Lists of structure factors, anisotropic displacement parameters and complete geometry of the non-H atoms have been deposited with the IUCr (Reference: BK1004). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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trans-Bis(acetato-*O*)bis(4-methylpyridine-*N*)copper(II)

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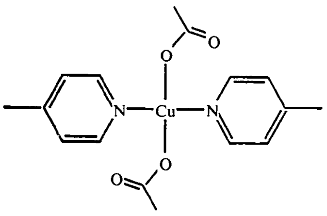
Abstract

The structure of *trans*-bis(acetato-*O*)bis(4-methylpyridine-*N*)copper(II), $[Cu(C_2H_3O_2)_2(C_6H_7N)_2]$, reported herein, represents a monomeric parent acetate complex with a distorted square-planar arrangement of acetate and 4-methylpyridine ligands around the Cu atom with the following distances and angles: Cu—N = 2.027 (4) and Cu—O1 = 1.950 (3) Å; O1—Cu—N = 89.1 (2) and O1—Cu—N′ = 90.9 (2)°. The Cu atom resides on a center of inversion. The most important dihedral angles are the angle between the 4-methylpyridine plane and the acetate plane (O1, O2, C21 and C22), 78.2°, and the angle between the 4-methylpyridine ring and the coordination plane (Cu, N, O1), 31.6°.

Comment

The title compound, (I), was prepared by the reaction of gallium sulfide with copper(I) acetate in 4-methylpyridine solution. A solution of copper(I) acetate (0.31 g, 2.4 mmol) and gallium sulfide (0.37 g, 3.6 mmol) in 25 ml of 4-methylpyridine was stirred for 3 days at 293 K under argon. All manipulations were performed in a drybox or on a vacuum line under an inert atmosphere using standard Schlenk techniques. Filtration and layering of the 4-methylpyridine solution with 30 ml of hexanes produced prismatic blue crystals of the title compound (I).



(I)

X-ray structures of the two following copper(II) acetate complexes have been determined: *trans*-bis[(chloroacetato)(α-picoline)]copper(II) and *trans*-bis[(dichloroacetato)(α-picoline)]copper(II) (Davey & Stephens, 1971*a*,*b*). The complex reported herein represents the unchlorinated compound. The Cu atom is surrounded by four ligands in a virtually square-planar arrangement with an O atom (O2) of the acetate group efficiently blocking the two remaining axial sides of the Cu atom above and below the coordination plane defined by atoms Cu, O1, O1′, N and N′. The Cu—O2 distance of 2.623 (4) Å is indicative of a weak interaction between the two atoms. The two 4-methylpyridine rings, as well as the two acetato groups, are forced to be coplanar by a center of symmetry residing on the Cu atom. The dihedral angle between the 4-methylpyridine plane and the acetate plane is 78.2°. Steric interactions force the 4-methylpyridine ring to be skewed at an angle of 31.6° with respect to the coordination plane. The C21—O2 distance of 1.227 (7) Å is shorter than the C21—O1 distance of 1.279 (6) Å, which suggests more double-bond character for the C21—O2 bond (Davey & Stephens, 1971*a*,*b*). The O1—C21—O2 angle of 122.7 (5)° is significantly smaller than the O—C—O angles of 126.6 and 128.0° in the dimeric copper(II) acetate complex $[Cu_2(C_2H_2ClO_2)_4(C_6H_7N)_2]$ (Davey & Stephens, 1970). All angles and bonds within the 4-methylpyridine rings are as expected.

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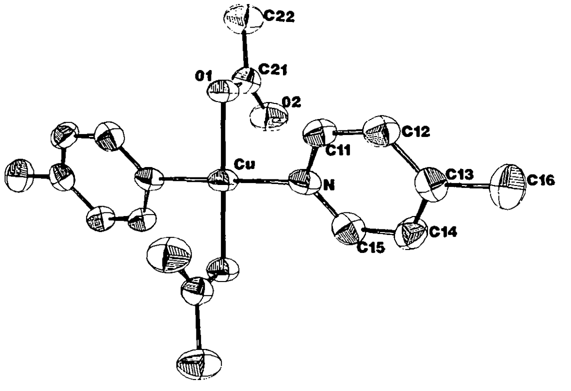

Fig. 1. *ORTEP* (Johnson, 1976) drawing representing the stereochemistry of the $[Cu(C_2H_3O_2)_2(C_6H_7N)_2]$ molecule and the atomic labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

