metal-organic papers

Bis(4-methoxy-2-oxidoacetophenone)copper(II)

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Key indicators

Single-crystal X-ray study
$T = 298$ K
Mean σ(C–C) = 0.007 Å
R factor = 0.052
wR factor = 0.161
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 crystal structure of the title compound, [Cu(C$_9$H$_9$O$_3$)$_2$], the Cu^{II} atom, lying on a center of symmetry, has a square-planar coordination formed by two paeonol anions.

Comment

Paeonol, or 2-hydroxy-4-methoxyacetophenone, is an effective component of many traditional Chinese medicines, and its derivatives have attracted considerable attention because of their potential biological properties (Liu *et al.*, 2000; Xu *et al.*, 2005). As part of our ongoing investigation on paeonol derivatives (Xu *et al.*, 2006), we present here the structure of the title Cu^{II} complex, (I).
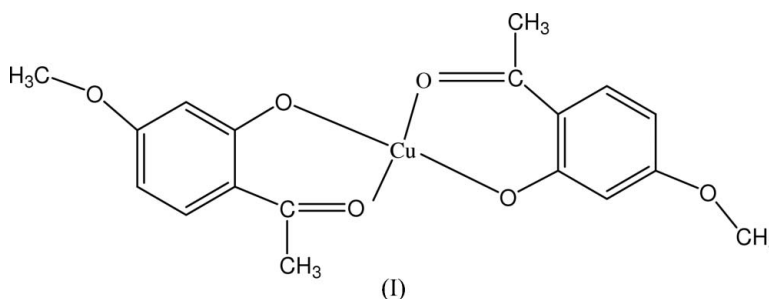
The Cu^{II} atom is coordinated in a square-planar geometry by the four O atoms of the paeonol anions, in which the hydroxyl groups are deprotonated (Fig. 1 and Table 1). Similar complexes commonly adopt a square-planar coordination geometry (Sillanpaa, 1991). The molecule is almost planar, the dihedral angle between the Cu1/O1/O2/C2/C3/C4 chelate ring and the benzene ring being 3.2 (2)°.

Experimental

To a stirred solution of Cu(ClO$_4$)$_2$·6H$_2$O (0.5 mmol) in 25 ml absolute methanol was added dropwise a solution of paeonol (1.0 mmol) in 10 ml absolute methanol at room temperature. After stirring for 3 h at 320 K, the precipitate was filtered off, washed with methanol and dried *in vacuo* but this was not suitable for X-ray diffraction analysis. Single crystals of (I) were obtained by slow evaporation of the filtrates at ambient temperature after 10 d.

Crystal data

[Cu(C$_9$H$_9$O$_3$)$_2$]	$Z = 2$
$M_r = 393.86$	$D_x = 1.643$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 8.871$ (4) Å	$\mu = 1.41$ mm^{-1}
$b = 13.763$ (6) Å	$T = 298$ (2) K
$c = 6.523$ (3) Å	Prism, green
$\beta = 90.824$ (6)°	$0.32 \times 0.24 \times 0.21$ mm
$V = 796.4$ (6) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	3980 measured reflections
φ and ω scans	1394 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)	1007 reflections with $I > 2\sigma(I)$
$T_{min} = 0.651$, $T_{max} = 0.744$	$R_{int} = 0.038$
	$\theta_{max} = 25.0°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0933P)^2 + 1.4385P]$
$R[F^2 > 2\sigma(F^2)] = 0.052$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.161$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.02$	$\Delta\rho_{max} = 0.46$ e Å^{-3}
1394 reflections	$\Delta\rho_{min} = -0.51$ e Å^{-3}
115 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.877 (4)	O2—C2	1.246 (6)
Cu1—O2	1.941 (3)	O3—C6	1.345 (6)
O1—C4	1.308 (6)	O3—C9	1.429 (6)
O1—Cu1—O2^i	88.32 (14)	O1—Cu1—O2	91.68 (14)

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

Methyl H atoms were placed in calculated positions (C—H = 0.96 Å) and torsion angles were refined, with $U_{iso}(H) = 1.5U_{eq}(C)$. Aromatic H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics:
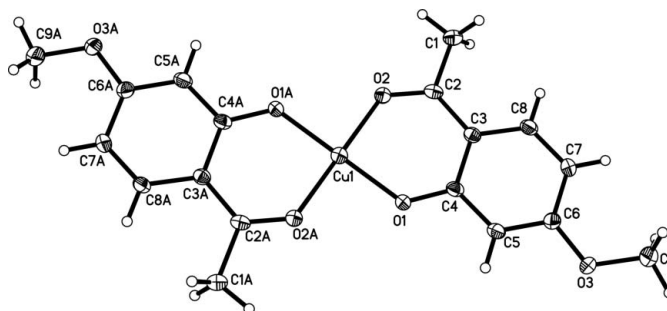

Figure 1
The molecular structure of (I) with 30% probability displacement ellipsoids. The suffix A corresponds to symmetry code (i) in Table 1.

SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

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