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Key indicators

Single-crystal X-ray study
 $T = 295$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.037
 wR factor = 0.115
Data-to-parameter ratio = 18.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Diethanol(2-hydroxy-2,2-diphenylacetato)-
pyridinecopper(II)

In the title mononuclear complex, $[\text{Cu}(\text{C}_{14}\text{H}_{11}\text{O}_3)_2(\text{C}_5\text{H}_5\text{N})_2(\text{C}_2\text{H}_6\text{O})_2]$, the Cu atom has a distorted octahedral environment, formed by the N atoms of two pyridine molecules, carboxylate O atoms belonging to two 2-hydroxy-2,2-diphenylacetate ligands and O atoms of two ethanol molecules. The molecule of the complex occupies a special position on a twofold axis, which passes through the Cu atom as well as the N and *para*-C atoms of each of the two pyridine ligands. One crystallographically independent intermolecular hydrogen bond, involving the OH group of the hydroxy-diphenylacetate ligand and a carbonyl O atom of another acetate ligand of a neighbouring complex, is responsible for the formation of infinite chains running along the a axis of the crystal structure.

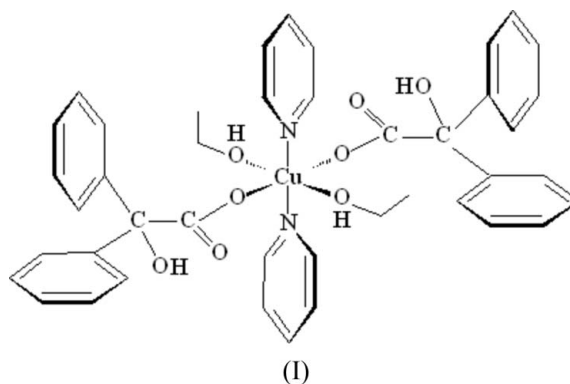
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Comment

2-Hydroxy-2,2-diphenylacetic acid (also known as benzoic acid) is a potentially multidentate ligand, which can bind to a metal centre through its carboxyl and/or hydroxy O atoms. The structural chemistry and biochemistry of α -hydroxy acids and their derivatives, such as benzoic acid, have attracted considerable interest (Barucki *et al.*, 2000; Cervilla *et al.*, 1995; Herrmann *et al.*, 1994; Kusthardt *et al.*, 1986; Chasteen *et al.*, 1969). In order to explore further the coordination behaviour of various metals with respect to benzoic acid, we synthesized a new copper complex, $[\text{Cu}(\text{C}_{14}\text{H}_{11}\text{O}_3)_2(\text{C}_5\text{H}_5\text{N})_2(\text{C}_2\text{H}_5\text{OH})_2]$, (I), by the reaction of copper(II) acetate, benzoic acid and pyridine in an ethanol solution. The crystal structure of (I) is reported here.



The crystal structure of (I) contains neutral mononuclear Cu^{II} complexes. The molecule of the complex (Fig. 1) occupies a special position on the twofold axis that passes through the central Cu1, as well as atoms N1, C17, N2 and C20 of the two pyridine ligands. Atom Cu1 has an octahedral environment

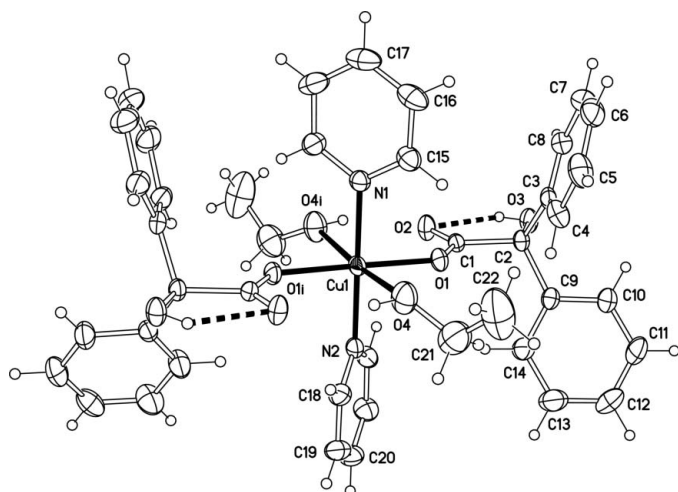


Figure 1
ORTEP (Johnson, 1976) plot of (I), with 30% probability displacement ellipsoids; H atoms are shown as small circles of arbitrary radii. Intramolecular hydrogen bonds are shown as dashed lines [symmetry code (i): $1 - x, y, \frac{3}{2} - z$].

