Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(2-acetyl-5-hydroxyphenolato-κ^2O,O')copper(II)

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

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

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

Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.036
wR factor = 0.117
Data-to-parameter ratio = 14.3

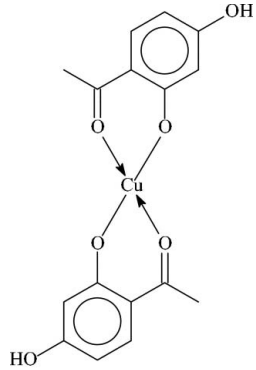
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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

The Cu atom in the title compound, $[Cu(C_8H_7O_3)_2]$, lies on a center of inversion and exists in a square-planar enviroment that is defined by the four chelating O atoms. Intermolecular O—H···O hydrogen bonds [O···O = 2.711 (3)Å] link adjacent molecules into a layer structure.

Comment

The deprotonated 2-hydroxyacetophenone anion has been used to chelate to a number of divalent transition metal ions; the copper(II) derivatives include, for example, (2-acetylphenolato)(2,2′-bipyridyl)perchloratocopper (Elmali *et al.*, 2002) and bis(2-acetylphenolato)(4-methylpyridine)copper (Duckworth & Stephenson, 1969). In the second example, the metal atom is coordinated by two 4-picoline molecules; the title compound, (I) (Fig. 1), crystallizes from pyridine without any solvent. The anion chelates to the metal atom which lies on an inversion center, with different Cu—O distances (Table 1). The Cu atom exists in a square-planar geometry, and adjacent molecules are linked by intermolecular O—H···O hydrogen bonds (Table 2) into a layer structure.



(I)

Experimental

2,4-Dihydroxyacetophenone (0.50 g, 3.6 mmol) and 4-nitroaniline (0.50 g, 3.6 mmol) were reacted in boiling ethanol, and to the mixture was added copper acetate monohydrate (0.36 g, 1.8 mmol). The heating was continued for an hour. The solid that was isolated upon removal of the solvent was recrystallized from pyridine.

Crystal data

$[Cu(C_8H_7O_3)_2]$
M_r = 365.81
Orthorhombic, *Pbca*
a = 7.022 (1) Å
b = 13.667 (2) Å
c = 15.192 (2) Å
V = 1458.1 (3) Å^3
Z = 4
D_x = 1.666 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 766 reflections
θ = 2.7–27.0°
μ = 1.53 mm^{-1}
T = 295 (2) K
Prism, dark brown

0.24 × 0.14 × 0.11 mm

Data collection

Bruker SMART area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.724, T_{max} = 0.850
8105 measured reflections
1591 independent reflections
1057 reflections with $I > 2\sigma(I)$
R_{int} = 0.061
θ_{max} = 27.0°
$h = -6 \rightarrow 8$
$k = -17 \rightarrow 17$
$l = -18 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.117
S = 1.04
1591 reflections
111 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0694P)^2 + 0.0274P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.912 (2)	Cu1—O2	1.883 (2)
O1—Cu1—O1^{i}	180	O1—Cu1—O2^{i}	87.47 (8)
O1—Cu1—O2	92.53 (8)		

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
O3—H3*o*···O2^{ii}	0.83 (1)	1.90 (1)	2.710 (3)	166 (4)

Symmetry code: (ii) $x-\frac{1}{2}, -y+\frac{3}{2}, -z+1$.

The C-bound H atoms were positioned geometrically (C—H = 0.93Å for the aromatic H atoms and 0.98Å for the methyl H atoms) and were included in the refinement in the riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(parent atom) for the aromatic C atoms and 1.5U_{eq} for the methyl H atoms. The methyl group was rotated to fit the electron density. The hydroxy H atom was located in a difference Fourier map, and was refined with a distance restraint of O—H = 0.85 (1) Å.

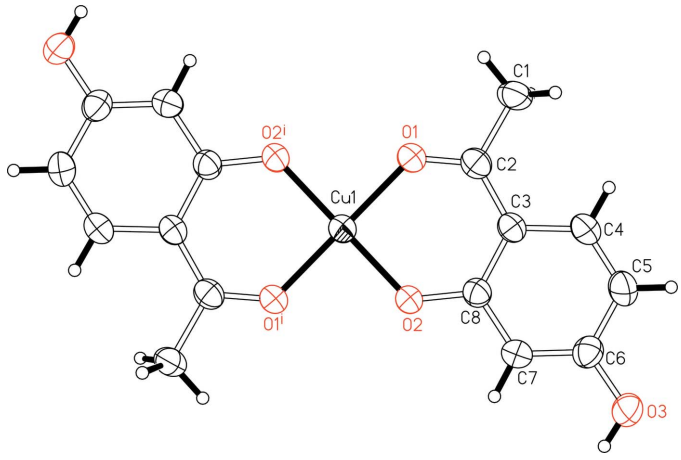


Figure 1
ORTEPII plot (Johnson, 1976) of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii. The Cu atom lies at the center of inversion ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$) [symmetry code: (i) $1-x, 1-y, 1-z$].

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

Bruker (1999). *SADABS*, *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Duckworth, V. F. & Stephenson, N. C. (1969). *Acta Cryst.* B**25**, 2245-2254.
Elmali, A., Elerman, Y. & Svoboda, I. (2002). *Z. Naturforsch. Teil B*, **57**, 1129-1132.
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.