

## Aquabis(2-formyl-6-methoxyphenolato)copper(II)

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## Key indicators

Single-crystal X-ray study  
 $T = 295$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.038  
 $wR$  factor = 0.109  
Data-to-parameter ratio = 13.0

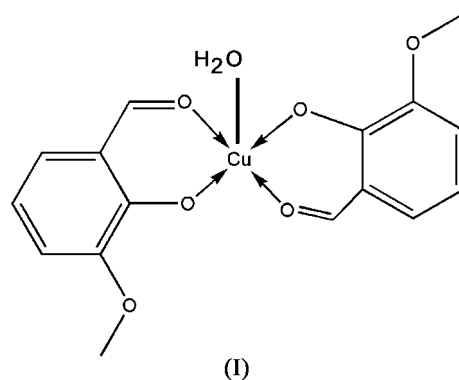
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the title mononuclear complex,  $[\text{Cu}(\text{C}_8\text{H}_7\text{O}_3)_2(\text{H}_2\text{O})]$ , the  $\text{Cu}^{\text{II}}$  atom is five-coordinated by four O atoms from two 2-formyl-6-methoxyphenolate ligands and one O atom from a water molecule, to form a slightly distorted square-pyramidal coordination geometry. Centrosymmetric dimers are formed through intermolecular  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds, and these dimers are further linked by weak  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds to form a three-dimensional network.

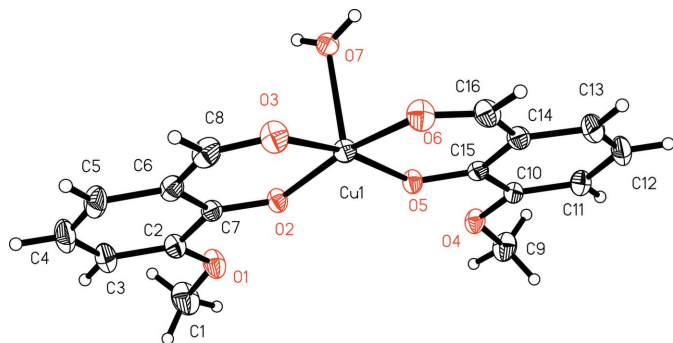
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## Comment

Schiff base metal complexes have been of interest in coordination chemistry for many years because of their facile synthesis and wide applications (Garnovskii *et al.*, 1993). These complexes make a significant contribution in the development of catalysis and enzymatic reactions, magnetism, molecular architectures and materials chemistry (Archer, 1993; Ziesel, 2001). In an attempt to obtain an *o*-vanillin Schiff base complex, copper acetate and hydrazine-1,2-diylidene-bis(methan-1-yl-1-ylidene)bis(2-methoxyphenol) were reacted in an ethanol solution, but after slow evaporation of a solution of the product, crystals of the unexpected title compound, (I), were formed.



2-Hydroxy-3-methoxybenzaldehyde is a potential bidentate ligand with versatile binding modes. However, reported crystal structures of metal complexes with *o*-vanillin are rare. In the molecular structure of (I) (Fig. 1), the  $\text{Cu}^{\text{II}}$  atom is coordinated in a slightly distorted square-pyramidal geometry by four O atoms from two bidentate 2-formyl-6-methoxyphenolate ligands in the basal plane and an O atom from the coordinated water molecule in the apical position. The dihedral angle between the planes of the two benzene rings is  $5.66(4)^\circ$ . The  $\text{Cu}-\text{O}$  bond lengths and  $\text{O}-\text{Cu}-\text{O}$  angles (Table 1) are within the expected ranges (Alcock *et al.*, 1996; Morshedi *et al.*, 2006). In the crystal structure, the coordinated water



**Figure 1**  
The molecular structure of (I), showing displacement ellipsoids drawn at the 30% probability level.

molecule forms intermolecular hydrogen bonds (Table 2) with the carboxyl and methoxy groups of a symmetry-related molecule to form a centrosymmetric dimer. These dimers are, in turn, linked by weak C—H...O hydrogen bonds to form a three-dimensional network (Fig. 2).

## Experimental

Cu(CH<sub>3</sub>COO)<sub>2</sub> (1 mmol, 181 mg) and hydrazine-1,2-diylidenebis(methan-1-yl-1-ylidene)bis(2-methoxyphenol) (1 mmol, 300 mg) were dissolved in an ethanol solution (20 ml), and the mixture was then refluxed for 3 h with stirring. The resulting clear yellow solution was kept in air and, after slow evaporation of the solvent over a period of a week, black crystals of (I) were formed at the bottom of the vessel. The crystals were isolated, washed three times with ethanol and dried in a vacuum desiccator using anhydrous CaCl<sub>2</sub> (yield 38%). Analysis calculated for C<sub>16</sub>H<sub>16</sub>CuO<sub>7</sub>: C 50.07, H 4.20%; found: C 50.36, H 4.52%.

