

The structure was solved by the heavy-atom method. Of two perchlorate anions, one was found disordered (Cl2) and was refined with two positions of its O atoms, the geometry of which with respect to the Cl2 atom was restrained to be similar to the geometry of the ordered anion (Cl1). O atoms of the disordered perchlorate were refined isotropically with a common U_{iso} value. The occupation factors of O atoms in two positions converged to 0.550 (9) and 0.450 (9) for those O atoms with labels appended by A and B, respectively. The absorption correction transmission factors derived from ΔF are in good agreement with those obtained via ψ scan method.

Data collection: *CAD-4 Software* (Enraf-Nonius, 1989). Cell refinement: *CAD-4 Software*. Data reduction: *Xtal3.0* (Hall & Stewart, 1990). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *ORTEPII* (Johnson, 1976), *PLUTO* (Motherwell & Clegg, 1978). Software used to prepare material for publication: *SHELXL93*.

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Lists of structure factors, least-squares-planes data, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: FG1115). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Bis[2-(2-pyridylmethylaminomethyl)-phenol]copper(II) Diacetate Trihydrate [Cu(HBPA)₂](CH₃COO)₂·3H₂O

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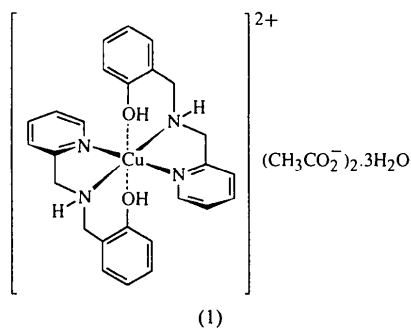
Abstract

The mononuclear [Cu(HBPA)₂]²⁺ cation within the title compound, [Cu(C₁₃H₁₄N₂O)₂](CH₃COO)₂·3H₂O, has a tetragonally elongated coordination polyhedron and represents a rare example of a copper complex in which two phenolic O atoms are axially coordinated to the Cu^{II} centre without deprotonation.

Comment

In recent years copper complexes of ligands containing phenolic hydroxy groups have received a great deal of attention because of their relevance to copper enzymes such as tyrosinase (Himmelwright, Eickman, LuBien, Lerch & Solomon, 1980) and galactose oxidase (Kosman, 1984). Recently, the crystal structure of galactose oxidase (Ito *et al.*, 1991) was determined. The geometry of the active site reveals a unique mononuclear copper site with two histidine N atoms, a tyrosine O atom and an acetate ion forming an almost perfect square and another tyrosine O atom in the axial position completing the square pyramid. In this work, we report the synthesis

and crystal structure of a new mononuclear copper(II) complex with N and O donor ligands, (1), which mimics the active site of this metalloenzyme.



The structure of (1) consists of discrete mononuclear $[\text{Cu}^{\text{II}}(\text{HBPA})_2]^{2+}$ cations and uncoordinated acetate anions. In the molecular structure of the cation, two tridentate HBPA ligands are equatorially coordinated to the metal ion through the nitrogen donors, with atoms of the same type [two N(amine) and two N(pyridine)] occupying *trans* positions with respect to each other. The remaining phenolic O atoms of HBPA occupy the axial positions to complete the coordination sphere in a facial conformation. The equatorial plane is planar within 0.012 (5) Å and the Cu—O1 and Cu—O2 bonds are almost perpendicular to this plane, with the O1—Cu—O2 angle being 177.6 (1)°. The Cu^{II} ion is displaced slightly out of the mean plane towards the Cu—O2 bond [by 0.057 Å]. The two six-membered chelate rings (CuNOC₃) adopt chair conformations with torsion angles N1—C1—C12—C11 of -72.3 (7) and N2—C2—C22—C21 of 72.8 (7)°. The remaining five-membered rings formed by the pendant 2-pyridylmethyl groups are closely planar, with the sum of interior angles being 528.3° for ring Cu—N31—C32—C3—N1 and 530.2° for Cu—N41—C42—C4—N2. The two pyridine rings are planar and the dihedral angle between them is 17.8 (5)°.