Experimental

Crystal data

$[Cu(C_2H_3O_2)_2(C_6H_7N)_2]$
$M_r = 367.89$
Monoclinic
$P2_1/c$
$a = 6.194\ (2)$ Å
$b = 16.474\ (6)$ Å
$c = 8.270\ (3)$ Å
$\beta = 92.02\ (3)°$
$V = 843.5\ (9)$ Å^3
$Z = 2$
$D_x = 1.448$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 2.44–15.8°$
$\mu = 1.295$ mm^{-1}
$T = 293$ K
Prism
$0.34 \times 0.32 \times 0.30$ mm
Blue

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega–2\theta$ scans
Absorption correction: empirical ψ scans (North, Phillips & Mathews, 1968)
$T_{\min} = 0.878$, $T_{\max} = 0.999$
1689 measured reflections
1478 independent reflections

873 observed reflections $[I > 3\sigma(I)]$
$R_{\rm int} = 0.39$
$\theta_{\max} = 25°$
$h = 0 \rightarrow 7$
$k = 0 \rightarrow 19$
$l = -9 \rightarrow 9$
3 standard reflections
frequency: 60 min
intensity variation: <5.1%

Refinement

Refinement on F
$R = 0.040$
$wR = 0.053$
$S = 1.142$
873 reflections
107 parameters
H-atom parameters not refined
$w = 1/\sigma^2(F_o)$
$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.300$ e Å^{-3}
$\Delta\rho_{\min} = -0.355$ e Å^{-3}
Extinction correction: $F_c = F_o/(1 + gI_c)$
Extinction coefficient: 2.1×10^{-6}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$$B_{\rm eq} = (1/3)\Sigma_i\Sigma_jB_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$B_{\rm eq}$
Cu	0	0	0	2.78 (1)
O1	0.1063 (6)	0.0795 (2)	−0.1527 (4)	3.13 (7)
O2	−0.1468 (7)	0.1486 (3)	−0.0336 (5)	4.78 (9)
N	0.2071 (7)	0.0459 (3)	0.1721 (4)	3.02 (9)
C11	0.1522 (8)	0.0462 (3)	0.3287 (6)	3.0 (1)
C12	0.2840 (9)	0.0783 (3)	0.4486 (6)	3.3 (1)
C13	0.4796 (9)	0.1142 (3)	0.4149 (6)	3.1 (1)
C14	0.5371 (8)	0.1127 (4)	0.2539 (7)	3.6 (1)
C15	0.3977 (8)	0.0798 (3)	0.1379 (6)	3.4 (1)
C16	0.626 (1)	0.1506 (4)	0.5428 (7)	4.6 (1)
C21	0.0045 (9)	0.1453 (3)	−0.1251 (6)	3.3 (1)
C22	0.080 (1)	0.2195 (4)	−0.2095 (7)	4.8 (1)

Table 2. *Selected geometric parameters* (Å, °)

Cu—N	2.027 (4)	N—C15	1.346 (7)
Cu—O1	1.950 (3)	C11—C12	1.367 (7)
Cu—O2	2.623 (4)	C12—C13	1.386 (8)
Cu—N	2.027 (4)	C13—C14	1.392 (8)
O1—C21	1.279 (6)	C13—C16	1.492 (8)
O2—C21	1.227 (7)	C14—C15	1.378 (7)
N—C11	1.351 (6)	C21—C22	1.492 (8)
O1—Cu—N	89.1 (2)	C11—C12—C13	121.5 (5)
O2—Cu—O1	55.2 (2)	C12—C13—C14	116.2 (5)
O2—Cu—N	93.8 (2)	C12—C13—C16	122.8 (5)
Cu—O1—C21	105.8 (3)	C14—C13—C16	121.0 (5)
Cu—N—C11	120.0 (3)	C13—C14—C15	119.8 (5)
Cu—N—C15	123.0 (3)	N—C15—C14	123.4 (5)
C11—N—C15	116.9 (4)	O1—C21—O2	122.7 (5)
N—C11—C12	122.2 (5)	O1—C21—C22	116.5 (5)
O2—C21—C22	120.8 (5)		

Profile analysis was performed on all reflections (Lehman & Larsen, 1974; Grant & Gabe, 1978). Intensities were corrected for Lorentz–polarization effects. Because of a center of inversion residing on the Cu atom, one formula unit is obtained from two asymmetric units. All calculations were performed using a PDP-11/60 microcomputer and the *SDP-Plus* (Enraf–Nonius, 1985) structure determination package.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and root-mean-squares data have been deposited with the IUCr (Reference: HH1030). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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