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Synthesis and crystal structure of bis(5-methyl-2-aldehyde-phenolato- $\kappa^2 O^1, O^2$)copper(II), $C_{16}H_{14}CuO_4$

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Abstract

$C_{16}H_{14}CuO_4$, monoclinic, $P2_1/c$ (no. 14), $a = 12.7831(4)$ Å, $b = 4.71970(10)$ Å, $c = 12.1802(4)$ Å, $\beta = 114.557(1)^\circ$, $Z = 2$, $V = 668.39(3)$ Å³, $R_{gt}(F) = 0.0211$, $wR_{ref}(F^2) = 0.0624$, $T = 173(2)$ K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

Synthesis of the copper(II) complex: All reagents and starting materials were obtained from commercial suppliers and used as received without further purification. Copper(II) acetate monohydrate (0.100 g, 0.5 mmol) dissolved in MeOH (5 mL) was added dropwise to 2-hydroxy-4-methylbenzaldehyde (0.136 g, 1 mmol) in CH_2Cl_2 (5 mL) at room temperature. The mixture was stirred for 2 h. The filtrate was allowed to stand for a week in a quiet environment. Several clear brown crystals were obtained. **FT-IR** (KBr, cm^{-1}): 3051, 3032, 2976, 1646, 1593, 1510, 1446, 1249, 1134, 861, 820, 563, 440.

Table 1: Data collection and handling.

Crystal:	Brown block
Size:	$0.27 \times 0.25 \times 0.24$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	1.65 mm^{-1}
Diffractometer, scan mode:	Bruker D8 Venture, φ and ω
$\theta_{\max}$, completeness:	26.7° , >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	11890, 1404, 0.038
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1263
$N(\text{param})_{\text{refined}}$:	98
Programs:	Bruker [1], SHELX [2, 3], Olex2 [4]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.500000	0.000000	0.000000	0.01914(11)
O2	0.47072(10)	0.0462(3)	0.14249(11)	0.0226(3)
C1	0.31714(13)	−0.3799(4)	−0.02213(14)	0.0183(3)
C2	0.31923(13)	−0.2933(3)	0.09076(13)	0.0173(3)
O1	0.38532(10)	−0.2783(3)	−0.06802(10)	0.0242(3)
C6	0.23503(14)	−0.5868(4)	−0.08870(15)	0.0207(3)
H6	0.232815	−0.649175	−0.163798	0.025*
C5	0.15819(13)	−0.7009(3)	−0.04815(14)	0.0204(3)
C4	0.16245(15)	−0.6131(4)	0.06510(15)	0.0235(4)
H4	0.110343	−0.691580	0.094193	0.028*
C3	0.24106(14)	−0.4168(4)	0.13212(15)	0.0211(3)
H3	0.243585	−0.361293	0.208154	0.025*
C7	0.39609(14)	−0.0839(4)	0.16436(14)	0.0186(3)
H7	0.390374	−0.037679	0.237581	0.022*
C8	0.07076(15)	−0.9159(4)	−0.12187(16)	0.0258(4)
H8A	0.073919	−0.937917	−0.200441	0.039*
H8B	−0.006194	−0.852138	−0.133847	0.039*
H8C	0.087456	−1.098163	−0.079471	0.039*

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment

Transition metal complexes play an important role in coordination chemistry, because they have excellent properties in many fields [5]. According to a literature review reported

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earlier, copper(II) complexes are particular important in the fields of catalysis, fluorescence and supramolecular chemistry [6–8]. Thus copper(II) complexes have received extensive attention. So far, we have designed and prepared a series of copper(II) complex [9, 10].

In this paper, we prepared a new copper(II) complex, whose structure was determined by X-ray crystallography. The copper(II) atom is located at an inversion center, and is four-coordinated four oxygen atoms from two symmetry-equivalent bidentate phenolato ligands. The Cu1–O1 bond length is 1.8845(11) Å and the Cu1–O2 bond length is 1.9338(12) Å. The angles of O1–Cu1–O2 and O1–Cu1–O1ⁱ are 93.89(5)° and 180.0°, respectively. All geometric parameters are within typical ranges [11, 12].

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