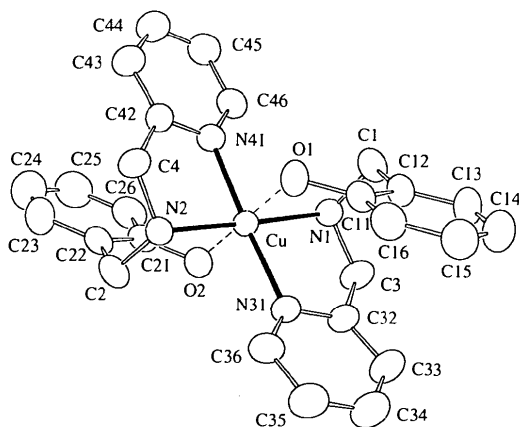


Fig. 1. Perspective view of the cation of (1) with the atomic numbering scheme. The displacement ellipsoids are drawn at the 50% probability level.

The Cu—N(amine) [average 2.003 (5) Å] and the Cu—N(pyridine) [average 2.051 (6) Å] bond lengths in the equatorial plane agree very well with those generally found in square-planar (Tamburini, Vigato & Casellato, 1989), square-pyramidal (Rajendran, Viswanathan, Palaniandavar & Lakshminarayanan, 1992) and distorted octahedral (Ranfod, Sadler & Tocher, 1993) complexes. In addition, the Cu^{II} ion makes two axial Cu—O contacts to the O atoms of the two phenolic groups of the HBPA ligands. These contacts [Cu—O1 = 2.494 (6) and Cu—O2 = 2.449 (6) Å] are significantly longer than that detected in the neutral complex $[\text{Cu}(\text{BPNP})\text{Cl}]$ [Cu—O(phenolate) = 2.268 Å] {HBPNP = 2-[bis(2-pyridylmethyl)aminomethyl]-4-nitrophenol}, in which the *p*-nitrophenolate group is coordinated in the axial position in the square-pyramidal species (Rajendran *et al.*, 1992). From this information and from the fact that (1) is a 2+ charged species we can assign a structure involving two axial copper(II)—phenol-OH bonds. To the best of our knowledge, this is the first structural example of a Cu^{II} complex in which two phenolic O-atom donors are axially coordinated to Cu^{II} without deprotonation, although a square-pyramidal complex with a Cu^{II}—OH bond of 2.6 Å in the apical position has been reported (Masuda, Odani & Yamauchi, 1989).

Finally, the acetate anions are ordered and do not show any serious distortions from planar geometry. The C—O and C—C bonds range from 1.240 (7) to 1.266 (7) Å and from 1.53 (1) to 1.55 (1) Å, respectively, while the O—C—O angles vary between 115.9 (6) and 125.3 (7)°.

Experimental

The reaction of $\text{Cu}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$ with (2-hydroxybenzyl)(2-pyridylmethyl)amine (HBPA) (Neves *et al.*, 1993) (1:2) in methanol afforded a purple microcrystalline precipitate which was filtered off and washed with cold methanol and ether. Single crystals of (1) suitable for X-ray crystallography were obtained by recrystallization from a methanol solution. Analysis: calculated for $\text{CuC}_{30}\text{H}_{40}\text{N}_4\text{O}_9$ C 54.25, H 6.07, N 8.44%; found C 54.31, H 5.95, N 8.37%.

Crystal data

$[\text{Cu}(\text{C}_{13}\text{H}_{14}\text{N}_2\text{O}_2)_2] \cdot (\text{C}_2\text{H}_3\text{O}_2)_2 \cdot 3\text{H}_2\text{O}$

$M_r = 664.21$

Triclinic

$P\bar{1}$

$a = 11.356 (1) \text{ \AA}$

$b = 11.862 (1) \text{ \AA}$

$c = 12.989 (1) \text{ \AA}$

$\alpha = 106.88 (1)^\circ$

$\beta = 102.95 (1)^\circ$

$\gamma = 94.38 (1)^\circ$

$V = 1612.8 (1) \text{ \AA}^3$

$Z = 2$

$D_x = 1.368 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 25

reflections

$\theta = 9.70\text{--}15.36^\circ$

$\mu = 0.732 \text{ mm}^{-1}$

$T = 298 \text{ K}$

0.55 × 0.45 × 0.40 mm

Violet

Data collection

Nonius CAD-4 diffractometer	4550 observed reflections
	[$F > 6\sigma(F)$]
$\omega/2\theta$ scans	$R_{\text{int}} = 0.0160$
Absorption correction:	$\theta_{\text{max}} = 24.97^\circ$
ψ scan (North, Phillips & Mathews, 1968)	$h = -13 \rightarrow 13$
$T_{\text{min}} = 0.969$, $T_{\text{max}} = 1.000$	$k = 0 \rightarrow 14$
	$l = -15 \rightarrow 14$
5668 measured reflections	2 standard reflections
5367 independent reflections	frequency: 120 min
	intensity decay: 3.6%

