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Bis{μ-(*E*)-5-methoxy-2-[1-(3-oxidopropylideneamino)ethyl]phenolato}copper(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.053
wR factor = 0.144
Data-to-parameter ratio = 13.0

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

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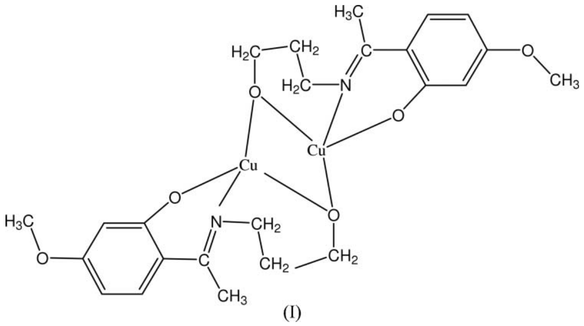
The title dimeric Cu^{II} complex, [$Cu_2(C_{12}H_{15}NO_3)_2$], is centrosymmetric. Two Cu^{II} atoms related by an inversion center are bridged by two O atoms of propanolamine. The Cu^{II} atom assumes a distorted square-planar geometry.

Comment

Paeonol, or 2-hydroxy-4-methoxyacetophenone, is an effective component of Chinese traditional medicines. As part of our ongoing investigation on Schiff base compounds of paeonol, we present here the structure of the title Cu^{II} complex, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. While the 5-methoxy-2-[1-(3-oxidopropylideneamino)ethyl]phenolate dianion chelates to an individual Cu^{II} atom through the amino and two diprotonated hydroxy groups, the deprotonated hydroxy atom O3 bridges two Cu^{II} atoms, forming a centrosymmetric dimeric complex. The Cu^{II} atom assumes a distorted square-planar coordination (Table 1). Within the dimeric complex, the Cu$\cdots$Cu separation is 3.0299 (11) Å.

Experimental

To a stirred solution of paeonol (1.0 mmol) and $Cu(ClO_4)_2\cdot6H_2O$ (1.0 mmol) in 25 ml absolute methanol was added dropwise a solution of propanolamine (1.0 mmol) in 10 ml absolute methanol at room temperature. After stirring for 3 h at 320 K, the resulting precipitate was filtered off, washed with methanol and dried *in vacuo*. Single crystals of (I) were obtained by slow evaporation of the filtrate after 5 d.

Crystal data

[$Cu_2(C_{12}H_{15}NO_3)_2$]	*Z* = 2
M_r = 569.6	D_x = 1.624 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo *K*α radiation
a = 6.774 (1) Å	μ = 1.87 mm^{-1}
b = 6.703 (1) Å	*T* = 293 (2) K
c = 25.775 (4) Å	Prism, blue
β = 95.493 (2)°	0.21 × 0.08 × 0.05 mm
V = 1165.1 (3) Å^3	

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Data collection

Bruker SMART APEX area-dectector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
$T_{\min} = 0.695$, $T_{\max} = 0.912$
5982 measured reflections
2034 independent reflections
1788 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.032$
$\theta_{\max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.144$
$S = 1.05$
2034 reflections
156 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0738P)^2 + 3.3311P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.74$ e Å^{-3}
$\Delta\rho_{\min} = -0.54$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.873 (3)	N1—C8	1.302 (6)
Cu1—O3$^{\rm i}$	1.935 (3)	N1—C10	1.475 (6)
Cu1—O3	1.912 (3)		
O1—Cu1—O3$^{\rm i}$	92.16 (15)	O3—Cu1—N1	98.56 (16)
O1—Cu1—O3	167.99 (15)	O3$^{\rm i}$—Cu1—N1	174.31 (16)
O1—Cu1—N1	93.28 (16)	Cu1$^{\rm i}$—O3—Cu1	103.93 (16)
O3$^{\rm i}$—Cu1—O3	76.07 (16)		

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

Methyl H atoms were placed in calculated positions, with C—H = 0.96 Å, and torsion angles were refined to fit the electron density [$U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C)]. Other H atoms were positioned geometrically, with C—H = 0.93 (aromatic) and 0.97 Å (methylene), and refined as riding, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C).

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

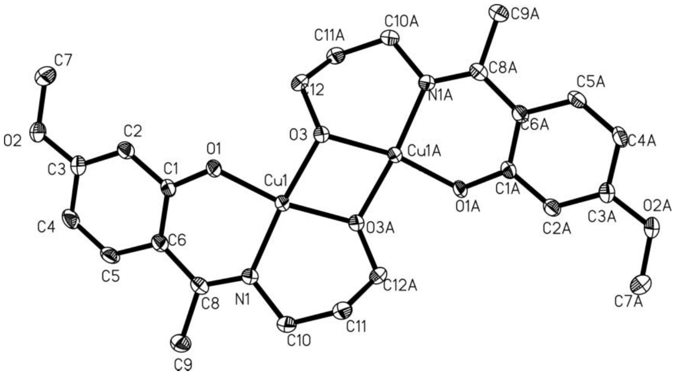

Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids [symmetry code: (i) $-x, -y, -z$]. H atoms have been omitted.

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