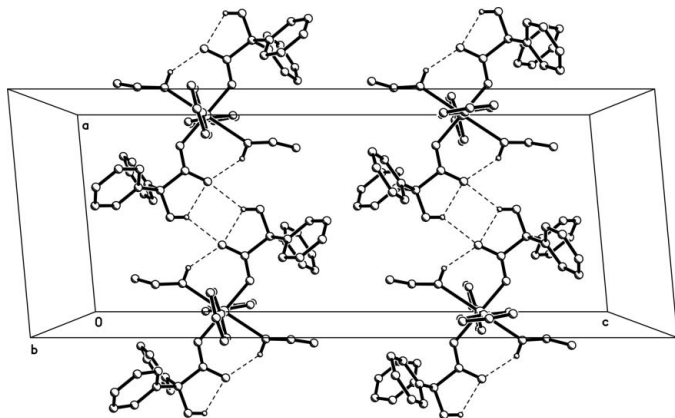


Figure 2
The hydrogen-bonded chain structure of (I), viewed along the *b* axis, with the O—H...O hydrogen bonds shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

formed by the N atoms of two pyridine ligands [Cu1—N1 = 2.014 (2) Å and Cu1—N2 = 2.018 (2) Å], the O atoms of two ethanol molecules and the O atoms of two benzoate residues. The Cu1—O4 distance [2.476 (2) Å], involving the O atom of the ethanol ligand, is significantly longer than the Cu1—O1 bond involving the acetate group [1.9807 (13) Å], which is not uncommon for the geometry of ethanol–acetate–copper complexes (Chiari *et al.*, 1988). The mean planes of the two pyridine ligands, N1/C15/C16/C17 and N2/C18/C19/C20, form a dihedral angle of 82.08 (2)° with each other; in accordance with the symmetry of the complex, these planes are also orthogonal to the plane through the four O atoms coordinating the Cu atom.

There are two ‘active’ H atoms in the molecule of complex (I). The ethanol OH group forms an intermolecular hydrogen bond with the carboxylate carbonyl O atom, whereas the hydroxy group of the benzoic acid residue participates in both intramolecular and intermolecular hydrogen bonds (Table 2).

The intermolecular bond is responsible for the formation of infinite chains, running along the *a* axis of the crystal structure (Fig. 2).

Experimental

The title compound was prepared by addition of copper(II) acetate (5 mmol) and pyridine (1 ml) to an ethanol solution (40 ml) of benzoic acid (5 mmol). The mixture was stirred for 0.5 h at room temperature and then filtered. Blue single crystals were isolated from the solution after five days. Analysis calculated for $C_{42}H_{44}CuN_2O_8$: C 65.65, H 5.77, N 3.65%; found: C 65.68, H 5.75, N 3.67%.

Crystal data

[Cu(C ₁₄ H ₁₁ O ₃) ₂ (C ₅ H ₅ N) ₂ (C ₂ H ₆ O) ₂]	$D_x = 1.311 \text{ Mg m}^{-3}$
$M_r = 768.34$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 17527 reflections
$a = 9.7231 (19) \text{ \AA}$	$\theta = 3.0\text{--}27.5^\circ$
$b = 15.992 (2) \text{ \AA}$	$\mu = 0.61 \text{ mm}^{-1}$
$c = 25.143 (3) \text{ \AA}$	$T = 295 (2) \text{ K}$
$\beta = 95.23 (3)^\circ$	Prism, blue
$V = 3893.3 (10) \text{ \AA}^3$	$0.37 \times 0.25 \times 0.19 \text{ mm}$
$Z = 4$	

Data collection

Rigaku R-Axis RAPID diffractometer	4450 independent reflections
ω scans	3728 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$R_{\text{int}} = 0.018$
$T_{\text{min}} = 0.804, T_{\text{max}} = 0.892$	$\theta_{\text{max}} = 27.5^\circ$
18339 measured reflections	$h = -12 \rightarrow 12$
	$k = -20 \rightarrow 19$
	$l = -32 \rightarrow 32$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0732P)^2 + 1.3059P]$
$R[F^2 > 2\sigma(F^2)] = 0.037$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.115$	$(\Delta/\sigma)_{\text{max}} = 0.002$
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.43 \text{ e \AA}^{-3}$
4450 reflections	$\Delta\rho_{\text{min}} = -0.27 \text{ e \AA}^{-3}$
245 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (Å, °).

Cu1—O1	1.9807 (13)	O1—C1	1.258 (2)
Cu1—O4	2.476 (2)	O2—C1	1.239 (2)
Cu1—N1	2.014 (2)	O3—C2	1.4221 (19)
Cu1—N2	2.018 (2)		
O1—Cu1—O1 ⁱ	178.95 (7)	O4—Cu1—N2	93.00 (7)
O1—Cu1—N1	90.52 (4)	O4—Cu1—O1 ⁱ	96.49 (7)
O4—Cu1—O1	83.57 (6)	O4 ⁱ —Cu1—O4	174.00 (7)
O4—Cu1—N1	87.00 (7)	N1—Cu1—N2	180

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

Table 2

Hydrogen-bond geometry (Å, °).

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
O3—H23...O2	0.82	2.04	2.564 (2)	121
O3—H23...O2 ⁱⁱ	0.82	2.23	2.914 (2)	142
O4—H24...O2 ⁱ	0.82	2.04	2.745 (2)	144

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

The H atoms bonded to O atoms were located using circular difference Fourier syntheses [$O-H = 0.82 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$]. The other H atoms were placed in calculated positions [$C-H = 0.93 \text{ \AA}$ (aromatic) and 0.97 \AA (methylene), and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$; $C-H = 0.96 \text{ \AA}$ (methyl) and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(C_{\text{methyl}})$], and were included in the refinement in the riding-model approximation.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSK, 2002); 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*.

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