Refinement

Refinement on F	$w = 1/\sigma^2(F)$
$R = 0.0609$	$(\Delta/\sigma)_{\text{max}} = 0.252$
$wR = 0.0823$	$\Delta\rho_{\text{max}} = 0.801 \text{ e } \text{\AA}^{-3}$
$S = 1.96$	$\Delta\rho_{\text{min}} = -0.146 \text{ e } \text{\AA}^{-3}$
4550 reflections	Extinction correction: none
397 parameters	Atomic scattering factors
H-atom parameters not refined	from <i>MolEN</i> (Fair, 1990)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (\AA^2)

$$B_{\text{eq}} = (8\pi^2/3) \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	x	y	z	B_{eq}
Cu	0.22505 (7)	0.23005 (6)	0.24556 (6)	2.64 (1)
O1	0.4365 (4)	0.2653 (4)	0.3682 (4)	3.4 (1)
O2	0.0161 (4)	0.1874 (4)	0.1264 (4)	3.5 (1)
N1	0.2379 (5)	0.4055 (4)	0.2683 (4)	2.9 (1)
N2	0.2179 (5)	0.0567 (4)	0.2305 (4)	2.8 (1)
N31	0.3175 (5)	0.2315 (4)	0.1263 (4)	3.2 (1)
N41	0.1447 (4)	0.2336 (4)	0.3720 (4)	2.9 (1)
C1	0.3362 (6)	0.4777 (5)	0.3717 (5)	3.4 (1)
C2	0.1142 (6)	-0.0204 (6)	0.1374 (5)	3.5 (1)
C3	0.2533 (6)	0.4257 (6)	0.1634 (5)	3.6 (1)
C4	0.2176 (6)	0.0430 (5)	0.3416 (5)	3.3 (1)
C11	0.5106 (6)	0.3548 (5)	0.3563 (5)	3.1 (1)
C12	0.4643 (6)	0.4613 (5)	0.3574 (5)	3.2 (1)
C13	0.5379 (7)	0.5557 (6)	0.3480 (6)	4.5 (2)
C14	0.6569 (7)	0.5426 (7)	0.3365 (7)	5.3 (2)
C15	0.7016 (7)	0.4349 (7)	0.3340 (6)	4.9 (2)
C16	0.6285 (6)	0.3409 (6)	0.3446 (6)	4.0 (2)
C21	-0.0550 (6)	0.1068 (6)	0.1520 (5)	3.3 (1)
C22	-0.0090 (6)	0.0016 (6)	0.1590 (5)	3.4 (1)
C23	-0.0786 (7)	-0.0834 (7)	0.1852 (6)	4.8 (2)
C24	-0.1932 (8)	-0.0635 (8)	0.2050 (8)	6.2 (2)
C25	-0.2388 (8)	0.0435 (9)	0.1975 (7)	6.0 (2)
C26	-0.1696 (7)	0.1286 (7)	0.1710 (6)	4.6 (2)
C32	0.3308 (6)	0.3393 (5)	0.1122 (5)	3.2 (1)
C33	0.4099 (6)	0.3699 (6)	0.0537 (6)	4.2 (2)
C34	0.4784 (7)	0.2834 (7)	0.0079 (6)	5.0 (2)
C35	0.4652 (7)	0.1722 (7)	0.0233 (6)	4.9 (2)
C36	0.3833 (6)	0.1480 (6)	0.0829 (5)	4.1 (2)
C42	0.1528 (5)	0.1352 (5)	0.4033 (5)	2.9 (1)
C43	0.1058 (6)	0.1188 (6)	0.4894 (5)	3.9 (2)
C44	0.0444 (6)	0.2079 (7)	0.5421 (6)	4.4 (2)
C45	0.0322 (7)	0.3082 (7)	0.5066 (6)	4.4 (2)
C46	0.0831 (6)	0.3187 (6)	0.4208 (5)	3.7 (2)
O1a	0.5216 (4)	0.0669 (4)	0.3501 (5)	5.0 (1)
O2a	0.4114 (4)	-0.0727 (4)	0.1978 (4)	4.1 (1)
C1a	0.4879 (6)	-0.0397 (5)	0.2896 (6)	3.7 (1)
C2a	0.5450 (8)	-0.1336 (6)	0.3352 (7)	6.2 (2)
O1b	0.0933 (5)	-0.3572 (4)	-0.0892 (4)	5.3 (1)
O2b	-0.0108 (4)	-0.4929 (4)	-0.2487 (4)	4.2 (1)
C1b	0.0693 (6)	-0.4609 (6)	-0.1593 (6)	3.9 (2)
C2b	0.1477 (8)	-0.5529 (6)	-0.1281 (7)	6.3 (2)
Ow1	0.2450 (7)	0.8757 (7)	0.5039 (6)	8.9 (2)
Ow2	0.2716 (5)	-0.2989 (4)	0.1144 (4)	5.0 (1)
Ow3	0.1569 (6)	0.7123 (6)	0.2886 (5)	7.4 (2)

