABS*, *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

m1432 Ali *et al.* • $[\rm Cu(C_{14}H_6BrO_3)_2(C_5H_5N)_2]\cdot 2H_2O$ *Acta Cryst.* (2005). E**61**, m1431–m1432