### Crystal data

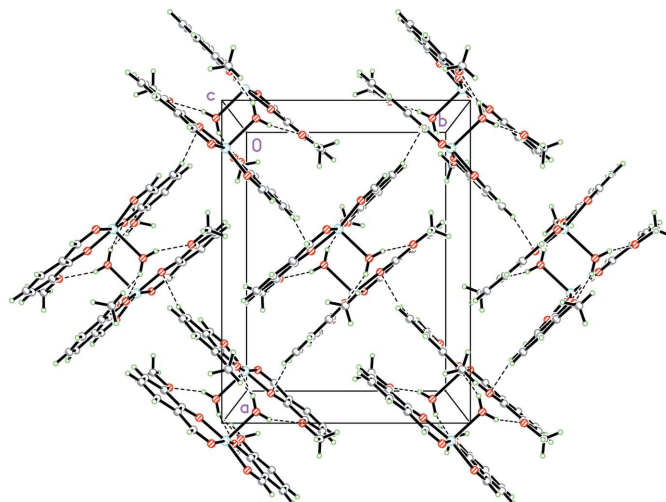
[Cu(C <sub>8</sub> H <sub>7</sub> O <sub>3</sub> ) <sub>2</sub> (H <sub>2</sub> O)]	Z = 8
<i>M<sub>r</sub></i> = 383.83	<i>D<sub>x</sub></i> = 1.571 Mg m <sup>-3</sup>
Orthorhombic, <i>Pbca</i>	Mo <i>K</i> α radiation
<i>a</i> = 15.2947 (12) Å	<i>μ</i> = 1.38 mm <sup>-1</sup>
<i>b</i> = 11.7932 (9) Å	<i>T</i> = 295 (2) K
<i>c</i> = 17.9949 (14) Å	Block, black
<i>V</i> = 3245.8 (4) Å <sup>3</sup>	0.24 × 0.22 × 0.18 mm

### Data collection

Siemens SMART CCD area-detector diffractometer	13485 measured reflections
<i>φ</i> and <i>ω</i> scans	2856 independent reflections
Absorption correction: multi-scan ( <i>SADABS</i> ; Sheldrick, 1996)	2323 reflections with <i>I</i> > 2σ( <i>I</i> )
<i>T<sub>min</sub></i> = 0.733, <i>T<sub>max</sub></i> = 0.789	<i>R<sub>int</sub></i> = 0.046
	<i>θ<sub>max</sub></i> = 25.0°

### Refinement

Refinement on <i>F</i> <sup>2</sup>	$w = 1/[\sigma^2(F_o^2) + (0.0669P)^2 + 0.1633P]$
$R[F^2 > 2\sigma(F^2)] = 0.038$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.109$	( $\Delta/\sigma$ ) <sub>max</sub> = 0.035
<i>S</i> = 1.04	$\Delta\rho_{\text{max}} = 0.44 \text{ e \AA}^{-3}$
2856 reflections	$\Delta\rho_{\text{min}} = -0.48 \text{ e \AA}^{-3}$
220 parameters	
H-atom parameters constrained	



**Figure 2**  
Crystal packing of (I), with O—H...O and C—H...O hydrogen bonds shown as dashed lines.

**Table 1**

Selected geometric parameters (Å, °).

Cu1—O2	1.9191 (17)	Cu1—O6	1.965 (2)
Cu1—O5	1.9207 (17)	Cu1—O7	2.2412 (19)
Cu1—O3	1.954 (2)		
O2—Cu1—O5	87.89 (7)	O3—Cu1—O6	85.83 (10)
O2—Cu1—O3	91.46 (9)	O2—Cu1—O7	99.05 (7)
O5—Cu1—O3	167.67 (9)	O5—Cu1—O7	98.15 (7)
O2—Cu1—O6	168.17 (9)	O3—Cu1—O7	94.11 (8)
O5—Cu1—O6	92.29 (9)	O6—Cu1—O7	92.64 (9)

**Table 2**

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O7—H7B...O4 <sup>i</sup>	0.85	2.27	2.893 (3)	130
O7—H7A...O1 <sup>i</sup>	0.82	2.44	2.908 (3)	117
O7—H7B...O5 <sup>i</sup>	0.85	2.15	2.896 (3)	146
C13—H13...O2 <sup>ii</sup>	0.93	2.43	3.346 (3)	168
C4—H4...O3 <sup>iii</sup>	0.93	2.56	3.325 (4)	140

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

H atoms bonded to C atoms were placed in calculated positions and were allowed to ride on their parent C atoms with a C—H distance of 0.93 Å for aromatic H atoms and 0.96 Å for methyl H atoms, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  or  $1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$ . The H atoms of the coordinated water molecule were placed in calculated positions and were allowed to ride on their parent O atom, with O—H = 0.85 Å, and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{iso}}(\text{O7})$ .

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINTE* (Siemens, 1996); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXL97*.

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