Table 2. Selected geometric parameters (\AA , $^\circ$)

Cu—N1	2.004 (5)	Cu—N41	2.042 (6)
Cu—N2	2.002 (5)	Cu···O1	2.494 (6)
Cu—N31	2.060 (6)	Cu···O2	2.449 (6)
N1—Cu—N2	177.1 (2)	N2—Cu—N31	97.8 (2)
N1—Cu—N31	83.3 (2)	N2—Cu—N41	83.0 (2)
N1—Cu—N41	95.7 (2)	N31—Cu—N41	176.0 (2)

Table 3. Hydrogen-bond distances (\AA)

O1···O1a	2.580	O2a···Ow2	2.791
O1a···Ow1 ⁱ	2.795	Ow2···Ow3 ⁱⁱⁱ	2.829
O1b···O2 ⁱⁱ	2.551	Ow3···O2b ⁱⁱ	2.822
O1b···Ow2	2.811	Ow3···Ow1	2.806

Symmetry codes: (i) $1-x, 1-y, 1-z$; (ii) $-x, -y, -z$; (iii) $x, y-1, z$.

The O atoms of the water molecules, acetates and phenolates are involved in hydrogen bonds, the contact distances and angles of which are deposited. One H atom of the water Ow2, one H atom of the water Ow3 and the H atoms attached to the phenol O atoms O1 and O2 were located from difference Fourier maps. The H atoms attached to the water O atoms were not found. All other H atoms were included at geometrically idealized positions. The H atoms were not refined in the least-squares calculations.

Data collection: *CAD-4-Express* (Nonius, 1993). Cell refinement: *MolEN* (Fair, 1990). Data reduction: *MolEN*. Program(s) used to solve structure: *SIR92* (Burla *et al.*, 1992). Program(s) used to refine structure: *MolEN*. Molecular graphics: *ORTEPII* (Johnson, 1976). Software used to prepare material for publication: *MolEN*.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: FG1104). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Clemizoledichlorozinc(II)

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Abstract

The crystal structure of the title compound, dichloro[1-(*p*-chlorophenylmethyl)-2-(1-pyrrolidinylmethyl)benzimidazole-*N,N'*]zinc(II), $[\text{ZnCl}_2(\text{C}_{19}\text{H}_{20}\text{ClN}_3)]$, is composed of independent molecules wherein clemizole acts as a bidentate ligand and is coordinated to zinc *via* pyrrolidinyl and imidazole N atoms. The geometry around zinc is distorted tetrahedral with bond distances Zn—N 2.029 (3) and 2.157 (3) Å, and Zn—Cl 2.196 (2) and 2.222 (2) Å.

Comment

The crystal structures of clemizole hydrochloride (Parvez, 1996) and clemizole in its free form (Parvez & Sabir, 1996) have been reported. We have now incorporated this important antihistamine into a transition metal complex to investigate the effects such complex formation may have on the conformation of the drug molecule. In this paper, we report the crystal structure of clemizoledichlorozinc(II), (1).

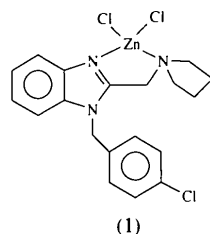


Fig. 1 shows an *ORTEP*II (Johnson, 1976) drawing of the title compound with the atomic numbering scheme. The drug molecule acts as a bidentate ligand and is coordinated *via* pyrrolidinyl and imidazole N atoms to zinc with Zn—N distances of 2.029 (3) and

2.157 (3) Å. The Zn atom is also bonded to two Cl atoms with distances of 2.196 (2) and 2.222 (2) Å. The geometry around zinc is distorted tetrahedral. Similar distances and geometries have been reported for a number of closely related zinc complexes, *e.g.* bis(antazoline)dichlorozinc(II) (Parvez & Rusiewicz, 1995), bis(xanthine)dichlorozinc(II) (Dubler, Hanggi & Schmale, 1992), bis(imidazole)dichlorozinc(II) (Lundberg, 1966), bis(1,2-dimethylimidazole)dichlorozinc(II) (Bharadwaj, Schugar & Potenza, 1991), bis{[3-(imidazol-1-yl)-1-oxopropyl]benzene-*N'*}dichlorozinc(II) (Bremer, Uhlenbrock, Pinkerton & Krebs, 1993) and (2,2'-bipyridine)dichlorozinc(II) (Khan & Tuck, 1984).

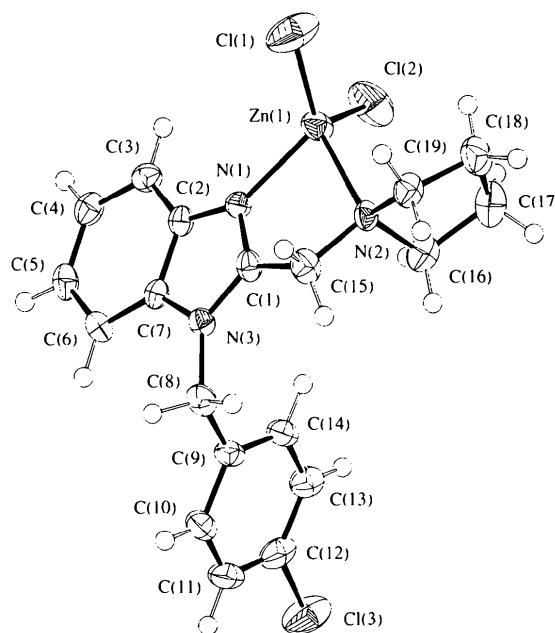


Fig. 1. *ORTEP*II (Johnson, 1976) drawing of the title compound with the atomic numbering scheme. Displacement ellipsoids are plotted at the 50% probability level and H atoms have been assigned arbitrary radii.

The molecular dimensions in the clemizole ligand are normal with bond distances $\text{C}_{sp^2}\text{—Cl}$ 1.748 (5) and C=N 1.321 (5) and mean $\text{C}_{sp^3}\text{—C}_{sp^2}$ 1.505 (7), $\text{C}_{sp^3}\text{—C}_{sp^3}$ 1.525 (8), $\text{C—C}_{\text{aromatic}}$ 1.386 (8), N—C_{sp^3} 1.476 (7), and N—C_{sp^2} (imidazole ring N atoms fused to benzene) 1.394 (4) Å; the N—C_{sp^2} distance $\text{C}(1)\text{—N}(3)$ [1.357 (5) Å] is significantly shorter than the other two corresponding distances.

The benzimidazole and the phenyl rings are essentially planar with maximum deviations of atoms from the least-squares planes being 0.015 (4) and 0.011 (4) Å, respectively. The dihedral angle between these planes is 81.1 (4)°; the corresponding angles in the crystal structures of clemizole hydrochloride and clemizole free base have been observed to be 82.8 (9) (Parvez, 1996) and 68.8 (6)° (Parvez & Sabir, 1996), respectively. The pyrrolidinyl ring has an N(2)-envelope conformation